Contemporary Mathematicians

Claude Brezinski
Ahmed Sameh
Editors

Walter Gautschi

Selected Works with Commentaries

Volume 2

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Walter Gautschi, Volume 2

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Erika and Walter Gautschi, 1974

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Part I

Commentaries

In all commentaries, reference numbers preceded by "GA" refer to the numbers in the list of Gautschi's publications; see Section 4, Vol. 1. Numbers in boldface type indicate that the respective papers are included in these selected works.

11

Orthogonal polynomials on the real line

Gradimir V. Milovanović

In about two dozen papers, Walter Gautschi developed the so-called *constructive theory of orthogonal polynomials on* $\mathbb{R}$, including effective algorithms for numerically generating orthogonal polynomials, a detailed stability analysis of such algorithms as well as several new applications of orthogonal polynomials. Furthermore, he provided software necessary for implementing these algorithms (see Section 23, Vol. 3) and applications.

Let $\mathcal{P}$ be the space of real polynomials and $\mathcal{P}_n \subset \mathcal{P}$ the space of polynomials of degree at most n. Suppose $\mathrm{d}\mu(t)$ is a positive measure on $\mathbb{R}$ with finite or unbounded support, for which all moments $\mu_k = \int_{\mathbb{R}} t^k \mathrm{d}\mu(t)$ exist and are finite, and $\mu_0 > 0$. Then the inner product

$$(p, q) = \int_{\mathbb{R}} p(t)q(t)\mathrm{d}\mu(t)$$

is well defined for any polynomials $p, q \in \mathcal{P}$ and gives rise to a unique system of monic orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; d\mu)$; that is,

$$\pi_k(t) \equiv \pi_k(t; \mathrm{d}\mu) = t^k + \text{terms of lower degree}, \quad k = 0, 1, \ldots,$$

and

$$(\pi_k, \pi_n) = ||\pi_n||^2 \delta_{kn} = \begin{cases} 0, & n \neq k, \\ ||\pi_n||^2, & n = k. \end{cases}$$

11.1. Three-term recurrence relation

Because of the property $(tp, q) = (p, tq)$, these polynomials satisfy a three–term recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2 \ldots, \tag{11.1}$$

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with $\pi_0(t) = 1$ and $\pi_{-1}(t) = 0$, where $(\alpha_k) = (\alpha_k(\mathrm{d}\mu))$ and $(\beta_k) = (\beta_k(\mathrm{d}\mu))$ are sequences of recursion coefficients which depend on the measure $\mathrm{d}\mu$. The coefficient β_0 may be arbitrary, but is conveniently defined by $\beta_0 = \mu_0 = \int_{\mathbb{R}} \mathrm{d}\mu(t)$. In the case of a *discrete measure* $\mathrm{d}\mu = \mathrm{d}\mu_N$, i.e., when $\mu(t)$ has only N points of increase, the system of polynomials $\{\pi_k\}$ consists of only N polynomials $\pi_0, \pi_1, \ldots, \pi_{N-1}$ (*discrete orthogonal polynomials*).

There are many reasons why the coefficients α_k and β_k in the three-term recurrence relation (11.1) are fundamental quantities in the constructive theory of orthogonal polynomials (for details see [GA**81**]). For example, α_k and β_k provide a compact way of representing and easily calculating orthogonal polynomials, their derivatives, and their linear combinations, requiring only a linear array of parameters.

The same recursion coefficients α_k and β_k appear also in the *Jacobi continued fraction associated with the measure* $\mathrm{d}\mu$,

$$F(z) = \int_{\mathbb{R}} \frac{\mathrm{d}\mu(t)}{z-t} \sim \frac{\beta_0}{z-\alpha_0-} \frac{\beta_1}{z-\alpha_1-} \cdots,$$

which is the *Stieltjes transform* of the measure $\mathrm{d}\mu$ (for details see [GAB3, p. 15], [17, p. 114]). The nth *convergent* of this continued fraction is easly seen to be

$$\frac{\beta_0}{z-\alpha_0-} \frac{\beta_1}{z-\alpha_1-} \cdots \frac{\beta_{n-1}}{z-\alpha_{n-1}} = \frac{\sigma_n(z)}{\pi_n(z)}, \tag{11.2}$$

where σ_n are the so-called *associated polynomials* defined by

$$\sigma_k(z) = \int_{\mathbb{R}} \frac{\pi_k(z) - \pi_k(t)}{z-t} \mathrm{d}\mu(t), \quad k \geq 0.$$

They satisfy the same fundamental relation (11.1), i.e.,

$$\sigma_{k+1}(z) = (z-\alpha_k)\sigma_k(z) - \beta_k \sigma_{k-1}(z), \quad k \geq 0,$$

with starting values $\sigma_0(z) = 0$, $\sigma_{-1}(z) = -1$.

The *functions of the second kind*,

$$\varrho_k(z) = \int_{\mathbb{R}} \frac{\pi_k(t)}{z-t} \mathrm{d}\mu(t), \quad k \geq 0, \tag{11.3}$$

where z is outside the spectrum of $\mathrm{d}\mu$ (the Stieltjes transforms of π_k), also satisfy the same three-term recurrence relation (11.1) and, under some mild conditions, represent its *minimal solution* (cf. Section 21, Vol. 3) normalized by $\varrho_{-1}(z) = 1$. This has been observed by Gautschi in [GA**75**] and is a remarkable result, very important for computation in the areas of orthogonal polynomials, special functions, and numerical analysis. Gautschi [GA**75**] showed that this minimal solution can be

computed accurately by means of his continued fraction algorithm presented in [GA**29**]. Namely, if one wishes to compute $\varrho_k(z)$ for $k = 0, 1, \ldots, n$, then for some $\nu > n$ one generates quantities $r_k^{(\nu)}$ and $\varrho_k^{(\nu)}$ by

$$r_\nu^{(\nu)} = 0, \quad r_{k-1}^{(\nu)} = \frac{\beta_k}{z - \alpha_k - r_k^{(\nu)}}, \quad k = \nu, \nu-1, \ldots, 1, 0,$$

$$\varrho_{-1}^{(\nu)} = 1, \quad \varrho_k^{(\nu)} = r_{k-1}^{(\nu)} \varrho_{k-1}^{(\nu)}, \quad k = 0, 1, \ldots, n.$$

The quantities $\varrho_k^{(\nu)}(z)$ then tend to $\varrho_k(z)$ when $\nu \to \infty$, for every $k = 0, 1, \ldots, n$. For some standard measures $\mathrm{d}\mu$, Gautschi also provides good estimates for the starting index ν, given n and the desired accuracy.

Notice that the rational function (11.2) has simple poles at the zeros $z = x_{n,k}$, $k = 1, \ldots, n$, of the polynomial $\pi_n(t)$. By $\lambda_{n,k}$ we denote the corresponding residues, i.e.,

$$\lambda_{n,k} = \lim_{z \to x_{n,k}} (z - x_{n,k}) \frac{\sigma_n(z)}{\pi_n(z)} = \frac{1}{\pi_n'(x_{n,k})} \int_{\mathbb{R}} \frac{\pi_n(t)}{t - x_{n,k}} \, \mathrm{d}\mu(t),$$

so that the continued fraction representation (11.2) assumes the form

$$\frac{\sigma_n(x)}{\pi_n(x)} = \sum_{k=1}^{n} \frac{\lambda_{n,k}}{x - x_{n,k}} \,. \tag{11.4}$$

The coefficients $\lambda_{n,k}$ play an important role in *Gauss–Christoffel quadrature formulae*, being the Christoffel numbers associated with $\mathrm{d}\mu$. Using procedures of numerical linear algebra, notably the QR or QL algorithm, one easily computes the zeros of the orthogonal polynomials π_n rapidly and efficiently as eigenvalues of the leading nth-order principal minor matrix of the *Jacobi matrix* associated with $\mathrm{d}\mu$,

$$J(\mathrm{d}\mu) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots \\ & & \ddots & \ddots \\ \mathbf{0} & & & \end{bmatrix}.$$

The first components of the corresponding normalized eigenvectors give also immediately the Christoffel numbers $\lambda_{n,k}$ (cf. [12, GA**65**]).

Unfortunately, the recursion coefficients are known explicitly only for some narrow classes of orthogonal polynomials. One of the most important classes for which these coefficients are known explicitly are surely the so-called *very classical orthogonal polynomials* (Jacobi, the generalized Laguerre, and Hermite polynomials), which appear frequently in applied analysis and computational science. Orthogonal

polynomials for which the recursion coefficients are not known we call *strongly nonclassical polynomials*. In this case, if we know how to compute the first n recursion coefficients α_k and β_k, $k = 0, 1, \ldots, n-1$, we can compute all orthogonal polynomials of degree $\leq n$ by a straightforward application of the three-term recurrence relation (11.1).

In [GA**81**] Walter Gautschi starts with an arbitrary positive measure $\mathrm{d}\mu(t)$, which is given explicitly, or implicitly via moment information, and considers the actual (numerical) construction of orthogonal polynomials to be a basic computational problem: *For a given measure* $\mathrm{d}\mu$ *and for given* $n \in \mathbb{N}$*, generate the first* n *coefficients* $\alpha_k(\mathrm{d}\mu)$ *and* $\beta_k(\mathrm{d}\mu)$*,* $k = 0, 1, \ldots, n-1$.

At that time, and even more so in the "pre-computer" era, the problem was given surprisingly little attention in the literature, probably because it has a straightforward theoretical solution. Indeed, if one knows the moments μ_k, $k \geq 0$, the polynomial $\pi_k(t; \mathrm{d}\mu)$ can be expressed in the form

$$\pi_k(t; \mathrm{d}\mu) = \frac{1}{\Delta_k} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-1} & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_k & t \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_k & \mu_{k+1} & \cdots & \mu_{2k-1} & t^k \end{vmatrix},$$

where the Hankel determinant

$$\Delta_k = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-1} \\ \mu_1 & \mu_2 & \cdots & \mu_k \\ \vdots & \vdots & & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-2} \end{vmatrix}$$

is nonvanishing. The coefficients in the three-term recurrence relation can also be expressed in terms of Hankel determinats (or by Darboux's formulae),

$$\alpha_k = \frac{\Delta'_{k+1}}{\Delta_{k+1}} - \frac{\Delta'_k}{\Delta_k} \left(= \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)} \right), \quad \beta_k = \frac{\Delta_{k-1}\Delta_{k+1}}{\Delta_k^2} \left(= \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})} \right), \tag{11.5}$$

where Δ'_k denotes the determinant obtained from Δ_k by replacing the last column $[\mu_{k-1}\ \mu_k \ldots \mu_{2k-2}]^T$ by $[\mu_k\ \mu_{k+1} \ldots \mu_{2k-1}]^T$.

Thus, the recursion coefficients α_k and β_k in (11.1) can be computed from (11.5) in terms of Hankel-type determinants, but this involves excessive complexity and is subject to extreme numerical instability. In the numerical construction of recursion coefficients an important aspect is the sensitivity of the problem with respect to small perturbations in the data (for example, perturbations in the first $2n$ moments μ_k, $k = 0, 1, \ldots, 2n-1$, when calculating the coefficients for $k \leq n-1$). There is a simple algorithm, due to Chebyshev, which transforms the moments to the desired recursion coefficients, $[\mu_k]_{k=0}^{2n-1} \mapsto [\alpha_k, \beta_k]_{k=0}^{n-1}$, but its viability is strictly dependent on the conditioning of this mapping. The latter is usually severely ill conditioned

so that these calculations via moments, in finite precision on a computer, are quite ineffective. The only salvation, in this case, is to either use symbolic computation, which however requires special resources and often is not possible, or else to use the explicit form of the measure. In the latter case, an appropriate discretization of the measure and subsequent approximation of the recursion coefficients is a viable alternative.

11.2. Basic procedures for generating the recursion coefficients

There are three well-known approaches for generating recursion coefficients: the *method of (modified) moments*, the *discretized Stieltjes–Gautschi procedure*, and the *Lanczos algorithm*.

11.2.1. Method of (modified) moments

In an attempt to avoid ill-conditioning, one can use the so-called modified moments $m_k = \int_{\mathbb{R}} p_k(t)\mathrm{d}\mu(t)$, $k = 0, 1, 2, \ldots$, where p_k are monic polynomials of degree k "close" in some sense to the desired polynomials π_k. Usually, the polynomials p_k satisfy a three-term recurrence relation of the form (11.1), with coefficients a_k ($\in \mathbb{R}$) and b_k (≥ 0) (instead of α_k and β_k). Then there is a unique map $K_n \colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ that takes the first $2n$ modified moments into the desired n recurrence coefficients α_k and β_k, i.e., $[m_k]_{k=0}^{2n-1} \mapsto [\alpha_k, \beta_k]_{k=0}^{n-1}$. An algorithm for realizing this map (*modified Chebyshev algorithm*) is formulated and summarized schematically in Gautschi [GA**81**]. In a somewhat different form, the algorithm has been first proposed by Sack and Donovan [29], and modified by Wheeler [33]. A derivation can also be found in [GA**64**]. For $a_k = b_k = 0$ we have $p_k(t) = t^k$ and the modified moments m_k reduce to the standard moments μ_k.

A rigorous and detailed analysis of the map K_n was given by Gautschi in [GA**81**] (see also [GA**94**] and especially his excellent survey [GA**146**] on applications and computational aspects of orthogonal polynomials). The novelty of his treatment consists in representing $K_n \colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ as a composition of two maps, $K_n = H_n \circ G_n$, where $G_n \colon [m_k]_{k=0}^{2n-1} \to [x_{n,k}, \lambda_{n,k}]_{k=1}^{n}$ is the map from the modified moments to the Gauss–Christoffel nodes and weights, and $H_n \colon [x_{n,k}, \lambda_{n,k}]_{k=1}^{n} \to [\alpha_k, \beta_k]_{k=0}^{n-1}$, the map from the Gauss–Christoffel quadrature rule

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\mu(t) = \sum_{k=1}^{n} \lambda_{n,k} f(x_{n,k}) + R_n(f), \quad R_n(\mathcal{P}_{2n-1}) = 0,$$

to the desired recursion coefficients. Notice that $x_{n,k}$, $k = 1, \ldots, n$, are the zeros of the orthogonal polynomial π_n associated with the measure $\mathrm{d}\mu$. The parameters $x_{n,k}$ and $\lambda_{n,k}$, $k = 1, \ldots, n$, also appear in (11.4).

The components H_n and G_n of the map K_n can be analyzed individually with regard to their numerical condition, which in turn yields a bound on the condition

of the composite map. The map H_n is usually fairly well conditioned, but G_n is the more sensitive one. The map K_n for standard moments, $[\mu_k]_{k=0}^{2n-1} \mapsto [\alpha_k, \beta_k]_{k=0}^{n-1}$, is severely ill conditioned when n is large. By using modified moments, the map may become better conditioned, very much so when the measure has finite support.

11.2.2. Discretization methods

The basic idea for these methods is an approximation of the given measure $\mathrm{d}\mu$ by a discrete N-point measure, usually through an appropriate quadrature rule,

$$\mathrm{d}\mu(t) \approx \mathrm{d}\mu_N(t) = \sum_{k=1}^{N} w_k \delta(t - x_k), \quad w_k > 0,$$

where δ is the Dirac delta function. Thereafter, the first n recursion coefficients are approximated by those of the discrete measure,

$$\alpha_k(\mathrm{d}\mu) \approx \alpha_k(\mathrm{d}\mu_N), \quad \beta_k(\mathrm{d}\mu) \approx \beta_k(\mathrm{d}\mu_N), \quad k = 1, 2, \ldots, n.$$

The approximate coefficients are computed by a discretized Stieltjes procedure. It takes $N \gg n$ and uses Darboux's formulae in (11.5) for $k \leq n-1$, computing the inner products as finite sums by

$$(p, q)_N = \int_{\mathbb{R}} p(t)q(t)\,\mathrm{d}\mu_N(t) = \sum_{k=1}^{N} w_k p(x_k)q(x_k).$$

All aspects of discretization methods, theoretical and practical, are carefully analyzed by Gautschi in [GA**81**] (questions of convergence, problems of computing recursion coefficients of discrete measures, appropriate choices of discretizations, numerical stability of the procedure, etc.). The idea of discretizing inner products appeared already in the 1968 paper [GA**31**], where the discretization is effected by the Fejér quadrature rule. Because of Gautschi's important contributions, the method is now known as the *discretized Stieltjes–Gautschi procedure*.

11.2.3. Lanczos algorithm

An alternative approach for obtaining the recursion coefficients of a discrete measure is the Lanczos algorithm, which is based on ideas of Lanczos and Rutishauser (for details see [GA**146**] and Gautschi's book from 2004 [GAB3, pp. 97–98]).

11.3. Examples of interesting classes of orthogonal polynomials

Walter's work and his contributions in the constructive theory of orthogonal polynomials allow the construction of many new classes of polynomials and their application in diverse areas of applied and numerical analysis (numerical integration,

interpolation processes, integral equations, probability, moment-preserving spline approximation, summation of slowly convergent series, approximation theory, etc.), as well as in many other areas of applied and computational science.

In this subsection we mention some interesting nonclassical measures $\mathrm{d}\mu(t) = w(t)\,\mathrm{d}t$ for which the recursion coefficients $\alpha_k(\mathrm{d}\mu)$, $\beta_k(\mathrm{d}\mu)$, $k = 0, 1, \ldots, n-1$, have been obtained in the literature and used in the construction of Gaussian quadratures and other applications of orthogonal polynomials. Many interesting examples, including discrete and continuous measures, were considered by Gautschi [GA**81**] in order to illustrate the strengths and weaknesses of the various constructive methods and to test the underlying theory.

1) Christoffel's example $\mathrm{d}\mu(t) = [(1-k^2t^2)(1-t^2)]^{-1/2}\,\mathrm{d}t$ on $[-1,1]$, $0 < k < 1$, was treated in [GA**81**, GA**94**] by the method of moments, using modified moments relative to Chebyshev polynomials of the first kind.

2) The logarithmic weight $w(t) = t^\alpha \log(1/t)$, $\alpha > -1$, on $(0,1)$ was first considered by Piessens and Branders [28] for some particular values of α. Gautschi [GA**81**, GA**117**] gave a complete stability analysis and used the modified moments relative to shifted Jacobi polynomials [GA**67**] in his construction, even for the more general measure $\mathrm{d}\mu(t) = t^\alpha(1-t)^\beta \log(1/t)\,\mathrm{d}t$, where $\alpha, \beta > -1$.

3) The half-range Hermite measure $\mathrm{d}\mu(t) = \exp(-t^2)\,\mathrm{d}t$ on $[0,\infty)$ was dealt with in [GA**81**] by using the discretized Stieltjes–Gautschi procedure. Orthogonal polynomials with respect to the same measure, but on a finite interval $[0,c]$ (Maxwell velocity distribution), were considered for $c = 1$ and $n = 10$ by Steen, Byrne, and Gelbard [30]. A stable construction is given by Gautschi in [GA**122**].

4) Polynomials orthogonal with respect to multiple-component distributions, e.g., $\mathrm{d}\mu(t) = [(1-t^2)^{-1/2} + a]\,\mathrm{d}t$ on $[-1,1]$, $a > 0$ (adding a multiple of the Legendre weight function to the Chebyshev weight function), was considered in [GA**81**].

5) In [GA**90**] Gautschi developed constructive methods for a class of polynomials orthogonal on two symmetric intervals with respect to the measure $\mathrm{d}\mu(t) = w(t)\,\mathrm{d}t$ on $[-1,1]$, where

$$w(t) = \begin{cases} |t|^\gamma (t^2-\zeta^2)^p (1-t^2)^q, & t \in [-1,-\zeta] \cup [\zeta,1], \\ 0 \text{ elsewhere}, & 0 < \zeta < 1,\ p > -1,\ q > -1,\ \gamma \in \mathbb{R}. \end{cases}$$

An analysis is given of certain phenomena of instability in connection with nonlinear recursions. The special case $\gamma = 1$, $p = q = -1/2$, $\zeta = (1-r)/(1+r)$ $(0 < r < 1)$ arises in the study of the diatomic linear chain (cf. J. C. Wheeler [34]). Gautschi showed how to use the recurrence relations for related polynomials orthogonal on $[\zeta,1]$ to generate the coefficients β_k in the desired three-term recurrence relation. For certain special values of the parameters p, q and γ, he obtained β_k explicitly in closed form. For general parameters, the theory of this class of polynomials has previously been studied by Barkov [2]. In 1989 Locher [14] obtained an explicit

representation of these polynomials in the case $\gamma = 0$ (and in some other cases where γ is an even integer), from which the recurrence relation can be derived.

6) The Airy weight $w(t) = \exp(-t^3/3)$ on $(0, +\infty)$ was considered in the chemistry literature [13], but the numerical results obtained were accurate to only $1-2$ decimal digits (cf. also Section 15.1). The inhomogeneous Airy functions $\mathrm{Hi}(t)$ and $\mathrm{Gi}(t)$ arise in theoretical chemistry (e.g. in harmonic oscillator models for large quantum numbers); their integral representations [13] are given by

$$\mathrm{Hi}(t) = \frac{1}{\pi}\int_0^{+\infty} w(x)e^{xt}\,dx,$$
$$\mathrm{Gi}(t) = -\frac{1}{\pi}\int_0^{+\infty} w(x)e^{-xt/2}\cos\Big(\frac{\sqrt{3}}{2}\,xt + \frac{2\pi}{3}\Big)\,dx.$$

These functions can effectively be evaluated by Gaussian quadrature relative to the Airy weight $w(t)$ once the orthogonal polynomials with respect to this weight are known. Gautschi [GA**84**] computed their recursion coefficients for $n = 15$ to 16 decimal digits after the decimal point, using standard double-precision arithmetic.

7) The reciprocal gamma function $w(t) = 1/\Gamma(t)$ as a weight function on $(0, +\infty)$ was considered by Gautschi in [GA**80**]. It could be useful as a probability density function in reliability theory (see Fransén [10]).

8) Einstein's and Fermi's weight functions on $(0, +\infty)$,

$$w_1(t) = \varepsilon(t) = \frac{t}{e^t - 1} \qquad \text{and} \qquad w_2(t) = \varphi(t) = \frac{1}{e^t + 1},$$

arise in solid state physics. (For this example, see also Section 15.5.) For $w_1(x)$, $w_2(x)$, $w_3(x) = \varepsilon(x)^2$ and $w_4(x) = \varphi(x)^2$, in a joint paper with Walter Gautschi [GA**93**], we determined the recursion coefficients α_k and β_k for $n = 40$ to 25 decimal digits, and gave an application of the respective Gauss–Christoffel quadratures to the summation of slowly convergent series whose general term is expressible in terms of a Laplace transform or its derivative. (For this, see also Section 25.2, Vol. 3) It was our first joint paper. The story of our collaboration has recently been told by Walter Gautschi [GA**201**] on the occasion of my 60th anniversary. Our collaboration has started in the mid eighties of the last century, just at the time when Walter developed his constructive theory of orthogonal polynomials. I was then in my thirties, so his influence on my scientific work and my further development was of crucial importance; for this I am very grateful to him.

9) For the hyperbolic weights on $(0, +\infty)$,

$$w_1(t) = \frac{1}{\cosh^2 t} \qquad \text{and} \qquad w_2(t) = \frac{\sinh t}{\cosh^2 t},$$

I constructed the recursion coefficients α_k, β_k for $n = 40$ to 30 decimal digits [19] using the discretized Stieltjes–Gautschi procedure with a discretization based on

the Gauss–Laguerre quadrature rule. The Gaussian quadratures relative to these weights were used in the summation of slowly convergent series (for details see [19–21]); see also Dahlquist [7–9] and [25] for related work.

10) The weight distribution $\mathrm{d}\mu(t) = t^{\alpha}K_0(t)\,\mathrm{d}t$ on $[0,\infty)$, $\alpha > -1$, where K_0 is the modified Bessel function, arose in work of R. Wong [35]. In [GA**81**] Gautschi showed how to decompose and discretize the inner product $(p,q) = \int_0^{\infty} p(t)q(t)\,\mathrm{d}\mu(t)$ in order to apply an appropriate Stieltjes–Gautschi procedure. Recently, Gautschi [GA**169**] described procedures for the high-precision calculation of the modified Bessel function $K_\nu(t)$, $0 < \nu < 1$, and the Airy function $\mathrm{Ai}(t)$, for positive arguments t, as prerequisites for generating Gaussian quadrature rules having these functions as a weight function.

Recent progress in symbolic computation and variable-precision arithmetic now makes it possible to generate the coefficients α_k and β_k in the three-term recurrence relation (11.1) directly by using the original Chebyshev method in sufficiently high precision. Respective symbolic/variable-precision software for orthogonal polynomials is available (Gautschi's package `SOPQ` in *Matlab* — see Section 23, Vol. 3 — and the *Mathematica* package `OrthogonalPolynomials` [5, 26]). Thus, all that is required is a procedure for the (symbolic) calculation of the moments in variable-precision arithmetic. Gautschi [GA**176**] illustrates this approach in the case of orthogonal polynomials having such unorthodox weight functions as $1 + \sin(1/t)$ on $[0,1]$, or $\exp(-t - 1/t)$ on $[0,\infty]$, which are respectively densely oscillating at one endpoint, or exponentially decaying at both. In each case the moments of the weight function are expressible in terms of special functions which can be evaluated to arbitrary precision. Similarly, in [GA**195**] Gautschi considered Freud and half-range Hermite polynomials, Bose–Einstein polynomials, and Fermi–Dirac polynomials.

Very recently, Gautschi [GA**205**] considered orthogonal polynomials relative to the Jacobi weight function $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha, \beta > -1$, but orthogonal on a strict subinterval $[-c,c]$ or $[-1,c]$, $0 < c < 1$, especially with regard to their numerical computation. Such sub-range Jacobi polynomials $\pi_k(x)$ can be expressed in terms of polynomials orthogonal on $[-1,1]$ relative to the weight function $w(ct)$ resp. $w(\frac{1}{2}(1+c)t - \frac{1}{2}(1-c))$ and constructed using a discretized Stieltjes–Gautschi procedure. Gautschi also considered corresponding Gaussian quadrature rules.

11.4. Christoffel modifications of the measure – modification algorithms

Let $\mathrm{d}\mu(t)$ be a positive measure with finite support $\mathrm{supp}(\mathrm{d}\mu) = [a,b]$,

$$u(t) = \pm\prod_{k=1}^{\ell}(t-u_k), \quad v(t) = \prod_{k=1}^{m}(t-v_k)$$

be two real polynomials, relatively prime and not vanishing on $[a, b]$, the sign + or − in $u(t)$ being chosen so that $u(t)/v(t) > 0$ on $[a, b]$. Define a new measure

$$\mathrm{d}\widehat{\mu}(t) = \frac{u(t)}{v(t)}\,\mathrm{d}\mu(t), \quad t \in [a, b]. \tag{11.6}$$

The main problem is to generate the three-term recurrence coefficients of the modified measure (11.6), $\widehat{\alpha}_k = \alpha_k(\mathrm{d}\widehat{\mu})$ and $\widehat{\beta}_k = \beta_k(\mathrm{d}\widehat{\mu})$, from those of the original measure, $\alpha_k = \alpha_k(\mathrm{d}\mu)$ and $\beta_k = \beta_k(\mathrm{d}\mu)$. Methods for implementing this transformation are known as *modification algorithms*. The first result in this area is due to Christoffel [4], who in 1858 expressed $u(t)\pi_n(t;\,\mathrm{d}\widehat{\mu})$, when $v \equiv 1$ and $\mathrm{d}\mu(t) = \mathrm{d}t$, in determinantal form as a linear combination of orthogonal polynomials $\pi_{n+\nu}(t;\,\mathrm{d}\mu)$, $\nu = 0, 1, \ldots, \ell$. The case with $v(t) \not\equiv 1$ was solved hundred years later by Uvarov [31].

Modifications by linear and quadratic factors and divisors play an important role in the computational use of orthogonal polynomials. Subsequent to a paper of Galant [11], who considered modification by a linear factor, Gautschi [GA**77**] in 1982 developed general modification algorithms for linear and quadratic factors $u(t) = t - x$ and $u(t) = (t - x)^2 + y^2$ and analogous divisors. Based on work by Verlinden [32], these methods can be simplified considerably and in this simplified form are included in Gautschi's book [GAB3, §2.4] along with *Matlab* software. An interesting quadratic factor is $u(t) = (t - x)^2$. It can be treated by techniques of numerical linear algebra (cf. [GA**170**]). Namely, in order to obtain $J_n(\,\mathrm{d}\widehat{\mu})$ one applies a single step of the QR algorithm with shift x to the Jacobi matrix $J_{n+2}(\,\mathrm{d}\mu)$ of order $n + 2$ and then discards the last two rows and columns of the resulting matrix.

In [GA**134**] Gautschi (with Shikang Li) considered $\mathrm{d}\widehat{\mu}(t) = [\pi_n(t;\,\mathrm{d}\mu)]^2\,\mathrm{d}\mu(t)$ and constructed the orthogonal polynomials $\pi_n(t;\,\mathrm{d}\widehat{\mu})$ and their recursion coefficients from the coefficients $\alpha_k(\mathrm{d}\mu)$ and $\beta_k(\mathrm{d}\mu)$ of the polynomials $\pi_n(t;\,\mathrm{d}\mu)$. They proposed a stable computational algorithm, which uses a sequence of QR steps with shifts, but for all four Chebyshev measures they obtained the desired coefficients analytically in closed form. These ideas have been used in [6] to develop a rational algorithm for quadratic Christoffel modification and to apply it to constrained L^2-approximation.

Recently, Gautschi [GA**206**] has developed algorithms for computing the recursion coefficients in the three-term recurrence relation of *repeatedly* modified orthogonal polynomials, the modifications involving division of the orthogonality measure by linear functions with real or complex coefficients. Several interesting examples are given, including Bose–Einstein distributions and the Szegő–Bernstein measure.

11.5. Sobolev-type orthogonal polynomials

In the last two decades, interest arose, and grew, in the development of orthogonal polynomials with respect to an inner product of Sobolev type, i.e., involving derivatives up to a given order with corresponding positive measures. There is a

growing literature on this kind of orthogonal polynomials, largely concerned with analytic and algebraic properties (cf. [15]). Computational aspects were first discussed systematically by Gautschi and his student M. Zhang [GA**145**], where the inner product considered is a bilinear functional involving derivatives up to some order s (≥ 1) with arbitrary positive measures $\mathrm{d}\mu_\nu$, $\nu = 0, 1, \ldots, s$,

$$(p, q)_{H_s} = \sum_{\nu=0}^{s} \int_{\mathbb{R}} p^{(\nu)}(t) q^{(\nu)}(t)\, \mathrm{d}\mu_\nu(t). \tag{11.7}$$

Here H_s denotes the Sobolev space $H_s(\mathbb{R}) = \{f : \sum_{\nu=0}^{s} \int_{\mathbb{R}} [f^{(\nu)}(t)]^2\, \mathrm{d}\mu_\nu(t) < \infty\}$. They developed two numerical methods for determining the coefficients in the (long) recurrence relation for orthogonal polynomials of Sobolev type,

$$\pi_{k+1}(t) = t\pi_k(t) - \sum_{\nu=0}^{k} \beta_\nu^k \pi_{k-\nu}(t), \quad k = 0, 1, \ldots.$$

The first is based on modified moments of the constitutive measures and generalizes what for ordinary orthogonal polynomials is known as "modified Chebyshev algorithm". The second is a generalized Stieltjes–Gautschi procedure. The numerical features of these methods are illustrated in the case of old, as well as new, Sobolev orthogonal polynomials. The coefficients in the recurrence relation can be used to compute the zeros of $\pi_n(t)$ as eigenvalues of an upper Hessenberg $n \times n$ matrix. Based on numerical experimentation, a number of conjectures are formulated with regard to the location and interlacing properties of the respective zeros.

In [GA**151**] Gautschi develops two recursive schemes for computing a special class of Sobolev-type orthogonal polynomials, considered previously by F. Marcellán and A. Ronveaux [16]. The inner product involves functions with an arbitrary positive measure $\mathrm{d}\mu(t)$ on $\mathbb{R}$, and a derivative of fixed order r with a one-point atomic measure, i.e., $[f, g] = (f, g) + f^{(r)}(c)g^{(r)}(c)$, $r \geq 1$, $c \in \mathbb{R}$, and $(f, g) = \int_{\mathbb{R}} f(t)g(t)\, \mathrm{d}\mu(t)$. Gautschi combines in an elegant way known algebraic properties of such Sobolev orthogonal polynomials with algorithmic ideas of his own to arrive at effective methods for computing these polynomials numerically. He illustrates them in the case of Hermite, Laguerre and Legendre measures, and uses them to explore numerically the zeros of the respective Sobolev-type orthogonal polynomials.

In the very interesting paper [GA**153**] Gautschi and Kuijlaars, using potential-theoretic methods, study the asymptotic distribution of zeros and critical points of Sobolev polynomials π_n orthogonal with respect to the inner product (11.7) with $s = 1$, assuming that $\mathrm{d}\mu_0$ and $\mathrm{d}\mu_1$ are compactly supported positive measures on the real line with finite total mass and infinite $\Sigma = \mathrm{supp}(\mu_0) \cup \mathrm{supp}(\mu_1)$. Under appropriate assumptions they show that the critical points (zeros of π_n') have a canonical asymptotic limit distribution supported on the real line. In certain cases the zeros themselves have the same asymptotic limit distribution. They also give a new result on zero distributions of asymptotically extremal polynomials.

11.6. Further extensions and applications

Gautschi's work on the constructive theory of orthogonal polynomials has had a great impact on the general development of the theory of orthogonal polynomials and led to many new applications of orthogonal polynomials in numerical integration, interpolation processes, approximation and optimization theory, spline theory, integral and differential equations, linear algebra, and in many other fields of applied and computational science. In particular, the development of appropriate software has encouraged a number of new applications. His article [GA**81**] alone is cited over 150 times (according to the Web of Science) in papers from the previously mentioned areas of mathematics, mechanics, computer science, physics, chemistry, engineering, etc.

In conclusion, I would like to mention a few generalizations and applications of Gautschi's ideas in my own work.

(a) *Construction of s-orthogonal polynomials.* These polynomials $\{\pi_{n,s}(t)\}_{n=0}^{\infty}$ (with a fixed $s \in \mathbb{N}$) are characterized by the nonlinear orthogonality relation

$$\int_{\mathbb{R}} t^{\nu}[\pi_{n,s}(t)]^{2s+1}\,\mathrm{d}\mu(t) = 0, \quad \nu = 0, 1, \ldots, n-1,$$

and play an important role in the construction of so-called Turán quadratures with multiple nodes (cf. [23]). In [18] we first reinterpret these relations as ordinary orthogonality conditions relative to the positive measure (implicitly defined) $\mathrm{d}\mu_{n,s}(t) = [\pi_{n,s}(t)]^{2s}\,\mathrm{d}\mu(t)$,

$$\int_{\mathbb{R}} t^{\nu}\pi_{n,s}(t)\,\mathrm{d}\mu_{n,s}(t) = 0, \quad \nu = 0, 1, \ldots, n-1,$$

and then apply Gautschi's idea of the discretized Stieltjes procedure to the corresponding system of nonlinear equations. In a joint paper with Walter Gautschi [GA**154**], and more recently in [GA211], the method was applied to construct Gauss–Turán quadrature formulae. (For this, see also Section 15.5.) These methods have led to further progress in the theory of quadratures with multiple nodes.

(b) *Orthogonal polynomials on radial rays.* In 1997 I introduced a class of polynomials orthogonal on radial rays in the complex plane [22]. For the numerical construction of the corresponding recurrence coefficients I used a generalized Stieltjes–Gautschi procedure [24].

(c) *Multiple orthogonal polynomials.* A nice survey of these polynomials, known also as Hermite–Padé polynomials, was given by Aptekarev [1]. In 2003, with my student Stanić, I gave an application of the generalized Stieltjes–Gautschi procedure to the numerical construction of a special class of multiple orthogonal polynomials (see [27]). Using these polynomials, we also described a method for the stable construction of Borges quadrature rules [3].

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12

Polynomials orthogonal on the semicircle

Lothar Reichel

In two papers, jointly with Henry J. Landau and Gradimir V. Milovanović, Walter Gautschi investigates polynomials that are orthogonal with respect to a non-Hermitian inner product defined on the upper half of the unit circle in the complex plane. For special choices of the weight function, these polynomials are related to Jacobi polynomials. Their recurrence relation and properties of their zeros are investigated, and applications to Gauss quadrature are explored. We first discuss the importance of orthogonal polynomials that satisfy recurrence relations with few terms, and then focus on the special properties of orthogonal polynomials on the semicircle.

12.1. Recurrence relations for orthogonal polynomials

Orthogonal polynomials are important in analysis, approximation theory, and computational mathematics. They provide a convenient basis both to express and compute polynomial approximants. The $n \times n$ matrix determined by the recursion coefficients for the first $n+1$ orthogonal polynomials is helpful for computing the nodes and weights of the n-point Gauss quadrature rule. Moreover, orthogonal polynomials form the foundation for numerous iterative methods in linear algebra, including the conjugate gradient method for the solution of large linear systems of equations with a symmetric positive definite matrix, and the symmetric Lanczos process for the computation of a few selected eigenvalues and associated eigenvectors of a large symmetric matrix. Very nice discussions of the many applications of orthogonal polynomials in scientific computation is provided by Gautschi in his survey article [GA**170**] as well as in his wonderful book [GAB3]. Further examples of usage of orthogonal polynomials in linear algebra can be found in the recent book by Golub and Meurant [8].

The symmetric Lanczos process is a manifestation of the Stieltjes procedure for generating the recursion coefficients for polynomials orthogonal with respect to an

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inner product on a real interval. These polynomials satisfy a three-term recurrence relation. The symmetric Lanczos process is the foundation for the conjugate gradient method for the iterative solution of large linear systems of equations with a symmetric positive definite matrix. The existence of a recurrence relation for the orthogonal polynomials with few terms reduces the computational effort and storage requirement for the conjugate gradient method. The availability of these recurrence relations also reduces the computational effort required by the symmetric Lanczos process for the computation of a few selected eigenvalues and associated eigenvectors of a large symmetric matrix. Analogously, the three-term recurrence relation for orthogonal polynomials is fundamental for the efficiency of the QR algorithm for the computation of all eigenvalues and possibly eigenvectors of a symmetric matrix. A variant of this algorithm is commonly applied to compute the nodes and weights of Gauss quadrature rules associated with a positive measure on a real interval; see, e.g., [GA**170**], [8, Secs. 6.2.3, 10]. The use of orthogonal polynomials for data-fitting is natural and the existence of a three-term recursion relation reduces the computational effort; see, e.g., Elhay et al. [7] and Gautschi [GA**170**, Sec. 4].

The above discussion illustrates that the existence of orthogonal polynomials that satisfy a recurrence formula with few terms is of significant interest in scientific computation. The aforementioned numerical methods use the three-term recurrence relations of polynomials that are orthogonal with respect to an inner product defined by a nonnegative measure on a real interval. Also matrix-valued polynomials that are orthogonal with respect to a symmetric positive definite matrix-valued measure satisfy a three-term recurrence relation and find applications in scientific computation; see, e.g., [2], [8, Sec. 2.7].

Polynomials that satisfy short recurrence relations different from three-term relations are of interest in computations as well. For instance, Szegő polynomials and the associated reversed polynomials satisfy pairs of short recurrence relations. Szegő polynomials find numerous applications in statistics and signal processing [10, 12], and their recurrence relations form the basis for an efficient QR algorithm for computing all eigenvalues, and possibly also all eigenvectors, of a unitary upper Hessenberg matrix [9, 19]. This QR algorithm can be applied to compute the nodes and weights of Gauss–Szegő quadrature rules associated with a positive measure on the unit circle [12]. The short recurrence relations of Szegő polynomials are important for the development of efficient algorithms for data-fitting applications as well; see, e.g., [1].

Orthogonal polynomials with respect to most inner products with support in the complex plane do not satisfy a short recurrence relation or pairs of short recurrence relations. For this reason the inner product sometimes is replaced by a bilinear form chosen to obtain families of polynomials that satisfy short recurrence relations. These polynomials give rise to oblique projection methods, such as the nonsymmetric Lanczos process, and they can be used in iterative methods for the solution of large linear systems of equations with a square nonsymmetric matrix, and for the computation of a few eigenvalues and associated eigenvectors of such

a matrix; see, e.g., Brezinski [3] for discussions and applications. A difficulty with these methods is that the recurrence formulas may break down and then require a special recovery procedure; see, e.g., Brezinski et al. [4] and references therein.

In 1985, before the publication of the first paper by Gautschi and Milovanović [GA**95**] on orthogonal polynomials on the semicircle, only polynomials orthogonal with respect to an inner product on an interval or on a circle were known to satisfy recurrence relations with few terms and not to suffer from the possibility of break down. The results of this paper and of the more complete investigations [GA**97**, GA**104**] therefore were quite surprising. The uncovering of the many nice properties of orthogonal polynomials on the semicircle was very important for analysis, approximation theory, and computational mathematics, and has spurred related work. The following subsection describes some important properties of orthogonal polynomials on the semicircle and the last subsection discusses some applications and more recent work.

12.2. Orthogonal polynomials on the semicircle

Let w be a weight function that is positive at infinitely many points in the open interval $(-1, 1)$, is integrable on this interval, and can be extended to a function $w(z)$ holomorphic in the open unit half disk $D_+ = \{z \in \mathbb{C} : |z| < 1, \operatorname{Im}(z) > 0\}$; the function w may be singular at ± 1. Introduce the inner product

$$(f, g) = \int_\Gamma f(z)g(z)w(z)(iz)^{-1}dz = \int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})d\theta, \tag{12.1}$$

where $i = \sqrt{-1}$ and Γ is the upper unit semicircle in the complex plane $\mathbb{C}$. Also define the inner product

$$[f, g] = \int_{-1}^1 f(x)\bar{g}(x)w(x)dx, \tag{12.2}$$

where the bar denotes complex conjugation. All integrals are assumed to exist, possibly as suitably defined improper integrals. The inner product (12.2) is positive definite. Therefore, there is a family of infinitely many monic orthogonal polynomials $\{p_j\}_{j=0}^\infty$ such that

$$[p_j, p_k] \begin{cases} > 0, & j = k, \\ = 0, & j \neq k, \end{cases} \qquad j, k = 0, 1, 2, \dots .$$

The inner product (12.1) is non-Hermitian. It therefore is not obvious that there is a family of infinitely many monic orthogonal polynomials $\{\pi_j\}_{j=0}^\infty$ such that

$$(\pi_j, \pi_k) \begin{cases} \neq 0, & j = k, \\ = 0, & j \neq k, \end{cases} \qquad j, k = 0, 1, 2, \dots .$$

Gautschi et al. [GA**104**] showed that under the mild restriction

$$\mathrm{Re}\,(1,1) = \mathrm{Re}\left(\int_0^\pi w(e^{i\theta})d\theta\right) \neq 0,$$

the orthogonal polynomials π_j exist. Moreover, they can be expressed in terms of the orthogonal polynomials p_j. Specifically, we have

$$\pi_k(z) = p_k(z) - i\theta_{k-1}p_{k-1}(z), \qquad k = 0, 1, 2, \dots\ , \quad p_{-1}(z) = 0, \tag{12.3}$$

where

$$\theta_{k-1} = \frac{\mu_0 p_k(0) + iq_k(0)}{i\mu_0 p_{k-1}(0) - q_{k-1}(0)}, \qquad k = 0, 1, 2, \dots\ .$$

The $q_k(0)$ denote the values of the associated polynomials

$$q_k(z) = \int_{-1}^{1} \frac{p_k(z) - p_k(x)}{z - x} w(x)dx, \qquad q_{-1}(z) = -1,$$

at the origin, and $\mu_0 = (1, 1)$ is the zeroth moment with respect to the inner product (12.1). Using the fact that the polynomials p_k satisfy a three-term recurrence relation, Gautschi et al. [GA**104**] obtain from (12.3) that the polynomials π_k satisfy a three-term recurrence relation of the form

$$\pi_{k+1}(z) = (z - i\alpha_k)\pi_k(z) - \beta_k\pi_{k-1}(z), \qquad k = 0, 1, 2, \dots\ , \tag{12.4}$$

with $\pi_{-1}(z) = 0$ and $\pi_0(z) = 1$.

The recursion formula (12.4) indicates that the eigenvalues of the tridiagonal matrix

$$J_k = \begin{bmatrix} i\alpha_0 & 1 & & & \mathrm{O} \\ \beta_1 & i\alpha_1 & 1 & & \\ & \beta_2 & i\alpha_2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & & 1 \\ \mathrm{O} & & & \beta_{k-1} & i\alpha_{k-1} \end{bmatrix} \in \mathbb{C}^{k\times k}$$

are the zeros of π_k.

If the weight function w satisfies $w(z) = w(-z)$ and $w(0) > 0$, then the subdiagonal entries of the matrix J_k are real, and J_k can be transformed to a real matrix. Moreover, Gautschi et al. [GA**104**, Thm. 6.2] show that all zeros of the orthogonal polynomials π_k live in the open upper half of the unit disk in $\mathbb{C}$ except possibly for a single zero on the positive imaginary axis.

Finally, Gautschi et al. [GA**104**, Thm. 6.2] discuss the special case of Jacobi- and Gegenbauer-type weight functions. The latter are given by

$$w(z) = (1 - z^2)^{\lambda-1/2}, \qquad \lambda > -\frac{1}{2}, \tag{12.5}$$

where the fractional powers are understood in terms of their principal branches. The zeros of the orthogonal polynomials π_k, $k \geq 2$, associated with a Gegenbauer-type weight function (12.5) are shown to be simple, distributed symmetrically with respect to the imaginary axis, and contained in the open upper unit half disk. Further results on the zeros of polynomials orthogonal on the semicircle are presented by Gautschi in [GA**113**].

12.3. Extensions and applications

A fairly natural modification of the work by Gautschi et al. [GA**97**, GA**104**] is to consider an inner product on a subarc of the upper half of the unit circle. De Bruin [6] investigated properties of polynomials orthogonal with respect to a possibly non-Hermitian inner product on an arc of the unit circle, symmetric with respect to the imaginary axis. Functions of the second kind and Stieltjes polynomials for such inner products are described by Milovanović and Rajković [17]. Milovanović [16] discusses Gauss quadrature rules and provides error bounds for integrals defined on the semicircle. Relations of polynomials orthogonal on the semicircle or on a circular arc to polynomials orthogonal with respect to an inner product on certain contours in $\mathbb{C}$ are explored by Milovanović and Rajković [15]. Applications of orthogonal polynomials on the semicircle to differentiation are described by Caliò et al. [5], and their use in zero-finders is commented on by Petković et al. [18]; see also Milovanović [13, 14] for discussions on applications. A recent account of orthogonal polynomials on the semicircle can be found in Gautschi [GAB3, Sec. 1.8].

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13

Chebyshev quadrature

Jaap Korevaar

Here we review Gautschi's work on Chebyshev quadrature, first his 1975 survey paper, and then original work by him and his colaborators.

13.1. Advances in Chebyshev quadrature

The paper [GA**55**] gives an account of the history and developments in Chebyshev quadrature, which is still quite valuable today. Gautschi begins by developing precise terminology. Let $d\mu$ be a positive measure on a finite or infinite interval J, with endpoints a, b, that has finite power moments $\mu_r = \int_J x^r d\mu(x)$ of all orders $r \geq 0$. One now considers quadrature formulas with equal weights,

$$\int_J f(x)d\mu(x) = \sum_{k=1}^{n} \frac{c}{n} f(x_k) + R_n(f), \quad c = c^{(n)},\ x_k = x_k^{(n)}. \tag{13.1}$$

Gautschi calls this a *Chebyshev quadrature rule* if $R_n(f) = 0$ for all polynomials of degree $\leq n$ (so that $c = \mu_0$), and all nodes x_k are *real*. He speaks of a Chebyshev quadrature rule *in the strict sense* if the nodes are distinct and contained in J. Finally, *any* formula (13.1) with real nodes is called a Chebyshev-*type* quadrature formula. The nodes need not be distinct and the rule need not be polynomially exact to any degree (not even degree zero).

The monic polynomial of degree n with zeros $x_k = x_k^{(n)}$ is denoted by $p_n(x; d\mu)$. For a Chebyshev quadrature rule, the polynomial can be obtained from the moments μ_r. They give the power sums of the roots up to degree n, so that the coefficients can be obtained by using symmetric functions. The roots may now be computed to any degree of accuracy. Formula (13.1) is a Chebyshev quadrature rule if and only if all roots of $p_n(x; d\mu)$ as obtained from $\mu_0, \ldots, \mu_n$ are real.

Gautschi first surveys the case (13.1) with $J = [-1, 1]$ and $d\mu(x) = dx$. Here Chebyshev computed the *classical* "Chebyshev quadrature rules" (with only real

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nodes) for $n = 2, 3, \ldots, 7$. A little later, Radau found such a rule for $n = 9$, and a formula involving nonreal nodes for $n = 8$. The ingenious work by Bernstein in the 1930s finally showed that for the measure $d\mu(x) = dx$, there are no cases with only real nodes beyond those that were known already. Subsequent authors have computed the formulas with complex nodes for larger n, and studied the distribution of the roots of $p_n(x; d\mu)$ in the complex plane.

Gautschi next discusses Chebyshev's construction of $p_n(z; d\mu)$ for the case $J = [-1, 1]$ and $d\mu(x) = (1 - x^2)^{-\frac{1}{2}} dx$. It leads to what is now called the Chebyshev polynomial $T_n(z)$ and to the corresponding Gauss-type quadrature formula with equal weights. Of course he also mentions Ullman's extension, which at the time came as quite a surprise. Next there is a thorough discussion of nonexistence results, also for other intervals and measures. In this area Gautschi published his paper [GA**50**]; see below. He also includes a simple proof of the fact that no Gauss-type quadrature formula on $[-1, 1]$, except the one mentioned above, is at the same time a Chebyshev formula for each n.

For Chebyshev-*type* quadratures the report surveys the maximum degree of polynomial exactness $p = p_n(d\mu)$. For $J = [-1, 1]$ and $d\mu(x) = dx$, Bernstein had already obtained the inequality $p < 4\sqrt{n}$. In this context one may now mention a 1993 paper by Kuijlaars [9].

The next subject is optimal Chebyshev-type quadratures of various kinds. Here it is natural that multiple nodes appear. In this area Gautschi published four papers: [GA**46**] (jointly with H. Yanagiwara), [GA**53**] (jointly with L.A. Anderson), [GA**57**] and [GA**58**] (jointly with G. Monegato), of which only the first and the last are reviewed separately. Here we also mention later work by the reviewer and Meyers [3].

Multidimensional Chebyshev-type quadrature problems have been considered by J. L. H. Meyers in his PhD thesis [10], and by the reviewer and Meyers in [4], [5]; cf. the reviewer's survey [6]. The problem of finding $\mathcal{O}(n^2)$ suitable nodes on the two-sphere (with area measure) is related to the Chebyshev-type problem for the interval $J = [-1, 1]$ and $d\mu(x) = dx$. In this connection one may mention the recent work [1] of Bondarenko, Radchenko and Viazovska on the sphere-conjecture of the reviewer and Meyers; cf. also (with thanks to Kuijlaars) the related work of Kane [2].

We finally mention papers by the reviewer and L. Bos [7], cf. [8], on a characterization of algebraic curves by Chebyshev quadrature.

13.2. Chebyshev-type quadratures

The paper [GA**46**] by Gautschi and Yanagiwara deals with Chebyshev-type quadrature for $J = [-1, 1]$ and $d\mu(x) = dx$. It ties in with Bernstein's result that formula (13.1) (with real nodes) can have algebraic degree of exactness $p = n$ only when $n \leq 7$ and $n = 9$. In that case the nodes are symmetric with respect to the origin,

so that in fact, $p = 2[n/2] + 1$. In order to obtain useful formulas for other degrees, the authors (primarily) deal with the following modified problem. Determine real symmetric nodes x_k which minimize

$$\left|R_n\left(x^{p+1}\right)\right| \quad \text{with } p = 2[n/2] - 1, \tag{13.1}$$

subject to the constraint that $R_n(x^j) = 0$ for $j = 1, 2, \ldots, p$. For $n = 8$ and $n \geq 10$, the authors show that every real solution must have multiple nodes, as was suggested by empirical work in the literature. By Bernstein's work there must be nonreal nodes when $n \geq 20$. For $n = 8$ and $10 \leq n \leq 19$ the authors compute symmetric nodes, and conclude that for $n = 12$ and $n \geq 14$, the modified problem has no solution with only real nodes.

In [GA**50**] Gautschi deals with Chebyshev-type quadratures on $[0, \infty)$ and $(-\infty, \infty)$. It was known that for Laguerre or Hermite weights, there cannot be Chebyshev formulas in the strict sense when $n \geq 3$, or for $n \geq 4$, respectively. Gautschi shows that for such weights, Chebyshev-type quadratures likewise exist only for certain severely limited values of n.

The paper [GA**58**] by Gautschi and Monegato is, in a sense, a continuation of [GA**46**]. In that paper the nodes were chosen so as to minimize $\left|R_n\left(x^{p+1}\right)\right|$ with $p = 2[n/2] - 1$. Here it is shown, among other things, that the same nodes in fact minimize $|R_n(x^j)|$ for every $j \geq p + 1$.

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14

Kronrod and other quadratures

Giovanni Monegato

This section is devoted to Gautschi's work on Kronrod quadratures and other special quadrature rules. For Gauss-type quadrature rules, see Section 15.

14.1. Kronrod rules

The most popular quadrature rules for the approximation of integrals, defined on bounded or unbounded intervals, are certainly the Gaussian ones. Given any "weight function" $w(x)$ having constant sign on the interval of integration (a, b) and finite moments, the Gaussian rule is an interpolatory formula of the form

$$\int_a^b w(x)f(x)dx = \sum_{i=1}^{n} w_{ni} f(x_{ni}) + R_n(f) =: G_n(f) + R_n(f)$$

whose nodes $\{x_{ni}\}$ coincide with the n zeros of the polynomial of degree n orthogonal on (a, b) with respect to $w(x)$. It is the unique quadrature rule having maximum degree of exactness $2n - 1$. Several representations for the remainder term $R_n(f)$ have been derived under different smoothness assumptions on the function f. While these are of interest for knowing the convergence behavior of the rule when the function f has a given smoothness property, they are of little help to obtain an error estimate for a given choice of the number n of nodes, not necessarily large.

A practical criterion commonly used to obtain such an estimate for any given value of n is

$$|R_n(f)| \approx |G_n(f) - G_m(f)|$$

with $m \approx n + 1$, when the function f is very smooth, and $m \approx 2n$ otherwise. Notice that the Gaussian rules associated with two different values of n may have at most one common node. This happens when both rules have an odd number of nodes symmetrically distributed in the interval (a, b), that is, when the weight function w is an even function with respect to the midpoint of the interval. Thus

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the computational cost of the above estimate runs from a minimum of $2n+1$ to a maximum close to $3n$ function evaluations. Notice also that to apply this criterion, one has to know *a priori* the degree of smoothness of the function f. Moreover, even if this is known, it may not be obvious how to choose $m \geq n+1$.

In 1964 A. S. Kronrod [5] proposed a practical and very efficient technique for estimating $R_n(f)$ in the case of the Gauss–Legendre rule. This new approach, taking $m = 2n+1$ regardless of the degree of smoothness of f and for $G_m(f)$ a $(2n+1)$-point quadrature rule, here denoted by $K_{2n+1}(f)$, has the abovementioned minimum (total) cost of $2n+1$ function evaluations. The rule $K_{2n+1}(f)$ is taken to be of interpolatory type and of the form

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} w_{ni}^{(1)} f(x_{ni}) + \sum_{j=1}^{n+1} w_{nj}^{(2)} f(y_{nj}) =: K_{2n+1}(f), \tag{14.1}$$

where the nodes $\{x_{ni}\}$ are those of the n-point Gauss–Legendre formula $G_n(f)$ while the additional nodes $\{y_{nj}\}$, and all weights, are chosen so that the degree of exactness of $K_{2n+1}(f)$ is at least $3n+1$ ($3n+2$ when n is odd). Kronrod constructed this rule for all $n \leq 40$. The tables he presented show that the new abscissas are real, symmetric, contained in $(-1,1)$, and alternate with the x_{ni}'s; moreover, all the weights are positive. Gautschi [GA177] in a short note published in 2005 pointed out that the same idea was suggested much earlier in 1894 by R. Skutsch.

Quadrature theory tells us that the polynomial $E_{n+1}(x)$ of degree $n+1$ having the nodes $\{y_{ni}\}$ as zeros must satisfy the orthogonality relations

$$\int_{-1}^{1} P_n(x)E_{n+1}(x)x^k dx = 0, \quad k = 0, 1, \ldots, n,$$

where $P_n(x)$ is the Legendre polynomial of degree n, whose zeros define the abscissas $\{x_{ni}\}$. It was I. P. Mysovskih [11] in 1964 and, independently, P. Barrucand [1] in 1970, who pointed out that such polynomials $E_{n+1}(x)$ have been studied already by Stieltjes [19] in 1894 and later in 1935 by G. Szegő [20] in the more general case of ultraspherical (or Gegenbauer) orthogonal polynomials $P_n^{(\lambda)}(x)$ with weight function $w(x) = (1-x^2)^{\lambda-1/2}$, $\lambda > -\frac{1}{2}$, on $(-1,1)$. Szegő in fact showed that for $0 < \lambda \leq 2$ the zeros of the corresponding polynomial $E_{n+1}^{(\lambda)}(x)$, now called *Stieltjes polynomial*, are all in $(-1,1)$, are distinct, and interlace with those of $P_n^{(\lambda)}(x)$. Thus, for the above values of the parameter λ, the Kronrod rule $K_{2n+1}^{(\lambda)}$, having degree at least $3n+1$, exists. Nothing was known, however, about the case $\lambda \notin (0,2]$, or the more general case of Jacobi weight functions $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha, \beta > -1$.

To my knowledge, Gautschi [GA**107**] has been the first to draw attention to the above (earlier) work of Mysovskih.

Concerning other types of classical weight functions, Ramskiĭ [17] in 1974 published a paper where the Kronrod idea was applied to the Gauss–Laguerre and

Gauss–Hermite quadrature rules. In particular, he constructed the new "extended" rules for all values of $n \leq 20$. In the Laguerre case, the additional nodes are real only for $n = 1$, although one being negative, and the associated weights are positive; for $2 \leq n \leq 20$ some of the nodes are complex. In the Hermite case, the Kronrod rule exists, with all nodes real, only when $n = 1, 2, 4$, and the weights in these cases are all positive. In that same year, this paper was reviewed by Walter Gautschi for Mathematical Reviews (MR0353638 (50#6121)).

At the end of August 1974, when I started my stay at Purdue University to do research under the supervision of Walter Gautschi, he showed me the review of Ramskiĭ's paper and proposed to prove a conjecture stated therein. This introduced me to Kronrod's work.

After several attempts without success, I gave up and started to examine some questions related to the Legendre case. Some preliminary results were published in 1976 (see [7]). But the major issue was the positivity of all the weights of Kronrod quadrature rules in the case of the ultraspherical weight. In 1977, when I had already returned to the University of Turin, I succeeded to prove positivity when $0 < \lambda \leq 1$ [8]. In that same year, a partial answer to the original research proposal made by Gautschi was given by David Kahaner and myself [4]. We were able, indeed, to prove nonexistence, except for the values of n stated by Ramskiĭ, of Kronrod extended rules with real nodes and positive weights. A proof in the case where positivity of the weights is not required is not yet known.

Some results on existence and nonexistence of Kronrod rules associated with the Gegenbauer and Jacobi weights are mentioned in my 1982 survey paper [9]. But it is in the Gautschi and Notaris paper [GA**109**] of 1988 that this question has been treated more systematically by numerical computation. For values of $n \leq 40$ the authors determined intervals in λ, resp. regions of the (α, β)-plane in the Jacobi case, for which the corresponding Kronrod rules exist and have all the desired properties. On the basis of this computational work, they made several conjectures concerning existence and properties of Kronrod rules, which gave some guidance for further research. A few of them have been proved later by F. Peherstorfer and his collaborators.

Indeed, in 2000, F. Peherstorfer and K. Petras [15] were able to show that in the ultraspherical case, for $\lambda > 3$ and n sufficiently large, the Stieltjes polynomials have only a few real zeros. On the other hand, for $\lambda = 3$ and n sufficiently large, all nodes of the Kronrod rules are real and have the desired interlacing property and some, but not all, of the weights are positive. The case $\lambda \in (2, 3)$ is still open. The same authors have also derived existence/nonexistence results in the Jacobi case for special choices of the parameters α, β. More recently, in 2007, Peherstorfer and de la Calle Ysern [16] examined the case $\lambda < 0$. They proved that all nodes of the Kronrod rules are real, contained in $(-1, 1)$ except for two of them, and interlace, and that all weights are positive.

Kronrod-type extended rules can also be associated with Gauss–Lobatto and Gauss–Radau rules; some results on their existence and properties are mentioned

in [9], where new Kronrod rules, defined on $(-1,1)$ and associated with the weight function

$$w(x) = \frac{\sqrt{1-x^2}}{1-\tau x^2}, \quad -\infty < \tau \leq 1,$$

were also considered, and their existence proved for all values of n, with all nodes in $(-1,1)$. For these, Gautschi and T. J. Rivlin [GA**111**] in 1988 proved that all the weights are positive; furthermore they produced explicit formulae for the weights. A year later, Gautschi and Notaris [GA**114**] considered the more general case of any one of the four Chebyshev weights divided by an arbitrary quadratic polynomial that remains positive in $[-1,1]$. They showed that, except for a very few identified exceptions, the Kronrod rules exist with all the desirable properties, and their degrees of exactness grow like $4n$, rather than $3n$, as in the usual case. Similar properties have been proved also in the case of a positive *linear* divisor polynomial. In 1990, it was shown independently by Notaris [12] and Peherstorfer [13] that Kronrod rules exist, with positive weights, even when the above divisor is an arbitrary (positive) polynomial of degree $m \leq n$.

In the same year, Perherstorfer [14] considered another large class of weight functions of the form

$$w(x) = \sqrt{1-x^2}|D(e^{i\theta})|^2, \quad x = \cos\theta,\ \theta \in [0,\pi],$$

where $D(z)$ is analytic, real on R, and $D(z) \neq 0$ for $|z| \leq 1$. Also for this class he showed that the associated Kronrod rules exist and have the desired properties for n sufficiently large.

In 1988 Gautschi [GA**107**] wrote a very nice and complete survey paper on Kronrod rules, which became a standard reference for researchers working on Stieltjes polynomials and Kronrod quadratures.

The last paper related to this topic was written by Walter Gautschi together with Walter Gander in 2000 (see [GA**160**]). It dealt with the construction of an adaptive automatic integration routine, based on two (successively) nested Kronrod extensions of a 4-point Gauss–Lobatto rule. The development of this new algorithm, which includes a particularly efficient stopping criterion, was motivated by some serious deficiencies the authors had detected in two adaptive integration routines provided at the time by Matlab. From the numerical testing performed by the authors, their new routine, for which they provided a Matlab code, showed excellent performance, even when compared with the best IMSL and NAG routines available at that time. The interest in this new routine is also evidenced by 135 (till now) citations in the Web of Science, with an average per year of more than 10. In most of the citing papers, the new routine is used to solve a variety of problems arising in several areas of engineering (including medical and biological engineering) and in mathematical finance, applied statistics, computational and physical sciences. The paper has also stimulated a few authors to search for further improvements. We mention in particular the works of T. O. Espelid [2], L. F. Shampine [18], and of P. Gonnet [3].

14.2. Quadratures for functions having singular or difficult behaviors

Another theme that has attracted the attention of Walter Gautschi has been the numerical integration of functions having singularities on or near the interval of integration that tend to adversely affect convergence of standard quadrature rules.

In the note [GA**30**] published in 1967, Gautschi examined the convergence of two well-known quadrature rules of interpolatory type already studied by L. Fejér in 1933. Their abscissas are the zeros of the Chebyshev polynomials of the first and second kind. Specifically, Gautschi showed that they converge not only for continuous functions, but also for functions having monotonic (integrable) singularities at one or both endpoints of the interval of integration.

In [GA**128**] he considered integrals extended over the half-infinite interval $(0, \infty)$, whose integrands have an algebraic singularity at the origin of type x^α, $\alpha > -1$, and behave like $x^{-\beta}$, $\beta > 1$, as $x \to \infty$, with $\beta - \alpha > 1$. For such integrals he examined two types of quadrature formulae, both of the form

$$\int_0^\infty w(x) f(x) dx \approx \sum_{k=1}^{n} w_k f(x_k). \tag{14.2}$$

The first, introduced earlier by R. Kumar and M. K. Jain in [6], is the Gaussian rule defined by the weight function

$$w(x) = \frac{x^\alpha}{(1+x)^\beta}\,. \tag{14.3}$$

Thus it has maximum polynomial degree of exactness $2n - 1$. In the second, Gautschi sets $w(x) = x^\alpha$ and determines the nodes and weights by requiring exactness of the rule for all of the following functions $f(x)$:

$$\frac{1}{(1+x)^{\beta+k}}\,, \quad k = 0, 1, \ldots, 2n-1.$$

The first rule has the severe limitation $2n < \beta - \alpha$ on the number n of nodes, and thus can be applied only when β is relatively large. Gautschi's rule does not have this drawback. In his paper, Gautschi has shown that both rules can be reduced to Gaussian formulae relative to appropriate Jacobi weight functions, and hence can be generated by standard mathematical software. Numerical testing recently performed in [10] confirms that the rule proposed by Gautschi, besides being very easy to construct, is indeed very efficient.

Gautschi's quadrature rule can also be interpreted as a formula of type (14.2), with $w(x)$ given by (14.3), which has the property that it integrates exactly the rational functions $(1+x)^{-k}$, $k = 0, 1, \ldots, 2n-1$. Thus it is a Gaussian rule based on rational interpolation. Quadrature formulas of this type have subsequently been

proposed and studied independently in [GA**137**] and by W. Van Assche and I. Vanherwegen in [21]. For additional work in this area, see Section 15.4.

Finally, in the 1993 paper [GA**136**], Gautschi examined the numerical evaluation of two integrals of interest in solid state physics and in many astrophysical problems, the generalized Fermi–Dirac integrals

$$F_k(\eta,\theta)=\int_0^\infty \frac{x^k\sqrt{1+\theta x/2}}{e^{-\eta+x}+1}dx,\quad \theta\ge 0,\ \eta\in\mathbb{R},$$

where $k=\frac{1}{2},\frac{3}{2},\frac{5}{2}$, and the associated Bose–Einstein integrals

$$G_k(\eta,\theta)=\int_0^\infty \frac{x^k\sqrt{1+\theta x/2}}{e^{-\eta+x}-1}dx,\quad \theta\ge 0,\ \eta\le 0.$$

Gautschi pointed out that two methods proposed 1989 and 1991 in the physics literature disregard the major obstacle to rapid convergence (when θ is relatively small), namely the presence of a sequence of (complex conjugate) poles at

$$x=\eta\pm(2\nu-1)\mathrm{i}\pi,\quad \nu=1,2,3,\dots,$$

in the case of F_k, and at

$$x=\eta\pm 2\nu\mathrm{i}\pi,\quad \nu=0,1,2,\dots,$$

for G_k. Starting from this observation, he then proposed a new and more efficient approach, based on a (rational) quadrature formula of the type

$$\int_0^\infty g(x)x^m e^{-x}dx\approx\sum_{r=1}^n w_r g(x_r),$$

which erases the adverse effects of the poles in the vicinity of the real line. In the case of F_k, he sets $m=k$ and (uniquely) defines the rule by requiring exact integration of all pairs of rational functions

$$g(x)=(1+\zeta_\nu x)^{-1},\quad g(x)=(1+\zeta_\nu^* x)^{-1},\quad \nu=1,2,\dots,n,$$

where

$$\zeta_\nu=-\frac{1}{\eta+(2\nu-1)\mathrm{i}\pi}$$

and the asterisk means complex conjugation. For G_k, he sets $m=k-1$ and proceeds as in the previous case, choosing

$$\zeta_\nu=-\frac{1}{\eta+2\nu i\pi}\ .$$

As shown by the author through numerical testing, the proposed rules are very satisfactory for high-precision calculation of Fermi–Dirac and Bose–Einstein integrals, in particular when this evaluation is required only for a few values of their parameters.

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15

Gauss–type quadrature

Walter Van Assche

Walter Gautschi's work in this area has had a profound impact, especially on the computational and practical aspects of Gauss quadrature. I have heard people refer to it as *Gautschian quadrature*, just to emphasize Walter's many contributions to the theory and computation.

To fix notation, suppose one wants to approximate the integral of a function f by a sum using only n evaluations of the function:

$$\int_a^b f(x)\,d\mu(x) = \sum_{k=1}^{n} \lambda_{k,n} f(x_{k,n}) + E_n(f). \tag{15.1}$$

Here the general case is considered where integration is with respect to a positive measure μ on the real line, supported on the finite or infinite interval $[a,b]$, but quite often only a weight function w on $[a,b]$ is used. If $\{x_{k,n} : 1 \le k \le n\}$ are the zeros of the nth-degree orthogonal polynomial p_n for the measure μ, i.e.,

$$\int_a^b p_n(x)x^k\,d\mu(x) = 0, \qquad 0 \le k \le n-1,$$

one can find weights $\{\lambda_{k,n} : 1 \le k \le n\}$ such that $E_n(f) = 0$ for every polynomial f of degree at most $2n-1$, and hence the quadrature gives the exact value of the integral for polynomials of degree less than or equal to $2n-1$. These weights are known as *Christoffel weights* or *Christoffel numbers*, and the quadrature formula is known as the *Gauss quadrature formula* or, as Walter Gautschi usually calls it, the *Gauss–Christoffel quadrature formula*. In his book [GAB3, §1.4.2] Gautschi uses the term Gauss-type quadrature to refer to this class of quadrature formulas, including those modified by Radau and Lobatto (cf. Section 15.2). Carl Friedrich Gauss originally (1816 [5]) considered the case where μ is the uniform measure on $[-1,1]$, for which the corresponding quadrature nodes are the zeros of the Legendre polynomial P_n; Elwin Bruno Christoffel [2] in 1877 extended this to more general weight functions.

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Szegő calls it *Gauss–Jacobi* mechanical quadrature in his book [10, §3.4], whereas Stroud and Secrest [9] refer to it as *Gaussian quadrature formulas* in their book (which contains many tables).

15.1. Construction of Gauss quadrature formulas

For the construction of Gauss quadrature formulas one basically needs to compute the n zeros $x_{1,n} < \cdots < x_{n,n}$ of the orthogonal polynomial p_n and the Christoffel numbers $\{\lambda_{j,n} : 1 \le j \le n\}$. The measure μ is given and one needs the first $2n$ moments $(\mu_k)_{0\le k\le 2n-1}$ of μ to find the zeros and the Christoffel numbers:

$$\mu_k = \int_a^b x^k \, d\mu(x) = \sum_{j=1}^{n} (x_{j,n})^k \lambda_{j,n}, \qquad 0 \le k \le 2n-1.$$

Gautschi shows in [GA**31**] that the map $(\mu_k)_{0\le k\le 2n-1} \mapsto (x_{j,n}, \lambda_{j,n})_{1\le j\le n}$ is ill conditioned and gives some lower bounds for the condition number κ_n showing that for a large class of weights on $[-1, 1]$ this κ_n grows exponentially like $(17+6\sqrt{8})^n = (1+\sqrt{2})^{4n}$ and he concludes that

> "The lesson to be learned from this analysis is evident: the moments are not suitable, as data, for constructing Gauss–Christoffel quadrature formulas of large order n. Apart from the fact that they are not always easy to compute, small changes in the moments (due to rounding, for example) may result in very large changes in the Christoffel numbers."

He proposes an alternative procedure in which the inner product involving the measure μ (or weight w) is replaced by a discrete inner product

$$\langle f, g\rangle_N = \sum_{k=1}^{N} w_{k,N} f(y_{k,N}) g(y_{k,N}), \qquad w_{k,N} > 0,$$

in such a way that

$$\lim_{N\to\infty} \langle f, g\rangle_N = \int_a^b f(x)g(x)\, d\mu(x)$$

for all polynomials f and g. In his later work he refers to this as the *discretized Stieltjes procedure* [GA**81**, §2.2], [GA**117**, §4.2]; it has since become known as the *discretized Stieltjes–Gautschi procedure* (cf. Section 11.2.2). The orthogonal polynomials $(\pi_{n,N})_{n\in\mathbb{N}}$ for this discrete inner product then have the property that

$$\lim_{N\to\infty} \pi_{n,N}(x) = p_n(x),$$

and the corresponding zeros and Christoffel numbers converge to the required quantities for the Gauss quadrature,

$$\lim_{N\to\infty} x_{j,n}^{(N)} = x_{j,n}, \quad \lim_{N\to\infty} \lambda_{j,n}^{(N)} = \lambda_{j,n}.$$

In order to be practical, one needs to find a suitable discrete inner product $\langle \cdot\,, \cdot \rangle_N$. Gautschi suggests using the Fejér quadrature formula (introduced by Fejér in 1933 [4] and studied by Gautschi in 1967 [GA**30**]) or the Gauss–Chebyshev quadrature formula to do the discretization. The convergence can be accelerated by Newton's method.

Another procedure was proposed by Sack and Donovan in 1969 and quickly picked up by Gautschi in [GA**40**]. Instead of starting from the moments

$$\mu_k = \int_a^b x^k \, d\mu(x),$$

it uses *modified moments*

$$\nu_k = \int_a^b q_k(x) \, d\mu(x),$$

where the $(q_n)_{n\in\mathbb{N}}$ are given orthogonal polynomials for a measure ν on $[\alpha, \beta]$,

$$\int_\alpha^\beta q_k(x) q_n(x) \, d\nu(x) = \delta_{k,n},$$

and hence satisfy a three-term recurrence relation

$$x q_k(x) = \alpha_{k+1} q_{k+1}(x) + \beta_k q_k(x) + \alpha_k q_{k-1}(x).$$

If one chooses the measure ν close to the measure μ (in particular with the same support $[a, b] = [\alpha, \beta]$), the mapping from the modified moments to the zeros and Christoffel numbers is often well conditioned. In [GA**40**] Gautschi gives an upper bound for the condition number and various asymptotic estimates for Jacobi weights. He also gives an algorithm for generating orthogonal polynomials $(p_n)_{n\in\mathbb{N}}$ for the measure μ, starting from the modified moments. Numerical examples (and tables of Gaussian quadrature on an accompanying microfiche supplement) show that this is indeed a very convenient way to construct Gauss quadrature formulas.

A very convincing way to show people that the mapping from moments to zeros and Christoffel numbers is ill conditioned is given in [GA**84**] where Gautschi displays a table for the nodes $\{x_{j,n} : 1 \le j \le n\}$ and Christoffel numbers $\{\lambda_{j,n} : 1 \le j \le n\}$ for $n = 15$ and weight $w(x) = e^{-x^3/3}$ on $[0, \infty)$, which appeared in the *Journal of Chemical Physics* in 1980. Table 1 shows 16 decimals but only the first two are correct. Gautschi also gives Table 2 with his own computation using a discretized Stieltjes procedure and a suitable partition of the infinite interval $[0, \infty)$ into eight subintervals. Instead of saying that the first table is wrong, Gautschi describes four tests which can be used to check the accuracy of the table and leaves it to the reader to decide that the second table is accurate to 16 decimals. He also explains why

Table 1 was thought to be accurate: it passes two of the tests. The first test is to check the quadrature formula on the moments, i.e., on the functions $f(x) = x^k$ with $0 \le k \le 2n-1$, and indeed both tables show that the quadrature formula produces the moments accurately to about 15 correct decimals. But this is an extreme case of correlation of errors. Test 2 suggested by Gautschi is to compute the coefficients in the recurrence relation

$$xp_k(x) = a_{k+1}p_{k+1}(x) + b_k p_k(x) + a_k p_{k-1}(x), \qquad k \ge 0,$$

of the orthogonal polynomials using the quadrature formula, and then to check whether

$$\mu_{2n} = \sum_{j=1}^{n} \lambda_{j,n} x_{j,n}^{2n} + a_1^2 a_2^2 \cdots a_n^2,$$

which follows from the formula for the error term $E_n(x^{2n})$ of the Gauss quadrature formula. This test too does not distinguish between the two tables. The two other tests show that Table 1 is not accurate but Table 2 is. Test 3 is to compute the recurrence coefficients using the quadrature formula and to check them with the explicit formulas in terms of Gram determinants (cf. Eq. (11.5) of Section 11.1). This test indeed shows that the accuracy of the recurrence coefficients decreases by one decimal in each step for Table 1, but remains stable for Table 2. Test 4 is to compute the sum of the nodes, which is the trace of the Jacobi matrix and which can be computed as the ratio of two determinants. This test also shows that Table 1 is only accurate to two decimals, whereas Table 2 gives 12 accurate decimals. I have computed the nodes and Christoffel numbers for this weight and $n = 15$ using Maple (which nowadays is a convenient way to perform multiprecision computations) and found that one needs to work with a precision of 45 decimals (`Digits:=45`) to produce Table 2 if one starts from the moments and uses the method with which Table 1 was generated. Gautschi's approach requires only double precision and hence is to be preferred. A Matlab suite for generating orthogonal polynomials and related quadrature rules can be found on his website `http://www.cs.purdue.edu/archives/2002/wxg/codes/` under the heading `OPQ`.

15.2. Gauss–Radau and Gauss–Lobatto quadrature

The Gauss quadrature formulas can be extended somewhat to include information of the function at the endpoints of the interval $[a, b]$. For *Gauss–Radau quadrature* one uses a fixed node at one of the endpoints a or b, and then n nodes in (a, b) are taken such that for every polynomial f of degree $\le 2n$

$$\int_a^b f(x)w(x)\,dx = \lambda_a f(a) + \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n}),$$

which is the Gauss–Radau quadrature rule with fixed left endpoint, or

$$\int_a^b f(x)w(x)\,dx = \lambda_b f(b) + \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n}),$$

which is the Gauss–Radau quadrature rule with fixed right endpoint. Even though these formulas use $n+1$ quadrature points, the effect of fixing one quadrature point is to reduce the degree of the polynomials which can be correctly integrated by one. Recall that the Gauss quadrature rule with $n+1$ points has degree of exactness $2n+1$, which is one higher than the Gauss–Radau rule. The n other nodes are all in the open interval (a,b) and turn out to be zeros of the orthogonal polynomial of degree n for the modified weight function $(x-a)w(x)$ when one fixes the left endpoint a, or $(b-x)w(x)$ when one fixes the right endpoint b. These orthogonal polynomials are known as kernel polynomials [1, §1.7] and can be expressed in terms of the Christoffel–Darboux formula.

For *Gauss–Lobatto quadrature* one uses both endpoints as fixed nodes and one looks for n nodes in (a,b) such that

$$\int_a^b f(x)w(x)\,dx = \lambda_a f(a) + \lambda_b f(b) + \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n})$$

for every polynomial f of degree $\leq 2n+1$. There are $n+2$ quadrature nodes, but two nodes are now fixed at a and b, resulting in the reduction of the polynomial degree of exactness by 2 (Gauss quadrature with $n+2$ nodes has degree of exactness $2n+3$). The n remaining nodes turn out to be the zeros of the orthogonal polynomial of degree n for the modified weight $(x-a)(b-x)w(x)$. These orthogonal polynomials can be expressed in terms of the orthogonal polynomials for the weight w by means of a formula of Christoffel [10, §2.5].

An e-mail from someone inquiring how to fix an underflow problem when computing high-order Gauss–Lobatto quadrature rules for the Legendre case $w(x)=1$ on $[-1,1]$ prompted Walter Gautschi to investigate the more general case of Jacobi weights $w(x)=(1-x)^\alpha(1+x)^\beta$ on $[-1,1]$ in [GA**163**]. The Gauss–Lobatto formula then uses the quadrature nodes ± 1 and the zeros of the orthogonal polynomials for the weight $(1-x^2)w(x)$, which is again a Jacobi weight but now with parameters $(\alpha+1,\beta+1)$. Gautschi first notes that underflow can be avoided by computing the two modified elements of the Jacobi matrix directly as functions of α and β, rather than by solving the usual 2×2 system of linear equations (which for large n becomes singular, numerically). He then gives explicit formulas for the weights λ_1 and λ_{-1} and for the interior weights in terms of the Jacobi polynomials $P_n^{(\alpha,\beta)}$ evaluated at the interior nodes. He compares the results obtained by direct computation using his formulas with the results obtained by computing the modified Jacobi matrix and the first components of the eigenvectors. The conclusion is that the direct computation using the explicit formulas is more accurate in 90% of all the 8,400 cases he investigated.

Gauss–Radau quadrature for the Jacobi weight is investigated in [GA**164**] where again explicit formulas are found for the weight at the boundary and for the interior weights in terms of the Jacobi polynomials evaluated at the interior nodes. No numerical results are presented but the explicit formula for the boundary weight is said to be more accurate than the result computed using the eigenvector of the modified Jacobi matrix. For the interior weights, however, in about two-thirds of the cases computed, the results of the direct computation are found less accurate than the results obtained by using the eigenvectors of the modified Jacobi matrix. [GA**164**] also deals with the Gauss–Radau formula for the Laguerre measure $w(x) = x^\alpha e^{-x}$ on $[0,\infty)$ and an explicit formula for the weight λ_0 is given, together with a formula for the interior weights in terms of the Laguerre polynomials evaluated at the interior nodes. Again no numerical results are presented but the conclusion is said to be much like in the case of the Jacobi weight, i.e., the boundary weight is always considerably more accurate by means of direct computation than via eigenvectors, whereas for the interior weights the result using the eigenvectors is generally more accurate than the explicit formula.

In [GA**126**] Walter Gautschi and Shikang Li extend the Gauss–Radau and Gauss–Lobatto idea by allowing the endpoints to appear with multiplicity 2. This amounts to using also the derivatives of f at the endpoints, i.e., for Gauss–Radau quadrature with fixed left endpoint

$$\int_a^b f(x)w(x)\,dx = \lambda_0 f(a) + \lambda_1 f'(a) + \sum_{j=1}^n \lambda_{j,n} f(x_{j,n}) + E_n^R(f).$$

If one takes for the n nodes $x_{j,n}$ the zeros of the orthogonal polynomial of degree n for the modified weight $(x-a)^2 w(x)$, then $E_n^R(f) = 0$ can be achieved for every polynomial of degree at most $2n+1$. Of course a similar formula can be constructed for the right endpoint. Gautschi and Li show that the weights in this quadrature formula are all positive and they give explicit formulas for the weights λ_0 and λ_1 when w is the Chebyshev weight function on $[-1,1]$ of any of the four kinds,

$$w(x) = (1-x)^{\pm 1/2}(1+x)^{\pm 1/2}.$$

They also handle the extension of Gauss–Lobatto quadrature, where

$$\int_a^b f(x)w(x)\,dx = \lambda_0 f(a) + \lambda_1 f'(a) + \sum_{j=1}^n \lambda_{j,n} f(x_{j,n}) + \mu_0 f(b) - \mu_1 f'(b) + E_n^L(f).$$

Note the negative sign before $\mu_1 f'(b)$. Choosing the n nodes $x_{j,n}$ as the zeros of the orthogonal polynomial of degree n for the weight $(x-a)^2(b-x)^2 w(x)$ then results in $E_n^L(f) = 0$ for every polynomial of degree at most $2n+3$. All the weights are again positive and the weights $\lambda_0, \lambda_1, \mu_0, \mu_1$ are explicitly given for the four Chebyshev weights. Their paper ends with various examples.

There is nothing really special about multiplicity two in Gauss–Radau or Gauss–Lobatto quadrature, so the natural next step is to consider having nodes of arbitrary multiplicity at one or both endpoints of the interval $[a, b]$. This is worked out in [GA**173**] in a general setting, and in [GA**194**] for Jacobi and Laguerre weight functions. The generalized Gauss–Radau formula has the form

$$\int_a^b f(x)w(x)\,dx = \sum_{k=0}^{r-1} \lambda_a^{(k)} f^{(k)}(a) + \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n}) + E_{n,r}^R(f),$$

where $r > 1$ is the multiplicity of the endpoint a. The degree of exactness is $2n-1+r$, i.e., one has $E_{n,r}^R(f) = 0$ for every polynomial of degree at most $2n-1+r$, if one takes for the internal nodes $\{x_{j,n} : 1 \le j \le n\}$ the zeros of the orthogonal polynomial of degree n for the weight function $(x-a)^r w(x)$. For the generalized Gauss–Lobatto quadrature, similarly,

$$\int_a^b f(x)w(x)\,dx = \sum_{k=0}^{r-1} \lambda_a^{(k)} f^{(k)}(a) + \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n}) + \sum_{k=0}^{r-1} (-1)^k \lambda_b^{(k)} f^{(k)}(b) + E_{n,r}^L(f),$$

where $E_{n,r}^L(f) = 0$ for every polynomial f of degree at most $2n-1+2r$ when the internal nodes are the zeros of the orthogonal polynomial of degree n for the weight $(x-a)^r(b-x)^r w(x)$. Note the alternating sign for the weights at the endpoint b. This is useful in the case of a symmetric weight $w(-x) = w(x)$ on a symmetric interval, where $\lambda_a^{(k)} = \lambda_b^{(k)}$ for $0 \le k \le r-1$. For questions regarding the positivity of the weights, see Section 7.6.2, Vol. 1.

Gautschi developed in [GA**173**] a routine for computing these generalized Gauss–Radau and Gauss–Lobatto formulas for arbitrary r, and Matlab routines are downloadable from his website `http://www.cs.purdue.edu/archives/2002/wxg/codes/` under the heading `HOGGRL`.

15.3. Error bounds for Gauss quadrature

So far we witnessed Gautschi's skills in constructing Gauss quadrature formulas. He also is a very skillful analyst able to find sharp bounds for the error $E_n(f)$ in Gauss quadrature on $[-1, 1]$ for functions f which are analytic in a domain D containing $[-1, 1]$. Together with Richard Varga he starts in [GA**85**] from the contour integral representation

$$E_n(f) = \frac{1}{2\pi i} \int_\Gamma K_n(z) f(z)\,dz,$$

where the kernel is

$$K_n(z) = \frac{1}{p_n(z)} \int_{-1}^{1} \frac{p_n(t)}{z-t}\,d\mu(t),$$

and Γ is a contour in D surrounding $[-1,1]$. A straightforward estimation gives

$$|E_n(f)| \le \frac{\ell(\Gamma)}{2\pi} \max_{z\in\Gamma} |K_n(z)| \max_{z\in\Gamma} |f(z)|,$$

where $\ell(\Gamma)$ is the length of the contour Γ. The first maximum depends only on μ and the second maximum only on the function f, thus separating the dependence of the error on the quadrature rule and on the function to be integrated. If Γ is the circle $\{|z| = r\}$ with $r > 1$, then Gautschi and Varga show that for a large class of measures μ the maximum of $|K_n(z)|$ is attained on the real line and is either $K_n(r)$ or $|K_n(-r)|$, and they show that it can be evaluated accurately and efficiently by recursion. This class of measures includes the Jacobi weights $d\mu(x) = (1-x)^\alpha(1+x)^\beta\,dx$ for arbitrary $\alpha, \beta > -1$. They also investigate elliptic contours $\Gamma = \{z = \frac{1}{2}(re^{i\theta} + \frac{1}{r}e^{-i\theta}), 0 \le \theta \le 2\pi\}$ for which they show that in the case of Chebyshev weights $\alpha = \beta = \pm\frac{1}{2}$ and $\alpha = -\frac{1}{2}$, $\beta = \frac{1}{2}$ the maximum of $|K_n(z)|$ is attained on the real positive axis, hence equal to $K_n((r+1/r)/2)$, except for the Chebyshev weight of the second kind ($\alpha = \beta = \frac{1}{2}$) for which the maximum is located on the imaginary axis when n is odd, and near the imaginary axis when n is even. The problem is much more complicated for general Jacobi weights; in this case some empirical results are worked out.

The problem for the elliptic contour and Chebyshev weights is taken up again in [GA**119**] with Tychopoulos and Varga, and a more detailed analysis is made for the Chebyshev weight $\alpha = \beta = \frac{1}{2}$ and n even. They show that for $r \ge r_{n+1}$, where $r_{n+1} > 1$ is the root of an explicitly stated algebraic equation, the maximum of $|K_n(z)|$ occurs on the imaginary axis while for $r < r_{n+1}$ it is near the imaginary axis within an angular distance less than $\pi/(2n+2)$. Furthermore, the sequence $(r_n)_{n\ge 2}$ decreases monotonically to 1.

A similar error bound analysis is done in [GA**123**] and [GA**121**] for Gauss–Radau quadrature and Gauss–Lobatto quadrature where the endpoints have multiplicity one and two, respectively, and integration is with respect to any of the Chebyshev weight functions. The original analysis can be carried over fairly well since most of the ingredients still involve orthogonal polynomials, albeit with a modified weight function. Furthermore, if one starts with a Chebyshev weight function, then the modified weights are still Jacobi weights and the corresponding orthogonal polynomials are linear combinations of Chebyshev polynomials.

15.4. Gauss quadrature for rational functions

The quadrature formulas so far are designed to integrate functions that are close to polynomials. If one deals with functions having poles (outside the interval of integration) or other singularities, then the best thing to do is to absorb that information in the weight function, or, which amounts to the same thing, to construct quadrature formulas that exactly integrate rational functions with prescribed location of the poles. This kind of rational quadrature is something I was interested in myself through the thesis of one of the PhD students in my department; see

[12], where we studied the case of poles of multiplicity one or two. The following characterization appears in [GA**137**] and [GA**167**]:

Theorem 1. *Let* $\{\zeta_k : 1 \le k \le M\}$ *be complex numbers such that* $-1/\zeta_k \notin [a,b]$ *and define*

$$\omega_m(x) = \prod_{k=1}^{M} (1+\zeta_k x)^{s_k}, \qquad m = \sum_{k=1}^{M} s_k,$$

where $s_k \in \mathbb{N}$. *Assume that the weight* $w(x)/\omega_m(x)$ *admits the* n*-point Gaussian quadrature formula*

$$\int_a^b f(x)\frac{w(x)}{\omega_m(x)}\,dx = \sum_{j=1}^{n} w_{j,n}^G f(x_{j,n}) + E_n^G(f),$$

with $E_n^G(f) = 0$ *for every polynomial* f *of degree at most* $2n-1$. *Then*

$$\int_a^b g(x)w(x)\,dx = \sum_{j=1}^{n} \lambda_{j,n} g(x_{j,n}) + E_n(g), \qquad \lambda_{j,n} = w_{j,n}^G \omega_m(x_{j,n}), \tag{15.2}$$

has the property that

$$E_n(g) = 0 \quad \text{if} \quad \begin{cases} g(x) = (1+\zeta_k x)^{-s}, & k = 1,2,\dots,M,\ s = 1,2,\dots,s_k, \\ g(x) = x^k, & k = 0,1,2,\dots,2n-m-1. \end{cases}$$

Hence one can construct n-point quadrature formulas for rational functions by using the n-point Gaussian quadrature formula for the weight $w(x)/\omega_m(x)$ which has prescribed poles outside $[a,b]$ with given multiplicities. Furthermore, Gautschi describes in [GA**137**] and [GA**167**] a way to compute the quadrature formula (15.2), either by a partial fraction decomposition and modification algorithms, or by the discretization method, which we described earlier. A number of examples illustrate the efficiency of the quadrature rule. Some other types of rational quadrature rules are also given in [GA**167**] such as the rational Fejér quadrature rule, rational Gauss–Kronrod quadrature, rational Gauss–Turán quadrature, and rational Cauchy principal value quadrature. The latter three are described in more detail in [GA**162**], where many numerical examples are given.

15.5. Gauss quadrature for special weights

The methods for constructing orthogonal polynomials, their recursion coefficients and the corresponding Gaussian quadrature, which were proposed by Gautschi, have been applied to a number of interesting explicit cases. In [GA**93**] Walter Gautschi and Gradimir Milovanović worked out the details for the weights

$$\epsilon_r(x) = \frac{x^r}{(e^x-1)^r}, \quad \varphi_r(x) = \frac{1}{(e^x+1)^r}, \qquad x \in [0,\infty),$$

for $r = 1$ and $r = 2$. The weight ϵ_1 is known as the *Einstein function* and φ_1 as the *Fermi function*. Integrals involving the functions ϵ_r occur in phonon statistics, lattice specific heats, and in the study of radiative recombination processes. Integrals involving the functions φ_r are encountered in the dynamics of electrons in metals and heavy doped semiconductors. For the weights ϵ_r $(r = 1, 2)$ they propose to compute the recursion coefficients of the orthogonal polynomials by means of a discretized Stieltjes–Gautschi procedure based on the Gauss–Laguerre quadrature rule, which uses the zeros of the Laguerre polynomial L_n as quadrature nodes. This indeed makes a lot of sense since $\epsilon_1(x) \sim xe^{-x}$ and $\epsilon_2(x/2) \sim x^2e^{-x}$ as $x \to \infty$, so that these weights behave near infinity as the weight $w(x) = e^{-x}$ for Laguerre polynomials, up to polynomial growth. A different procedure is suggested for the weights φ_r because the poles $\pm i\pi$ of these weights are closer to the real axis. Instead, a composite Fejér quadrature rule is proposed where the interval $[0,\infty)$ is decomposed into four subintervals $[0,10] \cup [10,100] \cup [100,500] \cup [500,\infty]$. These methods are illustrated by a number of numerical results. Tables of the recursion coefficients are included in the appendix of [GA**93**] and the quadrature nodes and quadrature weights are included in a supplement to [GA**93**]. A particularly interesting application is the summation of certain series $\sum_{n=1}^{\infty}(\pm 1)^n a_n$ where a_n is expressible as a Laplace transform or the derivative of a Laplace transform. Indeed, if

$$a_n = \int_0^\infty f(t)e^{-nt}\,dt,$$

then

$$\sum_{n=1}^{\infty}(-1)^{n-1}a_n = \int_0^\infty \frac{f(t)}{e^t+1}\,dt = \int_0^\infty f(t)\varphi_1(t)\,dt,$$

and when

$$a_n = \int_0^\infty tf(t)e^{-nt}\,dt = -\frac{d}{dx}\int_0^\infty f(t)e^{-xt}\,dt\bigg|_{x=n},$$

then

$$\sum_{n=1}^{\infty} a_n = \int_0^\infty f(t)\frac{t}{e^t-1}\,dt = \int_0^\infty f(t)\epsilon_1(t)\,dt.$$

Several examples of infinite series of this type are worked out, showing the efficiency of Gauss quadrature for evaluating slowly converging infinite series. Particularly useful is the advice they give for each example and ways to circumvent problems that occur.

In [GA**154**] Gautschi and Milovanović join forces again, but now their interest is in constructing *Gauss–Turán quadrature* rules, which are of the form

$$\int_{-1}^{1} f(x)\,dx = \sum_{i=0}^{k-1}\sum_{j=1}^{n} A_{i,j} f^{(i)}(x_{j,n}) + E_{n,k}(f),$$

using the derivatives $f^{(i)}$ for $0 \le i \le k-1$ at the quadrature nodes. Turán showed that for $k = 3$ the nodes can be chosen in such a way that the formula is exact for polynomials f of degree at most $4n-1$. In general one can choose the nodes $\{x_{j,n} : 1 \le j \le n\}$ in such a way that $E_{n,k}(f) = 0$ for polynomials of degree $\le (k+1)n-1$ whenever $k = 2s+1$ is odd, but this does not work when k is even. The nodes are zeros of the monic polynomial π_n that minimizes the L^{k+1} norm

$$\int_{-1}^{1} [\pi_n(x)]^{k+1}\,dx.$$

This can be extended to positive measures $d\mu$ on the real line and Gauss–Turán quadrature is possible for $k = 2s+1$ odd, with nodes being the zeros of the monic polynomial π_n minimizing the $L^{k+1}(\mu)$ norm. This minimization is equivalent to the conditions

$$\int_{\mathbb{R}} [\pi_n(x)]^{2s+1} x^r\,d\mu(x) = 0, \qquad r = 0, 1, \ldots, n-1,$$

and the corresponding polynomials π_n are known as *s-orthogonal polynomials*. Gautschi and Milovanović observe that these s-orthogonal polynomials are the polynomials $\pi_{n,n}$ from a sequence of orthogonal polynomials $(\pi_{k,n})_{k\le n}$ for the varying weight $[\pi_n(x)]^{2s}\,d\mu(x)$:

$$\int_{\mathbb{R}} [\pi_n(x)]^{2s} \pi_{k,n}(x) x^j\,d\mu(x) = 0, \qquad j = 0, 1, \ldots, k-1.$$

Note, however, that the s-orthogonal polynomials π_n are implicitly defined in this way, since the varying measure involves the polynomial π_n. Gautschi and Milovanović propose a method for computing the recurrence coefficients of the orthogonal polynomials starting from an initial guess for the unknown polynomial π_n and then applying an iterative procedure (Newton-Kantorovič method) to compute the recursion coefficients of the orthogonal polynomials $(\pi_{k,n})_{0\le k\le n}$, which in the end gives the required $\pi_n = \pi_{n,n}$. The elements in the Jacobian, which one needs for the Newton method, are integrals which can all be computed exactly by using Gaussian quadrature for the (nonvarying) measure μ taking $(s+1)n$ quadrature nodes. The procedure is illustrated with numerical examples. For the Chebyshev measure of the first kind on $[-1, 1]$, the monic polynomials minimizing

$$\int_{-1}^{1} \frac{|\pi_n(x)|^{k+1}}{\sqrt{1-x^2}}\,dx, \qquad k \ge 0,$$

are the monic Chebyshev polynomials of the first kind $T_n(x)/2^{n-1}$, hence the nodes for the Gauss–Turán formula are $\cos((2j-1)\pi/2n)$, $1 \le j \le n$.

In his most recent paper [GA211], Gautschi returns to Gauss–Turán quadrature, suggesting an improvement of the procedure described above in the case of Laguerre and Hermite weight functions.

Another example where Gautschi's construction of Gauss quadrature rules works well is Gauss quadrature for refinable weight functions, which appear in multiresolution analysis and wavelet analysis in particular. In [GA**161**] Gautschi worked with Laura Gori and Francesca Pitolli on Gaussian quadrature for a weight ϕ satisfying

$$\phi(x) = \sum_{j\in\mathbb{Z}} a_j \phi(2x-j),$$

where

$$a_j = 2^{-h}\left[\binom{m+1}{j} + 4(2^{h-m}-1)\binom{m-1}{j-1}\right], \qquad h \geq m \geq 2.$$

The function ϕ is only computable at dyadic points

$$x_k = -\frac{m+1}{2} + k\cdot 2^{-r}, \qquad k = 0,1,2,\ldots,(m+1)2^r,$$

hence these points are used for the discrete inner product needed for the discretization method. The inner product is taken as Simpson's quadrature. Numerical results and examples illustrate the proposed procedure.

The more recent paper [GA**198**] deals with weight functions with logarithmic factors, such as $v(x) = x^\alpha e^{-x}(x-1-\log x)$ on $[0,\infty)$ and $w(x) = (1-x)^\alpha(1+x)^\beta \log(2/(1+x))$ on $[-1,1]$, which are logarithmic modifications of the Laguerre weight and the Jacobi weight, respectively. The procedure is to use a (symbolic) modified Chebyshev algorithm based on ordinary as well as modified moments executed with sufficiently high precision. The natural choice for modified moments for the weight v is to use Laguerre polynomials,

$$\nu_k = \int_0^\infty x^\alpha e^{-x}(x-1-\log x)L_k^\alpha(x)\,dx,$$

and for w it is natural to make the change of variable $x = 2t-1$ and use the shifted Jacobi polynomials,

$$\nu_k = \int_0^1 t^\beta(1-t)^\alpha \log(1/t) P_k^{(\alpha,\beta)}(2t-1)\,dt.$$

These modified moments can be expressed explicitly in terms of special functions and evaluated to arbitrary precision. As usual, a number of examples illustrate the numerical results.

15.6. The circle theorem for Gauss-type quadrature

If one plots the n Gaussian weights (suitably normalized) against the n Gaussian nodes, one finds that, asymptotically as $n \to \infty$, they come to lie on a half circle when the weight is supported on a finite interval and satisfies a mild condition. This is known as the circle theorem and was first established by Davis and Rabinowitz [3] in 1961 for Jacobi weights $w(x) = (1-x)^\alpha(1+x)^\beta$ on $[-1,1]$.

Theorem 2. *Let w be a weight function on $[-1,1]$ in the Szegő class, i.e.,*

$$\int_{-1}^{1} \log w(x) \frac{dx}{\sqrt{1-x^2}} > -\infty$$

and suppose that $1/w \in L_1(\Delta)$ for a compact interval $\Delta \subset (-1,1)$. Then

$$\frac{n\lambda_{j,n}}{w(x_{j,n})} \sim \pi\sqrt{1-x_{j,n}^2}, \qquad n \to \infty,$$

for all nodes $x_{j,n}$ (and corresponding weights $\lambda_{j,n}$) that lie in Δ.

This theorem is useful if one wants to check whether the quadrature weights that one computed for a certain weight w are indeed reliable: if they don't follow the circle theorem, then one cannot trust the computed results. The circle theorem basically follows as a corollary of the asymptotic behavior of Christoffel functions

$$\lambda_n(x) = \frac{1}{\sum_{k=0}^{n-1} p_k^2(x)}$$

of a weight w, where $(p_n)_{n\in\mathbb{N}}$ are the orthonormal polynomials for w. Indeed, Nevai proved that

$$\lim_{n\to\infty} n\lambda_n(x) = \pi w(x)\sqrt{1-x^2} \tag{15.3}$$

holds almost everywhere in Δ under the conditions given in the theorem. The relation $\lambda_{j,n} = \lambda_n(x_{j,n})$ then gives the circle theorem. See [8, §4.5] for a discussion on asymptotics for the Christoffel functions, which shows that the idea of the circle theorem predates Davis and Rabinowitz [3]. The asymptotic behavior in (15.3) for weights w on $[-1,1]$ holds almost everywhere on an open interval $\Delta \subset [-1,1]$ under the weaker condition [7, Thm. 8]

$$\int_\Delta \log w(x)\, dx > -\infty.$$

Gautschi extends this circle theorem in [GA**180**] to Gauss–Radau and Gauss–Lobatto quadrature for weights w satisfying the conditions in Theorem 2. He also considers *Gauss–Kronrod quadrature*

$$\int_{-1}^{1} f(x)w(x)\,dx = \sum_{j=1}^{n} \lambda_{j,n} f(x_{j,n}) + \sum_{k=1}^{n+1} \lambda^*_{k,n} f(x^*_{k,n}) + E_n(f),$$

where $\{x_{j,n} : 1 \le j \le n\}$ are the Gaussian nodes and the Kronrod nodes $\{x^*_{k,n} : 1 \le k \le n+1\}$ and the weights $\{\lambda_{j,n} : 1 \le j \le n\}$ and $\{\lambda^*_{k,n} : 1 \le k \le n+1\}$ are such that $E_n(f) = 0$ whenever f is a polynomial of degree at least $3n-1$. (For Gauss–Kronrod quadrature, see also Section 14.1.) The Kronrod nodes are the zeros of the polynomial π_{n+1} which is the orthogonal polynomial of degree $n+1$ for the (nonpositive) weight $p_n(x)w(x)$, with p_n the orthogonal polynomial of degree n for the weight w:

$$\int_{-1}^{1} \pi_{n+1}(x)x^k p_n(x)w(x)\,dx = 0, \qquad k = 0, 1, 2, \ldots, n.$$

The Kronrod nodes are not necessarily in the interval $[-1, 1]$ and may in fact be complex, but when all the Kronrod nodes are real, distinct, in the interval $(-1, 1)$, and different from the Gauss nodes, there is indeed a chance for a circle theorem to hold. Gautschi proves such a circle theorem for Gauss–Kronrod quadrature for a restricted class of weights.

The function $\pi\sqrt{1-x^2}$ in the circle theorem and in (15.3) is in fact the reciprocal of the density of the equilibrium measure for the interval $[-1, 1]$ (the Chebyshev weight of the first kind). If one considers weights on a compact set E of the real line, then a variant of the circle theorem would be

$$\frac{n\lambda_{j,n}}{w(x_{j,n})} \sim \frac{1}{w_E(x_{j,n})},$$

where w_E is the density of the equilibrium measure of the compact set E. This holds, for instance, almost everywhere on $\Delta \subset E$ when E is a regular set and [11, Thm. 1]

$$\int_{\Delta} \log w(x)\,dx > -\infty.$$

Gautschi illustrates this when the weight w is supported on two disjoint intervals and remarks that the equilibrium measure is explicitly known for a set $E = T^{-1}([-1, 1])$, where T is a polynomial, referring to my joint work [6] with Jeff Geronimo in 1988.

Before concluding this presentation, this may be a good place to reaffirm that Walter Gautschi has written quite a few nice and interesting papers on Gauss-type quadrature, which are very influential and even essential when one plans to make numerical computations. Furthermore, he is very well aware of the existing literature, has a good taste in the choice of specific problems and examples, and

his papers are a pleasure to read. Some of the codes are available on his website `http://www.cs.purdue.edu/archives/2002/wxg/codes/` showing that he is willing to share his knowledge and results with the international community.

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Part II

Reprints

16

Papers on Orthogonal Polynomials on the Real Line

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67 On the preceding paper "A Legendre polynomial integral" by James L. Blue, Math. Comp. 33, 742–743 (1979)

75 Minimal solutions of three-term recurrence relations and orthogonal polynomials, Math. Comp. 36, 547–554 (1981)

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207 Neutralizing nearby singularities in numerical quadrature, Numer. Algorithms, DOI 10.1007/s11075-012-9672-9

16.1. [67] "On the Preceding Paper "A Legendre Polynomial Integral" by James L. Blue"

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[67] "On the Preceding Paper "A Legendre Polynomial Integral" by James L. Blue," *Math. Comp.* **33**, 742–743 (1979).

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On the Preceding Paper "A Legendre Polynomial Integral" by James L. Blue

By Walter Gautschi

Abstract. The modified moments of the distribution $d\sigma(x) = x^\alpha \ln(1/x)\,dx$ on $[0, 1]$, with respect to the shifted Legendre polynomials, are explicitly evaluated.

The result in the theorem of Section 2 of [1] can be generalized as follows: Let

$$\nu_n(\alpha) = \int_0^1 x^\alpha \ln(1/x) P_n^*(x)\,dx, \qquad \alpha > -1, \quad n = 0, 1, 2, \ldots,$$

where $P_n^*(x) = P_n(2x - 1)$ is the shifted Legendre polynomial of degree n. Then

$$(1)\quad \nu_n(\alpha) = \begin{cases} (-1)^{n-m}\,\dfrac{m!^2(n-m-1)!}{(n+m+1)!}, & \alpha = m < n,\ m \geqslant 0 \text{ an integer}, \\ \dfrac{1}{\alpha+1}\left\{\dfrac{1}{\alpha+1} + \displaystyle\sum_{k=1}^{n}\left(\frac{1}{\alpha+1+k} - \frac{1}{\alpha+1-k}\right)\right\}\displaystyle\prod_{k=1}^{n}\frac{\alpha+1-k}{\alpha+1+k}, & \text{otherwise.} \end{cases}$$

The result in [1] is the case $\alpha = 0$ of (1). For the proof, we note that

$$\begin{aligned} \nu_n(\alpha) &= -2^{-(\alpha+1)}\int_{-1}^{1}(1+t)^\alpha \ln(\tfrac{1}{2}(1+t))P_n(t)\,dt \\ &= -2^{-(\alpha+1)}\lim_{\nu\to n}\left\{\int_{-1}^{1}(1+t)^\alpha \ln(1+t)P_\nu(t)\,dt - \ln 2\cdot\int_{-1}^{1}(1+t)^\alpha P_\nu(t)\,dt\right\}, \end{aligned} \tag{2}$$

where $P_\nu(t)$ is the Legendre function of degree ν. It is well known [2, p. 316, Eq. (15)] that

$$\int_{-1}^{1}(1+t)^\alpha P_\nu(t)\,dt = \frac{2^{\alpha+1}\Gamma^2(\alpha+1)}{\Gamma(\alpha+\nu+2)\Gamma(\alpha+1-\nu)}, \qquad \alpha > -1. \tag{3}$$

Differentiating (3) with respect to α gives

$$\begin{aligned} &\int_{-1}^{1}(1+t)^\alpha \ln(1+t)P_\nu(t)\,dt \\ &= \frac{2^{\alpha+1}\Gamma^2(\alpha+1)}{\Gamma(\alpha+\nu+2)\Gamma(\alpha+1-\nu)}\{\ln 2 + 2\psi(\alpha+1) - \psi(\alpha+\nu+2) - \psi(\alpha+1-\nu)\}, \end{aligned} \tag{4}$$

with $\psi(x) = \Gamma'(x)/\Gamma(x)$ the logarithmic derivative of the gamma function. The assertion (1) now follows by inserting (3) and (4) in (2) and by using the recurrence relations $\Gamma(x+1) = x\Gamma(x)$, $\psi(x+1) = \psi(x) + 1/x$, together with the fact that for any integer

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$r \geqslant 0$,

$$\frac{\psi(-r+\epsilon)}{\Gamma(-r+\epsilon)} \longrightarrow (-1)^{r-1} r! \quad \text{as } \epsilon \longrightarrow 0.$$

The method of proof also allows the evaluation of integrals of the form

$$\nu_{n,k}(\alpha) = \int_0^1 x^\alpha [\ln (1/x)]^k P_n^*(x)\, dx,$$

by repeatedly differentiating (4) with respect to α.

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16.2. [75] "Minimal Solutions of Three-Term Recurrence Relations and Orthogonal Polynomials"

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Minimal Solutions of Three-Term Recurrence Relations and Orthogonal Polynomials*

By Walter Gautschi

Abstract. We observe that the well-known recurrence relation $p_{n+1}(z) = (z - a_n)p_n(z) - b_n p_{n-1}(z)$ for orthogonal polynomials admits a "minimal solution" if z is outside the spectrum of the mass distribution $ds(t)$ with respect to which the polynomials are orthogonal and if the moment problem for this distribution is determined. The minimal solution, indeed, is $f_n(z) = \int p_n(t)\, ds(t)/(z - t)$, and can be computed accurately by means of the author's continued fraction algorithm. An application is made to special Gauss-type quadrature formulas.

1. Introduction. Minimal solutions of three-term recurrence relations, and their computational implications, are discussed systematically in [7]. Effective algorithms for computing minimal solutions have been developed in [7], [16], [17] and continue to be the subject of further study (see, e.g., [14], [26], [5], [2], [24], [25], [3]). With these powerful algorithms at hand, it seems desirable to delineate large classes of recurrence relations for which the presence of minimal solutions can be ascertained and the minimal solution itself identified. Even more desirable is an understanding of the deeper reasons for the occurrence of minimal solutions, in terms of intrinsic features of the subject area in which they arise.

Few attempts have been made along these lines. The work of Thacher [22], [23] on power series solution of linear differential equations with polynomial coefficients may be considered a beginning, inasmuch as the presence of minimal solutions (of the recurrence relation satisfied by the expansion coefficients) is conjectured to be related in a specified way to the type of singularities in the differential equation. Here we wish to consider the recurrence relation

$$y_{n+1} = (z - a_n)y_n - b_n y_{n-1}, \qquad n = 1, 2, 3, \ldots, \ b_n > 0, \tag{1.1}$$

associated with the moment sequence of a mass distribution $ds(t)$ on the real line. We make the simple observation, apparently overlooked so far, that for any z outside the spectrum of $ds(t)$ *the recurrence relation* (1.1) *possesses a* (*readily identifiable*) *minimal solution whenever the moment problem for* $ds(t)$ *is determined* (Section 3). If the spectrum of $ds(t)$ is bounded (i.e., there is zero mass outside some finite interval), then the moment problem is always determined; hence a minimal solution always exists.

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Our observation opens up a large class of recurrence relations to which the algorithms mentioned above can be usefully applied. One such application (to special Gaussian quadrature rules) will be discussed in Section 4, and an appropriate algorithm in Section 5.

In the case of the Jacobi distribution on $[-1, 1]$, the existence of a minimal solution (when $z \notin [-1, 1]$) can easily be inferred from the asymptotic theory of difference equations [7, Theorem 2.3]. This is no longer the case for distributions on infinite intervals, such as the generalized Laguerre, or Hermite, distribution.

2. Orthogonal Polynomials and Associated Polynomials. Let $ds(t)$ be a mass distribution on the finite or infinite interval $[a, b]$ (i.e., $s(t)$ a nondecreasing function with infinitely many points of increase), and let $ds(t)$ admit finite moments of all orders,

$$m_n = \int_a^b t^n \, ds(t), \qquad n = 0, 1, 2, \ldots. \tag{2.1}$$

Let $\{p_n(z)\}$ be the (monic) polynomials orthogonal on $[a, b]$ with respect to $ds(t)$,

$$\int_a^b p_n(t)p_m(t) \, ds(t) = 0, \qquad n \neq m. \tag{2.2}$$

As is well known, they satisfy a three-term recurrence relation of the form

$$\begin{cases} p_{n+1}(z) = (z - a_n)p_n(z) - b_n p_{n-1}(z), & n = 0, 1, 2, \ldots, \\ p_{-1}(z) = 0, \qquad p_0(z) = 1, \end{cases} \tag{2.3}$$

where a_n are real, and $b_n > 0$, all n. (b_0 is arbitrary, but will be set equal to m_0.)

The polynomials

$$q_n(z) = \int_a^b \frac{p_n(z) - p_n(t)}{z - t} \, ds(t), \qquad n = 0, 1, 2, \ldots, \tag{2.4}$$

are called the polynomials *associated* with the orthogonal polynomials p_n. It is easily seen (and well known) that they also satisfy the recurrence relation (2.3), at least for $n > 1$. Indeed, by (2.3),

$$\begin{aligned} p_{n+1}(z) - p_{n+1}(t) &= zp_n(z) - tp_n(t) - a_n[p_n(z) - p_n(t)] - b_n[p_{n-1}(z) - p_{n-1}(t)] \\ &= (z - t)p_n(t) + (z - a_n)[p_n(z) - p_n(t)] - b_n[p_{n-1}(z) - p_{n-1}(t)], \end{aligned}$$

hence, dividing by $z - t$ and integrating,

$$\begin{cases} q_{n+1}(z) = \int_a^b p_n(t) \, ds(t) + (z - a_n)q_n(z) - b_n q_{n-1}(z), & n = 0, 1, 2, \ldots, \\ q_{-1}(z) = 0, \qquad q_0(z) = 0. \end{cases} \tag{2.5}$$

By orthogonality, the integral on the right of (2.5) vanishes if $n > 0$, and equals m_0 if $n = 0$. Consequently,

$$\begin{cases} q_{n+1}(z) = (z - a_n)q_n(z) - b_n q_{n-1}(z), & n = 1, 2, 3, \ldots, \\ q_0(z) = 0, \qquad q_1(z) = m_0. \end{cases} \tag{2.6}$$

((2.6) also holds for $n = 0$, if we redefine $q_{-1}(z) = -1$ and assume $b_0 = m_0$.) Since $p_0(z) = 1, p_1(z) = z - a_0$, hence the Wronskian of p_n, q_n is equal to m_0 at $n = 0$, we see that $\{p_n(z)\}$ and $\{q_n(z)\}$ are two linearly independent solutions of the recurrence relation (1.1).

3. Minimal Solutions and the Moment Problem. A solution f_n of the recurrence relation (1.1) is said to be minimal [7] if there exists a linearly independent solution, g_n, of the same recurrence relation such that

$$\lim_{n\to\infty} \frac{f_n}{g_n} = 0. \tag{3.1}$$

We show that the existence of a minimal solution is closely related to the determinacy of the moment problem for $ds(t)$.

Let

$$F(z) = \int_a^b \frac{ds(t)}{z - t}, \qquad z \notin [a, b]. \tag{3.2}$$

It is known [18, Satz 4.1] that the integral (3.2) has an "associated continued fraction"

$$F(z) \sim \frac{b_0}{z - a_0 -} \frac{b_1}{z - a_1 -} \frac{b_2}{z - a_2 -} \cdots (b_0 = m_0), \tag{3.3}$$

where a_n, b_n are the same coefficients as those appearing in the recurrence relation (1.1). Furthermore, the nth convergent of the continued fraction in (3.3) is equal to q_n/p_n, where p_n, q_n are defined in (2.3) and (2.6), respectively,

$$\frac{b_0}{z - a_0 -} \frac{b_1}{z - a_1 -} \cdots \frac{b_{n-1}}{z - a_{n-1}} = \frac{q_n(z)}{p_n(z)}, \qquad n = 1, 2, 3, \ldots. \tag{3.4}$$

We are interested in the case in which the continued fraction in (3.3) converges to the integral $F(z)$,

$$\lim_{n\to\infty} \frac{q_n(z)}{p_n(z)} = F(z), \qquad z \notin [a, b]. \tag{3.5}$$

If (3.5) holds true, then indeed

$$f_n(z) = F(z)p_n(z) - q_n(z) \tag{3.6}$$

is a minimal solution of (1.1). This follows at once by observing that (3.5) implies

$$\frac{f_n(z)}{p_n(z)} = F(z) - \frac{q_n(z)}{p_n(z)} \to 0 \quad \text{as } n \to \infty. \tag{3.7}$$

In view of (2.4) and (3.2), we can write f_n in the alternative form

$$f_n(z) = \int_a^b \frac{p_n(t)\, ds(t)}{z - t}, \qquad z \notin [a, b], \quad n = 0, 1, 2, \ldots. \tag{3.8}$$

If we define (see the parenthetic remark after (2.6)) $b_0 = m_0$, $q_{-1}(z) = -1$, then f_n in (3.6) satisfies (1.1) not only for $n \geq 1$, but also for $n = 0$, and we obtain the convenient starting value

$$f_{-1}(z) = 1. \tag{3.9}$$

Any condition which guarantees (3.5) is a sufficient condition for (3.8) to be a minimal solution of (1.1). We now recall some such conditions. If the interval $[a, b]$ is finite, then (3.5) always holds, by virtue of Markov's theorem [18, Satz 4.2]. If $[a, b]$ is a half-infinite interval, say $[0, \infty]$, we have (3.5) if the Stieltjes moment problem for the moment sequence (2.1) is determined [18, Satz 4.14 and Satz 4.10]. A sufficient condition for the latter, due to Carleman, is [20, Theorem 1.11]

$$\sum_{n=1}^{\infty} m_n^{-1/2n} = \infty.$$

Similarly, for the doubly-infinite interval $[-\infty, \infty]$ (in which case z in (3.5) is necessarily complex), the validity of (3.5) is assured if the Hamburger moment problem for the moment sequence (2.1) is determined [18, Satz 4.15 and Satz 4.11]. Sufficient conditions for the latter, due to Carleman, are [20, Theorem 1.10 and p. 59]

$$\sum_{n=1}^{\infty} m_{2n}^{-1/2n} = \infty, \quad \text{or} \quad \sum_{n=1}^{\infty} b_n^{-1/2} = \infty.$$

Since, for a finite interval $[a, b]$, the moment problem for (2.1) is always determined [20, Corollary 1.1], we may summarize by saying that *condition* (3.5) *is satisfied, hence* $f_n(z)$ *in* (3.8) *is a minimal solution of* (1.1), *whenever the moment problem for the moment sequence* (2.1) *is determined.* Most distributions $ds(t)$ that arise in practice indeed correspond to a determined moment problem.

4. Generation of Special Gaussian Quadrature Rules. Let $ds(t)$ be a mass distribution, as in Section 2, and assume first that its support is a (finite or infinite) subinterval $[a, b]$ of the real line. Let x be real, outside of $[a, b]$, and consider the new distribution

$$d\sigma(t) = \frac{ds(t)}{|x - t|}, \qquad a \leqslant t \leqslant b, \quad x \in \mathbf{R} \setminus [a, b]. \tag{4.1}$$

Given the recurrence relation (2.3) for the orthogonal polynomials $\{p_n\}$ associated with $ds(t)$ we are interested in constructing the (monic) orthogonal polynomials $\{\pi_n\}$ with respect to $d\sigma(t)$, and the corresponding Gaussian quadrature rules, all of which clearly exists uniquely.

A good general procedure for accomplishing our task consists in first determining the coefficients α_n, β_n for the desired polynomials,

$$\begin{cases} \pi_{n+1}(z) = (z - \alpha_n)\pi_n(z) - \beta_n \pi_{n-1}(z), & n = 0, 1, 2, \ldots, \\ \pi_{-1}(z) = 0, \qquad \pi_0(z) = 1, \end{cases} \tag{4.2}$$

in terms of the coefficients a_n, b_n of the given orthogonal polynomials and in terms of the "modified moments" of $d\sigma(t)$,

$$\nu_n = \int_a^b \frac{p_n(t)\, ds(t)}{|x - t|}, \qquad n = 0, 1, 2, \ldots, \tag{4.3}$$

and then to compute the eigenvalues and first components of the corresponding eigenvectors of the tridiagonal symmetric Jacobi matrix (with elements α_n, $n = 0, 1, 2, \ldots$, on the main diagonal, and elements $\sqrt{\beta_n}$, $n = 1, 2, 3, \ldots$, on the side diagonals), using the implicit QL algorithm. For details see [8, Section 5], [10],

[9]. Although this approach may not be the best possible, in terms of efficiency (for more direct methods, see [11], [19]), it has the distinct advantage of numerical stability, particularly when the interval $[a, b]$ is finite. Essential for the success of this approach, however, is the accurate determination of the modified moments in (4.3). These are seen to be identical with $f_n(x)$ (or $-f_n(x)$, if $x < a$) in (3.8)–a minimal solution of the recurrence relation (1.1), if the moment problem for $ds(t)$ is determined. An effective algorithm for the computation of this minimal solution will be discussed in Section 5.

A similar application can be made to weight distributions of the type (cf. also [12])

$$d\sigma(t) = \frac{ds(t)}{(x-t)^2 + y^2}, \qquad a < t < b, \quad x \in \mathbf{R}, \quad y > 0, \tag{4.4}$$

where the support $[a, b]$ of $ds(t)$ may or may not coincide with the whole real line. The modified moments, in this case, are given by

$$\nu_n = \int_a^b \frac{p_n(t)\, ds(t)}{(x-t)^2 + y^2}, \qquad n = 0, 1, 2, \ldots. \tag{4.5}$$

They are easily expressed in terms of $f_n(z)$ in (3.8). Indeed, letting $z = x + iy$, and observing that

$$\frac{1}{(x-t)^2 + y^2} = -\frac{1}{2iy}\left(\frac{1}{z-t} - \frac{1}{\bar{z}-t}\right),$$

one finds immediately

$$\nu_n = -\frac{\operatorname{Im} f_n(z)}{\operatorname{Im} z}. \tag{4.6}$$

Thus again, in the case of determinacy, we can generate ν_n accurately in terms of the minimal solution $f_n(z)$ of (1.1).

5. An Algorithm for Calculating the Minimal Solution $f_n(z)$. A number of algorithms are known for computing minimal solutions of a three-term recurrence relation: Miller's backward recurrence algorithm [1, p. xvii], the author's algorithm based on continued fractions [7], Olver's algorithm [16], and an economic reformulation of Olver's algorithm due to Van der Cruyssen [24]. Our experience with these algorithms, when applied to some typical minimal solutions $f_n(z)$, has been mixed. All algorithms, but the author's, have proved prone to overflow, particularly when x is moderately close to the half-infinite interval $[a, b] = [0, \infty]$ in (4.1), and $z = x + iy$ moderately close to $[a, b] = [-\infty, \infty]$ in (4.4). The algorithms converge very slowly in these cases. We have tried to combat overflow in Olver's algorithm by rewriting it in terms of appropriate ratios, but were not entirely successful. (An alternative way of dealing with the overflow problem, at the expense of approximately doubling the work, is to use extended-range arithmetic packages, as in [21], [13].) On the other hand, our own algorithm in [7], although not subject to overflow conditions, requires good estimates of the starting index (for backward recurrence) to remain competitive with the other algorithms. Fortunately, such estimates can be derived for the most common distributions $ds(t)$ occurring in practice. For this reason, in the present context, we tend to prefer the continued fraction algorithm of

[7] over the other algorithms mentioned. As "normalizing condition" we use the simple condition (3.9), which obviates the need of computing $f_0(z)$ separately.

Suppose, then, that we wish to compute $f_n(z)$ for $n = 0, 1, 2, \ldots, N$. Let $\nu > N$, and let quantities $r_n^{(\nu)}$ and $f_n^{(\nu)}$ be generated according to

$$(5.1)\qquad \begin{cases} r_\nu^{(\nu)} = 0, & r_{n-1}^{(\nu)} = \dfrac{b_n}{z - a_n - r_n^{(\nu)}}, \qquad n = \nu, \nu-1, \ldots, 1, 0, \\ f_{-1}^{(\nu)} = 1, & f_n^{(\nu)} = r_{n-1}^{(\nu)} f_{n-1}^{(\nu)}, \qquad n = 0, 1, 2, \ldots, N. \end{cases}$$

(Recall that $b_0 = m_0$.) If $f_n(z)$ is a minimal solution of (1.1), then [7, p. 39]

$$(5.2)\qquad \lim_{\nu\to\infty} f_n^{(\nu)} = f_n(z), \qquad n = 0, 1, 2, \ldots, N.$$

To implement (5.1), (5.2), one starts with some initial value of the index ν and keeps increasing ν, say by 5, until $|f_n^{(\nu+5)} - f_n^{(\nu)}| \leqslant \varepsilon |f_n^{(\nu+5)}|$ for all $n = 0, 1, 2, \ldots, N$, where ε is an appropriate (relative) error tolerance. (Alternatively, one could apply the convergence test on the $r_{n-1}^{(\nu)}$, rather than the $f_n^{(\nu)}$, and thus avoid the computation of $f_n^{(\nu)}$ for all but the final value of ν.)

For this algorithm to be effective, it is imperative that realistic estimates be available for the initial value of the index ν, given N and the error tolerance ε. Such estimates can be derived from known asymptotic results [6] concerning the behavior of $f_n(z)$ and $p_n(z)$ for large n.

To begin with, we recall from [7, (3.18)] that the relative errors can be approximated by

$$(5.3)\qquad \varepsilon_n^{(\nu)} \doteq \frac{f_{\nu+1}}{g_{\nu+1}}\left(g_{-1} - \frac{g_n}{f_n}\right), \qquad n = 0, 1, 2, \ldots, N,$$

where $\{g_n\}$ is any solution of (1.1) which is linearly independent of the (minimal) solution $\{f_n\}$. In view of (3.7), we may choose $g_n = p_n(z)$, in which case $g_{-1} = 0$. Since $|p_n/f_n| \to \infty$ as $n \to \infty$, we have, for N sufficiently large,

$$(5.4)\qquad \max_{1\leqslant n\leqslant N} |\varepsilon_n^{(\nu)}| \doteq |\varepsilon_N^{(\nu)}| \doteq \left|\frac{f_{\nu+1}}{p_{\nu+1}} \Big/ \frac{f_N}{p_N}\right|.$$

The ratios $f_{\nu+1}/p_{\nu+1}$ ($\nu > N$) and f_N/p_N in (5.4) can be estimated, at least for some common weight distributions $ds(t)$, from the asymptotic formulas for f_n/p_n given in the Appendix of [6].

For the *Jacobi distribution* $ds(t) = (1-t)^\alpha(1+t)^\beta\, dt$ on $[-1, 1]$, where $\alpha > -1$, $\beta > -1$, for example, using Eq. (A.1) in [6], one finds for z bounded away from $[-1, 1]$ that

$$(5.5)\qquad \frac{f_{\nu+1}(z)}{p_{\nu+1}(z)} \Big/ \frac{f_N(z)}{p_N(z)} \sim \left\{\frac{1}{z + (z-1)^{1/2}(z+1)^{1/2}}\right\}^{2(\nu+1-N)}, \qquad \nu > N \to \infty,$$

independently of α and β. (In evaluating the square roots in (5.5), the principal values of $\arg(z-1)$ and $\arg(z+1)$ are to be used.) For the maximum error in (5.4) to be less than ε, we thus find for ν the estimate

$$(5.6)\qquad \nu \geqslant N + \frac{\ln(1/\varepsilon)}{2\ln|z + (z-1)^{1/2}(z+1)^{1/2}|}.$$

This is applicable to modified moments of the type (4.5), with Jacobi distribution $ds(t)$, in which case $z = x + iy$ in (4.6) is complex, with $y > 0$. The estimate (5.6) also applies to (4.3), where $z = x$ is real outside of $[-1, 1]$, and can then be written in the simpler form

$$\nu > N + \frac{\ln(1/\varepsilon)}{2\ln\left(|x| + \sqrt{x^2 - 1}\right)}, \qquad x \in \mathbf{R} \setminus [-1, 1]. \tag{5.6'}$$

The contours in (5.6), i.e., the lines of constant $\left|z + \sqrt{z^2 - 1}\right| = \rho > 1$, are ellipses with foci at ± 1 and sum of semiaxes equal to ρ; cf. [4, p. 19].

In the case of *generalized Laguerre distributions* $ds(t) = t^{\alpha}e^{-t}\,dt$ on $[0, \infty]$, where $\alpha > 0$, we apply Eq. (A.6) in [6] and combine this with the well-known asymptotic formulas [15, 9.7.1 and 9.7.2] for modified Bessel functions, to obtain,

$$\frac{f_{\nu+1}(z)}{p_{\nu+1}(z)} \Big/ \frac{f_N(z)}{p_N(z)} \sim \exp\left\{-4\left[\sqrt{\nu + 1 - \frac{\alpha+1}{2}} - \sqrt{N + \frac{\alpha+1}{2}}\right](ze^{-i\pi})^{1/2}\right\}, \tag{5.7}$$

$$\nu > N \to \infty.$$

Here, z is assumed fixed in the complex plane cut along the positive real axis, and $0 < \arg z < 2\pi$. For our maximum error in (5.4) to be less than ε, it suffices to choose ν such that

$$\nu > \left[\sqrt{N + \frac{\alpha+1}{2}} + \frac{\ln(1/\varepsilon)}{4\sqrt{|z|}\cos\frac{1}{2}(\varphi - \pi)}\right]^2 - \frac{\alpha+1}{2}, \tag{5.8}$$

$$0 < \varphi = \arg z < 2\pi.$$

The contours in (5.8), i.e., the lines of constant $\sqrt{|z|}\cos\frac{1}{2}(\varphi - \pi) = \sqrt{\rho}$, are now parabolas with focus at the origin and vertex at $(-\rho, 0)$.

Finally, the case of Hermite distribution $ds(t) = e^{-t^2}\,dt$ on $(-\infty, \infty)$ can be reduced to the case $\alpha = \pm\frac{1}{2}$ of the generalized Laguerre distribution by observing that $H_{2n}(z) = L_n^{(-1/2)}(z^2)$, $H_{2n+1}(z) = zL_n^{(1/2)}(z^2)$, hence, for z nonreal,

$$\int_{-\infty}^{\infty} \frac{e^{-t^2}H_n(t)\,dt}{z - t} = \delta_n(z)\int_0^{\infty} \frac{e^{-t}t^{\pm 1/2}L_{[n/2]}^{(\pm 1/2)}(t)\,dt}{z^2 - t},$$

where $+$ or $-$ holds, depending on whether n is odd or even, and where $\delta_n(z) = 1$ for n odd, and $\delta_n(z) = z$ for n even. Proceeding as before, we now find for ν the estimate

$$\nu > 2\left(\sqrt{\frac{N}{2}} + \frac{\ln(1/\varepsilon)}{4|z|\sin\varphi}\right)^2, \qquad 0 < \varphi = \arg z < \pi. \tag{5.9}$$

The contours in (5.9) are straight lines parallel to the real axis.

Numerical experience has shown the estimates (5.6), (5.8), (5.9) to be quite realistic. In the majority of cases examined, one repetition of the algorithm (5.1) (with ν incremented by 5) suffices to confirm the desired accuracy. Occasionally,

two repetitions are required, and only rarely three (and this only when ν is quite large). On the other hand, when lowered by 5, the estimates, with few exceptions, proved inadequate to achieve the desired accuracy.

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POLYNOMIALS ORTHOGONAL WITH RESPECT TO THE RECIPROCAL GAMMA FUNCTION [1]

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In [1], [3] it is suggested that the reciprocal gamma function $1/\Gamma(t)$, $0 \leqq t < \infty$, properly normalized, may be useful in reliability theory as a probability density function. To evaluate the expected value

$$Ef = c\int_0^\infty f(t)dt/\Gamma(t), \qquad c = 1\Big/\int_0^\infty \Gamma^{-1}(t)dt,$$

of a function f, it will be necessary to apply appropriate quadrature schemes. Natural choices are the Gauss-Christoffel quadrature formulae with respect to the weight distribution $d\lambda(t) = dt/\Gamma(t)$ on $[0, \infty]$. These can readily be obtained once the recursion relation

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0, 1, 2, \ldots,$$

$$\pi_0(t) = 1, \qquad \pi_{-1}(t) = 0$$

is known for the respective (monic) orthogonal polynomials $\pi_k(\cdot\,; d\lambda)$ (see, e.g., [7], [5, § 5.1]).

We have computed the recursion coefficients α_k, β_k (where $\beta_0 = \int_0^\infty d\lambda(t)$) to 20 decimal digits for $0 \leqq k \leqq 39$, using a discretization procedure originally proposed in [4] and refined in [6, § 2.2]. The refinement consists in using a *composite* Fejér quadrature rule to discretize the required inner products

$$\int_0^\infty \pi_k^2(t)d\lambda(t), \qquad \int_0^\infty t\pi_k^2(t)d\lambda(t).$$

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The interval $[0, \infty]$ is decomposed into 10 subintervals,

$$[0, \infty] = \bigcup_{r=1}^{9} [5(r-1), 5r] \cup [45, \infty],$$

Table 1. *Recursion coefficients for the polynomials orthogonal on* $[0, \infty]$ *with respect to the weight distribution* $d\lambda t() = dt/\Gamma(t)$.

k	α_k	β_k
0	1.9345670421478847212	2.8077702420285193652
1	2.7879436158411281033	1.0939363340686113155
2	3.5739604354093584045	2.3372879608862272825
3	4.3091053098871069965	3.7441907365233042123
4	5.0058282584209047028	5.3119976010285601927
5	5.6727517332400777399	7.0335091327854930762
6	6.3158519817302918703	8.9011136859679101404
7	6.9393802176042965886	10.907913582772256131
8	7.5464565802642664718	13.047905143126414819
9	8.1394403777087012176	15.315898546377090832
10	8.7201633775933510257	17.707387474765001489
11	9.2900805740637845048	20.218427273043616394
12	9.8503704972102283522	22.845534195510892734
13	10.402003889465003792	25.585605138673464849
14	10.945791990799772276	28.435854235129588910
15	11.482421313858540088	31.393762617254118444
16	12.012479234667014793	34.457038306760120054
17	12.536473190369455701	37.623583882761530657
18	13.054845330588925070	40.891470158867125297
19	13.567983872331197187	44.258914541921217535
20	14.076232022477626524	47.724263073365304131
21	14.579895076761311877	51.285975395967277563
22	15.079246131908767385	54.942612066839360237
23	15.574530729178107620	58.692823769704697997
24	16.065970664623260125	62.535342077993342771
25	16.553767142458203825	66.468971494666667355
26	17.038103405347763134	70.492582551193826168
27	17.519146944326302125	74.605105791493263410
28	17.997051367989314956	78.805526500259759656
29	18.471957993324414724	83.092880061354758722
30	18.943997207459574857	87.466247852622676490
31	19.413289639591964888	91.924753599919767509
32	19.879947174626524801	96.467560126280306425
33	20.344073834028053459	101.09386644272912757
34	20.805766544658069470	105.80290513583357056
35	21.265115812622111611	110.59394001409378659
36	21.722206316167302173	115.46626398102261382
37	22.177117429273655261	120.41919710751600921
38	22.629923685647095095	125.45208488005816070
39	23.080695191249406477	130.56429660459561072

whereupon the Fejér quadrature rule (cf. [4]), suitably transformed, is applied to each subinterval. The decomposition is designed to make the contribution of the infinite interval $[45, \infty]$ sufficiently small so as to induce rapid convergence of the discretization process. The results, computed in double precision on the CDC 6500, are shown in Table 1.

Note that β_0 is the constant F computed in [3] to 61 decimal digits, and in [2] to 80 decimal digits. Table 1 permits the calculation of the orthogonal polynomials up to degree 40, hence the construction of Gauss-Christoffel formulae with up to 40 points.

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ON GENERATING ORTHOGONAL POLYNOMIALS*

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Abstract. We consider the problem of numerically generating the recursion coefficients of orthogonal polynomials, given an arbitrary weight distribution of either discrete, continuous, or mixed type. We discuss two classical methods, respectively due to Stieltjes and Chebyshev, and modern implementations of them, placing particular emphasis on their numerical stability properties. The latter are being studied by analyzing the numerical condition of appropriate finite-dimensional maps. A number of examples are given to illustrate the strengths and weaknesses of the various methods and to test the theory developed for them.

Key words. orthogonal polynomials, recurrence relations for orthogonal polynomials, Stieltjes procedure, discretized Stieltjes procedure, Chebyshev algorithm, modified Chebyshev algorithm, condition numbers

1. Introduction.

Let $d\lambda(t)$ be a nonnegative measure on the real line $\mathbb{R}$, with compact or infinite support, for which all *moments*

$$\mu_r = \int_{\mathbb{R}} t^r \, d\lambda(t), \qquad r = 0, 1, 2, \cdots, \tag{1.1}$$

exist and are finite, and $\mu_0 > 0$. With $d\lambda$ there is associated a unique system of (monic) *orthogonal polynomials*, i.e., a system of polynomials $\pi_r = \pi_r(\cdot\,; d\lambda)$ such that

(i) $\pi_r(t)$ has exact degree r and leading coefficient 1,

(ii) $$\int_{\mathbb{R}} \pi_r(t)\pi_s(t)\, d\lambda(t) \begin{cases} >0 & \text{if } r = s, \\ =0 & \text{if } r \neq s. \end{cases}$$

In general, the system $\{\pi_r\}$ consists of infinitely many polynomials, but reduces to a finite number N of polynomials $\pi_0, \pi_1, \cdots, \pi_{N-1}$, if $\lambda(t)$ has exactly N points of increase. We denote such a measure by $d\lambda_N(t)$, and call it a *discrete measure* and the associated polynomials *discrete orthogonal polynomials.*

The problem we wish to consider is the actual (numerical) construction of the polynomials $\pi_r(\cdot\,; d\lambda)$, given an arbitrary measure $d\lambda(t)$. The problem has received surprisingly little attention in the literature, even though orthogonal polynomials originated in connection with concrete questions of applied analysis (e.g., numerical integration, least squares approximation, series expansions, continued fractions, etc.). The reasons for this are probably twofold: In the first place, much of the practical work involving orthogonal polynomials is based on special measures $d\lambda(t)$ of the classical types, for which the orthogonal polynomials are explicitly known and the constructive aspects are therefore trivial. Secondly, even in the case of general measures, our problem has a straightforward mathematical solution: It is well known how to express, or how to compute, orthogonal polynomials in terms of the moments (1.1). This point of view, in fact, is typical for the "pre-computer" era; when executed in finite precision on a computer, however, the approach via moments is utterly ineffective on account of the explosive growth of rounding errors. Other more effective procedures have been proposed and analyzed by Forsythe [6] for discrete orthogonal polynomials, in connection with least-squares data fitting, and more recently by Sack

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and Donovan [25], Gautschi [11], [13] and Wheeler [29], for continuous distributions, in connection with the problem of Gaussian quadrature. It is our purpose, here, to bring this work into better historical perspective, to reorient it towards the problem of constructing orthogonal polynomials (rather than Gaussian quadrature rules), and to expand upon it and refine it in various directions.

First we must clarify what we mean by "constructing orthogonal polynomials." We take the position, here, that the fundamental quantities in the constructive theory of orthogonal polynomials are the coefficients in the basic three-term recurrence relation. As is well known, every system $\{\pi_r(\cdot\,; d\lambda)\}$ of (monic) orthogonal polynomials satisfies a recurrence relation of the form

$$\begin{aligned} &\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0, 1, 2, \cdots, \\ &\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1, \end{aligned} \tag{1.2}$$

where α_k, β_k are real constants with $\beta_k > 0$. It is the coefficients α_k, β_k that provide the key for the constructive use of orthogonal polynomials. There are many reasons for this, chief among which are the following:

(i) The coefficients α_k, β_k provide a compact way of representing orthogonal polynomials, requiring only a linear array of parameters. The coefficients of orthogonal polynomials, or their zeros, in contrast need two-dimensional arrays.

(ii) Knowing the coefficients α_k, β_k it is easy to compute the polynomials π_r and their derivatives recursively by (1.2) and the relations obtained from (1.2) by differentiation, for any fixed t within or without the spectrum of $d\lambda$. The procedure is not only straightforward, but also quite stable, much in contrast to the evaluation of π_r in terms of its coefficients.

(iii) Equally simple is the evaluation of finite sums $\sum c_r\pi_r(t)$ of orthogonal polynomials by Clenshaw's algorithm (see, e.g., [14, § 1.5.3]).

(iv) The functions of the second kind,

$$\rho_r(z) = \int_{\mathbb{R}} \frac{\pi_r(t)}{z-t}\, d\lambda(t), \qquad r = 0, 1, 2, \cdots, \tag{1.3}$$

where z is outside the spectrum of $d\lambda$, also satisfy the same recurrence relation as in (1.2) (where t is to be replaced by z), and in fact, under very weak assumptions on the measure $d\lambda$, represent the *minimal solution* of (1.2) normalized by $\rho_{-1}(z) = 1$. They, too, therefore can be calculated accurately by known algorithms (cf. [18]).

(v) From the coefficients α_k, β_k we can construct the *Jacobi matrix* associated with $d\lambda$, i.e., the symmetric tridiagonal matrix

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{1.4}$$

which in turn allows us to compute the zeros of π_n rapidly and efficiently as eigenvalues of the nth order segment of J, using modern procedures of numerical linear algebra, notably the QR (or QL) algorithm. The first components of the corresponding eigenvectors, indeed, also yield immediately the Christoffel numbers associated with $d\lambda$ (see, e.g., [20], [16]).

(vi) The coefficients α_k, β_k enter in Jacobi's continued fraction associated with the integral $\int_{\mathbb{R}} d\lambda(t)/(z-t)$, as well as in the corresponding Stieltjes continued fraction (cf. [14, § 1.4.2]).

(vii) The coefficients β_k determine the normalization constants by virtue of $\int_{\mathbb{R}} \pi_r^2(t)\, d\lambda(t) = \beta_0\beta_1 \cdots \beta_r$ (cf. [3, Chapt. 1, Thm. 4.2(b)] or (2.2)).

We thus consider the following problem to be fundamental in the constructive theory of orthogonal polynomials: *Given $d\lambda(t)$, compute as many of the coefficients α_k, β_k in* (1.2) *as are desired.*

The next important question concerns the "codification" of the measure $d\lambda$: In what form should $d\lambda(t)$ be given or what do we assume known about $d\lambda$? The classical way of codifying $d\lambda$ is through its moments (1.1). The problem then becomes: *Given, for some integer $n > 0$, the first $2n$ moments $\mu_0, \mu_1, \cdots, \mu_{2n-1}$ of $d\lambda$, compute the first n coefficients α_k, β_k, $k = 0, 1, \cdots, n-1$.* (It will be assumed throughout that $\beta_0 = \int_{\mathbb{R}} d\lambda(t) = \mu_0$, even though β_0 in (1.2) is arbitrary.) The solution of this problem gives us access to the first $n+1$ orthogonal polynomials $\pi_0, \pi_1, \cdots, \pi_n$.

There are several known procedures for solving this problem, of which two will be discussed in §§ 2.1 and 2.3. Unfortunately, the problem itself is highly sensitive to small perturbations in the moments, so that any algorithm which (theoretically) solves the problem will be subject to severe growth of errors when executed in finite precision. It is this unfortunate experience which motivates a careful study of the underlying (nonlinear) map $\mathbb{R}^{2n} \to \mathbb{R}^{2n}$, i.e., in the present case, the map from the first $2n$ moments μ_r to the first n recursion coefficients α_k, β_k. What we need to know is the *numerical condition* of this map, and of analogous maps for other related problems. This will be the subject of § 3, the particular map above being discussed in § 3.2. The novelty of our treatment, in part, consists in representing the respective map as a composition of two maps, the first being from the moments (or related quantities) to the Gaussian quadrature rule, the second from the Gaussian quadrature rule to the desired recursion coefficients. Each component map can be analyzed individually with regard to its numerical condition, which in turn yields a bound on the condition of the composite map.

A better codification of the measure $d\lambda$ was first proposed by Sack and Donovan [25] and involves the so-called *modified moments* $\nu_r = \int_{\mathbb{R}} p_r(t)\, d\lambda(t)$, where $\{p_r\}$ is an appropriate system of polynomials, often already orthogonal with respect to some classical measure. An algorithm that obtains the recursion coefficients from modified moments will be described in § 2.4. The condition of the underlying map is studied in § 3.3, where the principal result (Theorem 3.1) supersedes earlier results of ours, with regard to both generality and sharpness.

Methods based on the idea of discretizing the measure $d\lambda(t)$ were proposed in [11] and [19], and will be further dealt with in §§ 2.2, 2.5, and 3.4. They are applicable whenever $d\lambda$ has the form $d\lambda(t) = \omega(t)\, dt$, where ω is continuous on some open interval, or on the union of a finite number of open intervals, and zero on the complementary set in $\mathbb{R}$, whereby integrable singularities are allowed at the endpoints of the interval(s). The methods, in fact, are applicable to more general measures which in addition to the piecewise continuous component also contain a discrete point spectrum.

In § 4 the use and performance of the various methods discussed in § 2 will be illustrated by means of concrete and nontrivial examples involving orthogonal polynomials with respect to both discrete and continuous (also piecewise continuous) distributions $d\lambda$. Detailed comparisons are made between the actual performance of the algorithms and the expected performance based on the theory of § 3.

2. Basic procedures. There are essentially two classical procedures for generating the recursion coefficients of orthogonal polynomials. The first is based on the explicit inner product representation (2.2) of these coefficients, the constructive potential of which appears to have first been recognized by Stieltjes. We call the resulting method the *Stieltjes procedure.* The second method, due in the case of discrete orthogonal polynomials to Chebyshev, derives the desired coefficients directly from the moments of the underlying measure. We call this the *Chebyshev algorithm.*

Both procedures require substantial additional implementation work in order to make them effective tools of modern high-speed computation. The Stieltjes method can be implemented effectively by a discretization procedure proposed by Gautschi [11]. The resulting *discretized Stieltjes procedure,* especially in the refined form described at the end of § 2.2, is by far the most reliable and the most generally applicable procedure. Its major limitation is the possibility of relatively slow convergence, particularly in cases of integration measures with infinite support. Chebyshev's algorithm, in a more effective form involving modified moments, has been rediscovered by Sack and Donovan [25] and Wheeler [29]. We refer to their procedure as the *modified Chebyshev algorithm.* Its major difficulties are two-fold. First, there is the possibility of moderate to severe ill-conditioning, particularly, but not exclusively, in the case of infinite intervals of orthogonality. Secondly, the algorithm requires the accurate computation of modified moments, which is usually a highly nontrivial task. The latter difficulty can be alleviated to some extent by a suitable discretization, as is briefly proposed in [19, § 5.3] and further discussed in § 2.5. If modified moments are easily available and ill-conditioning poses no problem, the modified Chebyshev algorithm is certainly the method of choice, on account of its superior speed.

In the following subsections we present a more detailed description and discussion of each of these individual procedures. Applications to specific examples will be given in § 4.

2.1. Stieltjes procedure. It is well known that the system of (monic) polynomials orthogonal with respect to the measure $d\lambda(t)$ satisfies a three-term recurrence relation of the form

$$\begin{aligned} &\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \qquad k = 0, 1, 2, \cdots, \\ &\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1, \end{aligned} \tag{2.1}$$

where

$$\begin{aligned} \alpha_k &= \frac{\int_{\mathbb{R}} t\pi_k^2(t)\, d\lambda(t)}{\int_{\mathbb{R}} \pi_k^2(t)\, d\lambda(t)}, \qquad k = 0, 1, 2, \cdots, \\ \beta_k &= \frac{\int_{\mathbb{R}} \pi_k^2(t)\, d\lambda(t)}{\int_{\mathbb{R}} \pi_{k-1}^2(t)\, d\lambda(t)}, \qquad k = 1, 2, \cdots. \end{aligned} \tag{2.2}$$

In particular, $\beta_k > 0$ for all $k \geqq 1$; β_0 in (2.1) is arbitrary, but is conveniently defined as $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$.

The general formulas (2.1) were given already by Christoffel [4], who has different expressions for the α_k, β_k. The formulas in (2.2) are due, independently, to Darboux [5, pp. 411–413] and Stieltjes [26, Oeuvres I, p. 382]. Stieltjes observed how (2.1), (2.2) can be used to successively generate $\pi_1, \pi_2, \pi_3, \cdots$. Indeed, since $\pi_0 = 1$, the first coefficient α_0 can be computed from (2.2) with $k = 0$, which then allows us to obtain $\pi_1(t)$ from (2.1). Knowing π_0, π_1, we can get α_1, β_1 from (2.2), hence $\pi_2(t)$ from (2.1), etc. We call this procedure, alternating recursively between (2.1) and (2.2),

the *Stieltjes procedure.* Stieltjes did not elaborate on how to evaluate the integrals in (2.2). Presumably, he considered this a straightforward task, since, given the first $2k+2$ moments in (1.1) and given the coefficients of π_k and π_{k-1}, it is an easy matter to compute α_k and β_k in terms of these quantities, and then to obtain the coefficients of π_{k+1} from (2.1).

Unfortunately, in this form Stieltjes's procedure is practically useless, since rounding errors propagate very rapidly. As pointed out in [11], the rapid growth of errors is a reflection of the highly ill-conditioned nature of the map from the first $2n$ moments $\mu_0, \mu_1, \cdots, \mu_{2n-1}$ to the first n coefficients $\alpha_0, \cdots, \alpha_{n-1}, \beta_0, \cdots, \beta_{n-1}$. We will have more to say about this in § 3.2.

If the measure $d\lambda(t) = d\lambda_N(t)$ is a discrete N-point measure, the integrals in (2.2) become sums and can be computed directly, without recourse to moments. In this case, the Stieltjes procedure, also publicized by Forsythe [6], is generally quite stable, although it may happen that the coefficients α_k, β_k, when k is approaching N, and N is large, will suffer in accuracy (cf. Examples 4.1 and 4.3).

2.2. Discretized Stieltjes procedure. Suppose, to begin with, that

$$d\lambda(t) = \omega(t)\,dt \quad \text{on } (-1, 1), \tag{2.3}$$

where ω is a nonnegative weight function with finite moments $\mu_r = \int_{-1}^{1} t^r \omega(t)\,dt$, $r = 0, 1, \cdots, 2n-1$, and $\mu_0 > 0$. Our objective is to compute α_k, β_k, $k = 0, 1, \cdots, n-1$. In an attempt to escape ill-conditioning in the Stieltjes procedure we proposed in [11] to approximate the integrals in (2.2) by a suitable quadrature rule,

$$\int_{-1}^{1} p(t)\omega(t)\,dt = \sum_{m=1}^{N} w_m p(t_m)\omega(t_m) + R_N(p\omega), \qquad N > n, \tag{2.4}$$

with nodes $t_m = t_m^{(N)} \in (-1, 1)$ and weights $w_m = w_m^{(N)} > 0$. We require this rule to converge as $N \to \infty$ whenever p is a polynomial. It is easily seen that this procedure amounts to approximating the desired orthogonal polynomials π_k, $k = 0, 1, \cdots, n$, by the discrete orthogonal polynomials $\pi_{k,N}$, $k = 0, 1, \cdots, n$, orthogonal with respect to the N-point measure $d\lambda_N(t)$ having abscissas $t_m^{(N)}$ and jumps $w_m^{(N)}\omega(t_m^{(N)})$. In fact, under the assumption made, i.e., under the assumption

$$\int_{-1}^{1} p(t)\,d\lambda_N(t) \to \int_{-1}^{1} p(t)\,d\lambda(t), \qquad N \to \infty, \quad \text{all } p \in \mathbb{P}, \tag{2.5}$$

one can prove that [11]

$$\pi_{k,N}(t) \to \pi_k(t) \quad \text{as } N \to \infty,$$

for each fixed k, $0 \leqq k \leqq n^{-}$.

An attractive quadrature rule to be used in (2.4) is Fejér's rule, i.e., the interpolatory quadrature rule with nodes at the Chebyshev points $t_m^{(N)} = \cos((2m-1)\pi/2N)$. Among the considerations favoring this choice are the following:

(i) $t_m^{(N)}$ and $w_m^{(N)}$ are expressible in closed form in terms of trigonometric functions (cf. [11], [12]). Accordingly, the Fejér rule can be computed more rapidly than, say, the Gauss–Legendre quadrature rule. Some relevant timings are given in Table 2.1, where the method of Golub and Welsch [20] was used to generate the Gaussian rule.

(ii) Convergence (2.5) takes place not only for continuous functions ω, but also for functions ω that have singularities at the endpoints of $[-1, 1]$, provided they are monotonic and integrable [10].

TABLE 2.1
Timings (in seconds) for generating the n-point Fejér and the n-point Gauss–Legendre quadrature rule on the CDC 6500.

n	Fejér	Gauss
10	2.0 (−3)	4.3 (−2)
20	6.0 (−3)	1.5 (−1)
40	2.2 (−2)	5.5 (−1)
80	7.8 (−2)	2.1 (0)
160	2.9 (−1)	7.5 (0)
320	1.1 (0)	2.9 (1)
640	4.5 (0)	1.1 (2)

(Numbers in parentheses indicate decimal exponents.)

(iii) The discrete polynomials $\pi_{k,N}$, or rather, their coefficients $\alpha_{k,N}$, $\beta_{k,N}$, can be generated efficiently by the modified Chebyshev algorithm (see § 2.4), which ought to be quite stable on account of the point spectrum consisting of Chebyshev points (cf. Example 4.2).

(iv) If $\omega \in \mathbb{P}_s$ then $R_N(p\omega) = 0$ for all $p \in \mathbb{P}_{2n-1}$, whenever $N \geqq 2n+s$, and consequently our discretization process gives exact answers, when $N \geqq 2n+s$, except for rounding errors.

Nevertheless, when singularities are present, convergence in (2.5) can be rather slow. An example in point is the case of square-root singularities, say $\omega(t) = \omega_1(t)(1-t^2)^{-1/2}$, where ω_1 is smooth on $[-1, 1]$. In this case, the Fejér rule converges too slowly to be of practical use. Much more effective is the Gauss–Chebyshev rule

$$\int_{-1}^{1} p(t)\omega_1(t)(1-t^2)^{-1/2}\,dt = \frac{\pi}{N}\sum_{m=1}^{N} p(t_m)\omega_1(t_m) + R_N(p\omega_1),$$

where again $t_m = \cos((2m-1)\pi/2N)$. Similarly, one may wish to apply a Gauss–Jacobi rule in cases where $\omega(t) = \omega_1(t)(1-t)^{\alpha}(1+t)^{\beta}$, $\alpha > -1$, $\beta > -1$ (cf. Example 4.10).

If the basic interval is not $[-1, 1]$, but $[a, b]$, $-\infty \leqq a < b \leqq \infty$, we select a monotone function ϕ (a linear function, if $[a, b]$ is finite) which maps $[-1, 1]$ on $[a, b]$ and use

$$\int_a^b p(t)\omega(t)\,dt = \sum_{m=1}^{N} w_m p(\phi(t_m))\omega(\phi(t_m))\phi'(t_m) + R_N(p\omega) \tag{2.6}$$

in place of (2.4) (cf. [11]). This again leads to a discrete measure $d\lambda_N(t)$, the abscissas and jumps now being $\phi(t_m)$ and $w_m\omega(\phi(t_m))\phi'(t_m)$, respectively. In this way, arbitrary finite or infinite intervals can be handled.

The method described, actually, has still wider applicability. We may indeed allow $d\lambda(t)$ to be composed of a piecewise continuous weight distribution and a discrete distribution, whereby the former is supported on the union of a finite number of disjoint intervals, and the latter contains a finite number of distinct points. One or both of the extreme intervals of the piecewise continuous component may extend to infinity. To cope with this more general situation, all we need to do is to apply our discretization process, with suitable functions ϕ in (2.6), individually to each component interval, add up all the contributions, and then add to the resulting discrete measure the discrete measure of the given point spectrum. The convergence of the process, of course, is in no way affected by the addition of the given point spectrum, although its stability properties may be altered significantly (see Example 4.8).

As a simple example, suppose ω is piecewise constant on the continuous part of the spectrum. Then the process not only converges, but in fact is exact for $N \geqq 2n$, since each integral in (2.2) for $\alpha_k, \beta_k, 0 \leqq k \leqq n-1$, is integrated exactly by the composite N-point Fejér rule (cf. (iv) above; see also Example 4.7).

Our treatment of the piecewise continuous part of the spectrum can also be interpreted as expressing the weight function in the form of a sum of individual weight functions (each equal to zero, except in one of the component intervals). This suggests further generalizations, whereby the weight function is assumed to be a sum of weight functions, each supported on its own interval, and each treated by a separate quadrature rule. Some of these intervals may then in fact coincide. This will be very effective in cases where different components of the weight function (possibly on the same interval) must be dealt with by different quadrature rules; see Examples 4.6, 4.9 and 4.10 for illustrations.

2.3. Chebyshev algorithm. Chebyshev [2, Oeuvres I, p. 482], in the case of discrete orthogonal polynomials, observed that the coefficients α_k, β_k can be obtained directly in terms of the quantities

$$\sigma_{k,l} = \int_{\mathbb{R}} \pi_k(t) t^l \, d\lambda(t) \tag{2.7}$$

(for which Chebyshev used the symbol (k, l)), by means of

$$\begin{aligned} &\alpha_0 = \frac{\sigma_{0,1}}{\sigma_{0,0}}, \qquad \beta_0 = \sigma_{0,0}, \\ &\alpha_k = \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \qquad k = 1, 2, 3, \cdots. \\ &\beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}, \end{aligned} \tag{2.8}$$

The σ_{kl}, in turn, can be generated recursively from the moments μ_l by [2, Oeuvres I, p. 482]

$$\begin{aligned} &\sigma_{kl} = \sigma_{k-1,l+1} - \alpha_{k-1}\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l}, \qquad l = k, k+1, \cdots, 2n-k-1, \\ &\sigma_{-1,0} = 0, \qquad \sigma_{0l} = \mu_l. \end{aligned} \tag{2.9}$$

Given the first $2n$ moments $\mu_0, \mu_1, \cdots, \mu_{2n-1}$, this will produce the first n coefficients $\alpha_0, \cdots, \alpha_{n-1}$ and $\beta_0, \cdots, \beta_{n-1}$. We refer to (2.8), (2.9) as the *Chebyshev algorithm.*

Being based on the moments μ_r, the algorithm unfortunately suffers from the same effects of ill-conditioning as does the Stieltjes procedure, when implemented in terms of moments. In many cases it is possible, however, to stabilize the algorithm by introducing modified moments in place of ordinary moments.

2.4. Modified Chebyshev algorithm. Let $\{p_k(t)\}$ denote a system of (monic) polynomials satisfying a recurrence relation

$$\begin{aligned} &p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, 2, \cdots, \\ &p_{-1}(t) = 0, \qquad p_0(t) = 1, \end{aligned} \tag{2.10}$$

where a_k, b_k are assumed known. We then call

$$\nu_r = \int_{\mathbb{R}} p_r(t) \, d\lambda(t), \qquad r = 0, 1, 2, \cdots, \tag{2.11}$$

the *modified moments* of the measure $d\lambda$ relative to the polynomial system $\{p_r\}$. If $a_k = b_k = 0$ for all k, then $p_k(t) = t^k$, and the modified moments reduce to the ordinary moments (1.1).

Chebyshev's algorithm generalizes very naturally to the case of modified moments. One defines

$$\sigma_{kl} = \int_{\mathbb{R}} \pi_k(t) p_l(t)\, d\lambda(t), \tag{2.12}$$

and obtains the first n coefficients α_k, β_k, $k = 0, 1, \cdots, n-1$, from the first $2n$ modified moments ν_r, $r = 0, 1, \cdots, 2n-1$, by the following *modified Chebyshev algorithm.*

Initialization:

$$\begin{aligned} &\sigma_{-1,l} = 0, && l = 1, 2, \cdots, 2n-2, \\ &\sigma_{0,l} = \nu_l, && l = 0, 1, \cdots, 2n-1, \\ &\alpha_0 = a_0 + \frac{\nu_1}{\nu_0}, \\ &\beta_0 = \nu_0. \end{aligned} \tag{2.13_0}$$

Continuation: For $k = 1, 2, \cdots, n-1$

$$\begin{aligned} \sigma_{kl} &= \sigma_{k-1,l+1} - (\alpha_{k-1} - a_l)\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l} \\ &\quad + b_l\sigma_{k-1,l-1}, \qquad l = k, k+1, \cdots, 2n-k-1, \\ \alpha_k &= a_k + \frac{\sigma_{k,k+1}}{\sigma_{kk}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \\ \beta_k &= \frac{\sigma_{kk}}{\sigma_{k-1,k-1}}. \end{aligned} \tag{2.13_k}$$

The algorithm is summarized schematically in Fig. 2.1, where the "computing star" shows which of the σ_{kl} (indicated by black dots) are related to one another in the

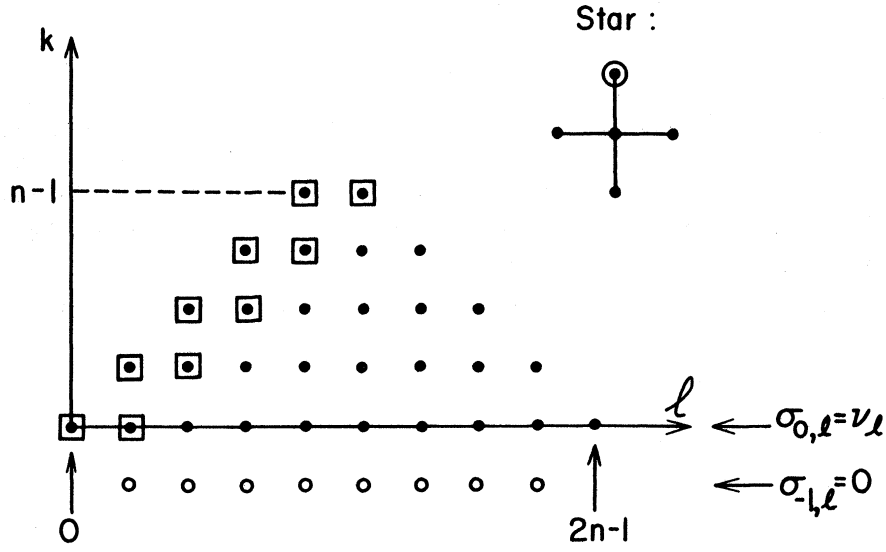

FIG. 2.1. *The modified Chebyshev algorithm (schematically for $n = 5$).*

identity (2.13_k). The circled dot indicates the quantity which is computed in terms of the others in the star. The entries in boxes are those used to compute α_k, β_k. The diagonal entries, incidentally, furnish the normalization constants

$$\sigma_{kk} = \int_{\mathbb{R}} \pi_k^2(t)\, d\lambda(t), \qquad k = 0, 1, \cdots, n-1. \tag{2.14}$$

(Chebyshev's algorithm proceeds similarly, except that it starts from the moments μ_l, and the left arm of the computing star is missing.) The algorithm (2.13), in a somewhat different form, was first proposed by Sack and Donovan [25], and in the form given here by Wheeler [29]. A derivation can also be found in [15].

The modified Chebyshev algorithm often proves to be exceptionally stable, particularly when π_k and p_k are orthogonal polynomials on finite intervals (see, e.g., Examples 4.4 and 4.5). On infinite intervals, disjoint intervals, and also in the case of discrete spectra, the underlying map, however, is likely to become ill-conditioned, sometimes even severely so (see, e.g., Examples 4.1, 4.3, 4.6, 4.7 and 4.8). Some new theoretical insights into these questions of condition are given in § 3.3.

2.5. Discretized (modified) Chebyshev algorithm. The tendency of becoming ill-conditioned is one of the limitations of the modified Chebyshev algorithm. Another is the difficulty inherent in the accurate calculation of the modified moments (2.11). It is possible, however, as suggested in [19, § 5.3], to apply the same discretization $d\lambda(t) \approx d\lambda_N(t)$ that was used in the Stieltjes procedure (cf. § 2.2) to the modified moments. One thus approximates ν_r by

$$\nu_{r,N} = \int_{\mathbb{R}} p_r(t)\, d\lambda_N(t), \tag{2.15}$$

and then calculates the associated recursion coefficients $\alpha_{k,N}$ and $\beta_{k,N}$ by the modified Chebyshev algorithm. The procedure converges under the same conditions as the discretized Stieltjes procedure. It is essential, however, that convergence (in relative accuracy) be tested on the $\beta_{k,N}$, and not on the $\nu_{r,N}$, since the latter may vanish and, besides, need not be required to have full relative precision (cf. Example 4.4). The range of applicability of this procedure can be extended, as in the case of the discretized Stieltjes procedure, to measures $d\lambda(t)$ composed of piecewise continuous components as well as point spectra. It is important to realize, however, that any ill-conditioning present in the modified Chebyshev algorithm will manifest itself also in its discretized version. There are fewer problems of this kind with the discretized Stieltjes procedure.

3. Questions of numerical condition. The modified Chebyshev algorithm of § 2.4 realizes the map $K_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ which associates to the first $2n$ modified moments ν_r the recursion coefficients α_k, β_k, $k = 0, 1, \cdots, n-1$, for the respective orthogonal polynomials:

$$\begin{gathered} K_n : \nu \to \rho, \\ \nu^T = [\nu_0, \nu_1, \cdots, \nu_{2n-1}], \qquad \rho^T = [\alpha_0, \cdots, \alpha_{n-1}, \beta_0, \cdots, \beta_{n-1}]. \end{gathered} \tag{3.1}$$

Throughout this section we assume that $\beta_0 = \int_{\mathbb{R}} d\lambda(t) = \nu_0$.

For the purpose of studying the numerical condition of the map K_n, it is convenient to think of K_n as the composition of two maps,

$$K_n = H_n \circ G_n, \tag{3.2}$$

where G_n is the map from the modified moments ν_r to the Gauss–Christoffel quadrature

rule,

$$G_n: \nu \to \gamma, \qquad \gamma^T = [\lambda_1, \cdots, \lambda_n, \tau_1, \cdots, \tau_n], \tag{3.3}$$

and H_n the map from the Gauss–Christoffel quadrature rule to the recursion coefficients,

$$H_n: \gamma \to \rho. \tag{3.4}$$

Here, $\lambda_\nu = \lambda_\nu^{(n)}$, $\tau_\nu = \tau_\nu^{(n)}$ are the Christoffel numbers and Gaussian abscissas (the zeros of $\pi_n(\cdot\,; d\lambda)$), respectively, associated with the measure $d\lambda(t)$, so that

$$\int_{\mathbb{R}} f(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \qquad R_n(\mathbb{P}_{2n-1}) = 0. \tag{3.5}$$

As one would expect, the map G_n is the more sensitive of the two. The map H_n is usually fairly well-conditioned; its condition is discussed in § 3.1. In § 3.2 we briefly recall the ill-conditioned nature of the map G_n when the vector ν consists of ordinary moments. The condition of G_n in the general case of modified moments is studied in § 3.3. As condition number of a map $M: x \to y$ from one finite-dimensional space into another we generally adopt the quantity (see, e.g., [15])

$$(\operatorname{cond} M)(x) = \frac{\|x\| \|J_M(x)\|}{\|y\|}, \qquad y = Mx, \tag{3.6}$$

where J_M is the Jacobian matrix of M, and $\|\cdot\|$ a suitable vector norm and subordinate matrix norm. In cases where the vector x (or y) has components of widely varying magnitude, this condition number may not be very meaningful on account of the falsification introduced by the factor $\|x\|$ (or $1/\|y\|$). In such cases we use more refined measures of the condition. Recall also that $\operatorname{cond}(H_n \circ G_n) \leqq \operatorname{cond}(H_n) \operatorname{cond}(G_n)$.

3.1. Condition of the map H_n. By virtue of (2.2) and (3.5), the map H_n can be described by

$$\begin{aligned} \alpha_k &= \frac{\sum_{\nu=1}^{n} \lambda_\nu \tau_\nu \pi_k^2(\tau_\nu)}{\sum_{\nu=1}^{n} \lambda_\nu \pi_k^2(\tau_\nu)}, \qquad k = 0, 1, 2, \cdots, n-1, \\ \beta_0 &= \sum_{\nu=1}^{n} \lambda_\nu, \\ \beta_k &= \frac{\sum_{\nu=1}^{n} \lambda_\nu \pi_k^2(\tau_\nu)}{\sum_{\nu=1}^{n} \lambda_\nu \pi_{k-1}^2(\tau_\nu)}, \qquad k = 1, 2, \cdots, n-1. \end{aligned} \tag{3.7}$$

We are here in a case where the condition number (3.6) is often not appropriate, since the Christoffel numbers λ_ν vary greatly in magnitude, particularly if the interval of orthogonality is infinite. We therefore use the one-dimensional equivalent of (3.6), applied to each α_k and β_k individually, considered as functions of one particular λ_ν or τ_ν. Thus, we write

$$(\operatorname{cond} \alpha_k)(\lambda_\nu) = \left| \frac{\lambda_\nu (\partial \alpha_k / \partial \lambda_\nu)}{\alpha_k} \right| \qquad (\text{if } \alpha_k \neq 0), \quad \text{etc.},$$

where in the case $\alpha_k = 0$ the division by α_k is omitted.

An elementary calculation then yields

$$
\begin{aligned}
&\sum_{\nu=1}^{n} (\operatorname{cond} \alpha_k)(\lambda_\nu) = d_k^{-1} \sum_{\nu=1}^{n} \lambda_\nu |\Delta_{\nu,k}| \pi_k^2(\tau_\nu), \\
&\sum_{\nu=1}^{n} (\operatorname{cond} \alpha_k)(\tau_\nu) = d_k^{-1} \sum_{\nu=1}^{n} \lambda_\nu |\tau_\nu| |\delta_k \pi_k^2(\tau_\nu) + 2\Delta_{\nu,k} \pi_k(\tau_\nu) \pi_k'(\tau_\nu)|, \\
&\sum_{\nu=1}^{n} (\operatorname{cond} \beta_k)(\lambda_\nu) = d_k^{-1} \sum_{\nu=1}^{n} \lambda_\nu |\pi_k^2(\tau_\nu) - \beta_k \pi_{k-1}^2(\tau_\nu)|, \\
&\sum_{\nu=1}^{n} (\operatorname{cond} \beta_k)(\tau_\nu) = 2 d_k^{-1} \sum_{\nu=1}^{n} \lambda_\nu |\tau_\nu| |\pi_k(\tau_\nu) \pi_k'(\tau_\nu) - \beta_k \pi_{k-1}(\tau_\nu) \pi_{k-1}'(\tau_\nu)|,
\end{aligned}
\tag{3.8}
$$

where

$$
d_k = \sum_{\nu=1}^{n} \lambda_\nu \pi_k^2(\tau_\nu) = \int_{\mathbb{R}} \pi_k^2(t)\, d\lambda(t), \qquad k = 0, 1, \cdots, n-1,
$$

$$
\delta_k = \begin{cases} \dfrac{1}{\alpha_k} & \text{if } \alpha_k \neq 0, \\ 1 & \text{if } \alpha_k = 0, \end{cases} \qquad \Delta_{\nu,k} = \begin{cases} \dfrac{\tau_\nu - \alpha_k}{\alpha_k} & \text{if } \alpha_k \neq 0, \\ \tau_\nu & \text{if } \alpha_k = 0. \end{cases}
$$

A suitable condition number, cond H_n, for the map H_n is now the maximum of all the numbers in (3.8), as k varies over $0, 1, \cdots, n-1$. Numerical values of this condition number, for some classical polynomials, are shown in Table 3.1.

TABLE 3.1
The numerical condition of the map H_n for some classical orthogonal polynomials.

n	Legendre	Chebyshev	Laguerre	Hermite
5	6.968 (0)	7.186 (0)	6.724 (0)	1.596 (1)
10	1.785 (1)	1.823 (1)	2.143 (1)	6.254 (1)
20	4.530 (1)	4.742 (1)	4.269 (1)	2.042 (2)
40	1.071 (2)	1.135 (2)	8.525 (1)	6.181 (2)
80	2.526 (2)	2.644 (2)	1.761 (2)	1.807 (3)

It is seen that the map H_n in these cases is relatively well-conditioned, cond H_n growing about linearly in n. The well-conditioning of H_n, however, is not always assured; see, e.g., Examples 4.1, 4.3 and 4.8.

The coefficients α_k, β_k are less sensitive to perturbations in the λ_ν than to perturbations in the τ_ν. Indeed, from (3.8) it follows immediately that

$$
\sum_{\nu=1}^{n} (\operatorname{cond} \alpha_k)(\lambda_\nu) \leqq \max_{\nu,k} |\Delta_{\nu,k}|, \qquad \sum_{\nu=1}^{n} (\operatorname{cond} \beta_k)(\lambda_\nu) \leqq 2.
$$

If the polynomials are orthogonal on $[-1, 1]$ with respect to a symmetric weight function, then the bound in the first inequality is <1.

Results in terms of the "global" condition number (3.6) are comparable to those in Table 3.1 in the case of Legendre and Chebyshev polynomials, but completely unrealistic in case of Laguerre and Hermite polynomials. For Laguerre polynomials, e.g., the condition numbers based on (3.6), using the uniform norm, range from 1.06×10^5 for $n = 5$ to 7.65×10^{61} for $n = 40$. This is a rather striking example of how

the introduction of inappropriate norms in the study of condition may completely distort the true nature of sensitivity.

3.2. Condition of the map G_n in case of ordinary moments. We assume in (3.3) that ν is the vector of ordinary moments,

$$\nu^T = [\mu_0, \mu_1, \cdots, \mu_{2n-1}], \qquad \mu_r = \int_{\mathbb{R}} t^r \, d\lambda(t).$$

The map G_n then amounts to solving the nonlinear system of equations,

$$\sum_{\nu=1}^{n} \lambda_\nu \tau_\nu^r = \mu_r, \qquad r = 0, 1, 2, \cdots, 2n-1. \tag{3.9}$$

If F_n is the map $\gamma \to \nu$ defined by (3.9), its Jacobian J_{F_n} is readily computed to be

$$J_{F_n} = T\Lambda,$$

where

$$\Lambda = \operatorname{diag}(1, \cdots, 1, \lambda_1, \cdots, \lambda_n),$$

$$T = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ \tau_1 & \cdots & \tau_n & 1 & \cdots & 1 \\ \tau_1^2 & \cdots & \tau_n^2 & 2\tau_1 & \cdots & 2\tau_n \\ \vdots & & \vdots & \vdots & & \vdots \\ \tau_1^{2n-1} & \cdots & \tau_n^{2n-1} & (2n-1)\tau_1^{2n-2} & \cdots & (2n-1)\tau_n^{2n-2} \end{bmatrix}.$$

Since $J_{G_n} = J_{F_n}^{-1}$, we have according to (3.6),

$$(\operatorname{cond} G_n)(\nu) = \frac{\|\nu\| \|\Lambda^{-1} T^{-1}\|}{\|\gamma\|}.$$

From the analysis in [11], in particular Theorem 2.1 and the discussion preceding it (which assumed [0, 1] as the support of $d\lambda(t)$, but extends easily to arbitrary measures on the *positive* real line), one gets

$$\operatorname{cond} G_n \geqq \frac{\|\nu\|}{\|\gamma\|} \frac{1}{\max_\nu \lambda_\nu} \cdot \max_\nu \left\{ (1+\tau_\nu) \prod_{\mu \neq \nu} \left(\frac{1+\tau_\mu}{\tau_\nu - \tau_\mu} \right)^2 \right\},$$

or, equivalently,

$$\operatorname{cond} G_n \geqq \frac{\|\nu\|}{\|\gamma\|} \frac{1}{\max_\nu \lambda_\nu} \cdot \frac{[\pi_n(-1)]^2}{\min_\nu \{(1+\tau_\nu)[\pi_n'(\tau_\nu)]^2\}}, \tag{3.10}$$

where $\|\nu\| = \max_{0 \leqq r \leqq 2n-1} \mu_r$, $\|\gamma\| = \max(\max_\nu \lambda_\nu, \max_\nu \tau_\nu)$ and $\operatorname{supp}(d\lambda) \in \mathbb{R}_+$. Since the point -1 is well outside the spectrum of $d\lambda$, the lower bound in (3.10) must be expected to grow rapidly to infinity as $n \to \infty$, on account of the asymptotic behavior of orthogonal polynomials outside the spectrum (for relevant results see, e.g. [27, Thms. 8.21.7, 8.22.3]).

Here also, the result (3.10) may be misleading if the interval of orthogonality is infinite, since the moments μ_r then likely grow rapidly. In analogy to § 3.1, it is better,

in these cases, to use the more refined condition numbers

$$\text{(3.11)}\qquad \begin{aligned} \sum_{r=0}^{2n-1} (\operatorname{cond} \lambda_\nu)(\mu_r) &= \sum_{r=0}^{2n-1} \frac{|\mu_r (T^{-1})_{\nu,r+1}|}{\lambda_\nu}, \\ \sum_{r=0}^{2n-1} (\operatorname{cond} \tau_\nu)(\mu_r) &= \sum_{r=0}^{2n-1} \frac{|\mu_r (T^{-1})_{n+\nu,r+1}|}{|\lambda_\nu \tau_\nu|}, \end{aligned} \qquad \nu = 1, 2, \cdots, n,$$

and take as cond G_n the maximum of these $2n$ quantities. Unfortunately, they no longer admit simple expressions in closed form, but can be readily computed, for example by means of the algorithm for T^{-1} in [8, § 4].

In Table 3.2 we illustrate the condition of the map G_n for the examples $d\lambda(t) = dt$ on $[0, 1]$, $d\lambda(t) = \ln(1/t)\, dt$ on $[0, 1]$, $d\lambda(t) = e^{-t}\, dt$ on $[0, \infty]$ and $d\lambda(t) = e^{-t^2}\, dt$ on $[0, \infty]$. The third column gives the lower bound in (3.10), the fourth column the maximum of the $2n$ condition numbers in (3.11), and the last one the actual error growth observed. The latter is taken to mean the largest relative error in the α_k, β_k, $k = 0, 1, \cdots, n-1$, divided by the machine precision, in our case 3.553×10^{-15}. The coefficients α_k, β_k were computed by Chebyshev's algorithm; cf. § 2.3. (Since the moments of the Laguerre distribution are integers, we first subjected them to random perturbations at the level of the machine precision before applying Chebyshev's algorithm.) In the first two examples, for $n = 12$ one of the β_k (the last one) came out to be negative; hence no results are shown for $n = 14$. Note that the second and fourth example involve nonclassical orthogonal polynomials.

It is seen that in the first two examples, where the interval of orthogonality is finite, the observed error magnification indeed follows the trend predicted by either of the two condition numbers. In the last two examples, involving infinite intervals of orthogonality, this is only true for the condition number based on (3.11); the other grossly overestimates the error growth, for reasons explained earlier.

TABLE 3.2

The condition of the map G_n in the case of ordinary moments and $d\lambda(t) = \omega(t)\, dt$.

$\omega(t)$	n	cond G_n (3.10)	cond G_n (3.11)	err. growth
1	2	1.997 (1)	4.132 (1)	2.400 (1)
on [0, 1]	5	6.803 (4)	3.802 (5)	6.280 (4)
	8	7.080 (8)	6.161 (9)	8.977 (8)
	11	1.111 (13)	1.302 (14)	2.108 (13)
	14	–	–	–
$\ln(1/t)$	2	4.863 (1)	1.932 (1)	2.655 (1)
on [0, 1]	5	2.133 (5)	7.071 (4)	2.411 (4)
	8	2.391 (9)	7.370 (8)	8.010 (7)
	11	3.889 (13)	1.156 (13)	3.851 (12)
	14	–	–	–
e^{-t}	2	1.665 (1)	1.549 (1)	3.500 (0)
on [0, ∞]	5	4.416 (6)	9.665 (3)	5.991 (2)
	8	7.006 (13)	5.968 (6)	1.600 (5)
	11	1.078 (22)	3.829 (9)	6.508 (7)
	14	8.170 (30)	2.521 (12)	9.164 (9)
e^{-t^2}	2	6.823 (0)	2.106 (1)	1.162 (2)
on [0, ∞]	5	2.698 (4)	4.691 (4)	8.070 (3)
	8	8.044 (8)	1.073 (8)	3.890 (6)
	11	6.445 (13)	2.555 (11)	3.274 (10)
	14	1.001 (19)	6.243 (14)	5.373 (13)

3.3. Condition of the map G_n in case of modified moments. We now assume in (3.3) that the vector ν contains the modified moments,

$$\nu^T = [\nu_0, \nu_1, \cdots, \nu_{2n-1}], \qquad \nu_r = \int_{\mathbb{R}} p_r(t)\, d\lambda(t),$$

where $\{p_k\}$ is a system of (monic) polynomials orthogonal with respect to some measure $dl(t)$,

$$\int_{\mathbb{R}} p_r(t)p_s(t)\, dl(t) = 0, \qquad r \neq s.$$

The support of $dl(t)$ may be finite or infinite, and need not necessarily coincide with the support of $d\lambda(t)$. The condition of the map G_n in this case has previously been studied in [13]. Our treatment here improves upon that work in several respects. First, we obtain considerably more realistic bounds for the condition number. Secondly, our new bound is valid irrespectively of whether $dl(t)$ has finite or infinite support, in contrast, e.g., to Theorem 2.1 of [13]. Finally, the bound can be evaluated exactly by Gaussian quadrature, in contrast, e.g., to the bound (2.33) in [13], where $L_{n,2}$, and hence $k_n^{(2)}$, does not allow exact evaluation by quadrature. The improvement is achieved by employing the more natural L_2-norm in place of the L_1-norm used in [13], and rests on the fact that for any real matrix A,

$$\|A\|_2 = \sqrt{\rho(A^TA)} \leqq \sqrt{\operatorname{tr}(A^TA)} = \|A\|_F, \tag{3.12}$$

where $\rho(\cdot)$ denotes the spectral radius, $\operatorname{tr}(\cdot)$ the trace, and $\|\cdot\|_F$ the Frobenius norm

$$\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2}, \qquad A = [a_{ij}].$$

As before, we let $\tau_\nu = \tau_\nu^{(n)}$, $\lambda_\nu = \lambda_\nu^{(n)}$ denote the Gaussian abscissas and Christoffel numbers, respectively, belonging to the measure $d\lambda(t)$. Furthermore,

$$\begin{aligned} h_\nu(t) &= l_\nu^2(t)[1 - 2l_\nu'(\tau_\nu)(t-\tau_\nu)], \\ k_\nu(t) &= l_\nu^2(t)(t-\tau_\nu), \end{aligned} \qquad \nu = 1, 2, \cdots, n \tag{3.13}$$

will denote the fundamental Hermite interpolation polynomials associated with the abscissas $\tau_1, \cdots, \tau_n$, i.e.,

$$\begin{aligned} h_\nu(\tau_\mu) &= \delta_{\nu\mu}, \qquad h_\nu'(\tau_\mu) = 0, \\ k_\nu(\tau_\mu) &= 0, \qquad k_\nu'(\tau_\mu) = \delta_{\nu\mu}, \end{aligned} \qquad \nu, \mu = 1, 2, \cdots, n, \tag{3.14}$$

where $\delta_{\nu\mu}$ is the Kronecker symbol and l_ν are the fundamental Lagrange interpolation polynomials.

It will be convenient to consider not the map $\nu \to \gamma$ in (3.3), but the map

$$\tilde{G}_n : \tilde{\nu} \to \gamma,$$

where $\tilde{\nu}$ is the vector of *normalized* modified moments

$$\tilde{\nu}_r = d_r^{-1/2}\nu_r, \qquad d_r = \int_{\mathbb{R}} p_r^2(t)\, dl(t), \qquad r = 0, 1, \cdots, 2n-1.$$

This has the theoretical advantage of making the $\tilde{\nu}_r$ independent of the normalization of the orthogonal polynomials $\{p_k\}$. For algorithmic purposes, however, the passage from ν to $\tilde{\nu}$ is not required, and in fact not recommended; cf. § 2.4. The additional

diagonal map introduced,

$$D_n : \nu \to \tilde{\nu},$$

of course, is harmless, since each individual transformation $\nu_r \to \tilde{\nu}_r$ involves just one multiplication and is therefore perfectly well-conditioned.

For the map $\tilde{G}_n$ we now have:

THEOREM 3.1. *The condition of the map $\tilde{G}_n$, in the sense of* (3.6), *with $\|\cdot\|$ the Euclidean norm, can be estimated as follows*:

$$(\text{cond } \tilde{G}_n)(\tilde{\nu}) \leqq \frac{\|\tilde{\nu}\|}{\|\gamma\|}\left\{\int_{\mathbb{R}} \sum_{\nu=1}^{n} \left(h_\nu^2(t) + \frac{1}{\lambda_\nu^2} k_\nu^2(t)\right) dl(t)\right\}^{1/2}, \tag{3.15}$$

where

$$\|\tilde{\nu}\|^2 = \sum_{r=0}^{2n-1} \tilde{\nu}_r^2, \qquad \|\gamma\|^2 = \sum_{\nu=1}^{n} (\lambda_\nu^2 + \tau_\nu^2). \tag{3.16}$$

Proof. The map $\tilde{G}_n$ amounts to solving the system of nonlinear equations

$$\Phi(\gamma) = \tilde{\nu},$$

where

$$\Phi_r(\gamma) = d_r^{-1/2} \sum_{\nu=1}^{n} \lambda_\nu p_r(\tau_\nu), \qquad r = 0, 1, \cdots, 2n-1.$$

The Jacobian $J_{\tilde{G}_n}(\tilde{\nu})$ of $\tilde{G}_n$, therefore, is the inverse of the Jacobian Φ_γ of Φ, so that

$$(\text{cond } \tilde{G}_n)(\tilde{\nu}) = \frac{\|\tilde{\nu}\|}{\|\gamma\|}\|\Phi_\gamma^{-1}(\gamma)\|. \tag{3.17}$$

An elementary calculation yields

$$\Phi_\gamma(\gamma) = D^{-1} P \Lambda,$$

where

$$D = \text{diag}\,(d_0^{1/2}, d_1^{1/2}, \cdots, d_{2n-1}^{1/2}), \qquad \Lambda = \text{diag}\,(1, \cdots, 1, \lambda_1, \cdots, \lambda_n),$$

and

$$P = \begin{bmatrix} p_0(\tau_1) & \cdots & p_0(\tau_n) & p_0'(\tau_1) & \cdots & p_0'(\tau_n) \\ p_1(\tau_1) & \cdots & p_1(\tau_n) & p_1'(\tau_1) & \cdots & p_1'(\tau_n) \\ \vdots & & \vdots & \vdots & & \vdots \\ p_{2n-1}(\tau_1) & \cdots & p_{2n-1}(\tau_n) & p_{2n-1}'(\tau_1) & \cdots & p_{2n-1}'(\tau_n) \end{bmatrix}.$$

Therefore, using (3.12),

$$\|\Phi_\gamma^{-1}(\gamma)\| = \|\Lambda^{-1} P^{-1} D\| \leqq \|\Lambda^{-1} P^{-1} D\|_F. \tag{3.18}$$

As previously observed in [13], the inverse of P can be expressed in terms of the expansion coefficients in

$$h_\nu(t) = \sum_{\mu=1}^{2n} a_{\nu\mu} p_{\mu-1}(t), \qquad k_\nu(t) = \sum_{\mu=1}^{2n} b_{\nu\mu} p_{\mu-1}(t)$$

as

$$P^{-1} = \begin{bmatrix} A \\ B \end{bmatrix}, \quad A = [a_{\nu\mu}], \quad B = [b_{\nu\mu}].$$

Since

$$(\Lambda^{-1}P^{-1}D)_{\nu,\mu} = d_{\mu-1}^{1/2}a_{\nu\mu}, \qquad (\Lambda^{-1}P^{-1}D)_{\nu+n,\mu} = \frac{1}{\lambda_\nu}d_{\mu-1}^{1/2}b_{\nu\mu},$$

one obtains

$$\|\Lambda^{-1}P^{-1}D\|_F^2 = \sum_{\nu=1}^{n}\sum_{\mu=1}^{2n} d_{\mu-1}\left(a_{\nu\mu}^2 + \frac{1}{\lambda_\nu^2}b_{\nu\mu}^2\right).$$

On the other hand,

$$\begin{aligned}\int_{\mathbb{R}} h_\nu^2(t)\,dl(t) &= \int_{\mathbb{R}} \sum_{\mu=1}^{2n} a_{\nu\mu}p_{\mu-1}(t) \sum_{\kappa=1}^{2n} a_{\nu\kappa}p_{\kappa-1}(t)\,dl(t)\\ &= \sum_{\mu,\kappa} a_{\nu\mu}a_{\nu\kappa}\int_{\mathbb{R}} p_{\mu-1}(t)p_{\kappa-1}(t)\,dl(t)\\ &= \sum_{\mu=1}^{2n} d_{\mu-1}a_{\nu\mu}^2,\end{aligned}$$

by virtue of the orthogonality of the p_r with respect to $dl(t)$. Similarly,

$$\int_{\mathbb{R}} k_\nu^2(t)\,dl(t) = \sum_{\mu=1}^{2n} d_{\mu-1}b_{\nu\mu}^2.$$

Therefore,

$$\|\Lambda^{-1}P^{-1}D\|_F^2 = \int_{\mathbb{R}} \sum_{\nu=1}^{n}\left(h_\nu^2(t) + \frac{1}{\lambda_\nu^2}k_\nu^2(t)\right) dl(t),$$

which in view of (3.17), (3.18) proves the theorem. □

We remark that the integral in (3.15), since the integrand is a polynomial of degree $\leqq 4n-2$, can be evaluated exactly (up to rounding errors) by the $2n$-point Gauss–Christoffel quadrature formula associated with $dl(t)$. This causes little problem, since dl is usually one of the standard integration measures and, besides, the integrand is positive. Furthermore, the integrand is conveniently evaluated in the form

$$\sum_{\nu=1}^{n}\left(h_\nu^2(t) + \frac{1}{\lambda_\nu^2}k_\nu^2(t)\right) = \frac{\sum_{\nu=1}^{n}[\rho_\nu(t-\tau_\nu)]^{-4}([1-2\sigma_\nu(t-\tau_\nu)]^2 + \lambda_\nu^{-2}(t-\tau_\nu)^2)}{(\sum_{\nu=1}^{n}[\rho_\nu(t-\tau_\nu)]^{-1})^4}, \tag{3.19}$$

where

$$\rho_\nu = \prod_{\substack{\mu=1\\ \mu\neq\nu}}^{n}(\tau_\nu - \tau_\mu), \qquad \sigma_\nu = \sum_{\substack{\mu=1\\ \mu\neq\nu}}^{n}\frac{1}{\tau_\nu - \tau_\mu},$$

as follows directly from (3.13) and the fact that $\sum_\nu l_\nu(t) = 1$ and $l_\nu(t) = \rho_\nu^{-1}\prod_{\mu\neq\nu}(t-\tau_\mu)$ for the Lagrange polynomials. Of course, the evaluation of (3.19), as well as of $\|\gamma\|$ in (3.16), requires knowledge of the Gaussian abscissas and Christoffel numbers for $d\lambda(t)$.

We will have occasion to comment further on the result (3.15), when we discuss specific examples in § 4. Suffice it to say, here, that Gaussian abscissas τ_ν that are distributed approximately uniformly (as they tend to be for discrete orthogonal polynomials based on an equally spaced point spectrum) give rise to integrals in (3.15) that are likely to be very large for large n on account of the violent oscillations of h_ν and k_ν near the extreme nodes τ_μ. Abscissas τ_μ, on the other hand, that are distributed

more like Chebyshev points are expected to yield much smaller values for these integrals, hence better condition for the map $\tilde{G}_n$.

The sharpness of (3.15) can be tested by considering $dl(t) = d\lambda(t)$, in which case the map $\tilde{G}_n$ essentially reduces to the (well-conditioned) map H_n^{-1}. The integral in (3.15), nevertheless, does not appear to allow an easy evaluation or estimation in simple form, except in special cases. One such special case is the Chebyshev measure $d\lambda(t) = (1-t^2)^{-1/2}\,dt$ on $[-1, 1]$, for which the integral in question can be evaluated by the Turán quadrature formula [28],

$$\int_{-1}^{1} f(t)(1-t^2)^{-1/2}\,dt = \sum_{\nu=1}^{n} [\lambda_\nu f(\tau_\nu) + \lambda'_\nu f'(\tau_\nu) + \lambda''_\nu f''(\tau_\nu)] + R_n(f),$$

where $\tau_\nu = \cos((2\nu-1)\pi/2n)$, which is exact for all $f \in \mathbb{P}_{4n-1}$ and known in closed form [22]:

$$\lambda_\nu = \frac{\pi}{n}, \quad \lambda'_\nu = -\frac{\pi}{4n^3}\tau_\nu, \quad \lambda''_\nu = \frac{\pi}{4n^3}(1-\tau_\nu^2).$$

One finds, in view of (3.14),

$$\int_{-1}^{1} \sum_{\mu=1}^{n} \left[h_\mu^2(t) + \frac{1}{\lambda_\mu^2} k_\mu^2(t)\right](1-t^2)^{-1/2}\,dt = \sum_{\nu=1}^{n} \left[\lambda_\nu + 2\lambda''_\nu\left(\frac{1}{\lambda_\nu^2} + h''_\nu(\tau_\nu)\right)\right]$$

$$\leqq \pi + 2\sum_{\nu=1}^{n} \frac{\lambda''_\nu}{\lambda_\nu^2} = \pi + \frac{2n^2}{\pi^2}\sum_{\nu=1}^{n} \lambda''_\nu,$$

since $h''_\nu(\tau_\nu) < 0$ for all ν. Observing that

$$\sum_{\nu=1}^{n} \lambda''_\nu = \frac{\pi}{4n^3}\sum_{\nu=1}^{n} \sin^2\left(\frac{2\nu-1}{2n}\pi\right) = \frac{\pi}{4n^3}\cdot\frac{n}{2} = \frac{\pi}{8n^2},$$

one gets

$$\int_{-1}^{1} \sum_{\mu=1}^{n} \left[h_\mu^2(t) + \frac{1}{\lambda_\mu^2} k_\mu^2(t)\right](1-t^2)^{-1/2}\,dt \leqq \pi + \frac{1}{4\pi}.$$

Finally, since $\nu_0 = \pi$, $\nu_r = 0$ for $r > 0$, hence $\tilde{\nu}_0 = \sqrt{\pi}$, $\tilde{\nu}_r = 0$ for $r > 0$, and since $\sum_{\nu=1}^{n}(\lambda_\nu^2 + \tau_\nu^2) = (\pi^2/n) + (n/2)$, we obtain

$$(\operatorname{cond} \tilde{G}_n)(\tilde{\nu}) \leqq \sqrt{\frac{\pi^2 + 1/4}{\pi^2/n + n/2}} \sim \sqrt{\frac{2\pi^2 + 1/2}{n}} \quad \text{as } n \to \infty,$$

admittedly a somewhat too optimistic result (made so by the factor $1/\|\gamma\|$ in (3.15)).

The same considerations apply to the example $dl(t) = (1-t^2)^{-1/2}\,dt$ on $[-1, 1]$ and $d\lambda(t) = d\lambda_N(t)$ the discrete N-point measure with abscissas at the Chebyshev points $t_m = \cos((2m-1)\pi/2N)$, $m = 1, 2, \cdots, N$, and jumps equal to π/N, provided that $n \leqq N$.

3.4. The condition underlying the discretized Stieltjes procedure. It is not entirely clear what should be the appropriate map that underlies the discretized Stieltjes procedure. In the simplest case $d\lambda(t) = \omega(t)\,dt$ on $[-1, 1]$, the input data surely include the values $\omega(t_m^{(N)})$ of the weight function at the discretization points $t_m^{(N)}$, $m = 1, 2, \cdots, N$, but may also include these points themselves, as well as the quadrature weights $w_m^{(N)}$. From these data the procedure then determines the desired coefficients α_k, β_k, $k = 0, 1, \cdots, n-1$, or more precisely, their discrete approximations

$\alpha_{k,N}, \beta_{k,N}$, $k = 0, 1, \cdots, n-1$. Analogous considerations apply to the more general measures $d\lambda(t)$ considered at the end of § 2.2.

The map in question, therefore, is similar to the map H_n considered in § 3.1, and in fact may be thought of as an approximation $H_{n,N}$ of H_n. Since our interest is in the condition of these maps, where orders of magnitude is all that matters, we may as well take the condition of H_n as indicative of the sensitivities inherent in the discretized Stieltjes procedure. It will be seen by numerical examples that cond H_n indeed agrees reasonably well with the actual error growth observed in the discretized Stieltjes procedure.

4. Examples. The purpose of this section is to illustrate the performance of the procedures of § 2, and the underlying theory of § 3, in a number of examples that we hope are representative. All computations reported were carried out on the CDC 6500 computer in single precision, except for the computation of errors, which was done in double precision.

4.1. Discrete orthogonal polynomials.

Example 4.1. The discrete orthogonal polynomials $t_r(x)$ of Chebyshev.

These are orthogonal with respect to the N-point discrete measure with abscissas at the integers $0, 1, \cdots, N-1$ and jumps equal to $1/N$:

$$\frac{1}{N}\sum_{k=0}^{N-1} t_r(k)t_s(k) = 0, \qquad r \neq s, \quad r, s = 0, 1, \cdots, N-1. \tag{4.1}$$

We prefer to deal with the (monic) polynomials

$$\pi_r(x) = \frac{r!^2}{(2r)!}N^{-r}t_r(Nx), \tag{4.2}$$

which satisfy the recurrence relation (2.1) with

$$\begin{aligned} &\alpha_k = \frac{1}{2}\left(1 - \frac{1}{N}\right), \qquad k = 0, 1, \cdots, N-1, \\ &\beta_0 = 1, \qquad \beta_k = \frac{1-(k/N)^2}{4(4-1/k^2)}, \qquad k = 1, 2, \cdots, N-1, \end{aligned} \tag{4.3}$$

and have their point spectrum on the interval $[0, 1]$. As $N \to \infty$, the polynomials (4.2) tend to the monic Legendre polynomials (shifted to the interval $[0, 1]$).

We first illustrate in Table 4.1 the ill-conditioning of the map G_n from the ordinary moments

$$\mu_r = \int_0^1 t^r\, d\lambda_N(t) = \frac{1}{N}\sum_{k=0}^{N-1}\left(\frac{k}{N}\right)^r, \qquad r = 0, 1, \cdots, 2n-1,$$

TABLE 4.1

The condition of the map G_n in the case of ordinary moments and discrete Chebyshev measure $d\lambda(t) = d\lambda_N(t)$, $N = 20$.

n	cond G_n (3.10)	cond G_n (3.11)	err. growth
2	1.957 (1)	4.110 (1)	2.456 (1)
5	6.109 (4)	5.047 (5)	2.110 (5)
8	5.318 (8)	1.768 (10)	1.028 (10)
11	4.366 (12)	1.406 (15)	3.286 (14)

with $N = 20$, to the n-point Gauss–Christoffel formula, in the format that was already used in Table 3.2. As is evident from Table 4.1, Chebyshev's original algorithm rapidly loses accuracy, at the rate of somewhat more than one decimal digit per degree!

More stable, though not entirely unproblematic, is the modified Chebyshev algorithm, which we illustrate in Table 4.2 by recording the bound (3.15) for the condition of $\tilde{G}_n$, as well as the actual error growth observed. The latter is now defined as the L_2-norm of the relative errors in the coefficients α_k, β_k, $k = 0, 1, \cdots, n-1$, divided by $\varepsilon\sqrt{2n}$, where ε is the machine precision. We feel that this is the appropriate measure, since the result (3.15) is based on the Euclidean norm. The modified moments chosen are those relative to the (monic) Legendre polynomials for the interval [0, 1].

TABLE 4.2

The condition of the map $\tilde{G}_n$ in the case of Legendre moments and discrete Chebyshev measure $d\lambda(t) = d\lambda_N(t)$, $N = 10, 20, 40, 80$.

N	n	cond $\tilde{G}_n$	err. growth	N	n	cond $\tilde{G}_n$	err. growth
10	5	2.515 (0)	4.713 (0)	40	15	2.020 (1)	1.679 (2)
	10	6.311 (4)	7.349 (4)		25	1.311 (6)	1.016 (7)
20	5	7.859 (−1)	3.537 (0)		35	5.015 (14)	1.110 (15)
	10	1.932 (1)	1.105 (2)	80	10	4.885 (−1)	3.126 (0)
	15	2.952 (4)	1.421 (5)		20	6.480 (0)	1.240 (2)
	20	3.328 (10)	9.646 (10)		30	3.936 (3)	8.320 (4)
40	5	6.463 (−1)	2.106 (0)		40	4.800 (7)	1.013 (9)
	10	9.953 (−1)	7.182 (0)		50	1.738 (13)	1.759 (16)

The magnitude of cond $\tilde{G}_n$ is solely determined by the integral in (3.15), since $\|\tilde{v}\|$ and $\|\gamma\|$ in this example both have order of magnitude 1. The steady growth of cond $\tilde{G}_n$ can be explained by the fact that as n approaches N, the Gaussian nodes of $d\lambda_N(t)$ become more and more equally distributed. (They are equally spaced when $n = N$.) The Hermite interpolation polynomials h_ν and k_ν in (3.13) therefore exhibit the violent oscillations characteristic of equally spaced nodes, which accounts for the large values of the integral in (3.15). Chebyshev nodes on [0, 1], according to this explanation, ought to result in substantially smaller conditions, a fact that will indeed be confirmed in the next example.

The error growth shown in Table 4.2 is consistently somewhat larger than what is indicated by cond $\tilde{G}_n$. This is because the growth of error in the coefficients α_k, β_k includes also the effects of the map H_n, the condition of which is shown in Table 4.3.

One might think that the large oscillations of h_ν and k_ν could be filtered out by choosing a measure $dl(t)$ in (3.15) which is very small (or even equal to zero) near the end zones of the interval [0, 1]. While this indeed reduces the magnitude of the bothersome integral, the other factor $\|\tilde{v}\|$ in (3.15) increases so much more that the condition of $\tilde{G}_n$ in fact gets worse.

Substantially more stable is the Stieltjes procedure, measured both in terms of the condition of the map H_n (cf. § 3.4) and in terms of actual performance. For $N = 10$ and 20, cond H_n is less than 22.08 and 50.80, respectively, for all $n \leqq N$, whereas the actual error growth observed is by factors of at most 10.86 and 16.66, respectively. For $N = 40$ and $N = 80$ we have the situation indicated in Table 4.3. It shows that ill-conditioning and consequent instability set in as n approaches N, relatively late for $N = 40$, but sooner for $N = 80$. The condition of H_n is seen to correctly predict the trend of instability, but overestimates it by several orders of magnitude.

TABLE 4.3
Stability of the Stieltjes procedure for the discrete Chebyshev measure $d\lambda(t) = d\lambda_N(t)$, $N = 40$ *and* 80.

N	n	cond H_n	err. growth	N	n	cond H_n	err. growth
40	≦35	≦7.2 (3)	≦2.4 (1)	80	≦50	≦2.6 (3)	≦1.95 (1)
	36	1.030 (5)	2.122 (2)		55	4.751 (6)	7.015 (3)
	37	1.755 (6)	3.835 (3)		60	2.937 (10)	4.284 (7)
	38	4.419 (7)	9.216 (4)		65	2.220 (12)	1.088 (12)
	39	1.641 (9)	3.361 (6)		70	2.172 (12)	1.668 (15)
	40	1.205 (11)	2.487 (8)		75	2.006 (12)	1.668 (15)

We report these results solely to illustrate the behavior of the various procedures in a typical case of a discrete measure involving equally spaced points. There is, of course, no need to apply these procedures, since the recurrence relation is known explicitly (cf. (4.3)).

Example 4.2. Polynomials orthogonal with respect to the discrete inner product

$$[p, q]_N = \sum_{k=1}^{N} w_k p(t_k) q(t_k),$$

where $t_k = t_k^{(N)}$ are the Chebyshev points on $[-1, 1]$ and $w_k = w_k^{(N)}$ the weights of the N-point Fejér quadrature rule. This example is of interest in connection with our discretization of the Stieltjes procedure (cf. § 2.2).

It seems natural, in this case, to run the modified Chebyshev algorithm with the modified moments relative to the (monic) Chebyshev polynomials of the first kind. The map $\tilde{G}_n$ then turns out to be perfectly well-conditioned; see Table 4.4. For $N = 10$, 20, 40, 80 and for selected values $n \leqq N$, we found cond $\tilde{G}_n$ never to exceed 1.2, and to be usually less than 1. The map H_n, likewise, appears to be quite well-conditioned. Accordingly, both the modified Chebyshev algorithm, as well as the Stieltjes procedure, perform exceedingly well. The respective error growths are shown in the last two columns of Table 4.4.

TABLE 4.4
Performance of the modified Chebyshev algorithm and the Stieltjes procedure in Example 4.2.

N	n	cond $\tilde{G}_n$	cond H_n	err. growth in Chebyshev algorithm	err. growth in Stieltjes procedure
10	5	1.169 (0)	6.968 (0)	1.969 (0)	3.750 (0)
	10	8.925 (−1)	2.133 (1)	1.969 (0)	1.472 (1)
20	5	1.169 (0)	6.968 (0)	1.969 (0)	6.000 (0)
	10	9.152 (−1)	1.785 (1)	1.994 (0)	9.969 (0)
	20	6.473 (−1)	5.054 (1)	1.045 (1)	2.053 (1)
40	10	9.152 (−1)	1.785 (1)	1.994 (0)	1.200 (1)
	20	6.684 (−1)	4.530 (1)	5.996 (0)	1.200 (1)
	40	4.597 (−1)	1.213 (2)	3.146 (1)	2.697 (1)
80	20	6.684 (−1)	4.530 (1)	5.996 (0)	2.300 (1)
	40	4.773 (−1)	1.071 (2)	9.998 (0)	2.300 (1)
	80	3.250 (−1)	2.827 (2)	7.948 (1)	8.435 (1)

Example 4.3. "Truncated Charlier polynomials", orthogonal with respect to the inner product

$$[p, q]_N = \sum_{k=0}^{N-1} \frac{e^{-a}a^k}{k!} p(k)q(k), \qquad a > 0.$$

For $N \to \infty$, these become the Charlier polynomials, whose recurrence formula is known explicitly.

The modified Chebyshev algorithm, at least when used in conjunction with modified moments based on Laguerre polynomials, performs rather poorly on this example. The main reason is the rapidly deteriorating condition of the respective map $\tilde{G}_n$. This is illustrated in Table 4.5 for the case $a = 1$ and $N = 40$. Practically identical results are obtained for larger N, and quite similar ones for smaller values of N.

TABLE 4.5
Performance of the modified Chebyshev algorithm with Laguerre moments in Example 4.3.

N	n	cond $\tilde{G}_n$	err. growth
40	2	4.113 (0)	0.0
	4	1.832 (3)	1.365 (2)
	6	3.963 (6)	5.622 (4)
	8	2.006 (10)	2.217 (9)
	10	1.793 (14)	2.907 (13)

For comparison we give in Table 4.6 some analogous information for the Stieltjes procedure.

TABLE 4.6
Performance of the Stieltjes procedure in Example 4.3.

N	n	cond H_n	err. growth
40	5	8.130 (0)	5.995 (0)
	10	2.740 (1)	1.027 (1)
	15	4.635 (1)	2.241 (1)
	20	6.661 (1)	3.547 (1)
	25	7.215 (5)	8.444 (7)
	30	1.532 (11)	7.290 (14)

4.2. Polynomials orthogonal on an interval.

Example 4.4. An example of Christoffel [4, Ex. 6]: $d\lambda(t) = \omega(t)\,dt$ with $\omega(t) = [(1-k^2t^2)(1-t^2)]^{-1/2}$ on $[-1, 1]$, $0 < k < 1$.

What intrigued Christoffel was the fact that the associated orthogonal polynomials $\{\pi_r(t)\}$, when considered as functions of $x = \int_0^t \omega(t)\,dt$, constitute a sequence of doubly periodic functions orthogonal in the sense

$$\int_{-K}^{K} \pi_r(t)\pi_s(t)\,dx = 0, \qquad r \neq s,$$

where K denotes the complete elliptic integral $K = \int_0^1 \omega(t)\,dt$.

Since $(1-k^2t^2)^{-1/2}$ is analytic in a neighborhood of the segment $[-1, 1]$, the desired polynomials must be "close" to the Chebyshev polynomials of the first kind.

This suggests the use of the latter as input to the modified Chebyshev algorithm, i.e., the construction of the desired recursion coefficients from the modified moments

$$\nu_r = \int_{-1}^{1} p_r(t)\omega(t)\,dt \tag{4.4}$$

with respect to the monic Chebyshev polynomials $p_0 = T_0$, $p_r(t) = T_r(t)/2^{r-1}$, $r = 1, 2, \cdots$. These moments can be computed as follows. Letting first $t = \cos\varphi$ in (4.4) gives

$$\nu_0 = \int_0^{\pi} \frac{d\varphi}{(1-k^2\cos^2\varphi)^{1/2}}, \qquad \nu_r = \frac{1}{2^{r-1}} \int_0^{\pi} \frac{\cos r\varphi}{(1-k^2\cos^2\varphi)^{1/2}}\,d\varphi, \qquad r \geqq 1. \tag{4.5}$$

Now put $\theta = \pi/2 - \varphi$ in the Fourier expansion

$$\frac{1}{(1-k^2\sin^2\theta)^{1/2}} = C_0(k^2) + 2\sum_{n=1}^{\infty} C_n(k^2)\cos 2n\theta$$

and substitute the result in (4.5). By the orthogonality of the cosine functions one immediately obtains

$$\begin{aligned} \nu_0 &= \pi C_0(k^2), \\ \nu_{2m} &= (-1)^m \frac{\pi}{2^{2m-1}} C_m(k^2), \qquad m = 1, 2, 3, \cdots, \end{aligned} \tag{4.6}$$

while of course $\nu_{2m-1} = 0$, $m = 1, 2, 3, \cdots$. On the other hand, $y_n = C_n(k^2)$, $n = 0, 1, 2, \cdots$, is a minimal solution of the three-term recurrence relation

$$\left(n+\frac{1}{2}\right) y_{n+1} + n\frac{1+q^2}{q} y_n + \left(n-\frac{1}{2}\right) y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots, \tag{4.7}$$

satisfying

$$y_0 + 2\sum_{n=1}^{\infty} y_n = 1, \tag{4.8}$$

where

$$q = \frac{k^2}{2-k^2+2(1-k^2)^{1/2}}$$

(see, e.g., Luke [23, p. 36]). Our algorithm in [9, Eq. (3.9)], in conjunction with the normalizing condition (4.8), then yields the Fourier coefficients $C_n(k^2)$, hence the modified moments (4.6), very accurately and efficiently. The algorithm works well even when k^2 is quite close to 1. Note, in fact, that (4.7) is a difference equation of the Poincaré type, with characteristic equation

$$u^2 + \frac{1+q^2}{q}u + 1 = 0, \qquad 0 < q < 1,$$

having two real roots u_1, u_2 with $|u_1| > 1 > |u_2|$ and

$$\left|\frac{u_1}{u_2}\right| = \frac{1}{q^2}.$$

(The minimal solution $y_n = C_n(k^2)$ "corresponds" to u_2.) If $k^2 = 1-\varepsilon$, $0<\varepsilon \ll 1$, then

$$\frac{1}{q^2} = \left(\frac{1+\sqrt{\varepsilon}}{1-\sqrt{\varepsilon}}\right)^2 = 1+4\sqrt{\varepsilon}+8\varepsilon+12\varepsilon\sqrt{\varepsilon}+16\varepsilon^2+o(\varepsilon^2), \qquad \varepsilon \to 0,$$

so that for $k^2 = .999$, for example, we have $\varepsilon = 10^{-3}$, hence

$$\left|\frac{u_1}{u_2}\right| \approx 1.13,$$

which is still an adequate separation of the roots.

In addition to the modified moments being accurately computable, it turns out that the modified Chebyshev algorithm is extremely stable. For all values of k^2 that we tried ($0<k^2\leqq .999$), and for degrees n up to 80, the error growth factor never exceeded 3.258, and the condition number cond $\tilde{G}_n$ never 3.153.

We have also used the discretized Stieltjes procedure, as well as the discretized modified Chebyshev algorithm (cf. §§ 2.2 and 2.5), with good success, using the Gauss–Chebyshev quadrature rule in place of Fejér's. The advantage of testing convergence on the relative accuracy of the coefficients $\beta_{k,N}$, rather than on that of the modified moments $\nu_{r,N}$ (cf. § 2.5), can be clearly demonstrated in this example. The modified moments indeed decrease very rapidly (unless k^2 is close to 1), so that insistence on high relative accuracy in these moments would not be meaningful. For example, if $k^2 = .5$, $n = 20$, we find that

$$\max_{0\leqq k\leqq n-1} \left|\frac{\beta_{k,N}-\beta_k}{\beta_k}\right| = 8.81\times 10^{-14} \quad \text{for } N = 60,$$

while for the same value of N,

$$\max_{\substack{0\leqq r\leqq 2n-1 \\ r \text{ even}}} \left|\frac{\nu_{r,N}-\nu_r}{\nu_r}\right| = 1.76\times 10^{1},$$

the maximum being attained for $r = 36$, where $\nu_r = 2.3825\cdots\times 10^{-25}$.

Example 4.5. Logarithmic singularity: $d\lambda(t) = \ln(1/t)\,dt$ on $[0, 1]$.

The modified moments relative to (shifted) Legendre and Jacobi polynomials are known explicitly for this measure, and even for more general measures such as $d\lambda(t) = t^{\alpha}(1-t)^{\beta}\ln(1/t)\,dt$, $\alpha, \beta > -1$ (cf. [1], [7], [17], [21]). The modified Chebyshev algorithm, based on Legendre moments, produces results which are essentially accurate to machine precision; the largest error growth factor observed in the range $1\leqq n\leqq 80$ is 2.82. The reason for this excellent performance is to be found in the well-conditioning of the maps $\tilde{G}_n$ and H_n, for which we show in Table 4.7 the bound (3.15) for cond $\tilde{G}_n$ and cond H_n computed on the basis of (3.8).

TABLE 4.7
The condition of the maps $\tilde{G}_n$ and H_n in Example 4.5.

n	cond $\tilde{G}_n$	cond H_n
5	5.903 (0)	7.835 (0)
10	1.090 (1)	2.040 (1)
20	2.058 (1)	4.623 (1)
40	3.981 (1)	1.095 (2)
80	7.818 (1)	2.548 (2)

The discretized Stieltjes procedure, in contrast, converges rather slowly, making it difficult to obtain an accuracy much higher than 6 or 7 significant decimal digits.

Example 4.6. Half-range Hermite measure $d\lambda(t) = e^{-t^2}\,dt$ on $[0, \infty]$.

Here, the map H_n is quite well-conditioned (cond $H_n \leqq 2.28 \times 10^2$ for $n \leqq 80$), in contrast to the map $\tilde{G}_n$, which becomes rapidly ill-conditioned if modified moments relative to Hermite or Laguerre polynomials are used, which appear to be natural choices. Interestingly, Laguerre polynomials give significantly worse conditionings than Hermite polynomials, which is also borne out by a correspondingly faster error growth in the coefficients α_k, β_k; see Table 4.8. Accordingly, the modified Chebyshev algorithm is not effective in this example. Acceptable results, with some effort, can be had by the discretized Stieltjes procedure, which for $n = 40$, e.g., produces α_k, β_k, $k = 0, 1, \cdots, n-1$, to about 12 correct decimal digits, requiring a discretization parameter $N = 560$. Much better results are obtained if the interval $[0, \infty]$ is decomposed as $[0, 3] \cup [3, 6] \cup [6, 9] \cup [9, \infty]$ and the discretized Stieltjes procedure is applied in the manner described at the end of § 2.2, using Fejér's quadrature rule (suitably transformed) in each subinterval. Again for $n = 40$, this will yield 15 correct decimal digits with $N = 80$. The method is similarly applicable to more general measures $d\lambda(t) = e^{-t^p}\,dt$ on $[0, \infty]$, $p > 1$.

TABLE 4.8
The condition of $\tilde{G}_n$ in Example 4.6 for modified moments based on Hermite and Laguerre polynomials.

n	Hermite moments		Laguerre moments	
	cond $\tilde{G}_n$	err. growth	cond $\tilde{G}_n$	err. growth
2	1.554 (1)	5.713 (0)	7.270 (1)	2.296 (1)
4	2.524 (3)	3.261 (2)	1.349 (6)	1.045 (6)
6	6.739 (5)	6.300 (4)	1.297 (11)	9.663 (10)
8	2.206 (8)	2.386 (8)	3.127 (16)	3.112 (16)
10	8.026 (10)	2.696 (11)	5.547 (21)	–

4.3. Polynomials orthogonal with respect to multiple component distributions. As already observed in § 2.2, the discretized Stieltjes procedure can also handle measures $d\lambda(t)$ of a more general type, for example, measures on a set of disjoint intervals or measures including a point spectrum. The discretized Stieltjes procedure in these circumstances is often far superior to the modified Chebyshev algorithm, which tends to become unstable. We illustrate this by a number of examples, of which Example 4.11 may prove useful in the numerical solution of large systems of linear algebraic equations by iterative methods [31].

Example 4.7. Piecewise constant weight function: $d\lambda(t) = \omega(t)\,dt$, where $\omega(t) = 1$ on $[-1, -\xi] \cup [\xi, 1]$ and $\omega(t) = 0$ elsewhere, $0 < \xi < 1$.

Equivalently, $d\lambda(t) = [\omega_1(t) + \omega_2(t)]\,dt$, where ω_1, ω_2 are the characteristic functions of the intervals $[-1, -\xi]$ and $[\xi, 1]$, respectively. The discretized Stieltjes procedure, as amended at the end of § 2.2, works extremely well, even for ξ relatively close to 1; the map H_n remains well-conditioned. Some relevant data are given in Table 4.9. (The discretized Stieltjes procedure in this example converges after one iteration, if the discretization parameter N is chosen appropriately; cf. § 2.2).

The modified moments ν_r, $r = 0, 1, \cdots, 2n-1$, based on Legendre polynomials are easily computed (exactly) by n-point Gauss–Legendre quadrature. The ensuing

TABLE 4.9
Performance of the discretized Stieltjes procedure in Example 4.7.

ξ	n	cond H_n	err. growth	ξ	n	cond H_n	err. growth
.3	5	7.683 (0)	8.233 (0)	.7	5	1.974 (1)	1.392 (1)
	10	2.138 (1)	9.956 (0)		10	5.520 (1)	1.392 (1)
	20	5.230 (1)	1.522 (1)		20	1.295 (2)	1.800 (1)
	40	1.248 (2)	1.937 (1)		40	3.072 (2)	1.803 (1)
.5	5	1.060 (1)	1.390 (1)	.9	5	6.585 (1)	2.463 (1)
	10	2.979 (1)	1.426 (1)		10	1.919 (2)	2.463 (1)
	20	7.159 (1)	1.426 (1)		20	4.469 (2)	3.894 (1)
	40	1.709 (2)	1.598 (1)		40	1.073 (3)	5.773 (1)

modified Chebyshev algorithm, however, becomes severely unstable, even for moderately large ξ, on account of ill-conditioned maps $\tilde{G}_n$. This is documented in Table 4.10. The same is true for the discretized modified Chebyshev algorithm.

TABLE 4.10
Performance of the modified Chebyshev algorithm in Example 4.7.

ξ	n	cond $\tilde{G}_n$	err. growth	ξ	n	cond $\tilde{G}_n$	err. growth
.3	5	1.335 (0)	2.118 (2)	.7	5	6.454 (1)	7.081 (2)
	10	7.754 (0)	1.955 (2)		10	6.457 (4)	4.198 (5)
	20	1.276 (3)	6.537 (3)		20	8.012 (11)	8.015 (12)
	40	1.169 (8)	7.077 (8)		40	3.748 (26)	9.648 (15)
.5	5	4.830 (0)	1.914 (2)	.9	5	9.263 (3)	1.244 (4)
	10	3.658 (2)	1.640 (3)		10	1.171 (9)	1.838 (9)
	20	7.650 (6)	4.445 (7)		20	2.630 (21)	8.940 (16)
	40	1.057 (16)	3.683 (14)		40	-	-

By virtue of symmetry, the orthogonal polynomials $\{\pi_r\}$ of Example 4.7 can be expressed in terms of polynomials orthogonal on a single interval. Indeed, letting $\pi_{2r}(t) = p_r^+(t^2)$, $\pi_{2r+1}(t) = tp_r^-(t^2)$, $r = 0, 1, 2, \cdots$, the polynomials $p_r^{\pm}(x)$ are orthogonal on $[\xi^2, 1]$ with respect to the weight function $\omega^{\pm}(t) = t^{\mp 1/2}$. If α_k^+, β_k^+ are the recursion coefficients for $\{p_r^+(x)\}$, then

$$\beta_0 = 2(1-\xi), \qquad \beta_1 = \alpha_0^+,$$

$$\beta_{2k} = \frac{\beta_k^+}{\beta_{2k-1}}, \qquad k = 1, 2, 3, \cdots$$

$$\beta_{2k+1} = \alpha_k^+ - \beta_{2k},$$

are those for the desired polynomials $\{\pi_r(t)\}$ (cf. [3, Chapt. I, §§ 8–9]). The discretized Stieltjes procedure could also be used to generate α_k^+, β_k^+, but would then require an infinite process, rather than the finite one when applied directly to the weight function ω.

Example 4.8. Adding a point spectrum to the distribution $d\lambda(t)$ of Example 4.7, where $\xi = .5$.

We make the distribution asymmetric if we add a point spectrum consisting of a single point, say at $t_1 = 2$, with jump $w_1 = 1$. The effect of this is a slight worsening of

the condition of $\tilde{G}_n$ and a profound impairment of cond H_n. As a result, one now has difficulty not only with the modified Chebyshev algorithm, but also with the discretized Stieltjes procedure, although the latter "survives" a bit longer; see Table 4.11.

TABLE 4.11
Performance of the modified Chebyshev algorithm and the discretized Stieltjes procedure in Example 4.8.

			Error growth	
n	cond $\tilde{G}_n$	cond H_n	mod. Chebyshev	discr. Stieltjes
4	1.612 (1)	2.021 (1)	6.621 (1)	2.898 (2)
8	1.174 (3)	4.088 (1)	1.146 (7)	4.627 (2)
12	9.217 (4)	6.658 (1)	4.712 (11)	5.700 (2)
16	6.950 (6)	4.218 (4)	4.686 (17)	1.876 (4)
20	5.120 (8)	4.334 (9)	-	1.910 (9)
24	2.135 (10)	2.833 (14)	-	4.456 (14)

Adding another point, $t_2 = -2$, with jump $w_2 = 1$, restores symmetry, but neither significantly improves, nor worsens, the condition of H_n.

We know of no stable method to compute orthogonal polynomials of the type introduced in Example 4.8.

Example 4.9.[1] Adding a constant to the Chebyshev weight function: $d\lambda(t) = [(1-t^2)^{-1/2} + a]\,dt$ on $[-1, 1]$, $a > 0$.

The discretized Stieltjes procedure applied directly to $d\lambda(t) = \omega(t)\,dt$, $\omega(t) = (1-t^2)^{-1/2} + a$ converges extremely slowly, regardless of whether the discretization is effected by Fejér's or the Gauss–Chebyshev quadrature rule. The reason for this is easily seen if one writes $\omega(t) = (1-t^2)^{-1/2}[1 + a(1-t^2)^{1/2}]$ and notes that the function in brackets has infinite derivatives at $t = \pm 1$. On the other hand, treating the two additive components of ω independently, as suggested at the end of § 2.2, and applying the Gauss–Chebyshev quadrature rule to the first, and Fejér's to the second, Stieltjes's procedure converges trivially. Results obtained for selected values of a in the range $0 \leqq a \leqq 1000$, and $0 \leqq n \leqq 80$, are accurate almost to machine precision, the largest error growth factor being 9.219(1). The condition numbers cond H_n are slowly decreasing as a function of a, from the values for Chebyshev polynomials, when $a = 0$, to those for Legendre polynomials, when $a \to \infty$ (cf. Table 3.1).

Equally accurate, but considerably faster (by a factor of more than 10 for $n = 80$) is the modified Chebyshev algorithm, based on Chebyshev moments

$$\nu_0 = \pi + 2a,$$

$$\nu_r = \frac{1}{2^{r-1}} \int_{-1}^{1} T_r(t)\,d\lambda(t) = -\frac{a}{2^{r-2}(r^2-1)}, \qquad r \text{ even} \neq 0,$$

$$\nu_r = 0, \qquad r \text{ odd}.$$

The maximum bound (3.15) for the condition of $\tilde{G}_n$ is found to be 6.748 (for $a = 1000$, $n = 80$), and the maximum error growth factor 1.146(1).

[1] This example was proposed to the author by Professor M. Golomb.

The recursion coefficients β_k, $k>0$, behave as expected, when a varies from 0 to ∞: There is a smooth (but not monotone) transition from the Chebyshev case to the Legendre case.

Example 4.10. A weight distribution involving a modified Bessel function: $d\lambda(t)=t^{\mu}K_0(t)\,dt$ on $[0,\infty]$, $\mu>-1$.

Gauss–Christoffel quadrature rules with this weight distribution are proposed by Wong [30] to obtain asymptotic approximations to oscillatory integrals.

It is known that

$$K_0(t)=\begin{cases}R(t)+I_0(t)\ln\left(\frac{1}{t}\right), & 0<t\leqq 1,\\ t^{-1/2}e^{-t}S(t), & 1\leqq t\leqq\infty,\end{cases}$$

where R and S are well-behaved smooth functions on their respective intervals and I_0 is the "regular" modified Bessel function. For R, S and I_0, high-accuracy rational approximations are available; see Russon and Blair [24]. Using the "multiple component" version of the discretized Stieltjes procedure, as described at the end of § 2.2, we decompose the inner product $(p,q)=\int_0^{\infty}t^{\mu}K_0(t)p(t)q(t)\,dt$ as follows,

$$(p,q)=\int_0^1 t^{\mu}[R(t)p(t)q(t)]\,dt+\int_0^1 t^{\mu}\ln\left(\frac{1}{t}\right)[I_0(t)p(t)q(t)]\,dt$$
$$+e^{-1}\int_0^{\infty}e^{-t}[(1+t)^{\mu-1/2}S(1+t)p(1+t)q(1+t)]\,dt,$$

and discretize the first integral by an N-point Gauss–Jacobi quadrature rule with parameters $\alpha=0$, $\beta=\mu$, the second by an N-point Gauss–Christoffel quadrature rule relative to the weight distribution $t^{\mu}\ln(1/t)\,dt$ on $[0,1]$, and the last one by an N-point Gauss–Laguerre quadrature rule. The first and last of these quadrature rules are easily obtained from the respective Jacobi matrices (see § 1, Eq. (1.4), and the remarks following this equation), while the second can be generated by the modified Chebyshev algorithm, as indicated in Example 4.5.

In this way, the desired orthogonal polynomials (and Gauss–Christoffel quadrature rules) can be generated accurately and in a stable manner. If $\mu=0$, or $\mu=-1/2$, for example, one gets the recursion coefficients α_k, β_k, $0\leqq k\leqq n$, accurately to 15 significant decimal digits by taking $N=100$ for $n=20$, and $N=160$ for $n=40$. In contrast, the discretized Stieltjes procedure based on the (transformed) Fejér quadrature rule requires $N=230$ for $\mu=0$ and $n=10$, just to get six correct decimal digits, and becomes prohibitively expensive for much larger values of n or higher accuracy.

Example 4.11. Find a polynomial $P_n(t)$ of degree $\leqq n$, with $P_n(1)=1$, such that $\int_0^1 P_n^2(t)\omega(t)\,dt=\min$, where $\omega(t)=\varepsilon$ on $[0,\xi]$, $\omega(t)=1$ on $[\xi,\eta]$, $\omega(t)=0$ on $[\eta,1]$, and $\varepsilon>0$, $0<\xi<\eta<1$.

The solution is known to be the polynomial orthogonal on $[0,1]$ with respect to the weight function $(1-t)\omega(t)$ (cf. [3, Chapt. I, § 7]). If $\pi_n(\cdot)=\pi_n(\cdot\,;(1-t)\omega(t)\,dt)$ denotes the monic orthogonal polynomial, then $P_n(t)=\pi_n(t)/\pi_n(1)$, and the desired minimum value is $\beta_0\beta_1\cdots\beta_n/\pi_n^2(1)$. The recursion coefficients α_k, β_k for $\{\pi_r\}$ are obtained in a stable manner by the discretized Stieltjes procedure, which can be made to converge after one iteration. Selected results (for the minimum value of $\int_0^1 P_n^2(t)\omega(t)\,dt$) in the case $\xi=1/3$, $\eta=2/3$, are shown in Table 4.12.

TABLE 4.12
Minimum values for the extremum problem of Example 4.11.

ε	n	$\min \int_0^1 P_n^2 \omega\, dt$	ε	n	$\min \int_0^1 P_n^2 \omega\, dt$
.0	5	4.890 (−9)	.6	5	7.984 (−7)
	10	1.107 (−16)		10	1.551 (−12)
	20	5.479 (−32)		20	5.733 (−24)
	40	1.317 (−62)		40	7.653 (−47)
.2	5	5.382 (−7)	.8	5	8.758 (−7)
	10	1.107 (−12)		10	1.707 (−12)
	20	4.038 (−24)		20	6.308 (−24)
	40	5.347 (−47)		40	8.420 (−47)
.4	5	6.950 (−7)	1.0	5	9.386 (−7)
	10	1.364 (−12)		10	1.842 (−12)
	20	5.030 (−24)		20	6.802 (−24)
	40	6.703 (−47)		40	9.075 (−47)

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16.5. [90] "ON SOME ORTHOGONAL POLYNOMIALS OF INTEREST IN THEORETICAL CHEMISTRY"

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ON SOME ORTHOGONAL POLYNOMIALS OF INTEREST IN THEORETICAL CHEMISTRY [1])

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To Germund Dahlquist on his 60th birthday

Abstract.

Constructive methods are developed for a class of polynomials orthogonal on two symmetric intervals. An analysis is given of certain phenomena of instability in connection with nonlinear recursions. Special cases arising in the study of the diatomic linear chain are worked out explicitly. In one of these cases the associated n-point Gauss-Christoffel quadrature formula has equal weights whenever n is even.

1. Introduction.

We consider constructive methods for orthogonal polynomials $\{\pi_r(\cdot\,; d\lambda)\}$ corresponding to the measure $d\lambda(t) = \omega(t)dt$ on $[-1, 1]$, where

$$\omega(t) = \begin{cases} |t|^\gamma (t^2-\xi^2)^p (1-t^2)^q, & t \in [-1, -\xi] \cup [\xi, 1], \\ 0 \text{ elsewhere}, & 0 < \xi < 1, p > -1, q > -1, \gamma \in \mathbb{R}. \end{cases} \tag{1.1}$$

The theory of such polynomials has previously been studied in [1] (for $\gamma = 1$), also in the more general (asymmetric) case where the factor $|t|$ is replaced by $|t+\alpha|$. The special case $\gamma = 1$, $p = q = -\frac{1}{2}$, $\xi = (1-r)/(1+r)$ $(0 < r < 1)$ of (1.1) arises in the study of the diatomic linear chain [13], where $r = m/M$ has the meaning of a mass ratio, m and M $(m < M)$ being the masses of the two kinds of particles alternating along the chain [2]). The object is to generate the coefficients β_k in the basic recurrence relation

$$\begin{aligned} &\pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \\ &\pi_{k+1}(t) = t\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \end{aligned} \tag{1.2}$$

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[2]) In reference [13] the basic interval is [0,1], rather than $[-1,1]$ as in (1.1).

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for the desired orthogonal polynomials. J. C. Wheeler in [13] employs the modified Chebyshev algorithm (cf. [6, §2.4]) for this purpose, using a rather ingenious choice of modified moments that induces numerical stability. Here we wish to point out (Sections 2–4) that the recursion coefficients of interest, even in the more general case indicated in (1.1), can be generated directly by simple nonlinear recursions. Care must be exercised, however, in the selection of these recursions to avoid numerical instability. In the special cases $\gamma = \pm 1$, $p = q = \pm\frac{1}{2}$, further manipulation of these recursions yields the coefficients of the basic recurrence relation in closed form (Section 5). Finally, in Section 6, we observe that the Gauss-Christoffel quadrature formula associated with the weight function (1.1) for $\gamma = 1$, $p = q = -\frac{1}{2}$ has equal weights whenever their number is even, and that this is the only symmetric Gauss-Christoffel quadrature formula with that property.

The author wishes to thank Professor J. C. Wheeler for letting him see a preprint of his paper [13].

2. Generation of the recurrence relation.

The weight function ω in (1.1) is even and its two support intervals are symmetric with respect to the origin. The associated orthogonal polynomials π_r are therefore even or odd depending on the parity of r, and they can be represented in terms of polynomials orthogonal on a single interval.

Letting

$$\pi_{2r}(t) = p_r^+(t^2), \qquad \pi_{2r+1}(t) = tp_r^-(t^2), \qquad r = 0, 1, 2, \ldots, \tag{2.1}$$

the polynomials $p_r^\pm(x)$ are orthogonal on $[\xi^2, 1]$ with respect to the weight function

$$\omega^\pm(x) = \omega(x^{1/2})x^{\mp 1/2} = x^{(\gamma \mp 1)/2}(x-\xi^2)^p(1-x)^q, \qquad \xi^2 < x < 1. \tag{2.2}$$

If we denote by α_k^+, β_k^+ the recursion coefficients for the (monic) polynomials $\{p_r^+(x)\}$,

$$p_{-1}^+(x) = 0, \quad p_0^+(x) = 1, \tag{2.3}$$

$$p_{k+1}^+(x) = (x-\alpha_k^+)p_k^+(x) - \beta_k^+ p_{k-1}^+(x), \quad k = 0, 1, 2, \ldots,$$

then the desired (monic) polynomials, as is well-known (cf. [2, Ch. I, §§8–9]), have the recursion coefficients

$$\left.\begin{aligned} \beta_1 &= \alpha_0^+ \\ \beta_{2k} &= \beta_k^+/\beta_{2k-1} \\ \beta_{2k+1} &= \alpha_k^+ - \beta_{2k} \end{aligned}\right\} \quad k = 1, 2, 3, \ldots. \tag{2.4$^+$}$$

Likewise, in terms of α_0^+ and the recursion coefficients α_k^-, β_k^- for the polynomials $\{p_r^-(x)\}$, we have

$$(2.4^-) \qquad \left.\begin{aligned} \beta_1 &= \alpha_0^+ \\ \beta_{2k} &= \alpha_{k-1}^- - \beta_{2k-1} \\ \beta_{2k+1} &= \beta_k^- / \beta_{2k} \end{aligned}\right\} \quad k = 1, 2, 3, \ldots.$$

On the other hand, if $\mathring{\alpha}_k^\pm$, $\mathring{\beta}_k^\pm$ are the recursion coefficients of the orthogonal polynomials with respect to the weight function (2.2) transformed to the standard interval $[-1, 1]$, i.e., with respect to

$$(2.5) \qquad \mathring{\omega}^\pm(t) = \left(t + \frac{1+\xi^2}{1-\xi^2}\right)^{(\gamma \mp 1)/2} (1+t)^p (1-t)^q, \quad -1 < t < 1,$$

then

$$(2.6^\pm) \qquad \begin{aligned} \alpha_k^\pm &= \tfrac{1}{2}(1-\xi^2)\mathring{\alpha}_k^\pm + \tfrac{1}{2}(1+\xi^2), && k = 0, 1, 2, \ldots, \\ \beta_k^\pm &= (\tfrac{1}{2}(1-\xi^2))^2 \mathring{\beta}_k^\pm, && k = 1, 2, 3, \ldots. \end{aligned}$$

The problem thus boils down to computing the recursion coefficients $\mathring{\alpha}_k^\pm$, $\mathring{\beta}_k^\pm$ for the weight function $\mathring{\omega}^\pm(t)$ in (2.5). Once obtained, they yield $\alpha_k^\pm$ and $\beta_k^\pm$ by means of $(2.6^\pm)$ and thus β_k by means of $(2.4^\pm)$. Either sign may be chosen, the choice depending on convenience or numerical stability.

Before discussing numerical stability, we prove

THEOREM 2.1. *There holds*

$$(2.7) \qquad \lim_{k\to\infty} \beta_{2k} = \tfrac{1}{4}(1-\xi)^2, \qquad \lim_{k\to\infty} \beta_{2k+1} = \tfrac{1}{4}(1+\xi)^2.$$

PROOF. The weight function (2.5) belongs to the Szegö class, i.e., it satisfies the conditions in [12, Theorem 12.1.2]. From [12, Eqs. (12.7.4), (12.7.6)] it then follows that

$$(2.8) \qquad \lim_{k\to\infty} \mathring{\alpha}_k^\pm = 0, \qquad \lim_{k\to\infty} \mathring{\beta}_k^\pm = \tfrac{1}{4},$$

regardless of the sign in (2.5). Consequently, by $(2.6^\pm)$,

$$(2.9) \qquad \lim_{k\to\infty} \alpha_k^\pm = \tfrac{1}{2}(1+\xi^2), \qquad \lim_{k\to\infty} \beta_k^\pm = (\tfrac{1}{4}(1-\xi^2))^2.$$

Now denote by γ_r, $\gamma_r^\pm$, and $\mathring{\gamma}_r^\pm$ the leading coefficient of the orthonormal polynomial of degree r relative to the weight function ω on $[-1, -\xi] \cup [\xi, 1]$, $\omega^\pm$ on $[\xi^2, 1]$, and $\mathring{\omega}^\pm$ on $[-1, 1]$, respectively. By (2.1) one has

$$(2.10) \qquad \gamma_{2r} = \gamma_r^+, \qquad \gamma_{2r+1} = \gamma_r^-,$$

and an elementary computation yields

$$(2.11)\qquad (\gamma_r^{\pm})^{-2} = \int_{\xi^2}^{1} [p_r^{\pm}(x)]^2 \omega^{\pm}(x)dx = (\tfrac{1}{2}(1-\xi^2))^{(\gamma \mp 1)/2 + 2r + p + q + 1} (\mathring{\gamma}_r^{\pm})^{-2}.$$

By a theorem of Szegö [12, Eq. (12.7.2)],

$$(2.12)\qquad \mathring{\gamma}_r^{\pm} \sim 2^r \mathring{\gamma}^{\pm} \qquad \text{as } r \to \infty,$$

where

$$(2.13)\qquad \mathring{\gamma}^{\pm} = \pi^{-1/2} \exp\left\{-(2\pi)^{-1} \int_{-1}^{1} \ln \mathring{\omega}^{\pm}(t)(1-t^2)^{-1/2}dt\right\}.$$

Now $\beta_r = \gamma_{r-1}^2/\gamma_r^2$, $r \geqq 1$, so that, using (2.10), (2.11),

$$\beta_{2k} = (\gamma_{2k-1}/\gamma_{2k})^2 = (\gamma_{k-1}^{-}/\gamma_k^{+})^2 = \tfrac{1}{2}(1-\xi^2)(\mathring{\gamma}_{k-1}^{-}/\mathring{\gamma}_k^{+})^2,$$

hence, by (2.12),

$$(2.14)\qquad \beta_{2k} \sim \tfrac{1}{8}(1-\xi^2)(\mathring{\gamma}^{-}/\mathring{\gamma}^{+})^2, \qquad k \to \infty.$$

Similarly,

$$(2.15)\qquad \beta_{2k+1} \sim \tfrac{1}{2}(1-\xi^2)(\mathring{\gamma}^{+}/\mathring{\gamma}^{-})^2, \qquad k \to \infty.$$

This shows that both limits in (2.7) exist. Letting $k \to \infty$ in (2.4$^+$), and noting (2.9), one sees, in fact, that these limits must be the roots of the quadratic equation $\beta^2 - \frac{1}{2}(1+\xi^2)\beta + (\frac{1}{4}(1-\xi^2))^2 = 0$, i.e., the quantities on the right in (2.7). It remains to identify roots with limits.

Using (2.13) in (2.14) gives

$$\begin{aligned}\mathring{\gamma}^{-}/\mathring{\gamma}^{+} &= \exp\left\{(2\pi)^{-1} \int_{-1}^{1} \ln[\mathring{\omega}^{+}(t)/\mathring{\omega}^{-}(t)](1-t^2)^{-1/2}dt\right\} \\ &= \exp\left\{-(2\pi)^{-1} \int_{-1}^{1} \ln(t+\varrho)(1-t^2)^{-1/2}dt\right\}, \quad \varrho = (1+\xi^2)/(1-\xi^2).\end{aligned}$$

But

$$\begin{aligned}\int_{-1}^{1} \ln(t+\varrho)(1-t^2)^{-1/2}dt &= \int_{0}^{1} \ln(\varrho^2 - t^2)(1-t^2)^{-1/2}dt \\ &= \pi \ln \varrho + \int_{0}^{1} \ln(1-\varrho^{-2}t^2)(1-t^2)^{-1/2}dt \\ &= \pi \ln \varrho + \pi \ln[\tfrac{1}{2}(1+(1-\varrho^{-2})^{1/2})] = \pi \ln[\tfrac{1}{2}(\varrho + (\varrho^2-1)^{1/2})],\end{aligned}$$

where Gradshteyn & Ryzhik [9, Eq. (4.295.29)] has been used for the last integral. There follows

$$(\mathring{\gamma}^-/\mathring{\gamma}^+)^2 = 2/(\varrho+(\varrho^2-1)^{1/2}) = 2(1-\xi)/(1+\xi),$$

which, together with (2.14), yields $\beta_{2k} \sim \frac{1}{4}(1-\xi)^2$, as claimed. ■

We remark that Theorem 2.1 and its proof are valid for any symmetric weight function $\omega(t)$ supported on $[-1,-\xi] \cup [\xi,1]$, provided the weight function

$$(2.16)\quad \mathring{\omega}^{\pm}(t) = [t+(1+\xi^2)/(1-\xi^2)]^{\mp 1/2}\omega([\tfrac{1}{2}(1-\xi^2)t+\tfrac{1}{2}(1+\xi^2)]^{1/2}),\ -1<t<1,$$

belongs to the Szegö class.

A heuristic argument now shows that the limits in (2.7) represent, asymptotically, an "attracting" stationary point of (2.4^+). Indeed, replacing α_k^+, β_k^+ in (2.4^+) by their limits values (2.9), one finds that a small relative perturbation ε in the limit value of β_{2k-1} produces in β_{2k+1} a relative perturbation $((1-\xi)/(1+\xi))^2\varepsilon$ (to first order in ε), the same being true for perturbations in β_{2k}. The recursion (2.4^+) thus is "attracting" near the stationary point, hence numerically stable, the more so the closer ξ is to 1. Just the opposite holds in case of (2.4^-), where relative perturbations are being magnified by the factor $((1+\xi)/(1-\xi))^2$ and the stationary point (2.7) of (2.4^-) is "repelling", the stronger so the closer ξ is to 1. Interchanging the limits, on the other hand, produces an attracting fixed point of (2.4^-). In the presence of rounding errors, the recursion (2.4^-) is therefore not likely to converge to the correct limits, but rather to limits which are flipped over. Thus, (2.4^-) must be expected to become numerically unstable.

The choice of the sign in (2.5), therefore, may well be dictated by considerations of numerical stability.

3. The case of general γ, p and q.

For arbitrary γ, the weight function in (2.5) is a general Jacobi weight (with parameters $\alpha = q$, $\beta = p$) multiplied by a factor which has a singularity (branch point or pole) or a zero at $-(1+\xi^2)/(1-\xi^2)$ outside the interval $[-1,1]$. In the case of a branch point, the associated orthogonal polynomials (i.e., the coefficients $\mathring{\alpha}_k^{\pm}, \mathring{\beta}_k^{\pm}$) may be obtained by a discretized Stieltjes procedure (cf. [6, §2.2]), using a discretization of the inner product based on the Gauss-Jacobi quadrature rule (with parameters $\alpha = q$, $\beta = p$). This should work well if the branch point is far away from $[-1,1]$, i.e., if ξ is close to 1. In this case, it is also possible, and perhaps more efficient, to use the methods in [10, pp. 451–452], the multiplicative factor in question being well approximated by a polynomial. Otherwise, more refined quadrature rules must be employed that take proper account of the branch point close to $[-1,1]$. If $(\gamma \mp 1)/2$ is a

positive integer, one can make repeated use of the algorithm in [5, §4.1] or the procedures in [8], all of which are reputed to be stable. In the case of a pole, i.e. if $(\gamma \mp 1)/2$ is a negative integer, repeated use of the algorithm in [5, §5.1] or the procedure in [4, §4] is suggested according as the pole is close or farther away from $[-1, 1]$, respectively. Alternatively, one may develop special quadrature rules (with real nodes) which take the pole into account and use them in conjunction with the discretized Stieltjes procedure. The simplest case, of course, is $\gamma = \pm 1$, in which case $\mathring{\alpha}_k^{\pm}, \mathring{\beta}_k^{\pm}$ are simply the recursion coefficients of the appropriate Jacobi polynomials. This is considered in more detail in Sections 4 and 5.

4. The case $\gamma = 1$ and general p, q.

Consider first $\gamma = 1$. In this case it is convenient to use the upper sign in (2.5), that is $\mathring{\omega}^{+}(t)$, which clearly is a Jacobi weight function on the interval $[-1, 1]$. Therefore, $\mathring{\alpha}_k^{+} = \alpha_k^J$, $\mathring{\beta}_k^{+} = \beta_k^J$ are the recursion coefficients of the (monic) Jacobi polynomials (with parameters $\alpha = q$, $\beta = p$) on the standard interval $[-1, 1]$. Combining (2.6^{+}) and (2.4^{+}), and defining $\beta_0 = \int_{-1}^{1} \omega(t)dt$, we obtain

$$
\begin{aligned}
\beta_0 &= (1-\xi^2)^{p+q+1}\Gamma(p+1)\Gamma(q+1)/\Gamma(p+q+2), \\
\beta_1 &= \tfrac{1}{2}(1-\xi^2)\alpha_0^J + \tfrac{1}{2}(1+\xi^2) \qquad (\gamma = 1) \\
\beta_{2k} &= (\tfrac{1}{2}(1-\xi^2))^2 \beta_k^J/\beta_{2k-1} \\
\beta_{2k+1} &= \tfrac{1}{2}(1-\xi^2)\alpha_k^J + \tfrac{1}{2}(1+\xi^2) - \beta_{2k}
\end{aligned}
\qquad k = 1, 2, 3, \ldots . \tag{4.1}
$$

By symmetry, of course, $\alpha_k = 0$ for all $k \geqq 0$. Numerical evidence indicates that the recursion in (4.1) is quite stable for an extended range of the Jacobi parameters $\alpha = q$, $\beta = p$ and for all ξ in $0 < \xi < 1$, even very close to the end points. We have in fact the case of an attracting fixed point; cf. Theorem 2.1 and the discussion following it.

If $\gamma = -1$, it would seem most convenient to take the lower sign in (2.5), in which case again $\mathring{\alpha}_k^{-} = \alpha_k^J$, $\mathring{\beta}_k^{-} = \beta_k^J$, and (2.6^{-}) may be combined with (2.4^{-}) to give

$$
\begin{aligned}
\beta_0 &= (\tfrac{1}{2}(1-\xi^2))^{p+q} F(-(1+\xi^2)/(1-\xi^2)), \\
\beta_1 &= \alpha_0^{+} \qquad (\gamma = -1) \\
\beta_{2k} &= \tfrac{1}{2}(1-\xi^2)\alpha_{k-1}^J + \tfrac{1}{2}(1+\xi^2) - \beta_{2k-1} \\
\beta_{2k+1} &= (\tfrac{1}{2}(1-\xi^2))^2 \beta_k^J/\beta_{2k}
\end{aligned}
\qquad k = 1, 2, 3, \ldots, \tag{4.2}
$$

where

$$
F(z) = \int_{-1}^{1} (1+t)^p (1-t)^q (t-z)^{-1} dt \tag{4.3}
$$

is the Stieltjes transform of the Jacobi measure. Note that α_0^+ in (4.2) is given by

$$\alpha_0^+ = \frac{\int_{\xi^2}^1 x\cdot x^{-1}(x-\xi^2)^p(1-x)^q dx}{\int_{\xi^2}^1 x^{-1}(x-\xi^2)^p(1-x)^q dx} = \frac{2^{p+q}(1-\xi^2)\Gamma(p+1)\Gamma(q+1)}{\Gamma(p+q+2)F(-(1+\xi^2)/(1-\xi^2))}. \tag{4.4}$$

To compute $F(z)$ for $z\notin[-1,1]$ one can use the recursive algorithm in [4, §5], which works well unless z is very close to $[-1,1]$, i.e., ξ is very small.

Unfortunately, the recursion (4.2), unlike (4.1), exhibits the kind of instability discussed at the end of Section 2. It initially produces relatively accurate results (especially if ξ is small), but then deteriorates and ends up converging to the limits (2.7) flipped over. During the switchover, some of the β's even become negative! The limits (2.7) are now a repelling fixed point of (4.2).

The problem can be avoided by choosing the upper sign in (2.5) and by computing the coefficients $\mathring{\alpha}_k^+$, $\mathring{\beta}_k^+$ by the more elaborate methods discussed in Section 3.

5. The cases $\gamma = \pm 1$ and $p = q = \pm\frac{1}{2}$.

5.1. *The case* $p = q = -\frac{1}{2}$

Consider first $\gamma = 1$, which is the case of interest in the diatomic linear chain model [13]. Here, $\alpha_k^J = 0$ $(k \geqq 0)$, and $\beta_1^J = \frac{1}{2}, \beta_k^J = \frac{1}{4}$ $(k \geqq 2)$, so that (4.1) becomes

$$\begin{aligned}
\beta_0 &= \pi \\
\beta_1 &= \tfrac{1}{2}(1+\xi^2) \\
\beta_2 &= \tfrac{1}{4}(1-\xi^2)^2/(1+\xi^2) \\
\beta_3 &= \tfrac{1}{4}(1+6\xi^2+\xi^4)/(1+\xi^2) \\
\beta_{2k} &= (\tfrac{1}{4}(1-\xi^2))^2/\beta_{2k-1} \\
\beta_{2k+1} &= \tfrac{1}{2}(1+\xi^2)-\beta_{2k}
\end{aligned}\Bigg\} \quad k = 2, 3, 4, \ldots, \tag{5.1}$$

where the last relation (for β_{2k+1}) also holds when $k = 1$. We first consider the even-numbered coefficients.

Letting

$$a = (\tfrac{1}{4}(1-\xi^2))^2, \quad b = \tfrac{1}{2}(1+\xi^2), \tag{5.2}$$

we combine the last two relations in (5.1) to obtain $\beta_{2k} = a/(b-\beta_{2k-2})$, $k = 2, 3, \ldots$ This yields the finite continued fraction

$$-\beta_{2k} = \frac{-a}{b-}\,\frac{a}{b-}\cdots\frac{a}{b-\beta_2}, \qquad k \geqq 2, \tag{5.3}$$

with constant partial numerators $-a$ and constant partial denominators b (except for the last ones). Denoting by A_n, B_n the nth numerator and denominator, respectively, of (5.3), we have from the elementary theory of continued fractions,

$$\begin{aligned} &A_0 = 0, A_{-1} = 1; \; B_0 = 1, B_{-1} = 0, \\ &\left.\begin{aligned} A_n &= bA_{n-1} - aA_{n-2} \\ B_n &= bB_{n-1} - aB_{n-2} \end{aligned}\right\} \quad n = 1, 2, \ldots, k-1, \\ &A_k = A_{k-1} - \beta_2 A_{k-2}; \; B_k = B_{k-1} - \beta_2 B_{k-2} \end{aligned} \tag{5.4}$$

and

$$-\beta_{2k} = A_k/B_k, \qquad k = 2, 3, 4, \ldots. \tag{5.5}$$

Since the recursion in (5.4) for $n = 1, 2, \ldots, k-1$ represents a linear difference equation with constant coefficients, it can be solved explicitly by well-known methods. An elementary (but somewhat lengthy) computation then yields with $\eta = (1-\xi)/(1+\xi)$

$$\beta_{2k} = \tfrac{1}{4}(1-\xi)^2(1+\eta^{2k-2})/(1+\eta^{2k}), \qquad k = 1, 2, 3, \ldots \qquad (\gamma = 1). \tag{5.6}$$

For the odd-numbered coefficients one finds quite analogously,

$$\begin{aligned} \beta_1 &= \tfrac{1}{2}(1+\xi^2), \\ \beta_{2k+1} &= \tfrac{1}{4}(1+\xi)^2(1+\eta^{2k+2})/(1+\eta^{2k}), \qquad k = 1, 2, 3, \ldots. \end{aligned} \qquad (\gamma = 1), \tag{5.7}$$

Note that (5.6) and (5.7) confirm the limit relations established in Theorem 2.1. In the application considered in [13], where $\xi = (1-r)/(1+r)$, they yield $\lim_{k\to\infty}\beta_{2k} = (r/(1+r))^2$ and $\lim_{k\to\infty}\beta_{2k+1} = (1+r)^{-2}$, in agreement [3]) with what was conjectured in [13, Eq. (25)]. The relative deviations from the limits, moreover, are given by

$$\varepsilon_{2k} \sim (r^{-2}-1)e^{-2k\ln(1/r)}, \qquad \varepsilon_{2k+1} \sim -(r^{-1}-r)e^{-(2k+1)\ln(1/r)}, \qquad k \to \infty,$$

so that the limits are attained exponentially fast, with a decay rate $\ln(1/r)$ which becomes larger as r deviates away from unity. This, too, has been conjectured in [13] from numerical evidence.

Proceeding now to the case $\gamma = -1$ (with p and q still being $-\frac{1}{2}$ each), we first note that

$$F(-(1+\xi^2)/(1-\xi^2)) = \pi(1-\xi^2)/2\xi,$$

[3]) To transform to the interval $[0, 1]$ considered in reference [13], the coefficients β_k, $k \geqq 1$, must be multiplied by 1/4 and α_k set equal to $\frac{1}{2}$ for all $k \geqq 0$.

so that (4.2) and (4.4) become

$$
\begin{aligned}
\beta_0 &= \pi/\xi \\
\beta_1 &= \xi \\
\beta_2 &= \tfrac{1}{2}(1-\xi)^2 \\
\beta_3 &= \tfrac{1}{4}(1+\xi)^2 \\
\beta_{2k} &= \tfrac{1}{2}(1+\xi^2)-\beta_{2k-1} \\
\beta_{2k+1} &= (\tfrac{1}{4}(1-\xi^2))^2/\beta_{2k}
\end{aligned}
\Bigg\} \quad k = 2, 3, 4, \ldots . \tag{5.8}
$$

A computation very similar to the one in the case $\gamma = 1$ then yields the remarkably simple, but in the light of the discussion at the end of Section 2 understandable results

$$
\begin{aligned}
&\beta_2 = \tfrac{1}{2}(1-\xi)^2, \qquad \beta_{2k} = \tfrac{1}{4}(1-\xi)^2, \qquad k \geqq 2, \\
&\beta_1 = \xi, \qquad\qquad\quad \beta_{2k+1} = \tfrac{1}{4}(1+\xi)^2, \quad k \geqq 1,
\end{aligned}
\qquad (\gamma = -1). \tag{5.9}
$$

5.2. *The case* $p = q = \frac{1}{2}$

Following the same course of computation as outlined in Subsection 5.1, but now with $\beta_k^J = \frac{1}{4}$ for all $k \geqq 1$ and $F(-(1+\xi^2)/(1-\xi^2)) = \pi(1-\xi)/(1+\xi)$, one finds, when $\gamma = 1$, and with $\eta = (1-\xi)/(1+\xi)$ as before,

$$
\begin{aligned}
&\beta_{2k} = \tfrac{1}{4}(1-\xi)^2(1-\eta^{2k})/(1-\eta^{2k+2}), \qquad k = 1, 2, 3, \ldots, \\
&\beta_{2k+1} = \tfrac{1}{4}(1+\xi)^2(1-\eta^{2k+4})/(1-\eta^{2k+2}), \qquad k = 0, 1, 2, \ldots,
\end{aligned}
\qquad (\gamma = 1). \tag{5.10}
$$

Similarly, when $\gamma = -1$,

$$
\beta_{2k} = \tfrac{1}{4}(1-\xi)^2, \quad k \geqq 1, \quad \beta_{2k+1} = \tfrac{1}{4}(1+\xi)^2, \quad k \geqq 0 \quad (\gamma = -1). \tag{5.11}
$$

The orthogonal polynomials associated with (5.11) are used in [13] to define "modified moments".

One could, of course, continue and treat in the same manner further special cases, for example $p = \frac{1}{2}$, $q = -\frac{1}{2}$, but we refrain from doing this here.

6. Equally weighted Gaussian quadrature formulae.

By a classical result, due to Posse [11], the Chebyshev measure $d\lambda(t) = (1-t^2)^{-1/2}dt$ on $[-1, 1]$ is the only measure, up to a linear transformation, for which the n-point Gauss-Christoffel formula

$$
\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f), \qquad R_n(\mathbb{P}_{2n-1}) = 0, \tag{6.1}
$$

has equal weights

$$\lambda_1^{(n)} = \lambda_2^{(n)} = \cdots = \lambda_n^{(n)} \tag{6.2}$$

for each $n = 1, 2, 3, \ldots$. We point out, here, that other equally weighted Gauss-Christoffel quadrature formulae exist if the equicoefficient property (6.2) is required to hold only for even values of n. In fact, we determine all such quadrature formulae which are symmetric, i.e., in which the support of $d\lambda(t)$ is symmetric with respect to the origin and $d\lambda(t) = \omega(t)dt$ with $\omega(t)$ an even nonnegative function.

Let $f(t) = p(t^2)$, where $p \in \mathbb{P}_{n-1}$ is an arbitrary polynomial of degree $\leqq n-1$. Then (6.1) holds with zero error, and by symmetry, assuming $\tau_1^{(n)} > \tau_2^{(n)} > \cdots > \tau_n^{(n)}$, and n even,

$$\int_{\mathbb{R}_+} p(t^2)\omega(t)dt = \sum_{\nu=1}^{n/2} \lambda_\nu^{(n)} p([\tau_\nu^{(n)}]^2), \qquad p \in \mathbb{P}_{n-1}.$$

Substituting $t^2 = x$, and letting $m = n/2$, this gives

$$\int_{\mathbb{R}_+} p(x)\omega(x^{1/2})x^{-1/2}dx = 2\sum_{\nu=1}^{m} \lambda_\nu^{(2m)} p([\tau_\nu^{(2m)}]^2), \quad p \in \mathbb{P}_{2m-1}, m = 1, 2, 3, \ldots. \tag{6.3}$$

If (6.2) holds for $n = 2m$, $m = 1, 2, 3, \ldots$, then Posse's result implies that $\omega(x^{1/2})x^{-1/2}dx$ is a Chebyshev measure on some finite interval on $\mathbb{R}_+$. Normalizing this interval to have the right end point at 1, the left end point may be any nonnegative number less than 1, say ξ^2, $0 \leqq \xi < 1$. Up to a constant factor, therefore,

$$\omega(x^{1/2})x^{-1/2} = (x-\xi^2)^{-1/2}(1-x)^{-1/2}, \qquad \xi^2 < x < 1,$$

and thus

$$\omega(t) = \begin{cases} |t|(t^2-\xi^2)^{-1/2}(1-t^2)^{-1/2}, & t \in [-1, -\xi] \cup [\xi, 1], \\ 0 \text{ elsewhere.} \end{cases} \tag{6.4}$$

This is precisely the weight function (1.1) with $\gamma = 1$ and $p = q = -\frac{1}{2}$. If $\xi = 0$, it reduces of course to the Chebyshev weight function.

The quadrature formula in question is

$$\int_{[-1,-\xi]\cup[\xi,1]} f(t)|t|(t^2-\xi^2)^{-1/2}(1-t^2)^{-1/2}dt = \lambda^{(n)} \sum_{\nu=1}^{n} f(\tau_\nu^{(n)}) + R_n(f), \tag{6.5}$$

n even,

where

$$\tau_\nu^{(n)} = \left[\frac{1-\xi^2}{2}\cos\frac{2\nu-1}{n}\pi + \frac{1+\xi^2}{2}\right]^{1/2} \qquad \nu = 1, 2, \ldots, n/2. \tag{6.6}$$

$$\tau_{n-\nu+1}^{(n)} = -\tau_\nu^{(n)}, \qquad \lambda^{(n)} = \pi/n$$

In terms of Chebyshev quadrature, we can say that the measure $\omega(t)dt$ in (6.4) has property T^∞ and its T-sequence is $T = \{2, 4, 6, 8, \ldots\}$ (cf. [3, §5]). Other measures are known having the same T-sequence [7], but the associated Chebyshev quadrature rules, of course, cannot be Gaussian at the same time. The weight function (6.4), however, is contained as a special case ($a = 0$) in [7, Eq. (3.1)].

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16.6. [145] “Computing orthogonal polynomials in Sobolev spaces”

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Computing orthogonal polynomials in Sobolev spaces*

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Summary. Numerical methods are considered for generating polynomials orthogonal with respect to an inner product of Sobolev type, i.e., one that involves derivatives up to some given order, each having its own (positive) measure associated with it. The principal objective is to compute the coefficients in the increasing-order recurrence relation that these polynomials satisfy by virtue of them forming a sequence of monic polynomials with degrees increasing by 1 from one member to the next. As a by-product of this computation, one gains access to the zeros of these polynomials via eigenvalues of an upper Hessenberg matrix formed by the coefficients generated. Two methods are developed: One is based on the modified moments of the constitutive measures and generalizes what for ordinary orthogonal polynomials is known as "modified Chebyshev algorithm". The other — a generalization of "Stieltjes's procedure" — expresses the desired coefficients in terms of a Sobolev inner product involving the orthogonal polynomials in question, whereby the inner product is evaluated by numerical quadrature and the polynomials involved are computed by means of the recurrence relation already generated up to that point. The numerical characteristics of these methods are illustrated in the case of Sobolev orthogonal polynomials of old as well as new types. Based on extensive numerical experimentation, a number of conjectures are formulated with regard to the location and interlacing properties of the respective zeros.

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1. Introduction

Let $d\lambda_\sigma$, $\sigma = 0, 1, \ldots, s$, be positive measures on the real line $\mathbb{R}$ having bounded or unbounded support. We consider the Sobolev space

$$H_s(\mathbb{R}) = \{f : \sum_{\sigma=0}^{s} \int_{\mathbb{R}} [f^{(\sigma)}]^2 d\lambda_\sigma < \infty\}$$

of functions f whose successive derivatives of order $\sigma \le s$ are square integrable against the respective measures $d\lambda_\sigma$. We assume that these measures are such that the space of polynomials $\mathbb{P}$ is a subspace of $H_s(\mathbb{R})$. We equip $\mathbb{P}$ with the inner product

$$\begin{aligned}(p,q)_{H_s} = &\int_{\mathbb{R}} p(x)q(x)d\lambda_0(x) + \int_{\mathbb{R}} p'(x)q'(x)d\lambda_1(x) + \cdots \\ &+ \int_{\mathbb{R}} p^{(s)}(x)q^{(s)}(x)d\lambda_s(x), \qquad p, q \in \mathbb{P},\end{aligned} \tag{1.1}$$

and associated norm $\|p\|_{H_s}^2 = (p,p)_{H_s}$. To stay away from unessential complications, we assume that $d\lambda_0$ has infinitely many points of increase. The inner product (1.1) is then positive definite on $\mathbb{P}$, and therefore defines a unique sequence of (monic) orthogonal polynomials $\pi_0, \pi_1, \pi_2, \ldots$:

$$\begin{aligned}&(\pi_k, \pi_\ell)_{H_s} = 0, \quad k \ne \ell, \quad k, \ell = 0, 1, 2, \ldots, \\ &\pi_k(x) = x^k + \text{ lower-degree terms}, \ k = 0, 1, 2, \ldots \ .\end{aligned} \tag{1.2}$$

We call them *orthogonal polynomials of Sobolev type*. Like any sequence of monic polynomials whose degrees increase by 1 from one member to the next, they must satisfy a recurrence relation of the form

$$\pi_{k+1}(x) = x\pi_k(x) - \sum_{j=0}^{k} \beta_j^k \pi_{k-j}(x), \qquad k = 0, 1, 2, \ldots \ . \tag{1.3}$$

One of our objects in this paper is to develop, and discuss, computational methods for generating the recursion coefficients β_j^k. These coefficients are important not only for the recursive computation of the desired orthogonal polynomials by means of (1.3), but also for computing the zeros of π_n as eigenvalues of an $n \times n$ upper Hessenberg matrix. Indeed, if

$$B_n = \begin{bmatrix} \beta_0^0 & \beta_1^1 & \beta_2^2 & \cdots & \beta_{n-2}^{n-2} & \beta_{n-1}^{n-1} \\ 1 & \beta_0^1 & \beta_1^2 & \cdots & \beta_{n-3}^{n-2} & \beta_{n-2}^{n-1} \\ 0 & 1 & \beta_0^2 & \cdots & \beta_{n-4}^{n-2} & \beta_{n-3}^{n-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \beta_0^{n-2} & \beta_1^{n-1} \\ 0 & 0 & 0 & \cdots & 1 & \beta_0^{n-1} \end{bmatrix} \tag{1.4}$$

and

$$\pi^{\mathrm{T}}(x) = [\pi_0(x), \pi_1(x), \ldots, \pi_{n-1}(x)], \tag{1.5}$$

then the zeros $\xi_1, \xi_2, \ldots, \xi_n$ of π_n are precisely the eigenvalues of B_n, with $\pi^{\mathrm{T}}(\xi_\nu)$ being a left eigenvector belonging to the eigenvalue ξ_ν. This follows readily from the relations (1.3) for $k = 0, 1, \ldots, n-1$ if we write them in matrix form as

$$x\pi^{\mathrm{T}}(x) = \pi^{\mathrm{T}}(x)B_n + \pi_n(x)e_n^{\mathrm{T}}, \qquad e_n^{\mathrm{T}} = [0, 0, \ldots, 1] \in \mathbb{R}^n.$$

Putting $x = \xi_\nu$ and noting that $\pi_n(\xi_\nu) = 0$ then yields

$$\xi_\nu \pi^{\mathrm{T}}(\xi_\nu) = \pi^{\mathrm{T}}(\xi_\nu)B_n, \tag{1.6}$$

which proves our assertion, since $\pi^{\mathrm{T}}(\xi_\nu)$ is a nonzero vector, its first component being $\pi_0(\xi_\nu) = 1$.

Classical orthogonal polynomials (on the line) correspond to the case $s = 0$ and have an inner product (1.1) satisfying

$$(xp, q)_{H_s} = (p, xq)_{H_s} \ (s = 0). \tag{1.7}$$

As a consequence, all coefficients β_j^k with $j > 1$ vanish, i.e., (1.3) is a three-term recurrence relation. In contrast, when $s > 0$, then (1.7) no longer holds, and we must expect a recurrence relation of the extended type (1.3).

Almost all cases studied in the literature refer to $s = 1$; prominent among these is the subcase in which

$$d\lambda_0(x) = d\lambda(x), \qquad d\lambda_1(x) = \gamma d\lambda(x), \qquad \gamma > 0, \tag{1.8}$$

where $d\lambda$ is a positive measure and γ a positive constant. The original motivation for considering orthogonal polynomials of this and similar types comes from the least squares approximation problem. Here, e.g., a given function f and its derivative f' are to be approximated simultaneously by a polynomial $\pi = \hat{\pi}$ of degree n minimizing

$$\| \pi - f \|_{H_1}^2 = \int_{\mathbb{R}} [\pi(x) - f(x)]^2 d\lambda(x) + \gamma \int_{\mathbb{R}} [\pi'(x) - f'(x)]^2 d\lambda(x) \tag{1.9}$$

over all $\pi \in \mathbb{P}_n$. Expanding π in the respective Sobolev-type orthogonal polynomials then yields, in the usual way, the Fourier approximation $\hat{\pi}$ of f and f'. The first work known to us, discussing this type of approximation, is the 1947 paper by D.C. Lewis [21], where the main emphasis, however, is on the remainder term of the approximation (expressed by means of the Peano kernel, as it were). Least squares approximation is also the motivation behind the work of P. Althammer [2], who was the first to initiate a detailed study of the associated orthogonal polynomials in the "Legendre case" $d\lambda(x) = dx$ on [–1,1] of (1.8). Rather remarkably, he has shown, among other things, that, as in the classical case, each π_n has n distinct zeros located in the interior of [–1,1], for all $\gamma > 0$. This is not true, however, for arbitrary positive measures $d\lambda$, as is shown in [2] by a counterexample; see also [34] and Sect. 3.2 below. The same polynomials, but normalized to the interval [0,1], have also been studied by W. Gröbner [14], who uses a variational approach and derives an interesting version of Rodrigues's formula for π_n. Alternative representations in terms of Legendre polynomials, and simplified proofs, are given by F.W. Schäfke [36]. P. Lesky [20] generalizes Gröbner's work to inner products (1.1) with $s \geq 1$ and $d\lambda_\sigma(x) = \gamma_\sigma dx$, $\gamma_\sigma > 0$. The example (1.8) with $d\lambda(x) = \mathrm{e}^{-x} dx$ on $[0,\infty]$ was dealt with by J. Brenner in his thesis [6] (see also [7]). This again is an example where all zeros of π_n can be shown (by an argument similar to Althammer's) to be simple and positive. When $d\lambda(x) = \mathrm{e}^{-x^2} dx$ on $[-\infty, \infty]$, the polynomials π_n are just the (monic) Hermite polynomials [6, Satz 2.3.1]. Some of the results of Althammer and Gröbner are generalized to Gegenbauer measures $d\lambda(x) = (1 - x^2)^{\alpha - \frac{1}{2}} dx$ in [27]. The example $d\lambda_0(x) = dx$ on [–1, 3] and $d\lambda_1(x) = \gamma \chi_{[-1,1]}(x) dx + dx$ on [–1, 3], discussed in [34] and generalizing an example of Althammer, is insofar of interest as for γ sufficiently large, π_n has at most two real zeros.

The application to least squares approximation on the interval [–1,1] in the case $d\lambda(x) = dx$ of (1.8) is further studied in A. Iserles et al. [15], where explicit formulae are derived not only for the respective polynomials π_n, but also for the Fourier coefficients. An example is given showing the advantage of Sobolev projections ($\gamma > 0$) over ordinary Legendre projections ($\gamma = 0$). In [16], the same authors study least squares approximation for the more general inner product (1.1) (with $s = 1$) with measures $d\lambda_0 = d\varphi$, $d\lambda_1 = \gamma d\psi$, where $(d\varphi, d\psi)$ forms a "coherent" pair — in a sense they define — and it is found, surprisingly, under proper normalizations, that all expansion coefficients except the last of π_n in terms of the classical polynomials $\{\pi_k(\,\cdot\,; d\varphi)\}$ are independent of n and indeed (as functions of γ) themselves orthogonal with respect to some (in general unknown) measure. They also develop an efficient algorithm for computing the expansion coefficients, which requires nothing beyond the calculation of classical expansion coefficients in the polynomials $\{\pi_k(\,\cdot\,; d\varphi)\}$ and $\{\pi_k(\,\cdot\,; d\psi)\}$, provided again that $d\varphi$ is coherent with $d\psi$. The zeros of the respective Sobolev orthogonal polynomials are studied by Meijer in [33].

Subsequent to work of H.L. Krall, A.M. Krall, L.L. Littlejohn, T.H. Koorwinder, T.S. Chihara and others, who inserted mass points of variable strengths at the endpoints of the support interval of classical measures, there has recently

been a flurry of activity regarding orthogonal polynomials of Sobolev type for an inner product (1.1) with $s = 1$ in which $d\lambda_0 = d\lambda_0^{\mathrm{ac}} + d\lambda_0^{\mathrm{d}}$ is a measure containing an absolutely continuous component $d\lambda_0^{\mathrm{ac}}$ and a discrete component $d\lambda_0^{\mathrm{d}}$, while $d\lambda_1 = d\lambda_1^{\mathrm{d}}$ is a discrete measure. The emphasis is generally on analytic and algebraic properties, and representations of the respective polynomials, but there are also many results on zeros. Thus, H. Bavinck and H.G. Meijer [3, 4] consider the case where $d\lambda_0^{\mathrm{ac}}$ is a Gegenbauer measure on [–1,1] and $d\lambda_0^{\mathrm{d}}$, $d\lambda_1^{\mathrm{d}}$ are both supported at the endpoints ± 1, each with equal weights. M. Alfaro et al. [1], F. Marcellán, T.E. Pérez and M.A. Piñar [26], and T.E. Pérez and M.A. Piñar [35] take $d\lambda_0^{\mathrm{ac}}$ to be an arbitrary absolutely continuous measure and $d\lambda_0^{\mathrm{d}}$, $d\lambda_1^{\mathrm{d}}$ both one-point measures supported at the same point inside, on the boundary, or outside the support of $d\lambda_0^{\mathrm{ac}}$. The special case of $d\lambda_0^{\mathrm{ac}}$ being the generalized Laguerre measure and $d\lambda_0^{\mathrm{d}}$, $d\lambda_1^{\mathrm{d}}$ supported (with different weights) at the origin is studied recently by R. Koekoek and H.G. Meijer [19] and R. Koekoek [18] and generalized to arbitrary measures $d\lambda_0^{\mathrm{ac}}$ on $[0, \infty]$ by H.G. Meijer [31]. For the analogous case with $s + 1$ discrete measures $d\lambda_0^{\mathrm{d}}, d\lambda_1^{\mathrm{d}}, \ldots, d\lambda_s^{\mathrm{d}}$ $(s > 1)$, see [17]. Higher-order derivatives are also considered in the papers [30] and [23], where $d\lambda_1 \equiv \cdots \equiv d\lambda_{s-1} \equiv 0$, and $d\lambda_s$ is supported at a single point c, viz. $c = 0$ in the former, and c arbitrary real in the latter. See also [8]. The case of an arbitrary measure $d\lambda_0$ on $\mathbb{R}$ and $d\lambda_1^{\mathrm{d}}$ supported on an arbitrary point $c \in \mathbb{R}$ is studied in [32] and an analogous case involving linear functionals in [5]. For measures $d\lambda_0^{\mathrm{ac}}$ in the Nevai class and $d\lambda_1^{\mathrm{d}}$ supported at a single point, and for more general Sobolev-type inner products, an asymptotic comparison between the Sobolev-type orthogonal polynomials and those orthogonal with respect to $d\lambda_0^{\mathrm{ac}}$ is made in [39, Ch.7], [24] and [22]. Many of the examples mentioned in this paragraph are special cases of Sobolev orthogonal polynomials relative to a pair of "semiclassical" measures $d\lambda_0$, $d\lambda_1$ studied in [28].

For a recent survey of Sobolev-type orthogonal polynomials we refer to [25].

In this paper, we first develop, in Sect. 2, a computational algorithm for generating the recursion coefficients β_j^k in (1.3), which extends to Sobolev-type orthogonal polynomials the "modified Chebyshev algorithm" (cf. [11, Sect. 2.4]) for ordinary orthogonal polynomials. Numerical experience with this algorithm, and computational results, are reported in Sect. 3. Particular attention is given to the zeros of the respective Sobolev-type orthogonal polynomials, for which a number of conjectures are formulated in the case of Jacobi measures (with and without discrete components) and generalized Laguerre measures. Finally, in Sect. 4, we describe a version of "Stieltjes's algorithm" appropriate for orthogonal polynomials of Sobolev type.

2. The modified Chebyshev algorithm

We now consider the general inner product (1.1) with $s \geq 1$,

$$(p, q)_{H_s} = \sum_{i=0}^{s} \int_{\mathbb{R}} p^{(i)}(x) q^{(i)}(x) d\lambda_i(x), \qquad p, q \in \mathbb{P}. \tag{2.1}$$

Our objective, in this section, similarly as in [11, Sects. 2.3, 2.4], is to use moment information about the measures $d\lambda_0, d\lambda_1, \ldots, d\lambda_s$ to generate the desired recursion coefficients β_j^k in (1.3). Since ordinary moments are expected to yield ill-conditioning, we adopt *modified moments*, and for simplicity define them relative to a single sequence of polynomials $\{p_k\}$, i.e.,

$$\nu_k^{(i)} = \int_{\mathbb{R}} p_k(x) d\lambda_i(x), \qquad k = 0, 1, 2, \ldots; \qquad i = 0, 1, \ldots, s. \tag{2.2}$$

As in [11], we assume that the polynomials p_k satisfy a three-term recurrence relation

$$\begin{aligned} p_{k+1}(x) &= (x - a_k)p_k(x) - b_k p_{k-1}(x), \qquad k = 0, 1, 2, \ldots, \\ p_0(x) &= 1, \qquad p_{-1}(x) = 0, \end{aligned} \tag{2.3}$$

with known coefficients a_k, b_k. The case of ordinary moments is included herein, with the choice $a_k = b_k = 0$. Normally, however, the a_k are real, not necessarily zero, and $b_k > 0$.

In what follows, we shall use the notation

$$(p, q)_{d\lambda_i} = \int_{\mathbb{R}} p(x)q(x)d\lambda_i(x), \qquad i = 0, 1, \ldots, s, \tag{2.4}$$

so that

$$(p, q)_{H_s} = \sum_{i=0}^{s} (p^{(i)}, q^{(i)})_{d\lambda_i}. \tag{2.5}$$

Definition 2.1. For $k, \ell = 0, 1, 2, \ldots$ and $u, v = 0, 1, \ldots, s$, we define

$$\sigma_{k,\ell} = (\pi_k, p_\ell)_{H_s}, \tag{2.6}$$

$$\mu_{k,\ell,i}^{(u,v)} = (\pi_k^{(u)}, p_\ell^{(v)})_{d\lambda_i}, \qquad i = 1, 2, \ldots, s, \tag{2.7}$$

where $\{\pi_k\}$ is the sequence of orthogonal polynomials of Sobolev type associated with the inner product (2.1), and $\{p_\ell\}$ are the polynomials (2.3) defining the modified moments (2.2). We will need the quantities (2.7) only for $u \le i$ and $v \le i$ (cf. (2.8)).

The following propositions are formulated with an algorithm in mind that generates the recursion coefficients β_j^k in (1.3) for $k = 0, 1, \ldots, n-1; j = 0, 1, \ldots, k$, hence the desired orthogonal polynomials up to degree n. This will generalize what we have called the Modified Chebyshev Algorithm in [11, Sect. 2.4].

Proposition 2.2. *We have, for* $k = 1, 2, \ldots, n-1$; $\ell = k, k+1, \ldots, 2n-k-1$,

$$\sigma_{k,\ell} = \sigma_{k-1,\ell+1} + a_\ell \sigma_{k-1,\ell} + b_\ell \sigma_{k-1,\ell-1} + \sum_{i=1}^{s} i(\mu_{k-1,\ell,i}^{(i-1,i)} - \mu_{k-1,\ell,i}^{(i,i-1)}) - \sum_{j=0}^{k-1} \beta_j^{k-1} \sigma_{k-1-j,\ell}. \tag{2.8}$$

Proof. By (2.6), (2.5) and (1.3) (with k replaced by $k-1$), we have

$$\sigma_{k,\ell} = (\pi_k, p_\ell)_{H_s} = (x\pi_{k-1}, p_\ell)_{d\lambda_0} + \sum_{i=1}^{s} ((x\pi_{k-1})^{(i)}, p_\ell^{(i)})_{d\lambda_i} - \sum_{j=0}^{k-1} \beta_j^{k-1} \sigma_{k-1-j,\ell}.$$

We write the first term on the right as $(\pi_{k-1}, xp_\ell)_{d\lambda_0}$, and for the second term note that

$$\begin{aligned} ((x\pi_{k-1})^{(i)}, p_\ell^{(i)})_{d\lambda_i} &= (x\pi_{k-1}^{(i)} + i\pi_{k-1}^{(i-1)}, p_\ell^{(i)})_{d\lambda_i} \\ &= (\pi_{k-1}^{(i)}, xp_\ell^{(i)})_{d\lambda_i} + i(\pi_{k-1}^{(i-1)}, p_\ell^{(i)})_{d\lambda_i} \\ &= (\pi_{k-1}^{(i)}, (xp_\ell)^{(i)})_{d\lambda_i} + i(\mu_{k-1,\ell,i}^{(i-1,i)} - \mu_{k-1,\ell,i}^{(i,i-1)}). \end{aligned}$$

Now we use (2.3) and its differentiated version in the form

$$xp_\ell = p_{\ell+1} + a_\ell p_\ell + b_\ell p_{\ell-1}, \qquad (xp_\ell)^{(i)} = p_{\ell+1}^{(i)} + a_\ell p_\ell^{(i)} + b_\ell p_{\ell-1}^{(i)}$$

to obtain (2.8). □

In all subsequent propositions, empty sums are assumed to be zero by definition.

Proposition 2.3. *We have, for* $i = 1, 2, \ldots, s$; $u = 0, 1, \ldots, i$, $v = 0, 1, \ldots, i$; $k = 1, 2, \ldots, n-1$, $\ell = k, k+1, \ldots, 2n-k-2$,

$$\begin{aligned} \mu_{k,\ell,i}^{(u,v)} &= \mu_{k-1,\ell+1,i}^{(u,v)} + a_\ell \mu_{k-1,\ell,i}^{(u,v)} + b_\ell \mu_{k-1,\ell-1,i}^{(u,v)} \\ &+ u\mu_{k-1,\ell,i}^{(u-1,v)} - v\mu_{k-1,\ell,i}^{(u,v-1)} - \sum_{j=0}^{k-1-u} \beta_j^{k-1} \mu_{k-1-j,\ell,i}^{(u,v)}, \end{aligned} \tag{2.9}$$

where the fourth and fifth terms on the right are zero if $u = 0$ *resp.* $v = 0$.

Proof. By definition (2.7) and (1.3), we have

$$\mu_{k,\ell,i}^{(u,v)} = (\pi_k^{(u)}, p_\ell^{(v)})_{d\lambda_i} = ((x\pi_{k-1})^{(u)}, p_\ell^{(v)})_{d\lambda_i} - \sum_{j=0}^{k-1} \beta_j^{k-1} (\pi_{k-1-j}^{(u)}, p_\ell^{(v)})_{d\lambda_i}.$$

By the product rule of differentiation,

$$((x\pi_{k-1})^{(u)}, p_\ell^{(v)})_{d\lambda_i} = (x\pi_{k-1}^{(u)} + u\pi_{k-1}^{(u-1)}, p_\ell^{(v)})_{d\lambda_i}$$

$$= (x\pi_{k-1}^{(u)}, p_\ell^{(v)})_{d\lambda_i} + u(\pi_{k-1}^{(u-1)}, p_\ell^{(v)})_{d\lambda_i}.$$

We write the first term on the right as $(\pi_{k-1}^{(u)}, xp_\ell^{(v)})_{d\lambda_i}$, add and subtract $vp_\ell^{(v-1)}$, and note that

$$xp_\ell^{(v)} + vp_\ell^{(v-1)} = (xp_\ell)^{(v)}.$$

Since $\pi_{k-1-j}^{(u)} = 0$ if $u > k-1-j$, the last terms with $j > k-1-u$ in the above summation may be deleted, and we obtain

$$\mu_{k,\ell,i}^{(u,v)} = (\pi_{k-1}^{(u)}, (xp_\ell)^{(v)})_{d\lambda_i} + u(\pi_{k-1}^{(u-1)}, p_\ell^{(v)})_{d\lambda_i}$$
$$-v(\pi_{k-1}^{(u)}, p_\ell^{(v-1)})_{d\lambda_i} - \sum_{j=0}^{k-1-u} \beta_j^{k-1}(\pi_{k-1-j}^{(u)}, p_\ell^{(v)})_{d\lambda_i}.$$

Continuing as in the proof of Proposition 2.2 gives (2.9). □

Proposition 2.4. *We have*

$$\beta_0^0 = \frac{\sigma_{0,1}}{\sigma_{0,0}} + a_0, \tag{2.10$_0$}$$

and, for $k = 1, 2, \ldots, n-1$,

$$\begin{aligned}
\beta_0^k &= \tfrac{\sigma_{k,k+1}}{\sigma_{k,k}} + a_k - \tfrac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \\
\beta_{k-j}^k &= \tfrac{\sigma_{j,k+1}}{\sigma_{j,j}} + a_k \tfrac{\sigma_{j,k}}{\sigma_{j,j}} + b_k \tfrac{\sigma_{j,k-1}}{\sigma_{j,j}} - \tfrac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1} \beta_{\ell-j}^\ell \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}, \\
&\qquad\qquad j = k-1, k-2, \ldots, 1 \quad (\text{if } k \geq 2), \\
\beta_k^k &= \tfrac{\sigma_{0,k+1}}{\sigma_{0,0}} + a_k \tfrac{\sigma_{0,k}}{\sigma_{0,0}} + b_k \tfrac{\sigma_{0,k-1}}{\sigma_{0,0}} - \sum_{\ell=0}^{k-1} \beta_\ell^\ell \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}.
\end{aligned} \tag{2.10}$$

Proof. Using $(\pi_j, \pi_j)_{H_s} = (\pi_j, p_j)_{H_s} = \sigma_{j,j}$, we have

$$p_k = \pi_k + \sum_{j=0}^{k-1} \frac{\sigma_{j,k}}{\sigma_{j,j}} \pi_j, \qquad k = 0, 1, 2, \ldots. \tag{2.11}$$

Combining this with (2.3) and Definition 2.1, we obtain

$$\begin{aligned}
\sigma_{j,k+1} &= (\pi_j, p_{k+1})_{H_s} = (\pi_j, xp_k)_{H_s} - a_k\sigma_{j,k} - b_k\sigma_{j,k-1} \\
&= \left(\pi_j, x\left(\pi_k + \sum_{\ell=0}^{k-1} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}} \pi_\ell\right)\right)_{H_s} - a_k\sigma_{j,k} - b_k\sigma_{j,k-1} \\
&= (\pi_j, x\pi_k)_{H_s} + \sum_{\ell=0}^{k-1} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}} (\pi_j, x\pi_\ell)_{H_s} - a_k\sigma_{j,k} - b_k\sigma_{j,k-1}.
\end{aligned}$$

Since, by (1.3),

$$\beta_{k-j}^{k} = \frac{(\pi_j, x\pi_k)_{H_s}}{(\pi_j, \pi_j)_{H_s}}, \qquad j \le k, \tag{2.12}$$

we get

$$\sigma_{j,k+1} = \beta_{k-j}^{k}\sigma_{j,j} + \sum_{\ell=0}^{k-1} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}(\pi_j, x\pi_\ell)_{H_s} - a_k\sigma_{j,k} - b_k\sigma_{j,k-1}, \quad j \le k.$$

Letting $j = k = 0$ immediately gives (2.10_0), since $\sigma_{0,-1} = 0$. If $j = 0 < k$, then $(\pi_0, x\pi_\ell)_{H_s} = \beta_\ell^\ell\ \sigma_{0,0}$ by (2.12), and the last relation in (2.10) follows. We may thus assume $1 \le j \le k$. Then, since $(\pi_j, x\pi_\ell)_{H_s} = 0$ if $\ell + 1 < j$, we obtain by using $(\pi_j, x\pi_{j-1})_{H_s} = (\pi_j, \pi_j)_{H_s} = \sigma_{j,j}$ and (2.12) that

$$\sigma_{j,k+1} = \beta_{k-j}^{k}\sigma_{j,j} + \frac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}}\sigma_{j,j} + \sum_{\ell=j}^{k-1} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}\beta_{\ell-j}^{\ell}\sigma_{j,j} - a_k\sigma_{j,k} - b_k\sigma_{j,k-1}.$$

Dividing both sides of the equation by $\sigma_{j,j}$ and solving for β_{k-j}^{k}, we get

$$\beta_{k-j}^{k} = \frac{\sigma_{j,k+1}}{\sigma_{j,j}} + a_k\frac{\sigma_{j,k}}{\sigma_{j,j}} + b_k\frac{\sigma_{j,k-1}}{\sigma_{j,j}} - \frac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1}\beta_{\ell-j}^{\ell}\frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}},$$

where, for $j = k$, the last sum is empty, hence equal to zero, and $\sigma_{k,k-1} = 0$. This proves the remaining relations in (2.10). □

In order to initialize the modified Chebyshev algorithm, we note that, by Definition 2.1,

$$\sigma_{0,k} = \nu_k^{(0)}, \quad k = 0, 1, \ldots, 2n-1,$$

$$\mu_{0,k,i}^{(0,0)} = \nu_k^{(i)}, \quad k = 0, 1, \ldots, 2n-2,\ i = 1, 2, \ldots, s,$$

which are the input moments (2.2) relative to the measures $d\lambda_0, d\lambda_1, \ldots, d\lambda_s$. We will show in Corollary 2.6 how to obtain

$$\mu_{0,k,i}^{(0,v)} = (\pi_0, p_k^{(v)})_{d\lambda_i} = \int_{\mathbb{R}} p_k^{(v)}(x)\,d\lambda_i(x), \qquad k = 1, 2, \ldots, 2n-2,$$

$$i = 1, 2, \ldots, s,\ v = 1, 2, \ldots, i.$$

The quantities $\mu_{0,k,i}^{(u,0)}$, $u = 1, 2, \ldots, i$, of course, are all zero. We begin by expressing p_k' as a linear combination of the p_j,

$$p_k'(x) = \sum_{j=0}^{k-1} \tau_j^k p_j(x), \tag{2.13}$$

and establish a recurrence relation for the τ_j^k. We define $\tau_j^k = 0$ if $j \geq k$ or $j < 0$.

Proposition 2.5. *We have, for* $k = 0, 1, \ldots, 2n-3$; $j = 0, 1, \ldots, k$,

$$\tau_j^{k+1} = \tau_{j-1}^k + \tau_{j+1}^k b_{j+1} + \tau_j^k (a_j - a_k) - b_k \tau_j^{k-1} + \delta_{j,k},$$

where $\delta_{j,k}$ *is the Kronecker delta.*

Proof. By differentiating (2.3) and using (2.13), we have

$$\begin{aligned} p'_{k+1} &= p_k(x) + (x - a_k)p'_k(x) - b_k p'_{k-1}(x) \\ &= p_k(x) + \sum_{j=0}^{k-1} \tau_j^k (x - a_k) p_j(x) - b_k \sum_{j=0}^{k-2} \tau_j^{k-1} p_j(x). \end{aligned}$$

By (2.3),

$$\begin{aligned} (x - a_k)p_j(x) &= (x - a_j)p_j(x) + (a_j - a_k)p_j(x) \\ &= p_{j+1}(x) + b_j p_{j-1}(x) + (a_j - a_k)p_j(x). \end{aligned}$$

Thus,

$$\begin{aligned} p'_{k+1} &= p_k(x) + \sum_{j=0}^{k-1} \tau_j^k (p_{j+1}(x) + b_j p_{j-1}(x) + (a_j - a_k)p_j(x)) - b_k \sum_{j=0}^{k-2} \tau_j^{k-1} p_j(x) \\ &= p_k(x) + \sum_{j=1}^{k} \tau_{j-1}^k p_j(x) + \sum_{j=0}^{k-2} b_{j+1} \tau_{j+1}^k p_j(x) + \sum_{j=0}^{k-1} \tau_j^k (a_j - a_k) p_j(x) \\ &\quad - b_k \sum_{j=0}^{k-2} \tau_j^{k-1} p_j(x) \\ &= (1 + \tau_{k-1}^k) p_k(x) + (\tau_{k-2}^k + \tau_{k-1}^k (a_{k-1} - a_k)) p_{k-1}(x) \\ &\quad + \sum_{j=1}^{k-2} (\tau_{j-1}^k + b_{j+1} \tau_{j+1}^k + \tau_j^k (a_j - a_k) - b_k \tau_j^{k-1}) p_j(x) \\ &\quad + (b_1 \tau_1^k + \tau_0^k (a_0 - a_k) - b_k \tau_0^{k-1}) p_0(x). \end{aligned}$$

Comparing coefficients of like terms with (2.13), where k is replaced by $k+1$, we get

$$\tau_k^{k+1} = 1 + \tau_{k-1}^k \quad \text{if} \quad k \geq 0,$$

$$\tau_{k-1}^{k+1} = \tau_{k-2}^k + \tau_{k-1}^k (a_{k-1} - a_k) \quad \text{if} \quad k \geq 1,$$

and for $j = 1, 2, \ldots, k-2$, $k \geq 3$,

$$\tau_j^{k+1} = \tau_{j-1}^k + b_{j+1}\tau_{j+1}^k + \tau_j^k(a_j - a_k) - b_k\tau_j^{k-1},$$

and

$$\tau_0^{k+1} = b_1\tau_1^k + \tau_0^k(a_0 - a_k) - b_k\tau_0^{k-1} \quad \text{if} \quad k \geq 2. \qquad \square$$

With the coefficients τ_j^k on hand, we can now evaluate $\mu_{0,k,i}^{(0,v)} = \int_{\mathbb{R}} p_k^{(v)}(x)d\lambda_i(x)$ as follows.

Corollary 2.6. *We have, for* $k = 1, 2, \ldots, 2n-2$,

$$\mu_{0,k,i}^{(0,v)} = \sum_{j=v-1}^{k-1} \tau_j^k \mu_{0,j,i}^{(0,v-1)}, \qquad v = 1, 2, \ldots, i.$$

Proof. By (2.7) and (2.13),

$$\mu_{0,k,i}^{(0,v)} = (\pi_0, p_k^{(v)})_{d\lambda_i} = (\pi_0, (p_k')^{(v-1)})_{d\lambda_i} = \sum_{j=0}^{k-1} \tau_j^k (\pi_0, p_j^{(v-1)})_{d\lambda_i}.$$

Since $p_j^{(v-1)} = 0$ if $v - 1 > j$, and using again (2.7), one gets the assertion. $\square$

In summary, we have the following

Modified Chebyshev algorithm

Objective: Given $n \geq 1$, compute the coefficients $\{\beta_j^k\}_{0\leq j\leq k}$ in (1.3) for $k = 0, 1, \ldots, n-1$, using the recursion coefficients a_j, b_j, $0 \leq j \leq 2n-2$ for the polynomials $\{p_k\}$ and the modified moments $\nu_j^{(0)}$, $0 \leq j \leq 2n-1$, and $\nu_j^{(i)}$, $0 \leq j \leq 2n-2$ (if $n \geq 2$), $i = 1, 2, \ldots, s$.

Notational convention: $\tau_j^k = 0$ if $j \geq k$ or $j < 0$; empty sums equal zero

Initialization:

for $\ell = 0, 1, \ldots, 2n-1$ do $\sigma_{0,\ell} = \nu_\ell^{(0)}$

$\beta_0^0 = \frac{\sigma_{0,1}}{\sigma_{0,0}} + \alpha_0$

if $n = 1$ then stop

$\tau_0^1 = 1$

for $k = 1, 2, \ldots, 2n-3$ do

  for $j = 0, 1, \ldots, k$ do

    $\tau_j^{k+1} = \tau_{j-1}^k + \tau_{j+1}^k b_{j+1} + \tau_j^k (a_j - a_k) - b_k \tau_j^{k-1} + \delta_{j,k}$

for $i = 1, 2, \ldots, s$

  for $u = 0, 1, \ldots, i$

    for $v = 0, 1, \ldots, i$

      for $k = 0, 1, \ldots, 2n-2$

        if $u = 0$ then

          if $v = 0$ then

            $\mu_{0,k,i}^{(u,v)} = \nu_k^{(i)}$

          else

            $\mu_{0,k,i}^{(u,v)} = \sum_{j=v-1}^{k-1} \tau_j^k \mu_{0,j,i}^{(0,v-1)}$

          end if

        else

            $\mu_{0,k,i}^{(u,v)} = 0$

        end if

Continuation:

$$
\begin{array}{l}
\text{for } k = 1, 2, \ldots, n-1 \text{ do} \\
\quad \text{for } \ell = k, k+1, \ldots, 2n-k-1 \text{ do} \\
\quad \sigma_{k,\ell} = \sigma_{k-1,\ell+1} + a_\ell \sigma_{k-1,\ell} + b_\ell \sigma_{k-1,\ell-1} + \sum_{i=1}^{s} i(\mu_{k-1,\ell,i}^{(i-1,i)} - \mu_{k-1,\ell,i}^{(i,i-1)}) \\
\qquad\qquad - \sum_{j=0}^{k-1} \beta_j^{k-1} \sigma_{k-1-j,\ell} \\
\beta_0^k = \frac{\sigma_{k,k+1}}{\sigma_{k,k}} + a_k - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}} \\
\quad \text{for } j = k-1, k-2, \ldots, 1 \text{ (if } k \geq 2) \text{ do} \\
\quad \beta_{k-j}^k = \frac{\sigma_{j,k+1}}{\sigma_{j,j}} + a_k \frac{\sigma_{j,k}}{\sigma_{j,j}} + b_k \frac{\sigma_{j,k-1}}{\sigma_{j,j}} \\
\qquad\qquad - \frac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1} \beta_{\ell-j}^{\ell} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}} \\
\beta_k^k = \frac{\sigma_{0,k+1}}{\sigma_{0,0}} + a_k \frac{\sigma_{0,k}}{\sigma_{0,0}} + b_k \frac{\sigma_{0,k-1}}{\sigma_{0,0}} - \sum_{\ell=0}^{k-1} \beta_\ell^{\ell} \frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}} \\
\text{if } k < n-1 \text{ then} \\
\quad \text{for } i = 1, 2, \ldots, s \text{ do} \\
\quad \text{for } u = 0, 1, \ldots, i \text{ do} \\
\quad \text{for } v = 0, 1, \ldots, i \text{ do} \\
\quad \text{for } \ell = k, k+1, \ldots, 2n-k-2 \text{ do} \\
\quad \mu_{k,\ell,i}^{(u,v)} = \mu_{k-1,\ell+1,i}^{(u,v)} + a_\ell \mu_{k-1,\ell,i}^{(u,v)} + b_\ell \mu_{k-1,\ell-1,i}^{(u,v)} + u \mu_{k-1,\ell,i}^{(u-1,v)} \\
\qquad\qquad - v \mu_{k-1,\ell,i}^{(u,v-1)} - \sum_{j=0}^{k-1-u} \beta_j^{k-1} \mu_{k-1-j,\ell,i}^{(u,v)}
\end{array}
$$

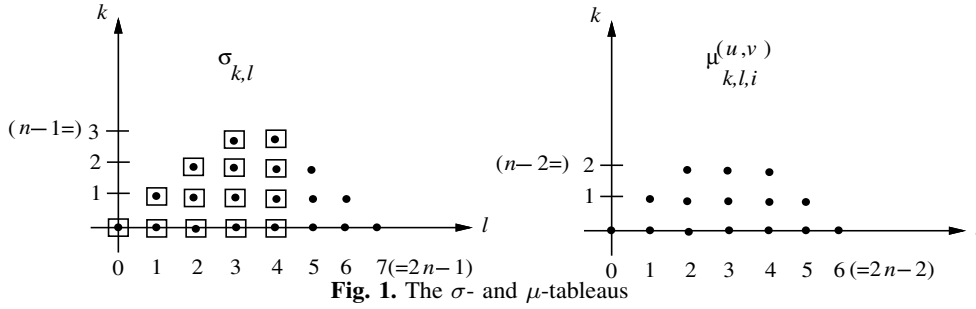

Fig. 1. The σ- and μ-tableaus

The scheme generates trapezoidal tableaus for $\sigma_{k,\ell}$ and $\mu_{k,\ell,i}^{(u,v)}$ as illustrated in Fig. 1 for $n = 4$. The boxed quantities in the σ-tableau are those used to compute β_{k-j}^{k}. The computing stencil for both tableaus is shown in Fig. 2.

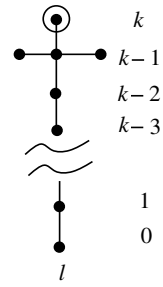

Fig. 2. The computing stencil for the σ- and μ-tableaus (the circled quantity is computed in terms of the others)

The algorithm described is considerably more complicated than the one for ordinary orthogonal polynomials (cf. [11, Sect. 2.4]), but this seems to be in the nature of things. In particular, its complexity is $O(n^3)$, rather than $O(n^2)$. Although it is not immediately evident, it can be shown by mathematical induction, that our present scheme reduces to the earlier one when $s = 0$.

3. Numerical examples

We report here on numerical experience with the modified Chebyshev algorithm for the special case $s = 1$ and mostly with measures $d\lambda_0, d\lambda_1$ as in (1.8). We experiment with both modified and ordinary moments. As was to be expected, the latter yield poor results as n becomes moderately large. Modified moments, on the other hand, produce rather satisfactory results, even for n large, when the measures are supported on finite intervals, but work less well for measures with infinite support.

All computations were done on the Cyber 205 in single precision ($\approx 7.1 \times 10^{-15}$) and double precision ($\approx 5.1 \times 10^{-29}$).

3.1. The polynomials of Althammer

These correspond to the inner product (1.8) with $d\lambda(x) = dx$ on [–1,1]; we will denote them here by $\pi_n(\cdot) = \pi_n(\,\cdot\,;\gamma)$ to indicate their dependence on the positive parameter γ. As $\gamma \to 0$ they of course approach the (monic) Legendre polynomials, and as $\gamma \to \infty$, up to the factor $x^2 - 1$, the (monic) Jacobi polynomials $\pi_{n-2}^{(1,1)}$ with parameters $\alpha = \beta = 1$ (cf. [10]):

$$\pi_n(x;\gamma) \to (x^2 - 1)\pi_{n-2}^{(1,1)}(x) \quad \text{as} \quad \gamma \to \infty, \quad n \geq 2. \tag{3.1}$$

The latter is illustrated numerically in Table 1, where $\beta_k^{(1,1)}$ are the recursion coefficients in $\pi_{k+1}^{(1,1)}(x) = x\pi_k^{(1,1)}(x) - \beta_k^{(1,1)}\pi_{k-1}^{(1,1)}(x)$, and β_j^k the coefficients in (1.3) for the polynomial $\pi_{k+1}(\,\cdot\,;\gamma)$ with $\gamma = 100$.

Table 1. The behavior of β_j^k for large $\gamma\,(= 100)$

k	β_1^k	$\max_{2\le j\le k}\lvert\beta_j^k\rvert$	$\beta_{k-2}^{(1,1)}$
5	.23813...	3.62(–5)	.23809...
10	.247680...	8.96(–7)	.247678...
15	.24904270...	1.80(–7)	.24904214...
20	.24948046...	6.34(–8)	.24948024...

In order to get a feel for the numerical stability of the Chebyshev algorithm, we ran it in single and double precision and determined ϵ_j^k, the modulus of the difference between the double- and single-precision value of β_j^k divided by $|\beta_j^k|$ if $|\beta_j^k| > 1$, as an indicator of single-precision accuracy. We let $\epsilon_{\max} = \max_{0\le k\le n-1}\max_{0\le j\le k}\epsilon_j^k$, and show the results in Table 2, where $n = 80$ was used for modified moments, and $n = 20$ for ordinary moments. As modified moments we took those relative to monic Legendre polynomials, so that $\nu_0^{(0)} = 2$, $\nu_0^{(1)} = 2\gamma$, and $\nu_k^{(i)} = 0$ for all $k > 0$ and $i = 0, 1$. Predictably, ordinary moments do poorly, in contrast to modified moments, which yield results accurate to almost machine precision. The maximum of the ϵ_j^k is consistently attained for $j = 1$ and for $k \approx 70$ (except when $\gamma = 0$) and $k = 19$, respectively.

Table 2. The accuracy of the modified Chebyshev algorithm

γ	mod. moments ($n = 80$)	ord. moments ($n = 20$)
	$\epsilon_{\max}$	$\epsilon_{\max}$
0.0	7.03(–15)	9.59(–4)
0.1	8.50(–14)	1.21(–3)
0.5	9.55(–14)	3.48(–3)
1.0	1.06(–13)	3.59(–3)
10.0	5.94(–14)	1.36(–3)
100.0	8.60(–14)	6.27(–4)

Similar and somewhat more accurate results have been observed for the Gröbner polynomials (orthogonal on [0,1]).

The coefficients β_j^k are rational functions of γ, which for $k = 0, 1, \ldots, 6$ are exhibited in [40] for the polynomials of Gröbner. These explicit formulae served as benchmarks for testing our computer routines.

While it is known that Althammer's polynomials have their zeros in (–1,1), for all $\gamma > 0$, it is an open question [10] as to whether they interlace, i.e., whether the zeros of π_{n+1} alternate with those of π_n. We examined this question numerically and found convincing evidence for interlacing to hold. We computed the zeros in double precision as eigenvalues of the respective matrix B

of (1.4), for $n = 2(1)40$ and $\gamma = .1, .5, 1., 10., 100.$, using the EISPACK routine HQR (cf. [38, p. 330]) and a double-precision version thereof (kindly supplied to us by Professor J. Demmel). We needed double precision, since some of the eigenvalues, for n large, are fairly ill-conditioned, causing a loss of as much as 10–12 decimal digits. Still, it was possible in this way to verify the interlacing property for all zeros except the very extreme ones (closest to ± 1), where even double precision did not provide sufficient resolution to demonstrate the separation of zeros when n and/or γ is large. Part of the difficulty has to do with the fact (cf. (3.1)) that these extreme zeros tend rapidly to ± 1 as $\gamma \to \infty$.

3.2. Jacobi weight functions

Letting $d\lambda(x) = w^{(\alpha,\beta)}(x)dx$ in (1.8), where $w^{(\alpha,\beta)}(x) = (1-x)^\alpha(1+x)^\beta$ is the Jacobi weight function on $[-1, 1]$, we denote the corresponding orthogonal polynomials of Sobolev type by $\pi_n^{(\alpha,\beta)}(\,\cdot\,;\gamma)$. It suffices to consider $\beta \geq \alpha > -1$, since an easy computation shows that

$$\pi_n^{(\beta,\alpha)}(x;\gamma) = (-1)^n \pi_n^{(\alpha,\beta)}(-x;\gamma). \tag{3.2}$$

We used the modified Chebyshev algorithm in single and double precision, as in Sect. 3.1, to generate the recursion coefficients β_j^k for the polynomials $\pi_n^{(\alpha,\beta)}(\,\cdot\,;\gamma)$ and the errors ϵ_j^k. The modified moments used were those relative to the (monic) Jacobi polynomials. In Table 3 we show, for $n = 40$, the maximum and minimum of $\epsilon_{\max}$ taken over $\alpha = -.75(.25)1.00$, $\beta = \alpha(.25)1.00$. The values of α and β for which the maximum resp. minimum is attained are shown in the columns headed by α and β.

Table 3. The accuracy of the modified Chebyshev algorithm for Jacobi weight functions

γ	$\max \epsilon_{\max}$	α	β	$\min \epsilon_{\max}$	α	β
0.0	9.47(–15)	–.75	–.75	5.28(–15)	0.00	.75
0.1	6.65(–12)	–.75	.75	1.37(–14)	.50	.50
0.5	1.48(–11)	–.75	–.25	1.28(–14)	.50	.50
1.0	1.77(–11)	–.75	–.25	1.37(–14)	.50	.50
10.0	2.01(–11)	–.75	–.50	1.56(–14)	.50	.50
100.0	2.60(–11)	–.75	–.50	1.61(–14)	.50	.50

Little is known about the zeros of $\pi_n^{(\alpha,\beta)}(\,\cdot\,;\gamma)$ when $\gamma > 0$ and α, β are not both equal to zero. It is of interest, therefore, to explore these zeros numerically. We have done so (in double precision) for the γ-values $\gamma = .1, .5, 1., 10., 100.$ and parameter values ranging over $\alpha = -.75(.25)5.00$, $\beta = \alpha(.5)5.0$ when $n = 2(1)20$, and $\alpha = -.5(.5)1.0$, $\beta = \alpha(.5)1.0$ when $n = 25(5)40$. Based on these computations, we are confident that the following conjectures are true.

Conjecture 3.1 (Location of the zeros of $\pi_n^{(\alpha,\beta)}(\,\cdot\,;\gamma)$, $\alpha > -1$, $\beta > -1$, $\gamma > 0$).

(i) *For each n, all zeros are real and distinct.*

(ii) *If* $\alpha \geq 0$, $\beta \geq 0$, *all zeros are contained in* (–1,1).
(iii) *If* $\alpha < 0$, $\beta \geq 0$, *then all zeros are in* (–1,1) *except, from some n on, one zero, which is larger than* 1.
(iv) *If* $\alpha < 0$, $\beta < 0$, *then all zeros are in* (–1,1) *except, from some n on, two zeros — one larger than* 1, *the other less than* –1.

Conjecture 3.2 (Interlacing of the zeros). *The zeros of* $\pi_{n+1}^{(\alpha,\beta)}(\,\cdot\,;\gamma)$ *interlace with those of* $\pi_n^{(\alpha,\beta)}(\,\cdot\,;\gamma)$ *except for the extreme zeros outside of* (–1,1) *in case* (iii) *and case* (iv) *of Conjecture* 3.1.

Conjecture 3.1(i),(ii),(iv) has recently been proved in the Gegenbauer case $\alpha = \beta$ by F. Marcellán et al. [27]. These authors also prove an "interlacing property" of the zeros of $\pi_n^{(\alpha,\alpha)}(\,\cdot\,;\gamma)$ with those of $\pi_n^{(\alpha,\alpha)}(\,\cdot\,;0)$. (Cf. (3.3) below.)

3.3. Generalized Laguerre weight functions

We denote by $\pi_n^{(\alpha)}(\,\cdot\,;\gamma)$ the orthogonal polynomials of Sobolev type belonging to the generalized Laguerre weight function $w^{(\alpha)}(x) = x^\alpha \mathrm{e}^{-x}$ on $(0,\infty)$, i.e., $d\lambda(x) = w^{(\alpha)}(x)dx$ in (1.8). Here the modified Chebyshev algorithm, using Laguerre moments, gradually deteriorates in accuracy as n increases, presumably because of effects of ill-conditioning. This is illustrated for $n = 10$ in Table 4, which shows, in the notation of the previous sections, the values of $\epsilon_{\max} = \max_{0\leq k\leq n-1} \max_{0\leq j\leq k} \epsilon_j^k$ for selected α and γ. By the time $n = 15$, these values become about five orders of magnitude larger, except when $\gamma = 0$.

Table 4. The accuracy of the modified Chebyshev algorithm for generalized Laguerre weight functions

$\gamma\backslash^{\alpha}$	–.5	0	.5	1.0	2.0	5.0
0.0	2.27(–14)	2.53(–14)	1.90(–14)	2.02(–14)	2.27(–14)	2.53(–14)
0.1	3.43(–7)	1.05(–7)	2.42(–8)	1.29(–8)	2.92(–9)	2.51(–10)
0.5	7.54(–7)	1.35(–7)	5.58(–8)	1.72(–8)	3.99(–9)	2.34(–10)
1.0	9.42(–7)	1.70(–7)	7.06(–8)	2.18(–8)	5.09(–9)	2.99(–10)
10.0	1.83(–5)	6.82(–6)	2.61(–6)	1.44(–6)	5.16(–7)	3.83(–8)
100.0	1.57(–5)	4.10(–6)	1.84(–6)	9.36(–7)	3.74(–7)	2.91(–7)

Although we are limited to relatively small values of n, there is sufficient computational evidence for the validity of the following conjectures.

Conjecture 3.3 (Location of the zeros of $\pi_n^{(\alpha)}(\,\cdot\,;\gamma)$, $\alpha > -1$, $\gamma > 0$).

(i) *For each n, all zeros are real and distinct.*
(ii) *If* $\alpha \geq 0$, *all zeros are positive.*
(iii) *If* $\alpha < 0$, *all zeros are positive except, from some n on, one zero, which is negative.*

Conjecture 3.4 (Interlacing of zeros). *The zeros of* $\pi_{n+1}^{(\alpha)}(\,\cdot\,;\gamma)$ *interlace with those of* $\pi_n^{(\alpha)}(\,\cdot\,;\gamma)$ *except for the negative zeros, if* $\alpha < 0$, *for which the interlacing property does not hold from some n on.*

After these computations had been done, we learned that Conjecture 3.3 was proved by F. Marcellán et al. [29]. They have also proved an "interlacing" property which relates the zeros of $\pi_n^{(\alpha)}(\,\cdot\,;\gamma)$ to the zeros of the generalized Laguerre polynomial $L_n^{\alpha}(\,\cdot\,)$ of the *same* degree. If the former, in increasing order, are $\xi_1 < \xi_2 < \cdots < \xi_n$, and the latter $x_1 < x_2 < \cdots < x_n$, then indeed

$$\xi_1 < x_1 < \xi_2 < x_2 < \cdots < \xi_n < x_n. \tag{3.3}$$

3.4. The Jacobi weight function combined with discrete measures

In this example, the two measures $d\lambda_0$ and $d\lambda_1$ in (2.1) are essentially different, the former being a Jacobi weight function with a discrete measure supported on $\pm c$ ($c > 0$) added to it, while the latter is just a discrete measure, also supported on $\pm c$. More precisely,

$$\begin{aligned} d\lambda_0(x) &= \frac{1}{\beta_0} w^{(\alpha,\beta)}(x)dx + \gamma_0[\delta(x-c) + \delta(x+c)]dx, \\ d\lambda_1(x) &= \gamma_1[\delta(x-c) + \delta(x+c)]dx, \quad \alpha,\beta > -1, \quad \gamma_0 \geq 0, \quad \gamma_1 > 0, \end{aligned} \tag{3.4}$$

where $\delta(\cdot)$ denotes the Dirac delta function, $w^{(\alpha,\beta)}$ the Jacobi weight function on [–1,1] (cf. Sect. 3.2), and

$$\beta_0 = \int_{-1}^{1} w^{(\alpha,\beta)}(x)dx. \tag{3.5}$$

This example was studied algebraically and analytically by H. Bavinck and H.G. Meijer [3, 4] in the (symmetric) Gegenbauer case $\alpha = \beta$ and for $c = 1$. In their second paper, they proved, in particular, that all zeros of π_n (located, of course, symmetrically with respect to the origin) are real and simple, and that for n sufficiently large, there is exactly one pair of real zeros outside of the interval (–1,1). The purpose of our numerical investigation is to make "sufficiently large" more concrete, and also to experiment with the cases $\alpha \neq \beta$ and $c \neq 1$ not (to our knowlege) treated in the literature.

We apply the modified Chebyshev algorithm with the choice $p_k = \hat{P}_k^{(\alpha,\beta)}$, the monic Jacobi polynomials, in the definition (2.2) of the modified moments. This then yields for the modified moments immediately

$$\begin{aligned} \nu_k^{(0)} &= \delta_{k,0} + \gamma_0[\hat{P}_k^{(\alpha,\beta)}(1) + \hat{P}_k^{(\alpha,\beta)}(-1)] \quad (\delta_{k,0} = \text{ Kronecker delta}), \\ \nu_k^{(1)} &= \gamma_1[\hat{P}_k^{(\alpha,\beta)}(1) + \hat{P}_k^{(\alpha,\beta)}(-1)], \end{aligned} \tag{3.6}$$

which is most easily calculated by the basic recurrence relation for Jacobi polynomials. (Expressions in terms of the gamma function are also available, but since the recursion coefficients for Jacobi polynomials are needed anyway in Chebyshev's algorithm, we might as well use them to compute the Jacobi polynomials by recurrence.) Thus, all the input quantities to the modified Chebyshev

algorithm are readily computable. The zeros of π_n are then computed as before as eigenvalues of the matrix B_n in (1.4) produced by the modified Chebyshev algorithm.

It appears that the presence of mass points has a deteriorating effect on the accuracy attainable with the Chebyshev algorithm. This is demonstrated in Table 5, which shows the maximum and minimum of $\varepsilon_{\max}$ taken over $\alpha = -.75(.25)1.00$, $\beta = \alpha(.25)1.00$ and γ_0, $\gamma_1 = .1, .5, 1.0, 2.0, 5.0, 10.0$, and the values of γ_0 and γ_1 for which the maximum resp. minimum is attained. Table 5 should be compared with Table 3 of Sect. 3.2 (where $n = 40$).

Table 5. The accuracy of the modified Chebyshev algorithm for Jacobi weight functions in the presence of mass points

n	c	max $\varepsilon_{\max}$	γ_0	γ_1	min $\varepsilon_{\max}$	γ_0	γ_1
5	.1	1.87(–10)	.5	10.0	7.93(–14)	10.0	.1
	.5	4.15(–11)	.1	10.0	3.03(–14)	5.0	.5
	1.0	1.64(–10)	.1	10.0	2.34(–14)	1.0	.1
	5.0	2.17(–10)	10.0	.1	2.30(–11)	.1	1.0
	10.0	1.24(–9)	10.0	.1	2.25(–11)	.1	5.0
10	.1	3.67(–9)	1.0	10.0	1.30(–12)	10.0	.1
	.5	3.40(–9)	.1	10.0	1.36(–12)	5.0	.1
	1.0	1.20(–7)	.1	10.0	2.17(–12)	1.0	.1
	5.0	3.89(–1)	.1	10.0	3.45(–5)	.1	.1
20	.1	1.69(–7)	.1	10.0	1.63(–9)	.5	.1
	.5	1.20(–7)	.1	10.0	3.16(–11)	2.0	.1
	1.0	2.61(–4)	.1	10.0	9.92(–10)	10.0	.1

As far as zeros are concerned, extensive testing that included values of $\alpha = \beta$ = –.75, –.5 , –.25, 0., .5, 1.0, 2.0, 5.0, 10.0, all combinations of γ_0, γ_1 over the values .5, 1.0, 2.0, 5.0, 10.0, and n as large as $n = 20$, lead us to conjecture the following refinement of the results of Bavinck and Meijer.

Conjecture 3.5. *When $\alpha = \beta > -1$ and $\gamma_1 > 0$, then for all $n \geq 3$ the Sobolev-type orthogonal polynomial π_n belonging to the measure* (2.1), (3.3) *has exactly one pair of real zeros outside of* (–1,1) *and all others inside. The exceptional pair approaches the points ± 1 monotonically as n (≥ 4) tends to infinity.*

The fact that ± 1 are limit points of the exceptional zeros has been proved rigorously by Bavinck and Meijer [4]. The novelty of Conjecture 3.5 is, on the one hand, the presence of a pair of exceptional zeros *for all* $n \geq 3$, and, on the other, the monotonicty of convergence (except for the first two values of n, i.e., $n = 2$ and $n = 3$).

Experiments with $\alpha \neq \beta$, $-1 < \alpha \leq 1$, $\alpha \leq \beta \leq 1$, and $c = 1$, using $n = 10$ and running through all combinations of γ_0 and γ_1 as above, seem to suggest that Conjecture 3.5 remains true also in this more general Jacobi case, except for the monotonicity of the two zeros outside of [–1,1], which occasionally holds only for $n \geq 5$. When $c > 1$ (for example, $c = 2, 5, 10$), we observed that exceptional zeros (in the sense of not being contained in the interval $[-c, c]$) may occur only for $n \geq 4$, and sometimes there is only one such exceptional zero, which

invariably is the one $< -c$. Also, the onset of monotonicity is often delayed until $n = 5$. Finally, when $c < 1$ (for example, $c = .5, .1$), complex zeros make their appearance, with real parts always in (–1,1). The remaining real zeros are also in (–1,1), except for at most one on either end.

4. Stieltjes's algorithm

The procedure of Sect. 2 turned out to be relatively complicated because we limited ourselves to employing only *rational* operations on the input data. Indeed, the desired coefficients β_j^k are computed, entirely by rational operations, in terms of moment information for the measures $d\lambda_0$, $d\lambda_1$ and in terms of certain recursion coefficients. If the latter belong to one of these measures, they in turn depend rationally on the moments. If we are prepared to incur the extra costs of *algebraic* operations (i.e., solving algebraic equations), we can arrive at a simpler and more transparent, though less efficient, algorithm. In view of recent progress in constructive methods and software for orthogonal polynomials [11, 12], we are indeed inclined to do so and, in particular, to employ Gaussian quadrature for the measures $d\lambda_i$. For simplicity, we will consider the case $s = 1$ in (1.1), but the extension to $s > 1$ is relatively straightforward.

The obvious thing to do is to express $-\beta_j^k$ in (1.3) as the Fourier-Sobolev coefficients of $\pi_{k+1}(x) - x\pi_k(x)$, that is,

$$\beta_j^k = \frac{(x\pi_k, \pi_{k-j})_{H_1}}{\| \pi_{k-j} \|_{H_1}^2}, \qquad j = 0, 1, \ldots, k, \tag{4.1}$$

and to evaluate the inner products in both numerator and denominator exactly by Gaussian quadrature rules (or other appropriate rules). To be specific, let us assume the most important scenario in which each measure $d\lambda_0$, $d\lambda_1$ consists of an absolutely continuous measure with a discrete measure superimposed on it:

$$d\lambda_i(x) = d\lambda_i^{\mathrm{ac}}(x) + \sum_{\rho=1}^{r^{(i)}} y_\rho^{(i)} \delta(x - x_\rho^{(i)}) dx, \qquad y_\rho^{(i)} > 0, \qquad x_\rho^{(i)} \in \mathbb{R}, \quad i = 0, 1. \tag{4.2}$$

Here, $r^{(i)}$ are nonnegative integers; if $r^{(i)} = 0$, then $d\lambda_i$ has no discrete component.

If we restrict k to be less than n (as in Sect. 2), then both inner products in (4.1) involve polynomials of degree $\leq 2n - 1$, hence can be computed exactly (up to rounding errors) by the n-point Gaussian quadrature formulae for $d\lambda_0^{\mathrm{ac}}$ and $d\lambda_1^{\mathrm{ac}}$. Specifically,

$$\begin{aligned}(xp, q)_{H_1} &= \sum_{\nu=1}^{n} \omega_\nu \xi_\nu p(\xi_\nu) q(\xi_\nu) + \sum_{\rho=1}^{r} y_\rho x_\rho p(x_\rho) q(x_\rho) \\ &+ \sum_{\nu=1}^{n} \omega'_\nu [\xi'_\nu p'(\xi'_\nu) + p(\xi'_\nu)] q'(\xi'_\nu)\end{aligned} \tag{4.3}$$

$$+\sum_{\rho=1}^{r'} y'_\rho [x'_\rho p'(x'_\rho) + p(x'_\rho)] q'(x'_\rho), \qquad p, q \in \mathbb{P}_{n-1},$$

and similarly (in fact, simpler) for $(p,q)_{H_1}$, where ξ_ν, ω_ν resp. ξ'_ν, ω'_ν are the nodes and weights of the n-point Gauss formula for $d\lambda_0^{\mathrm{ac}}$ resp. $d\lambda_1^{\mathrm{ac}}$, and where we have written, for simplicity, $r^{(0)} = r$, $r^{(1)} = r'$, $x_\rho^{(0)} = x_\rho$, etc. The polynomials intervening in (4.1), on the other hand, are successively computed with the help of the recurrence formula (1.3) involving coefficients β_j^k already computed. This is precisely the analogue of an algorithm for ordinary orthogonal polynomials which we attributed to Stieltjes in [11]. We continue to adopt the same name in the context of Sobolev orthogonal polynomials.

Note that, for initialization,

$$\beta_0^0 \;=\; \frac{(x\pi_0, \pi_0)_{H_1}}{\| \pi_0 \|_{H_1}^2} \;=\; \frac{(x,1)_{d\lambda_0}}{(1,1)_{d\lambda_0}} \;=\; \alpha_0(d\lambda_0)\ .$$

The required Gauss formulae for $d\lambda_i^{\mathrm{ac}}$ are computable by well-known eigenvalue techniques (cf. [13, 12]) based on the $n \times n$ Jacobi matrix for the measure $d\lambda_i^{\mathrm{ac}}$, i.e., the symmetric tridiagonal matrix with $\alpha_0^{(i)}, \alpha_1^{(i)}, \ldots$ down the main diagonal, and $\sqrt{\beta_1^{(i)}}, \sqrt{\beta_2^{(i)}}, \ldots$ down the two side diagonals, where $\alpha_k^{(i)} = \alpha_k(d\lambda_i)$ and $\beta_k^{(i)} = \beta_k(d\lambda_i)$ are the coefficients in the recurrence relation

$$\begin{aligned} p_{k+1}(x) &= (x - \alpha_k^{(i)}) p_k(x) - \beta_k^{(i)} p_{k-1}(x), \qquad k = 0, 1, 2, \ldots, \\ p_0(x) &= 1, \qquad p_{-1}(x) = 0 \end{aligned} \tag{4.4}$$

for the (monic) orthogonal polynomials $p_k(\cdot) = p_k(\,\cdot\,; d\lambda_i^{\mathrm{ac}})$ associated with the measure $d\lambda_i^{\mathrm{ac}}$, $i = 0, 1$. Software is now available [12] to compute these recursion coefficients for essentially arbitrary measures $d\lambda_i^{\mathrm{ac}}$.

Evaluating $(p,q)_{d\lambda_i}$ for $p, q \in \mathbb{P}_{n-1}$ (exactly) by applying an n-point Gauss formula to the absolutely continuous component $d\lambda_i^{\mathrm{ac}}$ of $d\lambda_i$ can be interpreted as evaluating $(p,q)_{d\lambda_i}$ (exactly) by an $(n + r^{(i)})$-point quadrature rule, $i = 0, 1$. Alternatively, if $d\lambda_i^{\mathrm{ac}} \not\equiv 0$, we could construct an n-point Gauss formula for the complete measure $d\lambda_i$ in (4.2) (not just the partial measure $d\lambda_i^{\mathrm{ac}}$), which results in a simpler algorithm for computing the β_j^k (where all summations over ρ in (4.3) are absent) and shifts the burden of dealing with the discrete parts of the measures $d\lambda_i$ onto the generation of the respective recursion coefficients in (4.4). But software for this has already been developed [12, Sect. 4.3], which is the reason why we favor this alternative approach when applicable. For simplicity, it is this version of the algorithm that is described in the summary below.

As already mentioned, there are no essential difficulties of extending this algorithm to the more general inner product (1.1), where $s \geq 1$ is an arbitrary integer and each $d\lambda_i$ has the form (4.2). Replacing integrals against $d\lambda_i$ by sums, as above, one ends up, for each $i = 0, 1, \ldots, s$, with a set of abscissae $t_\nu^{(i)}$ and weights $w_\nu^{(i)}$, $\nu = 1, 2, \ldots, \nu_{\max}(i)$ (which includes those coming from the discrete

components of $d\lambda_i$), at which π_k, $x\pi_k$ and their derivatives must be evaluated. This is done by updating $\pi_k^{(i)}(t_\nu^{(i)})$, for each i, and for each $\nu = 1, 2, \ldots, \nu_{\max}(i)$, by means of

$$\pi_k^{(i)}(x) = (x\pi_{k-1})^{(i)}(x) - \sum_{\ell=0}^{k-1} \beta_\ell^{k-1} \pi_{k-1-\ell}^{(i)}(x), \tag{4.5}$$

and likewise $(x\pi_k)^{(i)}(t_\nu^{(j)})$, for each i and j, and for $\nu = 1, 2, \ldots, \nu_{\max}(j)$, by means of

$$(x\pi_k)^{(i)}(x) = x \cdot (x\pi_{k-1})^{(i)}(x) + i(x\pi_{k-1})^{(i-1)}(x) - \sum_{\ell=0}^{k-1} \beta_\ell^{k-1} (x\pi_{k-1-\ell})^{(i)}(x). \tag{4.6}$$

This becomes rather expensive, however, giving rise to an algorithm of complexity $O(n^4)$.

If the support points $t_\nu^{(i)}$ are the same for each i (as for example in measures of the type (1.8)), the computation in (4.6) can be simplified, as it does not require a double sweep over i and j; the over-all computing time, accordingly, is reduced by about 70%.

4.1. Modified Stieltjes algorithm

Objective: Given $n \geq 1$, compute the coefficients $\{\beta_j^k\}_{0 \leq j \leq k}$ in (1.3) for $k = 0, 1, \ldots, n-1$, using the n-point Gaussian quadrature rules $\{\xi_\nu^{(i)}, \omega_\nu^{(i)}\}_{\nu=1}^n$ for $d\lambda_i$, $i = 0, 1$.

Notational convention: $\xi_\nu = \xi_\nu^{(0)}$, $\xi'_\nu = \xi_\nu^{(1)}$, etc.

Initialization:

for $\nu = 1, 2, \ldots, n$ do

- set and store
- $\pi_0(\xi_\nu) = \pi_0(\xi'_\nu) = 1$
- $\pi'_0(\xi_\nu) = \pi'_0(\xi'_\nu) = 0$

$\beta_0^0 = \alpha_0(d\lambda_0)$

if $n = 1$ then stop

Continuation:

for $k = 1, 2, \ldots, n-1$ do

for $j = 0, 1, \ldots, k$ do

for $i = 0, 1$ do

for $\nu = 1, 2, \ldots, n$ do

compute and store

$$\pi_k(\xi_\nu^{(i)}) = \xi_\nu^{(i)}\pi_{k-1}(\xi_\nu^{(i)}) - \sum_{\ell=0}^{k-1}\beta_\ell^{k-1}\pi_{k-1-\ell}(\xi_\nu^{(i)})$$

$$\pi_k'(\xi_\nu^{(i)}) = \pi_{k-1}(\xi_\nu^{(i)}) + \xi_\nu^{(i)}\pi_{k-1}'(\xi_\nu^{(i)}) - \sum_{\ell=0}^{k-1}\beta_\ell^{k-1}\pi_{k-1-\ell}'(\xi_\nu^{(i)})$$

$$num = \sum_{\nu=1}^{n}\{\omega_\nu\xi_\nu\pi_k(\xi_\nu)\pi_{k-j}(\xi_\nu) + \omega_\nu'[\xi_\nu'\pi_k'(\xi_\nu') + \pi_k(\xi_\nu')]\pi_{k-j}'(\xi_\nu')\}$$

$$den = \sum_{\nu=1}^{n}\{\omega_\nu[\pi_{k-j}(\xi_\nu)]^2 + \omega_\nu'[\pi_{k-j}'(\xi_\nu')]^2\}$$

$$\beta_j^k = num/den$$

We have run Stieltjes's procedure on all examples of Sects. 3.2–3.4. As expected, it is much slower than the modified Chebyshev algorithm, even with the simplification mentioned after (4.6), but often provides better accuracy. For example, the computation for Jacobi measures summarized in Table 3 was redone in the case $n = 20$ with the (simplified) Stieltjes procedure. The CPU time (on the Cyber 205) was 237.685 seconds, as opposed to 21.248 seconds with the Chebyshev algorithm – an increase by a factor of more than 10. On the other hand, for $\gamma > 0$, Stieltjes's procedure returned results whose maximum errors are consistently smaller than those for the Chebyshev algorithm, by 1–2 orders of magnitude.

The computation of Table 4 for generalized Laguerre measures required about 2.445 seconds of CPU time, when the Chebyshev algorithm was used, and 4.943 seconds – about twice as much – when the (simplified) Stieltjes procedure was used. Individual timings of the algorithms, however, revealed that the latter takes about five times as long as the former (when $n = 10$). Again, Stieltjes's procedure is generally more accurate for $\gamma > 0$, by 2–3 orders of magnitude, except when $\alpha = 5$, in which case Chebyshev's algorithm happens to be more accurate, by 1–2 orders of magnitude.

For Jacobi measures with added point spectra (cf. Sect. 3.4), the severe deterioration in accuracy that was observed in Table 5 as the value of c increases, does not occur with the Stieltjes procedure, which maintains (at least for $n = 5$ and $n = 10$) an accuracy of about 10^{-10} and 10^{-9} for $c = 5$ and $c = 10$, respectively. As before, however, it is about five times slower than the Chebyshev algorithm (when $n = 10$).

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Orthogonal polynomials: applications and computation

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We give examples of problem areas in interpolation, approximation, and quadrature, that call for orthogonal polynomials not of the classical kind. We then discuss numerical methods of computing the respective Gauss-type quadrature rules and orthogonal polynomials. The basic task is to compute the coefficients in the three-term recurrence relation for the orthogonal polynomials. This can be done by methods relying either on moment information or on discretization procedures. The effect on the recurrence coefficients of multiplying the weight function by a rational function is also discussed. Similar methods are applicable to computing Sobolev orthogonal polynomials, although their recurrence relations are more complicated. The paper concludes with a brief account of available software.

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CONTENTS

0. Introduction

The subject of orthogonal polynomials, if not in name then in substance, is quite old, having its origin in the 19th-century theories of continued fractions and the moment problem. Classical orthogonal polynomials, such as those of Legendre, Laguerre and Hermite, but also discrete ones, due to Chebyshev, Krawtchouk and others, have found widespread use in all areas of science and engineering. Typically, they are used as basis functions in which to expand other more complicated functions. In contrast, polynomials orthogonal with respect to general, nonstandard, weight functions and measures have received much less attention in applications, in part because of the considerable difficulties attending their numerical generation. Some progress, nevertheless, has been made in the last fifteen years or so, both in novel applications of non-classical orthogonal polynomials and in methods of their computation. The purpose of this article is to review some of these recent developments.

In Part I, we outline a number of (somewhat disconnected) problem areas that have given rise to unconventional orthogonal polynomials. These include problems in interpolation and least squares approximation, Gauss quadrature of rational functions, slowly convergent series, and moment-preserving spline approximation. Part II then takes up the problem of actually generating the respective orthogonal polynomials. Since most applications involve Gauss quadrature in one way or another, the computation of these quadrature rules is discussed first. Constructive methods for generating orthogonal polynomials,

including those of Sobolev type, then follow, among them moment-based methods, discretization methods, and modification algorithms. We conclude by giving a brief account of available software.

The choice of topics treated here reflects the author's past interest and involvement in orthogonal polynomials. There are other applications and computational aspects that would deserve equal treatment. Foremost among these are applications to iterative methods of solving large (and usually sparse) systems of linear algebraic equations and eigenvalue problems. The pioneering work on this was done in the 1950s by Stiefel (1958) and Lanczos (1950); modern accounts can be found, for instance in Hageman and Young (1981), Golub and Van Loan (1989) and Freund, Golub and Nachtigal (1991). Among additional computational issues there is the problem of constructing the measure underlying a set of orthogonal polynomials, given their recursion coefficients. Some discussion of this can be found in Askey and Ismail (1984), and Dombrowski and Nevai (1986).

Before we start, we recall two items of particular importance in the constructive theory of orthogonal polynomials: the Gaussian quadrature formula, and the basic three-term recurrence relation. This will also provide us with an opportunity to introduce relevant notation.

0.1. Gauss-type quadrature rules

The concept of orthogonality arises naturally in the context of quadrature formulae, when one tries to maximize, or nearly maximize, their degree of exactness. Thus suppose we are given a positive measure[1] $d\lambda$ on the real line $\mathbb{R}$ with respect to which polynomials can be integrated, that is, for which $\int_{\mathbb{R}} t^k \, d\lambda(t)$ exists for each nonnegative integer $k \in \mathbb{N}_0$. A quadrature formula

$$\int_{\mathbb{R}} f(t) \, d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{0.1}$$

[1] For our purposes it suffices to assume that $d\lambda$ is either a discrete measure, $d\lambda(t) = d\lambda_N(t)$, concentrated on a finite number N of points $t_1 < t_2 < \cdots < t_N$, that is, $\lambda(t)$ is constant on each open interval (t_i, t_{i+1}), $i = 0, 1, \ldots, N$ (where $t_0 = -\infty$, $t_{N+1} = +\infty$), and has a positive jump $w_i = \lambda(t_i+0) - \lambda(t_i-0)$ at t_i, $i = 1, 2, \ldots, N$, or $d\lambda(t) = w(t)\,dt$ is an absolutely continuous measure, where $w \geq 0$ is integrable on $\mathbb{R}$ and $\int_{\mathbb{R}} w(t)dt > 0$, or a combination of both. Then for suitable functions f,

$$\int_{\mathbb{R}} f(t) \, d\lambda(t) = \begin{cases} \sum_{i=1}^{N} w_i f(t_i), & d\lambda \text{ discrete}, \\ \int_{\text{supp}(d\lambda)} f(t) w(t) \, dt, & d\lambda \text{ absolutely continuous}, \end{cases}$$

where $\text{supp}(d\lambda)$ denotes the support of $d\lambda$, typically an interval or a union of disjoint intervals.

with distinct nodes $\tau_\nu \in \mathbb{R}$ and real weights λ_ν, is said to have *degree of exactness* d if

$$R_n(p) = 0, \qquad \text{all } p \in \mathbb{P}_d, \tag{0.2}$$

where $\mathbb{P}_d$ is the set of polynomials of degree $\leq d$. It is well known that for given τ_ν we can always achieve degree of exactness $n-1$ by interpolating at the points τ_ν and integrating the interpolation polynomial instead of f. The resulting quadrature rule (0.1) is called the *Newton–Cotes formula* (relative to the points τ_ν and the measure $d\lambda$). Indeed, any quadrature formula having degree of exactness $d = n-1$ can be so obtained, and is therefore called *interpolatory*. A natural question to ask is: what conditions must the nodes τ_ν and weights λ_ν satisfy in order for (0.1) to have degree of exactness larger than $n-1$, say $d = n-1+m$, where $m > 0$ is a given integer? The complete answer is given by the following theorem, essentially due to Jacobi (1826).

Theorem 1 Given an integer $m > 0$, the quadrature rule (0.1) has degree of exactness $d = n-1+m$ if and only if the following two conditions are satisfied:

(i) The formula (0.1) is interpolatory.

(ii) The node polynomial $\omega_n(t) = \Pi_{\nu=1}^n (t - \tau_\nu)$ satisfies

$$\int_{\mathbb{R}} \omega_n(t) p(t)\, d\lambda(t) = 0 \qquad \text{for each } p \in \mathbb{P}_{m-1}. \tag{0.3}$$

Condition (ii) is clearly a condition involving only the nodes τ_ν of (0.1); it says that the node polynomial must be *orthogonal* to all polynomials of degree $\leq m-1$. Here, orthogonality is in the sense of the inner product

$$(u, v)_{d\lambda} = \int_{\mathbb{R}} u(t) v(t)\, d\lambda(t), \qquad u, v \in \mathbb{P}, \tag{0.4}$$

in terms of which (0.3) can be stated as $(\omega_n, p)_{d\lambda} = 0$ for every $p \in \mathbb{P}_{m-1}$. Once a set of distinct nodes τ_ν has been found that satisfies this orthogonality constraint, condition (i) then determines uniquely the weights λ_ν, for example by requiring that (0.1) be exact for each power $f(t) = t^k$, $k = 0, 1, \ldots, n-1$. This is a system of linear equations for the weights λ_ν whose matrix is a Vandermonde matrix in the nodes τ_ν, hence nonsingular, since they are assumed distinct.

It is clear that $m \leq n$; otherwise, we could take $p = \omega_n$ in (ii) and get $\int_{\mathbb{R}} \omega_n^2(t)\, d\lambda(t) = 0$, which is impossible if $d\lambda$ has more than n points of increase. (In the context of quadrature rules, $d\lambda$ indeed is usually assumed to be absolutely continuous and thus to have infinitely many points of increase.) Thus, $m = n$ is optimal and gives rise to the condition

$$(\omega_n, p)_{d\lambda} = 0, \qquad \text{all } p \in \mathbb{P}_{n-1}. \tag{0.5}$$

This means that ω_n must be orthogonal to all polynomials of lower degree, hence (see Section 0.2 below) is the unique (monic) *orthogonal polynomial* of degree n relative to the measure $d\lambda$. We will denote this polynomial by $\pi_n(\cdot) = \pi_n(\cdot\,; d\lambda)$. The formula (0.1) then becomes the n-point *Gaussian quadrature formula* (with respect to the measure $d\lambda$), that is, the interpolatory quadrature rule of maximum degree of exactness $d = 2n-1$ whose nodes are the zeros of $\pi_n(\cdot\,; d\lambda)$. It is known from the theory of orthogonal polynomials (Szegő 1975) that these zeros are all simple and contained in the smallest interval containing the support of $d\lambda$.

There are other interesting special cases of Theorem 1. We mention four:

(1) Assume that the infimum $a = \inf \operatorname{supp}(d\lambda)$ is a finite number. We choose one of the nodes τ_ν to be equal to a, say $\tau_1 = a$. Then $\omega_n(t) = (t-a)\omega_{n-1}(t)$, where $\omega_{n-1}(t) = \prod_{\nu=2}^{n}(t-\tau_\nu)$, and condition (ii) requires that

$$\int_a^\infty \omega_{n-1}(t)p(t)(t-a)\,d\lambda(t) = 0, \qquad \text{all } p \in \mathbb{P}_{m-1}. \tag{0.6}$$

The optimal value of m is now clearly $m = n-1$, in which case ω_{n-1} is the unique (monic) polynomial of degree $n-1$ orthogonal with respect to the modified measure $d\lambda_a(t) = (t-a)\,d\lambda(t)$ – also a positive measure – that is, $\omega_{n-1}(t) = \pi_{n-1}(\cdot\,; d\lambda_a)$. Again, all zeros of ω_{n-1} are distinct and larger than a; the resulting formula (0.1) is called the n-point *Gauss–Radau formula* (with respect to the measure $d\lambda$).

(2) Similarly, if both $a = \inf \operatorname{supp}(d\lambda)$ and $b = \sup \operatorname{supp}(d\lambda)$ are finite numbers, and $n \geq 2$, and if we want $t_1 = a$ and (say) $t_n = b$, then $\omega_n(t) = -(t-a)(b-t)\omega_{n-2}(t)$, and $\omega_{n-2}(\cdot) = \pi_{n-2}(\cdot\,; d\lambda_{a,b})$ for optimal $m = n-2$, where $d\lambda_{a,b}(t) = (t-a)(b-t)\,d\lambda(t)$ is again a positive measure. The formula (0.1) with the interior nodes being the (distinct) zeros of $\pi_{n-2}(\cdot\,; d\lambda_{a,b})$ then becomes the n-point *Gauss–Lobatto quadrature rule* (for the measure $d\lambda$).

(3) Replace n in (0.1) by $2n+1$, let $\tau_\nu = \tau_\nu^{(n)}$ be the zeros of $\pi_n(\cdot\,; d\lambda)$ for some positive measure $d\lambda$, and choose $n+1$ additional nodes $\hat{\tau}_\mu$ such that the $(2n+1)$-point formula (0.1) with nodes τ_ν and $\hat{\tau}_\mu$ has maximum degree of exactness $d \geq 3n+1$. By Theorem 1 (with n replaced by $2n+1$), the $n+1$ nodes $\hat{\tau}_\mu$ to be inserted must be the zeros of the (monic) polynomial $\hat{\pi}_{n+1}$ satisfying

$$\int_{\mathbb{R}} \hat{\pi}_{n+1}(t)p(t)\pi_n(t;\, d\lambda)\,d\lambda(t) = 0, \qquad \text{all } p \in \mathbb{P}_n. \tag{0.7}$$

Here, the measure of orthogonality is $d\hat{\lambda}(t) = \pi_n(t;\, d\lambda)\,d\lambda(t)$, which is no longer positive, but oscillatory. This calls for special techniques of computation; see, for instance, Monegato (1982), Kautsky and Elhay (1984), Caliò, Gautschi and Marchetti (1986, Section 2) and Laurie (1996). While $\hat{\pi}_{n+1}$ can be shown to exist uniquely, its zeros are not necessarily contained in

the support of $d\lambda$ and may even be complex. The resulting $(2n+1)$-point quadrature formula is called the *Gauss–Kronrod rule*. It has an interesting history and has received considerable attention in recent years. For surveys, see Monegato (1982), Gautschi (1988) and Notaris (1994).

(4) Consider $s > 1$ different measures $d\lambda_\sigma$, $\sigma = 1, 2, \ldots, s$, with common support, and for each an n-point quadrature rule (0.1) with a common set of nodes $\{\tau_\nu\}$ but individual weights $\{\lambda_{\nu,\sigma}\}, \sigma = 1, 2, \ldots, s$. Assume $n = ms$ to be an integer multiple of s. Find s such quadrature rules, each having degree of exactness $n-1+m$. (This is expected to be optimal since there are $n(s+1)$ unknowns and $(n+m)s = ns+s$ conditions imposed.) According to Theorem 1, each quadrature rule has to be interpolatory, and the node polynomial ω_n must be orthogonal to polynomials of degree $m-1$ with respect to each measure,

$$\int_{\mathbb{R}} \omega_n(t) p(t)\, d\lambda_\sigma(t) = 0, \qquad \text{all } p \in \mathbb{P}_{m-1}, \quad \sigma = 1, 2, \ldots, s. \tag{0.8}$$

One obtains the *shared-nodes quadrature rules* recently introduced by Borges (1994) in connection with computer graphics illumination models, where the models $d\lambda_\sigma$ are colour matching functions. Instead of assuming $n = ms$, one could require (0.8) to hold for $p \in \mathbb{P}_{m_\sigma - 1}$, where $\sum_{\sigma=1}^{s} m_\sigma = n$, and thus 'distribute' the degrees of exactness differently among the s measures $d\lambda_\sigma$. The construction of such quadrature rules calls for *quasi-orthogonal polynomials*, that is, polynomials that are only partially orthogonal, as in (0.8), and not fully orthogonal, as in (0.5).

0.2. The three-term recurrence relation

Next to the Gauss formula, another important fact about orthogonal polynomials is that they always satisfy a three-term recurrence relation. The reason for this is the basic property

$$(tu, v)_{d\lambda} = (u, tv)_{d\lambda} \tag{0.9}$$

satisfied by the inner product (0.4). Indeed, assume that $d\lambda$ has at least N points of increase. Then the system of orthogonal polynomials $\pi_k(\cdot\,; d\lambda)$, $k = 0, 1, \ldots, N-1$, is easily seen to form a basis of $\mathbb{P}_{N-1}$. For any integer $k \le N-1$, therefore, since the polynomial

$$\pi_{k+1}(t) - t\pi_k(t)$$

is a polynomial of degree $\le k$ (both π_{k+1} and $t\pi_k$ being monic of degree $k+1$), there exist constants α_k, β_k and γ_{kj} such that

$$\pi_{k+1}(t) - t\pi_k(t) = -\alpha_k \pi_k(t) - \beta_k \pi_{k-1}(t) + \sum_{j=0}^{k-2} \gamma_{kj} \pi_j(t), \qquad k = 0, 1, \ldots, N-1, \tag{0.10}$$

where it is understood that $\pi_{-1}(t) \equiv 0$ and empty sums are zero. To determine α_k, take the inner product of both sides of (0.10) with π_k; this yields, by orthogonality,

$$-(t\pi_k, \pi_k) = -\alpha_k(\pi_k, \pi_k),$$

hence

$$\alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}.$$

Similarly, forming the inner product with π_{k-1} $(k \geq 1)$ gives

$$-(t\pi_k, \pi_{k-1}) = -\beta_k(\pi_{k-1}, \pi_{k-1}).$$

This can be simplified by noting $(t\pi_k, \pi_{k-1}) = (\pi_k, t\pi_{k-1}) = (\pi_k, \pi_k + \cdots)$, where dots stand for a polynomial of degree $< k$. By orthogonality, then, $(t\pi_k, \pi_{k-1}) = (\pi_k, \pi_k)$, and we get

$$\beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}.$$

Finally, taking the inner product with π_i, $i < k-1$, in (0.10), we find

$$-(t\pi_k, \pi_i) = \gamma_{ki}(\pi_i, \pi_i).$$

It is here where (0.9) is crucially used to obtain $\gamma_{ki} = 0$, since $(\pi_i, \pi_i) \neq 0$ and $(t\pi_k, \pi_i) = (\pi_k, t\pi_i) = 0$ because of $t\pi_i \in \mathbb{P}_{k-1}$. Thus, we have shown that

$$\begin{gathered}\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0, 1, \ldots, N-1, \\ \pi_{-1}(t) = 0, \qquad \pi_0(t) = 1,\end{gathered} \tag{0.11}$$

where

$$\begin{aligned}\alpha_k &= \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \qquad k = 0, 1, \ldots, N-1, \\ \beta_k &= \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \qquad k = 1, 2, \ldots, N-1.\end{aligned} \tag{0.12}$$

This is the basic *three-term recurrence relation* satisfied by orthogonal polynomials. Since $\pi_{-1} = 0$, the coefficient β_0 in (0.11) can be arbitrary. It is convenient, however, to define it by

$$\beta_0 = (\pi_0, \pi_0) = \int_{\mathbb{R}} d\lambda(t). \tag{0.13}$$

Note that by construction, π_N is orthogonal to all polynomials of degree $< N$. If $d\lambda = d\lambda_N$ is a discrete measure with exactly N points of increase, there can be at most N orthogonal polynomials, $\pi_0, \pi_1, \ldots, \pi_{N-1}$, which implies that $(\pi_N, \pi_N) = 0$, that is, π_N vanishes at all the support points of $d\lambda_N$. On the other hand, if $N = \infty$, then (0.11) holds for all $k \in \mathbb{N}_0$. Vice versa, if (0.11) holds for all $k \in \mathbb{N}_0$, with $\beta_k > 0$, then by a well-known

theorem of Favard (see, for instance, Natanson 1964/65, Volume II, Chapter VIII, Section 6) the system of polynomials $\{\pi_k\}$ is orthogonal relative to some positive measure $d\lambda$ having infinitely many support points.

The recurrence relation (0.11) is generally quite stable, numerically, and indeed provides an excellent means of computing the orthogonal polynomials $\pi_k(\cdot\,; d\lambda)$, both inside and outside the interval of orthogonality. For discrete measures $d\lambda_N$, however, there is a good chance that the recurrence relation exhibits a phenomenon of 'pseudostability' (*cf.* Gautschi 1993a; Gautschi 1996b, Section 3.4.2), particularly if the support points of $d\lambda_N$ are equally spaced. As a consequence, the accuracy of the $\pi_k(\cdot\,; d\lambda_N)$, if computed by (0.11), may severely deteriorate as k approaches N.

PART I: APPLICATIONS

1. Interpolation

1.1. Extended Lagrange interpolation

Our interest here is in the convergence of Lagrange interpolation and quadrature processes on a finite interval $[-1,1]$, assuming only that the function to be interpolated is continuous on $[-1,1]$. A well-known negative result of Faber (see, for instance, Natanson 1965, Volume III, Chapter II, Theorem 2) tells us that there is no triangular array of nodes for which Lagrange interpolation would be *uniformly* convergent for every continuous function. In response to this, Erdős and Turán (1937) showed that if one considers convergence *in the mean*, then there indeed exist triangular arrays of nodes – for example the zeros of orthogonal polynomials – on which convergence holds for every continuous function. More precisely, given a positive weight function w on $(-1,1)$, we have

$$\lim_{n\to\infty} \| f - L_n f \|_w = 0, \qquad \text{for all } f \in C[-1,1], \tag{1.1}$$

where

$$\| u \|_w^2 = \int_{-1}^{1} u^2(t) w(t)\, dt, \tag{1.2}$$

and $L_n f$ is the Lagrange interpolation polynomial of degree $< n$ interpolating f at the n zeros $\tau_i = \tau_i^{(n)}$, $i = 1,2,\ldots,n$, of $\pi_n(\cdot\,; w)$, the nth-degree polynomial orthogonal on $[-1,1]$ relative to the weight function w. Convergence of the related quadrature process, that is,

$$\lim_{n\to\infty} \int_{-1}^{1} [f(t) - (L_n f)(t)] w(t)\, dt = 0 \qquad \text{for all } f \in C[-1,1], \tag{1.3}$$

also holds, since the quadrature rule implied by (1.3) is simply the Gaussian rule (see Section 0.1), which is known to converge for any continuous function.

With this as a backdrop, suppose we wish to improve on $L_n f$ by considering an extended set of $2n+1$ nodes,

$$\tau_i^{(n)}, \qquad i = 1, 2, \ldots, n; \qquad \hat{\tau}_j, \qquad j = 1, 2, \ldots, n+1, \tag{1.4}$$

the first n being as before the zeros of $\pi_n(\,\cdot\,; w)$, and forming the corresponding Lagrange interpolant $\hat{L}_{2n+1} f$ of degree $< 2n+1$. Is it true that (1.1) and/or (1.3) still hold if $L_n f$ is replaced by $\hat{L}_{2n+1} f$?

The answer cannot be expected to be an unqualified 'yes', as the choice of the added nodes $\{\hat{\tau}_j\}$ has a marked influence on the convergence behaviour. A natural choice for these nodes is the set of zeros of $\pi_{n+1}(\,\cdot\,; w)$, for which it has recently been shown (see Criscuolo, Mastroianni and Nevai (1993), Theorem 3.2; and Mastroianni and Vértesi (1993), Theorem 2.3) that the analogue of (1.1), when w is a 'generalized Jacobi weight' (see Section 6.1, Example 6.2), holds if and only if the Jacobi parameters α, β are both strictly between -1 and 0. The analogue of (1.3) holds for any weight function w since the underlying quadrature rule turns out to be simply the $(n+1)$-point Gaussian rule for w (all nodes τ_i receive the weight zero).

Another interesting choice for the nodes $\hat{\tau}_j$, first proposed by Bellen (1981, 1988), is the set of zeros of $\hat{\pi}_{n+1}(\,\cdot\,) = \pi_{n+1}(\,\cdot\,; \pi_n^2 w)$,

$$\pi_{n+1}(\hat{\tau}_j; \pi_n^2 w) = 0, \qquad j = 1, 2, \ldots, n+1 \qquad (\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; w)). \tag{1.5}$$

Here the polynomial $\hat{\pi}_{n+1}$ is the $(n+1)$st-degree polynomial of an infinite sequence of polynomials $\pi_m(\,\cdot\,; \pi_n^2 w)$, $m = 0, 1, 2, \ldots$, studied in Gautschi and Li (1993) and termed there orthogonal polynomials *induced* by π_n. Both questions (1.1) and (1.3), for $\hat{L}_{2n+1} f$, then become considerably more difficult, and no precise results are known except for the four Chebyshev weight functions $w^{(\alpha,\beta)}(t) = (1-t)^\alpha (1+t)^\beta$, $\alpha, \beta = \pm\frac{1}{2}$. For these it has been shown in Gautschi (1992) that (1.1) is false unless $\alpha = \beta = +\frac{1}{2}$, in which case $\pi_n \hat{\pi}_{n+1}$ is a constant multiple of the 2nd-kind Chebyshev polynomial of degree $2n+1$, and hence (1.1) (for $\hat{L}_{2n+1} f$) is a consequence of the Erdős–Turán result. More recently (Gautschi and Li 1996), the analogue of (1.3) was established for all four Chebyshev weight functions by showing that the respective quadrature rules are positive and therefore convergent, by a classical result of Pólya (1933). In the case $\alpha = \beta = -\frac{1}{2}$, for example, the weights of the quadrature rule are given by Gautschi and Li (1996, Theorem 1).

$$\begin{aligned} \lambda_i &= \tfrac{\pi}{3n}, \qquad i = 1, 2, \ldots, n, \\ \mu_j &= \frac{2\pi/3}{n + \frac{3}{9 - 8\hat{\tau}_j^2}}, \qquad j = 1, 2, \ldots, n+1. \end{aligned}$$

For Jacobi weight functions $w = w^{(\alpha,\beta)}$, there are only conjectural results,

obtained by extensive computation based on the methods of Section 7.2. From these it appears that the analogue of (1.1) for $\hat{L}_{2n+1}f$ holds in the Gegenbauer case $\underline{\alpha} \le \alpha = \beta \le \overline{\alpha}$, where $\underline{\alpha} = -.31$ and $\overline{\alpha} = 1.6$ (perhaps even in a slightly larger interval), and in the Jacobi case when $0 \le \alpha, \beta \le \overline{\alpha}$ (again possibly in some slightly larger domain; see Gautschi (1992, Conjectures 5.1–5.3). The case $\alpha < 0$ remains open. The analogue of (1.3) is conjectured to hold for Jacobi weight functions with $|\alpha| \le \frac{1}{2}$, $|\beta| \le \frac{1}{2}$ (Gautschi and Li 1996, Conjecture 3.1).

1.2. Rational interpolation

Given $N+1$ distinct points $\{t_i\}_{i=0}^N$ on $\mathbb{R}$ and corresponding function values $f_i = f(t_i)$, $i = 0, 1, \ldots, N$, the problem now is to find a rational function

$$r_{m,n}(t) = \frac{p(t)}{q(t)}, \qquad m+n = N, \tag{1.6}$$

with q assumed monic of degree n and p of degree $\le m$, such that

$$r_{m,n}(t_i) = f_i, \qquad i = 0, 1, \ldots, N. \tag{1.7}$$

To derive an algorithm, one starts from the interpolation conditions (1.7), written in the form

$$p(t_i) = f_i q(t_i), \qquad i = 0, 1, \ldots, N. \tag{1.8}$$

Now recall that the Nth divided difference of a function g can be represented in the form

$$[t_0, t_1, \ldots, t_N]g = \sum_{i=0}^{N} \frac{g(t_i)}{w_i}, \qquad w_i = \prod_{\substack{j=0 \\ j\neq i}}^{N} (t_i - t_j). \tag{1.9}$$

Letting $\psi_j(t) = t^j$, $j = 0, 1, \ldots, n-1$, multiplying (1.8) by $\psi_j(t_i)/w_i$ and summing, yields

$$\sum_{i=0}^{N} \frac{\psi_j(t_i)p(t_i)}{w_i} = \sum_{i=0}^{N} \frac{\psi_j(t_i)f_i q(t_i)}{w_i};$$

hence, by (1.9),

$$[t_0, t_1, \ldots, t_N](\psi_j p) = [t_0, t_1, \ldots, t_N](\psi_j f q), \qquad j = 0, 1, \ldots, n-1.$$

But $\psi_j p$ is a polynomial of degree $m+n-1 < N$, hence the divided difference on the left vanishes. The same is therefore true of the divided difference on the right, that is,

$$\sum_{i=0}^{N} \frac{f_i}{w_i} q(t_i)\psi_j(t_i) = 0, \qquad j = 0, 1, \ldots, n-1. \tag{1.10}$$

Defining the discrete measure $d\lambda_N$ to have support points $\{t_0, \ldots, t_N\}$, and jumps $\omega_i = f_i/w_i$ at t_i, we can write (1.10) as

$$\int_{\mathbb{R}} q(t)\psi(t)\, d\lambda_N(t) = 0, \qquad \text{all } \psi \in \mathbb{P}_{n-1}. \tag{1.11}$$

Thus, $q(\cdot) = \pi_n(\cdot\,; d\lambda_N)$ is the nth-degree monic polynomial orthogonal with respect to the (indefinite) measure $d\lambda_N$.

The denominator $q(\cdot) = \pi_n(\cdot\,; d\lambda_N)$, when generated by methods to be discussed in Section 6, can be checked to see whether it vanishes at any of the points t_i and, thus, whether the existence of the rational interpolant (1.6) is in doubt.

If all function values are different from zero, then the numerator polynomial p or, more precisely, its monic companion, $p_{\text{mon}} \in \mathbb{P}_m$, can also be characterized as a discrete orthogonal polynomial. Indeed, it is orthogonal relative to the measure $d\lambda_N^{(-1)}$ having the same support points as $d\lambda_N$, but jumps $\omega_i^{(-1)} = f_i^{-1}/w_i$ instead of f_i/w_i. This follows immediately from (1.8) if we write it in the form

$$q(t_i) = f_i^{-1} p(t_i), \qquad i = 0, 1, \ldots, N, \tag{1.12}$$

and apply the same reasoning as above to find

$$\int_{\mathbb{R}} p_{\text{mon}}(t)\varphi(t)\, d\lambda_N^{(-1)}(t) = 0, \qquad \text{all } \varphi \in \mathbb{P}_{m-1}. \tag{1.13}$$

To obtain p itself, it suffices to multiply $p_{\text{mon}}(\cdot) = \pi_m(\cdot\,; d\lambda_N^{(-1)})$ by a suitable normalization factor c, for example, $c = f_0 q(t_0)/p_{\text{mon}}(t_0)$ (assuming, of course, that $q(t_0) \neq 0$, $p_{\text{mon}}(t_0) \neq 0$).

The procedure described is particularly attractive if *all* rational interpolants $r_{m,n}$ with $m+n = N$ are to be obtained, since the numerator and denominator of $r_{m,n}$, being orthogonal polynomials, can be generated efficiently by the three-term recurrence relation (*cf.* 0.2). Some caution, nevertheless, is advised because of possible build-up of computational errors. These are caused by the indefiniteness of the inner product $(\cdot, \cdot)_{d\lambda_N}$, in particular by the fact that the weights ω_i and $\omega_i^{(-1)}$ typically alternate in sign. One expects these errors to be more prevalent the larger the moduli of these weights, hence the smaller the interval $[t_0, t_N]$.

Notes to Section 1

1.1. The potential failure of $\hat{L}_{2n+1} f$ to converge in the mean to f for the special choices of nodes studied here must not so much be regarded as a critique of these choices, but rather as a reflection of the very large class – $C[-1, 1]$ – of functions f. Adding only a slight amount of regularity, for example Lipschitz continuity with a parameter larger than one half, would restore (mean) convergence. For smoother

functions, numerical evidence presented in Gautschi (1992, Table 6.1) suggests very fast convergence.

An analogue of the Erdős–Turán result for a class of rational interpolants has been established in Van Assche and Vanherwegen (1993, Theorem 7).

Mean convergence of extended Lagrange interpolation with $\hat{\tau}_j$ the Gauss–Kronrod points is studied in Li (1994). Other types of extended Lagrange interpolation by polynomials are studied in Bellen (1981) for Lipschitz-continuous functions $f \in \operatorname{Lip}\gamma$, $\gamma > \frac{1}{2}$, and in Criscuolo, Mastroianni and Occorsio (1990, 1991) and Criscuolo, Mastroianni and Vértesi (1992) with a view toward uniform convergence; see also Criscuolo et al. (1993) and Mastroianni and Vértesi (1993). For yet other extended interpolation processes and their L_p-convergence for arbitrary continuous functions, see Mastroianni (1994).

1.2. There are well-established algorithms for constructing a rational interpolant when one exists; see, for instance, Stoer and Bulirsch (1980, Section 2.2) and Graves-Morris and Hopkins (1981). The approach described in this subsection, based on discrete orthogonal polynomials (though relative to an indefinite measure) can be traced back to Jacobi (1846) and has recently been advocated in Eğecioğlu and Koç (1989). A numerical example illustrating its weaknesses and strengths is given in Gautschi (1989).

2. Approximation

2.1. Constrained least squares approximation

The problem of least squares ties in with the early history of orthogonal polynomials. We thus begin by looking at the classical version of the problem.

Given a positive measure $\mathrm{d}\lambda$ on the real line $\mathbb{R}$ and a function f defined on the support of $\mathrm{d}\lambda$, we want to find a polynomial p of degree at most n minimizing the $L^2_{\mathrm{d}\lambda}$-error,

$$\text{minimize } \int_{\mathbb{R}} [p(t) - f(t)]^2 \, \mathrm{d}\lambda(t) : \qquad p \in \mathbb{P}_n. \tag{2.1}$$

Often, the measure $\mathrm{d}\lambda$ is a discrete measure $\mathrm{d}\lambda_N$ concentrated on N distinct points of $\mathbb{R}$, with $N > n$ (*cf.* footnote ([1]) of Section 0.1). If not, we must assume that f is in $L^2_{\mathrm{d}\lambda}$, and we will also assume that all polynomials are in $L^2_{\mathrm{d}\lambda}$. On the space $\mathbb{P}$ (of all real polynomials), respectively $\mathbb{P}_{N-1}$ (if $\mathrm{d}\lambda = \mathrm{d}\lambda_N$), we introduce the inner product (0.4),

$$(u, v)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t)v(t) \, \mathrm{d}\lambda(t), \qquad u, v \in \mathbb{P} \text{ (resp. } u, v \in \mathbb{P}_{N-1}), \tag{2.2}$$

which renders these spaces true inner product spaces. There exist, therefore, unique polynomials

$$\pi_k(t; \mathrm{d}\lambda) = t^k \; + \; \text{lower-degree terms} \, , \qquad k = 0, 1, 2, \ldots, \tag{2.3}$$

satisfying

$$(\pi_k, \pi_\ell)_{\mathrm{d}\lambda} \begin{cases} = 0 & \text{if } k \neq \ell, \\ > 0 & \text{if } k = \ell. \end{cases} \tag{2.4}$$

These are the (monic) *orthogonal polynomials* relative to the measure $\mathrm{d}\lambda$ (*cf.* Section 0.2). There are infinitely many of them if the support of $\mathrm{d}\lambda$ is infinite, and exactly N of them ($0 \leq k \leq N-1$ in (2.3)) if $\mathrm{d}\lambda = \mathrm{d}\lambda_N$. The solution of (2.1) is then given by

$$p(t) = \sum_{k=0}^{n} c_k \pi_k(t; \mathrm{d}\lambda), \qquad c_k = \frac{(f, \pi_k)_{\mathrm{d}\lambda}}{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}, \tag{2.5}$$

the $(n+1)$st partial sum of the Fourier series of f in the orthogonal system $\{\pi_k\}$.

Suppose now that we wish to minimize (2.1) among all polynomials $p \in \mathbb{P}_n$ satisfying the constraints

$$p(s_j) = f(s_j), \qquad j = 0, 1, \ldots, m; \qquad m < n, \tag{2.6}$$

where s_j are given distinct points on $\mathbb{R}$ where f is defined. It is then natural to seek p of the form

$$p(t) = p_m(t; f) + s_m(t)\delta(t), \tag{2.7}$$

where

$$s_m(t) = \prod_{j=0}^{m} (t - s_j), \tag{2.8}$$

$p_m(\cdot\,; f)$ being the unique polynomial in $\mathbb{P}_m$ interpolating f at the points $\{s_j\}_0^m$ and δ a polynomial of degree $n-m-1$. Every polynomial of the form (2.7) is indeed in $\mathbb{P}_n$ and satisfies the constraints (2.6). Conversely, every such polynomial can be written in the form (2.7). It thus remains to determine δ.

We have

$$\begin{aligned} \int_{\mathbb{R}} [p(t) - f(t)]^2 \, \mathrm{d}\lambda(t) &= \int_{\mathbb{R}} [p_m(t; f) + s_m(t)\delta(t) - f(t)]^2 \, \mathrm{d}\lambda(t) \\ &= \int_{\mathbb{R}} \left[\frac{f(t) - p_m(t; f)}{s_m(t)} - \delta(t) \right]^2 s_m^2(t) \, \mathrm{d}\lambda(t), \end{aligned}$$

so that our minimization problem (2.1), (2.6) becomes

$$\text{minimize} \int_{\mathbb{R}} [\Delta(t) - \delta(t)]^2 s_m^2(t) \, \mathrm{d}\lambda(t) : \qquad \delta \in \mathbb{P}_{n-m-1}, \tag{2.9}$$

where

$$\Delta(t) := \frac{f(t) - p_m(t; f)}{s_m(t)} = [s_0, s_1, \ldots, s_m, t]f. \tag{2.10}$$

Here, the expression on the far right is the divided difference of f of order

$m+1$ with respect to the points $s_0, s_1, \ldots, s_m, t$, and its equality with Δ is a consequence of the well-known remainder term of interpolation. We see that the desired polynomial δ is the solution of an *unconstrained* least squares problem, but for a new function, Δ, and a different measure, $s_m^2\,\mathrm{d}\lambda$. Therefore, the solution of the constrained least squares problem is given by (2.7) with

$$\delta(t) = \sum_{k=0}^{n-m-1} d_k \hat{\pi}_k(t), \qquad d_k = \frac{(\Delta, \hat{\pi}_k)_{s_m^2\,\mathrm{d}\lambda}}{(\hat{\pi}_k, \hat{\pi}_k)_{s_m^2\,\mathrm{d}\lambda}}, \tag{2.11}$$

where

$$\hat{\pi}_k(\cdot) = \pi_k(\cdot\,; s_m^2\,\mathrm{d}\lambda). \tag{2.12}$$

It is required, therefore, to construct the orthogonal polynomials relative to the measure $s_m^2\,\mathrm{d}\lambda$, assuming those for $\mathrm{d}\lambda$ are known. This is an instance of a *modification problem*; its solution by 'modification algorithms' will be discussed in Section 7.2.

The same idea can be applied to least squares approximation by a rational function

$$r(t) = \frac{p(t)}{q(t)}, \tag{2.13}$$

where q is a prescribed polynomial satisfying

$$q(t) > 0 \quad \text{for } t \in \operatorname{supp}(\mathrm{d}\lambda); \qquad q(s_j) \neq 0, \qquad j = 0, 1, \ldots, m. \tag{2.14}$$

One finds that

$$\text{minimize} \int_{\mathbb{R}} \left[\frac{p(t)}{q(t)} - f(t)\right]^2 \mathrm{d}\lambda(t) : \qquad p \in \mathbb{P}_n, \tag{2.15}$$

subject to the constraints

$$\frac{p(s_j)}{q(s_j)} = f(s_j), \qquad j = 0, 1, \ldots, m, \tag{2.16}$$

is now equivalent to

$$\text{minimize} \int_{\mathbb{R}} [\Delta(t) - \delta(t)]^2 \frac{s_m^2(t)}{q^2(t)}\,\mathrm{d}\lambda(t) : \qquad \delta \in \mathbb{P}_{n-m-1}, \tag{2.17}$$

where

$$\Delta(t) = \frac{q(t)f(t) - p_m(t; qf)}{s_m(t)} = [s_0, s_1, \ldots, s_m, t](qf). \tag{2.18}$$

With δ so obtained, the desired p in (2.13) is then given by

$$p(t) = p_m(t; qf) + s_m(t)\delta(t). \tag{2.19}$$

The modification of the measure now involves not only multiplication but

also division by a polynomial. This requires additional algorithms for generating the respective orthogonal polynomials, which will be the subject of Section 7.3.

2.2. Least squares approximation in Sobolev spaces

In order to approximate (in the least squares sense) not only functions, but also, simultaneously, some of their derivatives, we may pose the problem

$$\text{minimize} \int_{\mathbb{R}} \sum_{\sigma=0}^{s} [p^{(\sigma)}(t) - f^{(\sigma)}(t)]^2 \, d\lambda_\sigma(t) : \qquad p \in \mathbb{P}_n, \tag{2.20}$$

where $d\lambda_0, \ldots, d\lambda_s$ are positive measures on $\mathbb{R}$ and each derivative $f^{(\sigma)}$ is defined on the support of the corresponding measure $d\lambda_\sigma$. The natural scenario in which to consider this problem is the Sobolev space

$$H_s(\mathbb{R}) = \{f : \sum_{\sigma=0}^{s} \int_{\mathbb{R}} [f^{(\sigma)}]^2 \, d\lambda_\sigma < \infty\} \tag{2.21}$$

of functions f whose successive derivatives of order $\sigma \leq s$ are square integrable against the respective measures $d\lambda_\sigma$. If we assume that the measures $d\lambda_\sigma$ are such that the space $\mathbb{P}$ of polynomials is a subspace of $H_s(\mathbb{R})$, the problem (2.20) can be written as

$$\text{minimize} \ \| p - f \|_{H_s}^2 : \qquad p \in \mathbb{P}_n, \tag{2.22}$$

where the norm $\| u \|_{H_s} = \sqrt{(u,u)_{H_s}}$ is defined in terms of the inner product

$$(u,v)_{H_s} = \sum_{\sigma=0}^{s} \int_{\mathbb{R}} u^{(\sigma)}(t) v^{(\sigma)}(t) \, d\lambda_\sigma(t). \tag{2.23}$$

If $d\lambda_0$ has infinitely many points of increase, then, regardless of whether or not some or all of the other measures $d\lambda_\sigma$, $\sigma \geq 1$, are discrete, the inner product (2.23) is positive definite on $H_s(\mathbb{R})$ and therefore defines a unique set of (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; H_s)$, $k = 0, 1, 2, \ldots$, satisfying

$$(\pi_k, \pi_\ell)_{H_s} \begin{cases} = 0 & \text{if} \quad k \neq \ell, \\ > 0 & \text{if} \quad k = \ell. \end{cases} \tag{2.24}$$

These are called *Sobolev orthogonal polynomials.* In terms of these functions, the solution of (2.20), as in (2.5), is given by a finite Fourier series,

$$p(t) = \sum_{k=0}^{n} c_k \pi_k(t; H_s), \qquad c_k = \frac{(f, \pi_k)_{H_s}}{(\pi_k, \pi_k)_{H_s}}. \tag{2.25}$$

It is important to note that the inner product in (2.23), if $s > 0$, no longer satisfies the basic property (0.9), that is,

$$(tu, v)_{H_s} \neq (u, tv)_{H_s} \qquad (s > 0), \tag{2.26}$$

which means that we can no longer expect the orthogonal polynomials to satisfy a simple three-term recurrence relation. The numerical computation of Sobolev orthogonal polynomials (not to speak of their algebraic and analytic properties!) is therefore inherently more complicated; we will give a brief account of this in Section 8.

A widely used choice of measures is

$$d\lambda_\sigma(t) = \gamma_\sigma \, d\lambda(t), \qquad \sigma = 0, 1, 2, \ldots, s, \tag{2.27}$$

where $d\lambda$ is a (positive) 'base measure' and the $\gamma_\sigma > 0$ are positive constants with $\gamma_0 = 1$. The latter allow us to assign different weights to different derivatives. The most studied case, by far, is (2.27) with $s = 1$.

2.3. Moment-preserving spline approximation

Given a function f on $[0, \infty)$, we wish to approximate it by a spline function of degree m with n positive knots. The approximation is not to be sought in any of the usual L_p-metrics, but is to share with f as many of the initial moments as possible. This is a type of approximation favoured by physicists, since moments have physical meaning, and the approximation thus preserves physical properties.

The most general spline in question can be written in the form

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (\tau_\nu - t)_+^m, \tag{2.28}$$

where $m \geq 0$ is an integer, $u_+ = \max(0, u)$, a_ν are real numbers, and

$$0 < \tau_1 < \tau_2 < \cdots < \tau_n < \infty \tag{2.29}$$

are the knots of the spline. The arbitrary polynomial of degree m that one could add to (2.28) must be identically zero if the moments of $s_{n,m}$ are to be finite. Since we have $2n$ parameters to choose from – the n coefficients a_ν and the n knots τ_ν – we expect to be able to match the first $2n$ moments,

$$\int_0^\infty s_{n,m}(t) t^j \, dt = \int_0^\infty f(t) t^j \, dt, \qquad j = 0, 1, \ldots, 2n-1. \tag{2.30}$$

This problem, not surprisingly, leads to a problem of Gaussian quadrature. Assume, indeed, for fixed $n \in \mathbb{N}$ and $m \in \mathbb{N}_0$, that

(i) $f \in C^{m+1}[\mathbb{R}_+]$,
(ii) $\int_0^\infty f(t) t^j \, dt$ exists for $j = 0, 1, \ldots, 2n-1$,
(iii) $f^{(\mu)}(t) = o(t^{-2n-\mu})$ as $t \to \infty$, for $\mu = 0, 1, \ldots, m$,

and define the measure

$$d\lambda_m(t) = \frac{(-1)^{m+1}}{m!} t^{m+1} f^{(m+1)}(t) \, dt \qquad \text{on } \mathbb{R}_+. \tag{2.31}$$

Then we have the following result.

Theorem 2 Given a function f on $[0, \infty)$ satisfying assumptions (i)–(iii), there is a unique spline function $s_{n,m}$, (2.28), matching the first $2n$ moments of f, (2.30), if and only if the measure $d\lambda_m$ in (2.31) admits a Gaussian quadrature formula

$$\int_0^\infty g(t)\,d\lambda_m(t) = \sum_{\nu=1}^{n} \lambda_\nu^G g(t_\nu^G) + R_{n,m}^G(g), \qquad R_{n,m}^G(\mathbb{P}_{2n-1}) = 0, \tag{2.32}$$

having distinct positive nodes

$$0 < t_1^G < t_2^G < \cdots < t_n^G. \tag{2.33}$$

If that is the case, then the desired spline $s_{n,m}$ is given by

$$\tau_\nu = t_\nu^G, \qquad a_\nu = \frac{\lambda_\nu^G}{(t_\nu^G)^{m+1}}, \qquad \nu = 1, 2, \ldots, n. \tag{2.34}$$

Proof. Since τ_ν is positive, substituting (2.28) in (2.30) yields

$$\sum_{\nu=1}^{n} a_\nu \int_0^{\tau_\nu} t^j (\tau_\nu - t)^m\,dt = \int_0^\infty t^j f(t)\,dt, \qquad j = 0, 1, \ldots, 2n-1. \tag{2.35}$$

We now apply m (respectively $m+1$) integrations by parts to the integrals on the left (respectively right) of (2.35). On the left, we obtain

$$\begin{aligned} &m![(j+1)(j+2)\cdots(j+m)]^{-1} \sum_{\nu=1}^{n} a_\nu \int_0^{\tau_\nu} t^{j+m}\,dt \\ &= m![(j+1)(j+2)\cdots(j+m)(j+m+1)]^{-1} \sum_{\nu=1}^{n} a_\nu \tau_\nu^{j+m+1}. \end{aligned} \tag{2.36}$$

On the right, we carry out the first integration by parts in detail to exhibit the reasonings involved. We have, for any $b > 0$,

$$\int_0^b t^j f(t)\,dt = \frac{1}{j+1}\, t^{j+1} f(t)\Big|_0^b - \frac{1}{j+1} \int_0^b t^{j+1} f'(t)\,dt. \tag{2.37}$$

The integrated term clearly vanishes at $t = 0$ and tends to zero as $t = b \to \infty$ by assumption (iii) with $\mu = 0$, since $j + 1 \le 2n$. The integral on the left converges as $b \to \infty$ by assumption (ii); the same is true, therefore, for the integral on the right. We conclude that

$$\int_0^\infty t^j f(t)\,dt = -\frac{1}{j+1} \int_0^\infty t^{j+1} f'(t)\,dt.$$

Continuing in this manner, using assumption (iii) to show convergence to zero of the integrated term at the upper limit (its value at $t = 0$ always being zero) and the existence of $\int_0^\infty t^{j+\mu} f^{(\mu)}(t)\,dt$ already established to infer the

existence of $\int_0^\infty t^{j+\mu+1} f^{(\mu+1)}(t)\,\mathrm{d}t$, $\mu = 1, 2, \ldots, m$, we arrive at

$$\int_0^\infty t^j f(t)\,\mathrm{d}t = \frac{(-1)^{m+1}}{(j+1)(j+2)\cdots(j+m+1)} \int_0^\infty t^{j+m+1} f^{(m+1)}(t)\,\mathrm{d}t.$$

In particular, this shows that the first $2n$ moments of $\mathrm{d}\lambda_m$ all exist. Since the last expression obtained, by (2.35), must be equal to the one in (2.36), we see that (2.30) is equivalent to

$$\sum_{\nu=1}^{n} (a_\nu \tau_\nu^{m+1}) \tau_\nu^j = \int_0^\infty \frac{(-1)^{m+1}}{m!}\, t^{m+1} f^{(m+1)}(t) \cdot t^j\,\mathrm{d}t,$$
$$j = 0, 1, \ldots, 2n-1.$$

These are precisely the conditions for τ_ν to be the nodes of the Gauss formula (2.32) and for $a_\nu \tau_\nu^{m+1}$ to be the respective weights. Both, if indeed they exist, are uniquely determined. □

The measure $\mathrm{d}\lambda_m$ in (2.31) is neither one of the classical measures nor is it necessarily positive, in general. Thus we need constructive methods that also work for sign-changing measures.

The simplest example is the exponential function, $f(t) = e^{-t}$, in which case

$$\mathrm{d}\lambda_m(t) = \frac{1}{m!}\, t^{m+1} e^{-t}\,\mathrm{d}t \qquad (f(t) = e^{-t}) \tag{2.38}$$

is a generalized Laguerre measure with parameter $\alpha = m+1$, hence indeed one of the classical measures. Examples of positive measures $\mathrm{d}\lambda_m$ are furnished by completely monotone functions, that is, functions f satisfying

$$(-1)^k f^{(k)}(t) > 0 \qquad \text{on } \mathbb{R}_+, \qquad k = 0, 1, 2, \ldots\,. \tag{2.39}$$

The physically important example of the Maxwell velocity distribution, $f(t) = e^{-t^2}$, is an example leading to a sign-variable measure,

$$\mathrm{d}\lambda_m(t) = \frac{1}{m!}\, t^{m+1} H_{m+1}(t) e^{-t^2}\,\mathrm{d}t \qquad (f(t) = e^{-t^2}), \tag{2.40}$$

where H_{m+1} is the Hermite polynomial of degree $m+1$. If $m > 0$, then H_{m+1} has $\lfloor (m+1)/2 \rfloor$ positive zeros, hence the measure (2.40) changes sign that many times.

Although the spline $s_{n,m}$ was constructed to match the moments of f, it also provides a reasonably good pointwise approximation. Its error indeed can be shown to be related to the remainder $R_{n,m}^G$ of the Gauss formula (2.32) in the sense that for any $t > 0$ one has

$$f(t) - s_{n,m}(t) = R_{n,m}^G(h_{t,m}), \tag{2.41}$$

where

$$h_{t,m}(u) = u^{-(m+1)}(u-t)_+^m, \qquad 0 \le u < \infty. \tag{2.42}$$

From a known convergence theorem for Gauss quadrature on $[0, \infty)$ (*cf.* Freud (1971, Chapter 3, Theorem 1.1)) it follows, in particular, that for fixed m,

$$\lim_{n\to\infty} s_{n,m}(t) = f(t), \qquad t > 0,$$

if f satisfies the assumptions of Theorem 2 for all $n = 1, 2, 3, \ldots$ and if $\mathrm{d}\lambda_m$ is a positive measure for which the moment problem is determined.

Similar approximation problems can be posed on a finite interval, which then give rise to generalized Gauss–Lobatto and Gauss–Radau quadrature for a measure $\mathrm{d}\lambda_m$ which again depends on $f^{(m+1)}$.

Notes to Section 2

2.1. Least squares approximation by polynomials was considered as early as 1859 by Chebyshev (1859) in the case of discrete measures $\mathrm{d}\lambda = \mathrm{d}\lambda_N$. Although Chebyshev expressed the solution in the form (2.5), he did not refer to the polynomials $\pi_k(\cdot\,; \mathrm{d}\lambda_N)$ as 'orthogonal polynomials' – a concept unknown at the time – but characterized them, as did other writers of the period, as denominators of certain continued fractions. A more recent treatment of discrete least squares approximation by polynomials, including computational and statistical aspects, is Forsythe (1957). The idea of reducing the constrained least squares problem for polynomials to an unconstrained one involving a new objective function and a new measure can be found in Walsh (1969, p. 320). For the extension to rational functions, see Lin (1988).

2.2. In the case of measures (2.27) with $s = 1$, the Sobolev-type least squares approximation problem (2.20) was first considered by Lewis (1947), largely, however, with a view toward analysing the error of approximation (via the Peano kernel, as it were). The respective Sobolev orthogonal polynomials were studied later by Althammer (1962) and Gröbner (1967) in the case of the Legendre measure, $\mathrm{d}\lambda(t) = \mathrm{d}t$ in (2.27). Other choices of measures $\mathrm{d}\lambda_\sigma$ in (2.23), especially discrete ones for $\sigma \geq 1$, have been studied extensively in recent years. For surveys, see Marcellán, Alfaro and Rezola (1993), Marcellán, Pérez and Piñar (1995), and for a bibliography, Marcellán and Ronveaux (1995). Special pairs of measures $\{\mathrm{d}\lambda_0, \mathrm{d}\lambda_1\}$ in the case $s = 1$, termed 'coherent', are studied in Iserles, Koch, Nørsett and Sanz-Serna (1990; 1991) and shown to allow efficient evaluation not only of the Sobolev–Fourier coefficients c_k in (2.25), but also of the Sobolev polynomials $\pi_k(\cdot; H_1)$ themselves. For zeros of such polynomials, see Meijer (1993), and de Bruin and Meijer (1995).

An application of Sobolev-type least squares approximation to the solution of systems of linear algebraic equations is proposed in Moszyński (1992). Here, $s + 1$ is the dimension of the largest Jordan block in the matrix of the system.

2.3. Piecewise constant approximations on $\mathbb{R}_+$ to the Maxwell velocity distribution that preserve the maximum number of moments were used in computational plasma physics by Calder, Laframboise and Stauffer (1983), and Calder and Laframboise (1986), under the colourful name 'multiple-water-bag distributions'. The connection with Gaussian quadrature was pointed out in Gautschi (1984b). Since piecewise constant functions are a special case of polynomial spline functions, it is

natural to extend the idea of moment-preserving approximation to spline functions of arbitrary degree. This was done in Gautschi and Milovanović (1986), where one can find Theorem 2 and the error formulae (2.41), (2.42), along with their proofs. In the same paper, the sign-variable measure (2.40) was examined numerically and shown to lead, on occasion, to Gauss formulae with negative, or even conjugate complex, nodes. The analogous approximation on a finite interval, mentioned at the end of Section 2.3, was studied in Frontini, Gautschi and Milovanović (1987). Further extensions can be found in Milovanović and Kovačević (1988, 1992), Micchelli (1988), Frontini and Milovanović (1989), Gori and Santi (1989, 1992) and Kovačević and Milovanović (1996), with regard to both the type of spline function and the type of approximation.

3. Quadrature

3.1. Gauss quadrature for rational functions

Traditionally, Gauss quadrature rules (*cf.* Section 0.1) are designed to integrate exactly (against some measure) polynomials up to a maximum degree. This makes sense if one integrates functions that are 'polynomial-like'. Here we are interested in integrating functions that have poles, perhaps infinitely many. In this case, the use of rational functions, in combination with polynomials, seems more appropriate. The rational functions should be chosen so as to match the most important poles of the given function. This gives rise to the following problem.

Let $d\lambda$ be a (usually positive) measure on $\mathbb{R}$, and let there be given M nonzero complex numbers $\zeta_1, \ldots, \zeta_M$ such that

$$\zeta_\mu \neq 0, \qquad 1 + \zeta_\mu t \neq 0 \qquad \text{on supp } (d\lambda), \qquad \mu = 1, 2, \ldots, M. \tag{3.1}$$

For given integers m, n with $1 \leq m \leq 2n$, find an n-point quadrature rule that integrates exactly (against the measure $d\lambda$) the m rational functions

$$(1 + \zeta_\mu t)^{-s}, \qquad \mu = 1, 2, \ldots M, \qquad s = 1, 2, \ldots, s_\mu, \tag{3.2}$$

where $s_\mu \geq 1$ and

$$\sum_{\mu=1}^{M} s_\mu = m, \tag{3.3}$$

as well as polynomials of degree $\leq 2n - m - 1$. If $m = 2n$, a polynomial of degree -1 is understood to be identically zero. We then have the extreme case of $2n$ rational functions (with poles of multiplicities s_μ at $-1/\zeta_\mu$) being integrated exactly, but no nontrivial polynomials. The quadrature rule is then optimal for rational functions, just as the classical Gaussian rule is optimal for polynomials; *cf.* Section 0.1. The latter corresponds to the limit case $M = m = 0$.

In principle, it is straightforward to construct the desired quadrature rule according to the following theorem.

Theorem 3 Define

$$\omega_m(t) = \prod_{\mu=1}^{M} (1+\zeta_\mu t)^{s_\mu}, \tag{3.4}$$

by (3.3) a polynomial of degree m. Assume that the measure $d\lambda/\omega_m$ admits a (polynomial) n-point Gauss quadrature formula, that is,

$$\int_{\mathbb{R}} f(t)\,\frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu^G f(t_\nu^G) + R_n^G(f), \qquad R_n^G(\mathbb{P}_{2n-1}) = 0, \tag{3.5}$$

and define

$$t_\nu = t_\nu^G, \qquad \lambda_\nu = w_\nu^G \omega_m(t_\nu^G), \qquad \nu = 1,2,\ldots,n. \tag{3.6}$$

Then

$$\int_{\mathbb{R}} g(t)\,d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu g(t_\nu) + R_n(g), \tag{3.7}$$

where

$$R_n(g) = 0 \quad \text{if } g \in \mathbb{P}_{2n-m-1}, \text{ or } g(t) = (1+\zeta_\mu t)^{-s},\ 1 \le \mu \le M,\ 1 \le s \le s_\mu. \tag{3.8}$$

Once again, we are led to a modification problem that involves division by a polynomial, so that the algorithms of Section 7.3 become relevant.

Proof of Theorem 3. For $\mu = 1,2,\ldots,M$; $s = 1,2,\ldots,s_\mu$, define

$$q_{\mu,s}(t) = \frac{\omega_m(t)}{(1+\zeta_\mu t)^s}.$$

Since $m \le 2n$ and $s \ge 1$, we have $q_{\mu,s} \in \mathbb{P}_{m-s} \subset \mathbb{P}_{2n-1}$, and therefore, by (3.5),

$$\begin{aligned}\int_{\mathbb{R}} \frac{d\lambda(t)}{(1+\zeta_\mu t)^s} &= \int_{\mathbb{R}} q_{\mu,s}(t)\,\frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu^G q_{\mu,s}(t_\nu^G) \\ &= \sum_{\nu=1}^{n} w_\nu^G \frac{\omega_m(t_\nu^G)}{(1+\zeta_\mu t_\nu^G)^s} = \sum_{\nu=1}^{n} \frac{\lambda_\nu}{(1+\zeta_\mu t_\nu)^s},\end{aligned}$$

where (3.6) has been used in the last step. This proves the assertion in the top line of (3.8).

To prove the bottom part of (3.8), let p be an arbitrary polynomial in

$\mathbb{P}_{2n-m-1}$. Then, since $p\omega_m \in \mathbb{P}_{2n-1}$, again by (3.5) and (3.6),

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} p(t)\omega_m(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)}$$
$$= \sum_{\nu=1}^{n} w_\nu^G p(t_\nu^G)\omega_m(t_\nu^G) = \sum_{\nu=1}^{n} \lambda_\nu p(t_\nu).$$

□

The existence of the Gaussian quadrature formula in Theorem 3 is assured if it exists for the measure $\mathrm{d}\lambda$ and the polynomial ω_m has constant sign on supp $(\mathrm{d}\lambda)$. This is typically the case if the complex poles $-1/\zeta_\mu$ (if any) occur in conjugate complex pairs and the real ones are all outside the support interval of $\mathrm{d}\lambda$.

Quantum statistical distributions provide important examples of integrals amenable to rational Gauss-type quadrature. Thus, the Fermi–Dirac distribution gives rise to the generalized Fermi–Dirac integral

$$F_k(\eta,\theta) = \int_0^\infty \frac{t^k\sqrt{1+\frac{1}{2}\theta t}}{e^{-\eta+t}+1}\,\mathrm{d}t, \qquad \theta \geq 0, \qquad \eta \in \mathbb{R}, \tag{3.9}$$

where the k-values of physical interest are the half-integers $\frac{1}{2}$, $\frac{3}{2}$ and $\frac{5}{2}$. Similarly, Bose–Einstein distributions lead to the generalized Bose–Einstein integral

$$G_k(\eta,\theta) = \int_0^\infty \frac{t^k\sqrt{1+\frac{1}{2}\theta t}}{e^{-\eta+t}-1}\,\mathrm{d}t, \qquad \theta \geq 0, \qquad \eta \leq 0, \tag{3.10}$$

with the same values of k as before. For the integral in (3.9), the poles are located at

$$t = \eta \pm (2\mu-1)\,\mathrm{i}\pi, \qquad \mu = 1,2,3,\ldots, \tag{3.11}$$

whereas for the one in (3.10) they are at

$$t = \eta \pm 2\mu\,\mathrm{i}\pi, \qquad \mu = 0,1,2,\ldots\,. \tag{3.12}$$

This suggests taking for the ζ_μ in (3.1) the negative reciprocals of (3.11) and (3.12), respectively. If in the integral (3.9) we match the first n pairs of complex poles, we are led to apply Theorem 3 with $m = 2n$ and

$$\omega_{2n}(t) = \prod_{\mu=1}^{n}[(1+\xi_\mu t)^2 + \eta_\mu^2 t^2],$$

where ξ_μ and η_μ are the real and imaginary parts, respectively, of $\zeta_\mu = -(\eta + (2\mu-1)\,\mathrm{i}\pi)^{-1}$. Similarly for the integral (3.10), where we need to match the real pole (at η) and the first $n-1$ pairs of complex poles. This

calls for Theorem 3 with $m = 2n - 1$ and

$$\omega_{2n-1}(t) = (1 + \xi_0 t) \prod_{\mu=1}^{n-1} [(1 + \xi_\mu t)^2 + \eta_\mu^2 t^2],$$

where ξ_μ and η_μ are the real and imaginary parts of $\zeta_\mu = -(\eta + 2\mu i\pi)^{-1}$.

3.2. Slowly convergent series

It may seem strange, at first, to see infinite series dealt with in a section on quadrature. But infinite series are integrals relative to a discrete measure supported on the positive integers! It is not unnatural, therefore, to try to approximate such integrals by finite sums. We do this for a special class of series in which the general term can be expressed as the Laplace transform of some function evaluated at an integer. Such series exhibit notoriously slow convergence. We will show that they can be transformed into an integral containing a positive, but nonclassical, weight function and then apply Gauss quadrature to obtain an effective summation procedure.

Thus, suppose that

$$S = \sum_{k=1}^{\infty} a_k, \qquad a_k = (\mathcal{L}f)(k), \tag{3.13}$$

where $\mathcal{L}f$ is the Laplace transform of some (known!) function f, that is,

$$(\mathcal{L}f)(s) = \int_0^\infty e^{-st} f(t)\, dt. \tag{3.14}$$

Then by Watson's lemma (see, for example, Wong 1989, p. 20), if f is regular near the origin, except possibly for a branch point at $t = 0$, where $f(t) \sim t^\lambda$, $\lambda > 0$, as $t \to 0$, and if f grows at most exponentially at infinity, one has $a_k \sim k^{-\lambda-1}$ as $k \to \infty$, showing that convergence of the series (3.13) is slow unless λ is large. However, we can write

$$\begin{aligned} S &= \sum_{k=1}^{\infty} (\mathcal{L}f)(k) = \sum_{k=1}^{\infty} \int_0^\infty e^{-kt} f(t)\, dt \\ &= \int_0^\infty \sum_{k=1}^{\infty} e^{-(k-1)t} \cdot e^{-t} f(t)\, dt \\ &= \int_0^\infty \frac{1}{1 - e^{-t}} \cdot e^{-t} f(t)\, dt, \end{aligned}$$

assuming the interchange of summation and integration is legitimate. This yields the following integral representation:

$$S = \int_0^\infty \epsilon(t)\, \frac{f(t)}{t}\, dt \tag{3.15}$$

involving the weight function

$$\epsilon(t) = \frac{t}{e^t - 1} \qquad \text{on } [0, \infty). \tag{3.16}$$

Such integrals occur frequently in solid state physics, where ϵ is known as Einstein's function. (Of course, ϵ is also the generating function of the Bernoulli numbers.)

There are two approaches that suggest themselves naturally for evaluating the integral (3.15). One is Gaussian quadrature relative to the weight function ϵ, if $f(t)/t$ is sufficiently regular, or, if not, with respect to some modified weight function. The other is rational Gauss quadrature of the type discussed in Section 3.1, writing

$$S = \int_0^\infty \frac{t}{1 - e^{-t}} \frac{f(t)}{t} \cdot e^{-t}\, \mathrm{d}t, \tag{3.17}$$

letting $e^{-t}\,\mathrm{d}t = \mathrm{d}\lambda(t)$, and matching as many of the poles at $\pm 2\mu\,\mathrm{i}\pi$, $\mu = 1, 2, 3, \ldots$, as possible. Both approaches call for nonclassical orthogonal polynomials.

To give an example, consider the series

$$S = \sum_{k=1}^{\infty} \frac{k^{\nu-1}}{(k+a)^m}, \qquad 0 < \nu < 1, \qquad m \geq 1, \tag{3.18}$$

where a is a complex number with $\operatorname{Re} a > 0$, $\operatorname{Im} a \geq 0$. Writing the general term of the series as

$$k^{\nu-1} \cdot (k+a)^{-m} = (\mathcal{L}f)(k),$$

we note that

$$k^{\nu-1} = \left(\mathcal{L}\, \frac{t^{-\nu}}{\Gamma(1-\nu)}\right)(k), \qquad (k+a)^{-m} = \left(\mathcal{L}\, \frac{t^{m-1}}{(m-1)!}\, e^{-at}\right)(k),$$

so that the convolution theorem for Laplace transforms (see, for example, Widder 1941, Theorem 12.1a)

$$\mathcal{L}g \cdot \mathcal{L}h = \mathcal{L}g * h,$$

where

$$(g * h)(t) = \int_0^t g(\tau) h(t-\tau)\, \mathrm{d}\tau,$$

yields

$$f(t) = \frac{1}{(m-1)!\Gamma(1-\nu)} \int_0^t e^{-a(t-\tau)} (t-\tau)^{m-1} \tau^{-\nu}\, \mathrm{d}\tau.$$

After the change of variable $\tau = tu$, this becomes

$$f(t) = \frac{t^{m-\nu}e^{-at}}{(m-1)!\Gamma(1-\nu)} \int_0^1 e^{atu}(1-u)^{m-1}u^{-\nu}\,du.$$

The integral on the right, up to a constant factor, can be recognized as Kummer's function $M(\alpha,\beta,z)$ with parameters $\alpha = 1-\nu$, $\beta = m+1-\nu$ and variable $z = at$ (see Abramowitz and Stegun, eds, 1964, Equation 13.2.1). Thus,

$$f(t) = t^{1-\nu}g_{m-1}(t;a,\nu), \tag{3.19}$$

where

$$g_n(t;a,\nu) = \frac{t^n e^{-at}}{\Gamma(n+2-\nu)} M(1-\nu,n+2-\nu,at), \qquad n = 0,1,2,\ldots . \tag{3.20}$$

It is known that Kummer's function satisfies a recurrence relation relative to its second parameter (Abramowitz and Stegun, eds, 1964, Equation 13.4.2), from which one gets for $g_n(\,\cdot\,) = g_n(\,\cdot\,;a,\nu)$ the three-term recurrence relation

$$g_{n+1}(t) = \frac{1}{n+1}\left\{\left(t + \frac{n+1-\nu}{a}\right)g_n(t) - \frac{t}{a}\,g_{n-1}(t)\right\}, \qquad n \geq 0,$$
$$g_{-1}(t) = \frac{t^{-1}}{\Gamma(1-\nu)}\,. \tag{3.21}$$

To compute g_{m-1} in (3.19), it is enough, therefore, to compute $g_0(t) = e^{-at}M(1-\nu,2-\nu,at)/\Gamma(2-\nu)$ and then to apply (3.21). On the other hand, g_0 is expressible (Abramowitz and Stegun, eds, 1964, Equation 13.6.10) in terms of Tricomi's form of the incomplete gamma function (Abramowitz and Stegun, eds, 1964, Equation 6.5.4),

$$g_0(t;a,\nu) = e^{-at}\gamma^*(1-\nu,-at), \tag{3.22}$$

where

$$\gamma^*(\lambda,z) = \frac{z^{-\lambda}}{\Gamma(\lambda)} \int_0^z e^{-t}t^{\lambda-1}\,dt. \tag{3.23}$$

Since g_0 is known to be an entire function of all its variables (see Tricomi 1954, Chapter IV), it follows from (3.21) that each function $g_n(t)$ is an entire function of t. Putting (3.19) into (3.15), we thus finally arrive at

$$\sum_{k=1}^{\infty} \frac{k^{\nu-1}}{(k+a)^m} = \int_0^{\infty} t^{-\nu}\epsilon(t)\cdot g_{m-1}(t;a,\nu)\,dt,$$
$$\operatorname{Re} a > 0, \qquad 0 < \nu < 1, \qquad m \geq 1, \tag{3.24}$$

with ϵ given by (3.16) and g_{m-1} an entire function of t. We can now proceed evaluating the integral on the right as discussed above, either treating $t^{-\nu}\epsilon(t)$ as a weight function in ordinary Gaussian quadrature, or writing $t^{-\nu}\epsilon(t) = (t/(1-e^{-t}))\cdot t^{-\nu}e^{-t}$ and using $t^{-\nu}e^{-t}\,dt = d\lambda(t)$ in rational Gauss quadrature.

It is worth noting that in this way we can sum series of the more general form

$$S = \sum_{k=1}^{\infty} k^{\nu-1} r(k), \qquad 0 < \nu < 1, \tag{3.25}$$

where $r(k)$ is any rational function

$$r(s) = \frac{p(s)}{q(s)}, \qquad \deg p < \deg q. \tag{3.26}$$

It suffices to decompose r into partial fractions and to apply (3.24) to each of them. The parameter $-a$ in (3.24) then represents one of the zeros of q, and m its multiplicity. If the condition $\operatorname{Re} a > 0$ is not satisfied, we can sum a few of the initial terms directly until the condition holds for all remaining terms.

We remark that for series with alternating sign factors, that is,

$$S' = \sum_{k=1}^{\infty} (-1)^{k-1} a_k, \qquad a_k = (\mathcal{L}f)(k), \tag{3.27}$$

analogous techniques can be applied, with the result that

$$S' = \int_0^{\infty} f(t)\varphi(t)\,\mathrm{d}t, \tag{3.28}$$

where now

$$\varphi(t) = \frac{1}{e^t + 1} \tag{3.29}$$

is what is known in solid state physics as Fermi's function.

Notes to Section 3

3.1. Convergence of the quadrature rule (3.5), when $m = 2n$, $\operatorname{supp}(\mathrm{d}\lambda) = [-1, 1]$ and $\zeta_\mu \in (-1, 1)$ with $s_\mu = 1$, for functions f analytic in a domain containing the interval $[-1, 1]$ in its interior has been studied by López and Illán (1984). Theorem 3, in this case, is due to Van Assche and Vanherwegen (1993, Theorem 1). These authors also consider a quadrature rule of the type (0.1) with $\operatorname{supp}(\mathrm{d}\lambda) = [-1, 1]$ whose nodes are the zeros of the rational function $(1+\zeta_n t)^{-1} + \sum_{\mu=1}^{n-1} c_\mu (1+\zeta_\mu t)^{-1}$ orthogonal (in the measure $\mathrm{d}\lambda$) to 1 and to $(1+\zeta_\mu t)^{-1}$, $\mu = 1, 2, \ldots, n-1$, where $\zeta_\mu \in (-1, 1)$ are given parameters. This is no longer a 'Gaussian' formula, as would be the case for polynomials, but leads to polynomials orthogonal with respect to the measure $\mathrm{d}\lambda/(\omega_{n-1}\omega_n)$, where $\omega_m(t) = \prod_{\mu=1}^{m}(1+\zeta_\mu t)$. The use of conjugate complex parameters ζ_μ in the context of rational quadrature rules is considered in López and Illán (1987). Theorem 3 in the general form stated is from Gautschi (1993b), where one can also find numerical examples. The application of rational Gauss formulae to generalized Fermi–Dirac integrals (3.9) and Bose–Einstein integrals (3.10) is further discussed in Gautschi (1993c) and has proven to be very effective.

3.2. The use of Gaussian quadrature for the purpose of summing infinite series has already been proposed by Newbery (unpublished). Summation of series (3.13) and (3.27) involving the Laplace transform by means of Gaussian quadrature relative to Einstein and Fermi weight functions, respectively, was first proposed in Gautschi and Milovanović (1985). The technique has since been applied to series of the type (3.25), and to analogous series with alternating sign factors, in Gautschi (1991a), and was also used in Gautschi (1991b) to sum slowly convergent power series of interest in plate contact problems. For the latter, an alternative complementary treatment has been given in Boersma and Dempsey (1992). Series of the type (3.18) were encountered by Davis (1993) in his study of spirals, in particular in his attempt to smooth certain discrete spirals ascribed by him to the 4th-century BC mathematician Theodorus. The treatment given here is taken from Davis (1993, Appendix A), where one also finds numerical examples. Alternative approaches using special function theory can be found in Boersma and Dempsey (1992), and using Euler–Maclaurin summation in Lewanowicz (1994); see also Davis (1993, pp. 40–41). Series (3.13) and (3.27) in which the terms a_k are values $f(k)$ of certain analytic functions f are summed in Milovanović (1994) by Gaussian quadrature involving weight functions $\cosh^{-2}(t)$ and $\sinh(t)\cosh^{-2}(t)$ on $\mathbb{R}_+$. Applications to series of the type (3.18), also with alternating signs, and to the Riemann Zeta function, are given in Milovanović (1995).

PART II: COMPUTATION

4. Computation of Gauss-type quadrature rules

In many applications, as we have seen in Part I, the need for orthogonal polynomials arises via Gauss-type quadrature with respect to some measure $d\lambda$. We therefore begin by discussing the computational aspects of Gaussian quadrature rules.

4.1. Gaussian rules

We assume that $d\lambda$ is a positive measure whose support contains infinitely many points, and all moments of which exist. There then exists, for each integer $n \geq 1$, an n-point Gauss formula

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^G f(t_\nu^G) + R_n^G(f), \qquad R_n^G(\mathbb{P}_{2n-1}) = 0. \tag{4.1}$$

The connection with orthogonal polynomials is well known (*cf.* Section 0.1). The nodes t_ν^G are the zeros of $\pi_n(\,\cdot\,; d\lambda)$, while the weights λ_ν^G – also called the *Christoffel numbers* – can be expressed in various ways in terms of the same orthogonal polynomials. For purposes of computation, however, it is better to characterize both quantities in terms of an eigenvalue problem.

To describe this characterization, we recall (*cf.* Section 0.2) that every system of (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot\,; d\lambda)$ satisfies a three-term recurrence relation

$$\begin{aligned} \pi_{k+1}(t) &= (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0,1,2,\ldots, \\ \pi_{-1}(t) &= 0, \qquad \pi_0(t) = 1, \end{aligned} \tag{4.2}$$

where the coefficients $\alpha_k = \alpha_k(d\lambda)$, $\beta_k = \beta_k(d\lambda)$ are real numbers uniquely determined by the measure $d\lambda$, and each β_k is positive. With the recursion coefficients α_k, β_k we associate an infinite, symmetric, tridiagonal matrix

$$J_\infty = J_\infty(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & & \\ & & \ddots & \ddots & \ddots & \\ 0 & & & & & \end{bmatrix}, \tag{4.3}$$

the *Jacobi matrix* belonging to the measure $d\lambda$. Its $n \times n$ leading principal minor matrix will be denoted by

$$J_n = J_n(d\lambda) = [J_\infty(d\lambda)]_{n\times n}. \tag{4.4}$$

The Gaussian nodes and weights can then be expressed in terms of the eigenvalues and eigenvectors of $J_n(d\lambda)$ according to the following theorem.

Theorem 4 Let x_ν be the eigenvalues of $J_n(d\lambda)$, and u_ν the corresponding normalized eigenvectors, so that

$$J_n(d\lambda)u_\nu = x_\nu u_\nu, \qquad u_\nu^T u_\nu = 1, \qquad \nu = 1,2,\ldots,n. \tag{4.5}$$

Then the Gaussian nodes t_ν^G and weights λ_ν^G in (4.1) are given by

$$t_\nu^G = x_\nu, \qquad \lambda_\nu^G = \beta_0 u_{\nu,1}^2, \qquad \nu = 1,2,\ldots,n, \tag{4.6}$$

where $u_{\nu,1}$ is the first component of u_ν and $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$.

Thus, the Gauss formula can be generated by computing the eigenvalues and (first components of) eigenvectors of a symmetric tridiagonal matrix. This is a routine problem in numerical linear algebra and can be solved by powerful algorithms such as the QR algorithm with carefully selected shifts (see, for example, Parlett 1980, Sections 8.9–8.11). The approach via eigenvalues is generally more efficient than traditional methods based on polynomial rootfinding.

Note also that the positivity of the Gauss weights λ_ν^G is an immediate consequence of (4.6).

Proof of Theorem 4. Let $\tilde{\pi}_k(\cdot) = \tilde{\pi}_k(\cdot\,; d\lambda)$ denote the normalized orthogonal polynomials, so that $\pi_k = \sqrt{(\pi_k, \pi_k)_{d\lambda}}\,\tilde{\pi}_k$. Inserting this into (0.11), dividing

by $\sqrt{(\pi_{k+1}, \pi_{k+1})_{\mathrm{d}\lambda}}$, and using (0.12), we obtain

$$\tilde{\pi}_{k+1}(t) = (t - \alpha_k) \frac{\tilde{\pi}_k}{\sqrt{\beta_{k+1}}} - \beta_k \frac{\tilde{\pi}_{k-1}}{\sqrt{\beta_{k+1}\beta_k}},$$

or, multiplying through by $\sqrt{\beta_{k+1}}$ and rearranging,

$$t\tilde{\pi}_k(t) = \alpha_k \tilde{\pi}_k(t) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(t) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t), \quad k = 0, 1, 2, \ldots, n-1. \tag{4.7}$$

In terms of the Jacobi matrix $J_n = J_n(\mathrm{d}\lambda)$ we can write these relations in vector form as

$$t\tilde{\pi}(t) = J_n\tilde{\pi}(t) + \sqrt{\beta_n}\tilde{\pi}_n(t)e_n, \tag{4.8}$$

where $\tilde{\pi}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_{n-1}(t)]^T$ and $e_n = [0, 0, \ldots, 0, 1]^T$ are vectors in $\mathbb{R}^n$. Since t_ν^G is a zero of $\tilde{\pi}_n$, it follows from (4.8) that

$$t_\nu^G \tilde{\pi}(t_\nu^G) = J_n\tilde{\pi}(t_\nu^G), \qquad \nu = 1, 2, \ldots, n. \tag{4.9}$$

This proves the first relation in (4.6), since $\tilde{\pi}$ is a nonzero vector, its first component being

$$\tilde{\pi}_0 = \beta_0^{-1/2}. \tag{4.10}$$

To prove the second relation in (4.6), note from (4.9) that the normalized eigenvector u_ν is

$$u_\nu = \frac{1}{[\tilde{\pi}(t_\nu^G)^T\tilde{\pi}(t_\nu^G)]^{1/2}}\,\tilde{\pi}(t_\nu^G) = \left(\sum_{\mu=1}^{n} \tilde{\pi}_{\mu-1}^2(t_\nu^G)\right)^{-1/2} \tilde{\pi}(t_\nu^G).$$

Comparing the first component on the far left and right, and squaring, gives, by virtue of (4.10),

$$\frac{1}{\sum_{\mu=1}^{n} \tilde{\pi}_{\mu-1}^2(t_\nu^G)} = \beta_0 u_{\nu,1}^2, \qquad \nu = 1, 2, \ldots, n. \tag{4.11}$$

On the other hand, letting $f(t) = \tilde{\pi}_{\mu-1}(t)$ in (4.1), one gets, by orthogonality, using (4.10) again, that

$$\beta_0^{1/2}\delta_{\mu-1,0} = \sum_{\nu=1}^{n} \lambda_\nu^G \tilde{\pi}_{\mu-1}(t_\nu^G) \qquad (\delta_{\mu-1,0} = \text{ Kronecker delta}),$$

or, in matrix form,

$$P\lambda^G = \beta_0^{1/2} e_1, \tag{4.12}$$

where $P \in \mathbb{R}^{n\times n}$ is the matrix of eigenvectors, $\lambda^G \in \mathbb{R}^n$ the vector of Gauss weights, and $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n$. Since the columns of P are orthogonal,

we have

$$P^TP = D, \qquad D = \operatorname{diag}(d_1, d_2, \ldots, d_n), \qquad d_\nu = \sum_{\mu=1}^{n} \tilde{\pi}_{\mu-1}^2(t_\nu^G).$$

Now multiply (4.12) from the left by P^T to obtain

$$D\lambda^G = \beta_0^{1/2} P^T e_1 = \beta_0^{1/2} \cdot \beta_0^{-1/2} e = e, \qquad e = [1, 1, \ldots, 1]^T.$$

Therefore, $\lambda^G = D^{-1}e$, that is,

$$\lambda_\nu^G = \frac{1}{\sum_{\mu=1}^{n} \tilde{\pi}_{\mu-1}^2(t_\nu^G)}, \qquad \nu = 1, 2, \ldots, n.$$

Comparing this with (4.11) establishes the desired result. □

Similar techniques apply to generate Gauss–Radau and Gauss–Lobatto quadrature rules. This will be discussed in Sections 4.2 and 4.3. Before we do so, however, it is useful to pursue the connection between Gauss quadrature formulae and linear algebra just a bit further.

If $U = [u_1, u_2, \ldots, u_n]$ is the (orthogonal) matrix of the normalized eigenvectors of $J = J_n(\mathrm{d}\lambda)$, then, by (4.5) and the first relation in (4.6),

$$JU = UD_t, \qquad U^TU = I, \qquad D_t = \operatorname{diag}(t_1^G, t_2^G, \ldots, t_n^G) \tag{4.13}$$

provides the spectral resolution of J. The second formula in (4.6), on the other hand, can be written in matrix form as

$$\sqrt{\lambda}^T = \sqrt{\beta_0}\, e_1^T U, \qquad \sqrt{\lambda} = \left[\sqrt{\lambda_1^G}, \sqrt{\lambda_2^G}, \ldots, \sqrt{\lambda_n^G}\right]^T, \tag{4.14}$$

where $e_1 = [1, 0, \ldots, 0]^T$ is the first coordinate vector. Letting $Q = U^T$, we can summarize (4.13), (4.14) by

$$Q^T D_t Q = J, \qquad Q^T\sqrt{\lambda} = \sqrt{\beta_0}\, e_1.$$

We then have

$$\begin{aligned} &\begin{bmatrix} 1 & 0^T \\ 0 & Q^T \end{bmatrix} \begin{bmatrix} 1 & \sqrt{\lambda}^T \\ \sqrt{\lambda} & D_t \end{bmatrix} \begin{bmatrix} 1 & 0^T \\ 0 & Q \end{bmatrix} \\ &= \begin{bmatrix} 1 & \sqrt{\lambda}^T Q \\ Q^T\sqrt{\lambda} & Q^T D_t Q \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_0}\, e_1^T \\ \sqrt{\beta_0}\, e_1 & J \end{bmatrix}. \end{aligned} \tag{4.15}$$

Thus, the 'Gauss matrix' in the middle on the far left is connected with the (slightly extended) Jacobi matrix on the far right by the orthogonal similarity transformation (4.15). This is important for two reasons: it shows that the passage from the Gauss quantities (more precisely, the n square roots $(\lambda_\nu^G)^{1/2}$ and n nodes t_ν^G) to the recursion coefficients (more precisely, the $2n$ quantities $\beta_0^{1/2}, \beta_1^{1/2}, \ldots, \beta_{n-1}^{1/2}, \alpha_0, \alpha_1, \ldots, \alpha_{n-1}$) is a *stable* process in terms of linear

perturbations. (Orthogonal transformations leave the Euclidean length of vectors unchanged.) Secondly, (4.15) suggests *Lanczos-type algorithms* for computing the recursion coefficients (*cf.* Section 6.2).

4.2. Gauss–Radau rules

We write the Gauss–Radau formula in the form

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \lambda_0^R f(a) + \sum_{\nu=1}^{n} \lambda_\nu^R f(t_\nu^R) + R_n^R(f), \qquad R_n^R(\mathbb{P}_{2n}) = 0, \quad (4.16)$$

where $a = \inf \operatorname{supp}(\mathrm{d}\lambda)$ is assumed to be a finite number. (Everything below will also be valid if $a < \inf \operatorname{supp}(\mathrm{d}\lambda)$.) We recall from Section 0.1 (where n is to be replaced by $n+1$) that the nodes t_ν^R are the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda_a)$, that is,

$$\pi_n(t_\nu^R;\mathrm{d}\lambda_a) = 0, \qquad \nu = 1,2,\ldots,n, \quad (4.17)$$

where $\mathrm{d}\lambda_a(t) = (t-a)\,\mathrm{d}\lambda(t)$, and that, with the nodes so determined, the formula (4.16) must be interpolatory, that is, have degree of exactness n.

With $\tilde{\pi}_k(\,\cdot\,) = \tilde{\pi}_k(\,\cdot\,;\mathrm{d}\lambda)$ denoting, as before, the normalized orthogonal polynomials, we adjoin to the n relations (4.7) the additional relation

$$t\tilde{\pi}_n(t) = \alpha_n^*\tilde{\pi}_n(t) + \sqrt{\beta_n}\tilde{\pi}_{n-1}(t) + \sqrt{\beta_{n+1}}\pi_{n+1}^*(t). \quad (4.18)$$

Here, $\beta_n = \beta_n(\mathrm{d}\lambda)$, $\beta_{n+1} = \beta_{n+1}(\mathrm{d}\lambda)$, and α_n^* is a parameter to be determined; once α_n^* is known, (4.18) defines π_{n+1}^*. Letting

$$\tilde{\pi}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_n(t)]^T, \qquad e_{n+1} = [0,0,\ldots,1]^T \in \mathbb{R}^{n+1},$$

we write (4.7) and (4.18) in matrix form as

$$t\tilde{\pi}(t) = J_{n+1}^*\tilde{\pi}(t) + \sqrt{\beta_{n+1}}\pi_{n+1}^*(t)e_{n+1}, \quad (4.19)$$

where

$$J_{n+1}^* = J_{n+1}^*(\mathrm{d}\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \ddots & & \\ & \ddots & \ddots & \sqrt{\beta_{n-1}} & \\ & & \sqrt{\beta_{n-1}} & \alpha_{n-1} & \sqrt{\beta_n} \\ 0 & & & \sqrt{\beta_n} & \alpha_n^* \end{bmatrix}. \quad (4.20)$$

We now choose α_n^* in such a way that $\pi_{n+1}^*(a) = 0$. By (4.18), this requires that

$$a\tilde{\pi}_n(a) - \alpha_n^*\tilde{\pi}_n(a) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(a) = 0,$$

or, reverting to monic polynomials and recalling that $\tilde{\pi}_{n-1}/\tilde{\pi}_n = \beta_n^{1/2}\pi_{n-1}/\pi_n$,

$$\alpha_n^* = a - \beta_n \frac{\pi_{n-1}(a)}{\pi_n(a)} . \tag{4.21}$$

(The denominator $\pi_n(a)$ does not vanish by the assumption on a.) Therefore,

$$\pi_{n+1}^*(t) = (t-a)\omega_n(t), \qquad \omega_n \in \mathbb{P}_n, \tag{4.22}$$

and, by (4.19), the zeros $t_0 = a$, $t_1, t_2, \ldots, t_n$ of π_{n+1}^* are the eigenvalues of J_{n+1}^*, with $\tilde{\pi}(a)$, $\tilde{\pi}(t_1), \ldots, \tilde{\pi}(t_n)$ the corresponding eigenvectors. We now show that $t_\nu = t_\nu^R$, $\nu = 1, 2, \ldots, n$, that is, except for a constant factor,

$$\omega_n(t) = \pi_n(t; \mathrm{d}\lambda_a). \tag{4.23}$$

By (4.18) we have indeed

$$\begin{aligned} \sqrt{\beta_{n+1}}\pi_{n+1}^*(t) &= (t-\alpha_n^*)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t) \\ &= (t-\alpha_n)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t) + (\alpha_n - \alpha_n^*)\tilde{\pi}_n(t) \\ &= \sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) + (\alpha_n - \alpha_n^*)\tilde{\pi}_n(t), \end{aligned}$$

where in the last step we have used (4.7) for $k = n$. There follows, for any $p \in \mathbb{P}_{n-1}$,

$$\begin{aligned} \sqrt{\beta_{n+1}}\int_{\mathbb{R}} \pi_{n+1}^*(t)p(t)\,\mathrm{d}\lambda(t) &= \sqrt{\beta_{n+1}}\int_{\mathbb{R}} \omega_n(t)p(t)\cdot(t-a)d\lambda(t) \\ = \int_{\mathbb{R}} [\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) &+ (\alpha_n - \alpha_n^*)\tilde{\pi}_n(t)]p(t)\,\mathrm{d}\lambda(t) = 0, \end{aligned}$$

by the orthogonality of the $\tilde{\pi}_k$. This proves (4.23).

By reasonings virtually identical with those in the proof of Theorem 4, one finds that

$$\lambda_\nu^R = \beta_0 u_{\nu,1}, \qquad \nu = 0, 1, 2, \ldots, n, \tag{4.24}$$

where $u_{\nu,1}$ is the first component of the normalized eigenvector u_ν of J_{n+1}^* corresponding to the eigenvalue t_ν^R (where $t_0^R = a$). We thus have the following result.

Theorem 5 The Gauss–Radau nodes $t_0^R = a$ and $t_1^R, \ldots, t_n^R$ are the eigenvalues of the matrix $J_{n+1}^*(\mathrm{d}\lambda)$ in (4.20), where α_n^* is defined by (4.21). The Gauss–Radau weights λ_ν^R are given by (4.24), where $u_{\nu,1}$ is the first component of the normalized eigenvector u_ν of $J_{n+1}^*(\mathrm{d}\lambda)$ corresponding to the eigenvalue t_ν^R.

The same theorem also holds for Gauss–Radau formulae with the fixed node at the upper end of the support interval. That is, if $\mathrm{d}\lambda$ has a support bounded from above, the number a, both in the formulation of Theorem 5 and in (4.16) and (4.21), may be replaced by $b \geq \sup \mathrm{supp}(\mathrm{d}\lambda)$.

Computing α_n^* by (4.21) may raise some concern about the possibility of a

large cancellation error. The example of the Jacobi measure $d\lambda^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta\,dt$ on $[-1,1]$, however, suggests that this concern is unwarranted. In this case, say for $a=-1$, one indeed finds that

$$\beta_n \frac{\pi_{n-1}(-1)}{\pi_n(-1)} = -\frac{1+\frac{\alpha}{n}}{2\left(1+\frac{\alpha+\beta}{2n}\right)\left(1+\frac{\alpha+\beta+1}{2n}\right)} \qquad (d\lambda = d\lambda^{(\alpha,\beta)}),$$

which for $n\to\infty$ tends to $-\frac{1}{2}$, so that for large n at least, there is no danger of cancellation. It is also interesting to note that for the generalized Laguerre measure $d\lambda^{(\alpha)}(t) = t^\alpha e^{-t}\,dt$ on $[0,\infty)$, and $a=0$, one has $\alpha_n^* = n$.

4.3. Gauss–Lobatto rules

Assuming that $d\lambda$ has bounded support, we write the Gauss–Lobatto formula in the form

$$\int_{\mathbb{R}} f(t)\,d\lambda(t) = \lambda_0^L f(a) + \sum_{\nu=1}^{n} \lambda_\nu^L f(t_\nu^L) + \lambda_{n+1}^L f(b) + R_n^L(f), \qquad R_n^L(\mathbb{P}_{2n+1}) = 0, \tag{4.25}$$

where $a \le \inf\operatorname{supp}(d\lambda)$ and $b \ge \sup\operatorname{supp}(d\lambda)$. We recall from Section 0.1 that the interior nodes t_ν^L are the zeros of $\pi_n(\,\cdot\,; d\lambda_{a,b})$, that is,

$$\pi_n(t_\nu^L; d\lambda_{a,b}) = 0, \qquad \nu = 1,2,\dots,n, \tag{4.26}$$

where $d\lambda_{a,b}(t) = (t-a)(b-t)\,d\lambda(t)$, and that with these nodes so determined, the formula (4.25) must be interpolatory, that is, have degree of exactness $n+1$. We proceed similarly as in Section 4.2, but adjoin to the n relations (4.7) not one, but two additional relations:

$$\begin{aligned} t\tilde\pi_n(t) &= \alpha_n\tilde\pi_n(t) + \sqrt{\beta_n}\tilde\pi_{n-1}(t) + \sqrt{\beta_{n+1}^*}\pi_{n+1}^*(t), \\ t\pi_{n+1}^*(t) &= \alpha_{n+1}^*\pi_{n+1}^*(t) + \sqrt{\beta_{n+1}^*}\tilde\pi_n(t) + \sqrt{\beta_{n+2}}\pi_{n+2}^*(t), \end{aligned} \tag{4.27}$$

where α_{n+1}^*, β_{n+1}^* are parameters to be determined and $\alpha_n = \alpha_n(d\lambda)$, $\beta_n = \beta_n(d\lambda)$, $\beta_{n+2} = \beta_{n+2}(d\lambda)$. We now define

$$J_{n+2}^* = J_{n+2}^*(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \alpha_{n-1} & \sqrt{\beta_n} & \\ & & & \sqrt{\beta_n} & \alpha_n & \sqrt{\beta_{n+1}^*} \\ 0 & & & & \sqrt{\beta_{n+1}^*} & \alpha_{n+1}^* \end{bmatrix}, \tag{4.28}$$

so that, with the usual notation

$$\tilde\pi(t) = [\tilde\pi_0(t),\dots,\tilde\pi_n(t),\pi_{n+1}^*(t)]^T, \qquad e_{n+2} = [0,\dots,0,1]^T \in \mathbb{R}^{n+2},$$

the relations (4.7) and (4.27) can be written in matrix form as

$$t\tilde{\pi}(t) = J_{n+2}^*\tilde{\pi}(t) + \sqrt{\beta_{n+2}}\pi_{n+2}^*(t)e_{n+2}. \tag{4.29}$$

We now choose α_{n+1}^*, β_{n+1}^* such that $\pi_{n+2}^*(a) = \pi_{n+2}^*(b) = 0$. By the second relation in (4.27) this requires

$$(t - \alpha_{n+1}^*)\pi_{n+1}^*(t) - \sqrt{\beta_{n+1}^*}\tilde{\pi}_n(t) = 0 \qquad \text{for } t = a, b,$$

or, using the first relation in (4.27) to eliminate π_{n+1}^*,

$$(t - \alpha_{n+1}^*)[(t - \alpha_n)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] - \beta_{n+1}^*\tilde{\pi}_n(t) = 0 \qquad \text{for } t = a, b.$$

The expression in brackets, however, is $\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t)$; thus,

$$(t - \alpha_{n+1}^*)\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) - \beta_{n+1}^*\tilde{\pi}_n(t) = 0 \qquad \text{for } t = a, b.$$

Converting to monic polynomials, we obtain the 2×2 linear system

$$\begin{bmatrix} \pi_{n+1}(a) & \pi_n(a) \\ \pi_{n+1}(b) & \pi_n(b) \end{bmatrix} \begin{bmatrix} \alpha_{n+1}^* \\ \beta_{n+1}^* \end{bmatrix} = \begin{bmatrix} a\pi_{n+1}(a) \\ b\pi_{n+1}(b) \end{bmatrix}.$$

By assumption on a and b, we have $\operatorname{sgn}[\pi_{n+1}(a)\pi_n(b)] = (-1)^{n+1}$ and $\operatorname{sgn}[\pi_{n+1}(b)\pi_n(a)] = (-1)^n$, so that the determinant is nonzero and, in fact, has sign $(-1)^{n+1}$. The system, therefore, has a unique solution, namely

$$\begin{aligned} \alpha_{n+1}^* &= (a\pi_{n+1}(a)\pi_n(b) - b\pi_{n+1}(b)\pi_n(a))/\Delta_n, \\ \beta_{n+1}^* &= (b - a)\pi_{n+1}(a)\pi_{n+1}(b)/\Delta_n, \end{aligned} \tag{4.30}$$

where

$$\Delta_n = \pi_{n+1}(a)\pi_n(b) - \pi_{n+1}(b)\pi_n(a). \tag{4.31}$$

Since both Δ_n and $\pi_{n+1}(a)\pi_{n+1}(b)$ have the sign $(-1)^{n+1}$, we see that $\beta_{n+1}^* > 0$, so that π_{n+1}^* and π_{n+2}^* in (4.27) are uniquely determined real polynomials, and J_{n+2}^* in (4.28) a real symmetric tridiagonal matrix. Its eigenvalues, by (4.29), are the zeros of π_{n+2}^*, among them a and b. Writing

$$\pi_{n+2}^*(t) = (t - a)(b - t)\omega_n(t), \qquad \omega_n \in \mathbb{P}_n, \tag{4.32}$$

we now show that, up to a constant factor,

$$\omega_n(t) = \pi_n(t;\, \mathrm{d}\lambda_{a,b}), \tag{4.33}$$

so that the eigenvalues of J_{n+2}^* are precisely the nodes of the Gauss–Lobatto formula (4.25), including a and b (*cf.* (4.26)). Using in turn the second and first relation of (4.27), we have

$$\begin{aligned} \sqrt{\beta_{n+2}}\pi_{n+2}^*(t) &= (t - \alpha_{n+1}^*)\pi_{n+1}^*(t) - \sqrt{\beta_{n+1}^*}\tilde{\pi}_n(t), \\ \sqrt{\beta_{n+1}^*\beta_{n+2}}\pi_{n+2}^*(t) &= (t - \alpha_{n+1}^*)[(t - \alpha_n)\tilde{\pi}_n(t) - \sqrt{\beta_n}\tilde{\pi}_{n-1}(t)] - \beta_{n+1}^*\tilde{\pi}_n(t) \\ &= (t - \alpha_{n+1}^*)\sqrt{\beta_{n+1}}\tilde{\pi}_{n+1}(t) - \beta_{n+1}^*\tilde{\pi}_n(t). \end{aligned}$$

It follows that π^*_{n+2} is orthogonal relative to the measure $\mathrm{d}\lambda$ to polynomials of degree $< n$, which by (4.32) implies (4.33).

Since, again by (4.29), the eigenvectors of J^*_{n+2} are $\tilde{\pi}(t^L_\nu)$, $\nu = 0, 1, \ldots, n$, $n+1$, where $t^L_0 = a$, $t^L_{n+1} = b$, the now familiar argument (used previously in Sections 4.1 and 4.2) yields the following theorem.

Theorem 6 The Gauss–Lobatto nodes $t^L_0 = a$, $t^L_{n+1} = b$ and $t^L_1, \ldots, t^L_n$ are the eigenvalues of the matrix $J^*_{n+2}(\mathrm{d}\lambda)$ in (4.28), where α^*_{n+1}, β^*_{n+1} are defined by (4.30), (4.31). The Gauss–Lobatto weights λ^L_ν are given by

$$\lambda^L_\nu = \beta_0 u^2_{\nu,1}, \qquad \nu = 0, 1, 2, \ldots, n, n+1, \tag{4.34}$$

where $u_{\nu,1}$ is the first component of the normalized eigenvector u_ν of $J^*_{n+2}(\mathrm{d}\lambda)$ corresponding to the eigenvalue t^L_ν.

Since, as already noted, the two terms defining Δ_n in (4.31) are of opposite sign, there is no cancellation in the computation of Δ_n, nor is there any in computing β^*_{n+1}. For α^*_{n+1} this may no longer be true (indeed, $\alpha^*_{n+1} = 0$ for symmetric measures!), but here it is more the absolute error than the relative error that matters.

The construction of Gauss-type quadrature formulae is just one of several instances illustrating the importance of the recursion coefficients $\alpha_k(\mathrm{d}\lambda)$, $\beta_k(\mathrm{d}\lambda)$ for computational purposes. It is for this reason that all our constructive methods for orthogonal polynomials are directed toward computing these coefficients.

Notes to Section 4

4.1. The fact that Gauss quadrature nodes can be viewed as eigenvalues of a symmetric tridiagonal matrix – the Jacobi matrix – has long been known. The characterization of the Gauss weights in terms of eigenvectors seems more recent; it was noted in Wilf (1962, Chapter 2, Exercise 9) and previously, around 1954, by Goertzel (Wilf 1980), and has also been used by Gordon (1968). The importance of these characterizations for computational purposes has been emphasized by Golub and Welsch (1969), who give a detailed computational procedure based on Francis's QR algorithm. Alternative procedures that compute the Gauss nodes as zeros of orthogonal polynomials by Newton's method or other rootfinding methods not only require considerable care in the selection of initial approximations, but also tend to be slower (Gautschi 1979). Also of importance is the inverse problem (Boley and Golub 1987) – given the Gauss nodes and weights, find the corresponding Jacobi matrix – and its solution by Lanczos-type algorithms.

4.2, 4.3. The eigenvalue techniques described for generating Gauss–Radau and Gauss–Lobatto quadrature rules are due to Golub (1973); our derivation slightly differs from the one in Golub (1973).

5. Moment-based methods

The classical approach of generating orthogonal polynomials is based on the moments of the given measure $d\lambda$:

$$\mu_k = \mu_k(d\lambda) = \int_{\mathbb{R}} t^k \, d\lambda(t), \qquad k = 0, 1, 2, \ldots . \tag{5.1}$$

The desired recursion coefficients can be expressed in terms of Hankel determinants in these moments,

$$\left.\begin{aligned} \alpha_k(d\lambda) &= \frac{D'_{k+1}}{D_{k+1}} - \frac{D'_k}{D_k} \\ \beta_k(d\lambda) &= \frac{D_{k+1} D_{k-1}}{D_k^2} \end{aligned}\right\} \qquad k = 0, 1, 2, \ldots, \tag{5.2}$$

where $D_0 = D_{-1} = 1$, $D_1 = \mu_0$, $D'_0 = 0$, $D'_1 = \mu_1$ and D_m, D'_m, $m \geq 2$, are determinants whose first row consists of $\mu_0, \mu_1, \ldots, \mu_{m-1}$ and $\mu_0, \mu_1, \ldots, \mu_{m-2}, \mu_m$, respectively (the others having the subscripts successively increased by 1). Likewise, the orthogonal polynomials themselves admit the determinantal representation

$$\pi_n(t; d\lambda) = \frac{1}{D_n} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_n & \mu_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} & \mu_{2n-1} \\ 1 & t & \cdots & t^{n-1} & t^n \end{vmatrix} . \tag{5.3}$$

The trouble with these formulae is that the coefficients α_k, β_k, and with them π_n, become extremely sensitive to small changes (such as rounding errors) in the moments as k increases. In other words, the (nonlinear) map

$$K_n : \qquad \mathbb{R}^{2n} \to \mathbb{R}^{2n} \qquad \mu \mapsto \rho, \tag{5.4}$$

which maps the moment vector $\mu = [\mu_0, \mu_1, \ldots, \mu_{2n-1}]^T$ to the vector $\rho = [\alpha_0, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{n-1}]^T$ of recursion coefficients becomes extremely ill conditioned. Therefore it is important to study the condition of such moment-related maps.

A natural idea to overcome this difficulty is to use *modified moments* instead. That is, given a system of polynomials $\{p_k\}$, one uses

$$m_k = m_k(d\lambda) = \int_{\mathbb{R}} p_k(t) \, d\lambda(t), \qquad k = 0, 1, 2, \ldots, \tag{5.5}$$

in place of μ_k. One then has a new map K_n,

$$K_n : \qquad \mathbb{R}^{2n} \to \mathbb{R}^{2n} \qquad m \mapsto \rho, \tag{5.6}$$

where $m = [m_0, m_1, \ldots, m_{2n-1}]^T$, which one hopes is better conditioned than

the old map (5.4). We discuss the conditioning of these maps in Section 5.1. In Section 5.2 we develop an algorithm that implements the maps K_n in (5.4) and (5.6) when the polynomials p_k defining the modified moments (5.5) satisfy a three-term recurrence relation. An example will be given in Section 5.3.

5.1. The conditioning of moment maps

The analysis of the map K_n in (5.4) or (5.6) is facilitated if the map is thought of as a composition of two maps,

$$K_n = H_n \circ G_n, \tag{5.7}$$

where $G_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ maps μ (respectively m) into the Gaussian quadrature rule,

$$G_n : \ \mu \text{ (resp. } m) \mapsto \gamma, \qquad \gamma = [\lambda_1, \ldots, \lambda_n, t_1, \ldots, t_n]^T, \tag{5.8}$$

where $\lambda_\nu = \lambda_\nu^G$, $t_\nu = t_\nu^G$ (*cf.* (4.1)), and $H_n : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ maps the Gaussian quadrature rule into the recursion coefficients,

$$H_n : \qquad \gamma \mapsto \rho. \tag{5.9}$$

The reason for this is that the map H_n, as was seen at the end of Section 4.1, is well conditioned, and G_n is easier to analyse. For a direct study of the map K_n see, however, Fischer (1996).

Just as the sensitivity of a function $f\colon \mathbb{R} \to \mathbb{R}$ at a point x can be measured by the magnitude of the derivative f' at x, in the sense that a small change $\mathrm{d}x$ of x produces the change $\mathrm{d}f(x) = f'(x)\,\mathrm{d}x$, we can measure the sensitivity of the map $G_n\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ at a given vector μ (respectively m) by the magnitude of the Fréchet derivative at μ (respectively m). For finite-dimensional maps, this derivative is nothing but the linear map defined by the Jacobian matrix. We thus define

$$\text{cond } G_n = \| \partial G_n \|, \tag{5.10}$$

where by ∂G_n we denote the Jacobian matrix of the map G_n, and where for $\| \cdot \|$ we can take any convenient matrix norm. Note that this concept of condition is based on absolute errors; one could refine it to deal with relative errors as well, but we shall not do so here.

5.1.1. We begin with the map G_n for ordinary moments. Since the Gauss formula (4.1) is exact for the first $2n$ monomials t^j, $j = 0, 1, \ldots, 2n-1$, we have

$$\sum_{\nu=1}^{n} \lambda_\nu t_\nu^j = \int_{\mathbb{R}} t^j \,\mathrm{d}\lambda(t) = \mu_j, \qquad j = 0, 1, \ldots, 2n-1,$$

which can be written as

$$\Phi(\gamma) = \mu, \qquad \Phi_j(\gamma) = \sum_{\nu=1}^{n} \lambda_\nu t_\nu^j, \qquad j = 0, 1, \ldots, 2n-1. \tag{5.11}$$

The map G_n consists in solving this (nonlinear) system for the unknown vector γ, given the vector μ. The Jacobian ∂G_n, therefore, is the inverse of the Jacobian $\partial\Phi$ of Φ. This latter is readily computed to be

$$\partial\Phi = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ t_1 & \cdots & t_n & \lambda_1 & \cdots & \lambda_n \\ t_1^2 & \cdots & t_n^2 & 2\lambda_1 t_1 & \cdots & 2\lambda_n t_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ t_1^{2n-1} & \cdots & t_n^{2n-1} & (2n-1)\lambda_1 t_1^{2n-2} & \cdots & (2n-1)\lambda_n t_n^{2n-2} \end{bmatrix} = TD_\lambda,$$

where T is the confluent Vandermonde matrix

$$T = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ t_1 & \cdots & t_n & 1 & \cdots & 1 \\ t_1^2 & \cdots & t_n^2 & 2t_1 & \cdots & 2t_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ t_1^{2n-1} & \cdots & t_n^{2n-1} & (2n-1)t_1^{2n-2} & \cdots & (2n-1)t_n^{2n-2} \end{bmatrix} \tag{5.12}$$

and D_λ the diagonal matrix

$$D_\lambda = \operatorname{diag}(1, \ldots, 1, \lambda_1, \ldots, \lambda_n). \tag{5.13}$$

Therefore,

$$\partial G_n = D_\lambda^{-1} T^{-1}. \tag{5.14}$$

It is now convenient to work with the uniform vector and matrix norm $\| \cdot \| = \| \cdot \|_\infty$. Since $\sum_{\nu=1}^{n} \lambda_\nu = \mu_0$ implies $\lambda_\nu < \mu_0$, and $\lambda_\nu^{-1} > \mu_0^{-1}$, it follows readily from (5.14) that

$$\| \partial G_n \| > \min(1, \mu_0^{-1}) \, \| T^{-1} \| .$$

Since the factor on the right involving μ_0 is unimportant, we shall henceforth assume that $\mu_0 = 1$ (which amounts to a normalization of the measure $\mathrm{d}\lambda$). To obtain a particularly simple result, we further assume that $\mathrm{d}\lambda$ is supported on the positive real line,

$$\operatorname{supp}(\mathrm{d}\lambda) \subset \mathbb{R}_+.$$

It then follows from norm estimates for the inverse confluent Vandermonde matrix (see Gautschi 1963) that

$$\| \partial G_n \| > \frac{\prod_{\nu=1}^{n} (1+t_\nu)^2}{\min_{1 \le \nu \le n} \left\{ (1+t_\nu) \prod_{\substack{\mu=1 \\ \mu \ne \nu}}^{n} (t_\nu - t_\mu)^2 \right\}} .$$

By definition (5.10) of the condition of G_n, and because the $\{t_\nu\}$ are the zeros of $\pi_n(\cdot) = \pi_n(\cdot\,; \mathrm{d}\lambda)$, we can write this inequality more elegantly as

$$\text{cond } G_n \;>\; \frac{\pi_n^2(-1)}{\min_{1\le\nu\le n}\{(1+t_\nu)[\pi_n'(t_\nu)]^2\}} \,. \tag{5.15}$$

Elegant as this result may be, it is also quite disconcerting, since orthogonal polynomials are known to grow rapidly with the degree when the argument is outside the support interval. In (5.15), the argument is -1, a good distance away from $\mathbb{R}_+$, and squaring the polynomial does not help either! Since the denominator in (5.15) grows only moderately with n, we must conclude that G_n becomes rapidly ill conditioned as n increases.

To illustrate (5.15), consider the (normalized) Chebyshev measure $\mathrm{d}\lambda(t) = \frac{1}{\pi}[t(1-t)]^{-1/2}$ on $[0,1]$, for which $\pi_n = T_n^*$, the 'shifted' Chebyshev polynomial, except for normalization. It then follows from (5.15) by elementary calculations that

$$\text{cond } G_n \;>\; \frac{(3+\sqrt{8})^n}{64n^2} \qquad (\pi_n = T_n^*).$$

The lower bound happens to grow at the same exponential rate as the (Turing) condition number of the $n \times n$ Hilbert matrix!

5.1.2. We consider now the map $G_n : m \to \gamma$, where $m \in \mathbb{R}^{2n}$ is the vector of modified moments (5.5). We assume that the polynomials p_k defining these modified moments are themselves orthogonal, but relative to a measure, $\mathrm{d}s$, over which we can exercise control,

$$p_k(\cdot) = \pi_k(\cdot\,; \mathrm{d}s), \qquad k = 0, 1, 2, \ldots \,. \tag{5.16}$$

The hope is that by choosing $\mathrm{d}s$ 'close' to the target measure $\mathrm{d}\lambda$, there is little chance for things to go wrong during the 'short' transition from the p_k to the π_k.

In analysing the condition of G_n, one arrives at a more satisfying result if, instead of the modified moments m_k, one departs from the *normalized* modified moments

$$\tilde{m}_k \;=\; \frac{m_k}{\| p_k \|_{\mathrm{d}s}} \,, \qquad k = 0, 1, 2, \ldots; \qquad \| p_k \|_{\mathrm{d}s} = \sqrt{(p_k, p_k)_{\mathrm{d}s}} \,. \tag{5.17}$$

We thus consider the map

$$\tilde{G}_n : \qquad \mathbb{R}^{2n} \to \mathbb{R}^{2n} \qquad \tilde{m} \mapsto \gamma, \qquad \tilde{m} = [\tilde{m}_0, \tilde{m}_1, \ldots, \tilde{m}_{2n-1}]^T. \tag{5.18}$$

The preliminary map $m \mapsto \tilde{m}$ is a perfectly well-conditioned diagonal map, and therefore does not distort the condition of G_n.

Similarly, as in (5.11), the map $\tilde{G}_n$ amounts to solving the nonlinear system

$$F(\gamma) = \tilde{m}, \qquad F_j(\gamma) = s_j^{-1} \sum_{\nu=1}^{n} \lambda_\nu p_j(t_\nu), \qquad j = 0, 1, \ldots, 2n-1,$$

where $s_j = \| p_j \|_{ds}$, and

$$\partial \tilde{G}_n = (\partial F)^{-1}.$$

By an elementary computation,

$$\partial F = D_s^{-1} P D_\lambda,$$

where $D_s = \operatorname{diag}(s_0, s_1, \ldots, s_{2n-1})$, $D_\lambda = \operatorname{diag}(1, \ldots, 1, \lambda_1, \ldots, \lambda_n)$, and $P \in \mathbb{R}^{2n \times 2n}$ is a confluent Vandermonde matrix in the polynomials $\{p_k\}$, that is,

$$\operatorname{row}_j P = [p_j(t_1), \ldots, p_j(t_n), p_j'(t_1), \ldots, p_j'(t_n)], \qquad j = 0, 1, \ldots, 2n-1. \tag{5.19}$$

Therefore,

$$\partial \tilde{G}_n = D_\lambda^{-1} P^{-1} D_s. \tag{5.20}$$

In order to invert the matrix P in (5.19), we let h_ν, k_ν be the fundamental Hermite interpolation polynomials of degree $2n-1$ associated with the Gaussian abscissae $t_1, t_2, \ldots, t_n$:

$$\begin{aligned} h_\nu(t_\mu) &= \delta_{\nu\mu}, \quad h_\nu'(t_\mu) = 0; \\ k_\nu(t_\mu) &= 0, \quad k_\nu'(t_\mu) = \delta_{\nu\mu}, \end{aligned} \tag{5.21}$$

and expand them in the polynomials $\{p_k\}$,

$$h_\nu(t) = \sum_{\mu=1}^{2n} a_{\nu\mu} p_{\mu-1}(t), \qquad k_\nu(t) = \sum_{\mu=1}^{2n} b_{\nu\mu} p_{\mu-1}(t), \qquad \nu = 1, 2, \ldots, n. \tag{5.22}$$

Letting

$$A = [a_{\nu\mu}], \qquad B = [b_{\nu\mu}],$$

we can write the interpolation conditions (5.21), in conjunction with (5.19), in the form

$$AP = [I, O], \qquad BP = [O, I],$$

that is,

$$\begin{bmatrix} A \\ B \end{bmatrix} P = \begin{bmatrix} I & O \\ O & I \end{bmatrix},$$

which shows that

$$P^{-1} = \begin{bmatrix} A \\ B \end{bmatrix}.$$

We are now ready to compute the norm of $\partial \tilde{G}_n$ in (5.20). This time it turns out to be convenient to use the Frobenius norm $\| \cdot \| = \| \cdot \|_F$. Since

$$\begin{aligned} (D_\lambda^{-1} P^{-1} D_s)_{\nu\mu} &= s_{\mu-1} a_{\nu\mu}, \qquad & (D_\lambda^{-1} P^{-1} D_s)_{\nu+n,\mu} &= \lambda_\nu^{-1} s_{\mu-1} b_{\nu\mu}, \\ \nu &= 1, 2, \ldots, n; & \mu &= 1, 2, \ldots, 2n, \end{aligned}$$

one indeed obtains

$$\| \partial \tilde{G}_n \|^2 = \sum_{\nu=1}^{n} \sum_{\mu=1}^{2n} s_{\mu-1}^2 \left(a_{\nu\mu}^2 + \frac{1}{\lambda_\nu^2} b_{\nu\mu}^2 \right) \tag{5.23}$$

from (5.20). On the other hand, by (5.22),

$$\int_{\mathbb{R}} h_\nu^2(t)\, \mathrm{d}s(t) = \sum_{\mu,\kappa=1}^{2n} a_{\nu\mu} a_{\nu\kappa} \int_{\mathbb{R}} p_{\mu-1}(t) p_{\kappa-1}(t)\, \mathrm{d}s(t) = \sum_{\mu=1}^{2n} s_{\mu-1}^2 a_{\nu\mu}^2,$$

where the last equation follows from the orthogonality of the p_k. Similarly,

$$\int_{\mathbb{R}} k_\nu^2(t)\, \mathrm{d}s(t) = \sum_{\mu=1}^{2n} s_{\mu-1}^2 b_{\nu\mu}^2.$$

Hence, recalling (5.10), equation (5.23) finally yields

$$\operatorname{cond} \tilde{G}_n = \left\{ \int_{\mathbb{R}} \sum_{\nu=1}^{n} \left[h_\nu^2(t) + \frac{1}{\lambda_\nu^2} k_\nu^2(t) \right] \mathrm{d}s(t) \right\}^{1/2}. \tag{5.24}$$

This result clearly identifies the factors influencing the condition of $\tilde{G}_n$. On the one hand, we have the polynomial of degree $4n-2$,

$$g_n(t;\, \mathrm{d}\lambda) = \sum_{\nu=1}^{n} \left[h_\nu^2(t) + \frac{1}{\lambda_\nu^2} k_\nu^2(t) \right], \tag{5.25}$$

appearing in the integrand of (5.24), which depends only on the measure $\mathrm{d}\lambda$ (through the Gaussian nodes $t_\nu = t_\nu^G$). On the other hand, there is integration with respect to the measure $\mathrm{d}s$. It is a combination of both, namely the *magnitude of g_n on the support of* $\mathrm{d}s$, which determines the magnitude of $\operatorname{cond} \tilde{G}_n$.

We note from (5.21) and (5.25) that $g_n(\,\cdot\,) = g_n(\,\cdot\,;\, \mathrm{d}\lambda)$ is strictly positive on $\mathbb{R}$ and satisfies

$$g_n(t_\nu) = 1, \qquad g_n'(t_\nu) = 0, \qquad \nu = 1, 2, \ldots, n. \tag{5.26}$$

(By themselves, these conditions of course do not yet determine g_n.) Ideally, one would like g_n to remain ≤ 1 throughout the support of $\mathrm{d}s$, in which case $\operatorname{cond} \tilde{G}_n$ would be bounded by $s_0 = (\int_{\mathbb{R}} \mathrm{d}s(t))^{1/2}$, uniformly in n. Unfortunately, this is only rarely the case. One example in which this property is likely to hold, based on computation, is $\mathrm{d}\lambda_k(t) = [(1-k^2t^2)(1-t^2)]^{-1/2}\, \mathrm{d}t$ on $[-1,1]$, where $0 < k < 1$. For $k = 0$, it was shown in Fischer (1996) that $g_n \leq 1 + 2/\pi^2$ on $[-1,1]$. In other cases, such as $\mathrm{d}\lambda_\sigma(t) = t^\sigma \ln(1/t)$ on $[0,1]$, where $\sigma > -1$, the property $g_n(t) \leq 1$ holds over part of the interval, whereas in the remaining part, g_n, assumes relatively large peaks between consecutive nodes t_ν, but such that the integral in (5.24) (when $\mathrm{d}s(t) = 1$) is still of acceptable magnitude.

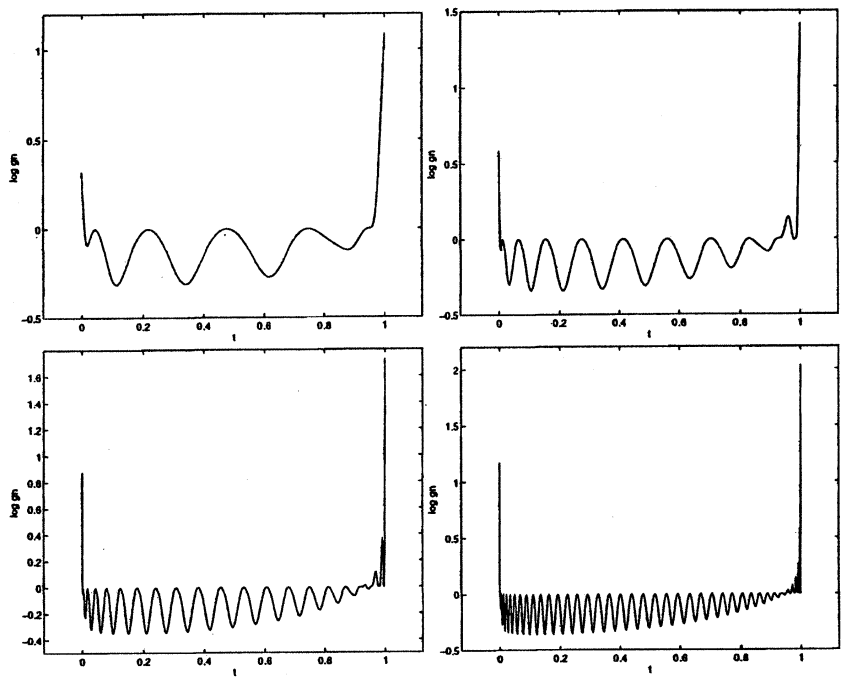

Fig. 1. The polynomial g_n, $n = 5, 10, 20, 40$, for the Maxwell measure with $c = 1$

An example of interest in quantum physics is the Maxwell velocity distribution

$$d\lambda(t) = e^{-t^2}\,dt \qquad \text{on } [0, c], \qquad 0 < c \leq \infty. \tag{5.27}$$

One finds by computation that g_n 'almost' satisfies $g_n \leq 1$ on $[0, c]$ when c is only moderately large, but develops larger and larger peaks, encroaching on an ever increasing portion of the interval, as c increases. This is illustrated in Fig. 1, which depicts $\log g_n$ for $n = 5, 10, 20, 40$ in the case $c = 1$, and in Fig. 2, where the analogous information is shown for $c = 5$. The respective condition numbers (when $ds(t) = dt$) are all less than 1 in the case $c = 1$, and range from 3.52×10^{12} to 8.57×10^{19} when $c = 5$. Fig. 2 is also representative for the case $c = \infty$. Arguably, Legendre moments ($ds(t) = dt$) are a poor choice in this case, but it has been observed in Gautschi (1996c) that even the best choice, $ds(t) = d\lambda(t)$, gives rise to very large condition numbers if c is large.

It has generally been our experience that cond $\tilde{G}_n$ becomes unacceptably large, even for moderately large n, when the support of $d\lambda$ is unbounded, as in the case $c = \infty$ of (5.27).

A final example of some interest in theoretical chemistry involves a measure $d\lambda$ of Chebyshev type supported on two separate intervals, say $[-1, -\xi]$ and $[\xi, 1]$, where $0 < \xi < 1$. Here, all nodes t_ν congregate on the two support intervals, at most one being located on the 'hole' $[-\xi, \xi]$ (see Szegő 1975, Theorem 3.41.2). As a consequence, g_n is likely to remain relatively small

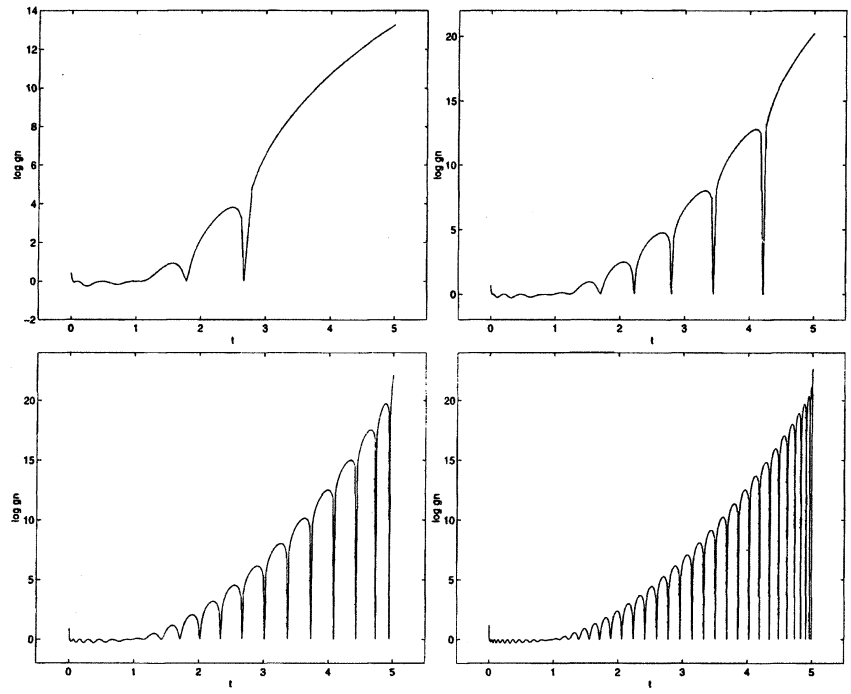

Fig. 2. The polynomial g_n, $n = 5, 10, 20, 40$, for the Maxwell measure with $c = 5$

(perhaps even ≤ 1) on the two support intervals, but may well become extremely large on the hole. To avoid a large condition number cond $\tilde{G}_n$, it is then imperative not to choose a measure $\mathrm{d}s$ for the modified moments that is supported on the whole interval $[-1, 1]$, but one that preferably has the same support as $\mathrm{d}\lambda$.

5.2. The modified Chebyshev algorithm

We assumed in Section 5.1.2 that the polynomials p_k defining the modified moments (5.5) are themselves orthogonal. We now assume only that they satisfy a three-term recurrence relation

$$\begin{aligned} &p_{-1}(t) = 0, \qquad p_0(t) = 1, \\ &p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \end{aligned} \tag{5.28}$$

with known coefficients a_k, b_k, where the b_k need not necessarily be positive. This, in particular, encompasses the case $a_k = b_k = 0$, leading to $p_k(t) = t^k$, hence to ordinary moments (5.1).

To formulate an algorithm that implements the map $K_n : m \mapsto \rho$, we introduce 'mixed moments'

$$\sigma_{k,\ell} = \int_{\mathbb{R}} \pi_k(t) p_\ell(t)\, \mathrm{d}\lambda(t), \qquad k, \ell \geq -1, \tag{5.29}$$

and immediately observe that, by orthogonality, $\sigma_{k,\ell} = 0$ for $k > \ell$, and

$$\int_{\mathbb{R}} \pi_k^2(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} \pi_k(t) t p_{k-1}(t)\,\mathrm{d}\lambda(t) = \sigma_{k,k}, \qquad k \geq 1. \tag{5.30}$$

The relation $\sigma_{k+1,k-1} = 0$, therefore, in combination with the recurrence relation (0.11) for the π_k, yields

$$0 = \int_{\mathbb{R}} [(t-\alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t)] p_{k-1}(t)\,\mathrm{d}\lambda(t) = \sigma_{k,k} - \beta_k \sigma_{k-1,k-1},$$

hence

$$\beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}, \qquad k = 1, 2, 3, \ldots . \tag{5.31}$$

(Recall that $\beta_0 = m_0$ by convention.) Similarly, $\sigma_{k+1,k} = 0$ gives

$$0 = \int_{\mathbb{R}} \pi_k(t) t p_k(t)\,\mathrm{d}\lambda(t) - \alpha_k \sigma_{k,k} - \beta_k \sigma_{k-1,k}.$$

Using (5.28) in the form $tp_k(t) = p_{k+1}(t) + a_k p_k(t) + b_k p_{k-1}(t)$, we can write this as

$$0 = \sigma_{k,k+1} + (a_k - \alpha_k)\sigma_{k,k} - \beta_k \sigma_{k-1,k},$$

which, together with (5.31) and $\sigma_{-1,k} = 0$, yields

$$\begin{cases} \alpha_0 = a_0 + \dfrac{\sigma_{0,1}}{\sigma_{0,0}}, \\ \alpha_k = a_k + \dfrac{\sigma_{k,k+1}}{\sigma_{k,k}} - \dfrac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \qquad k = 1, 2, 3, \ldots . \end{cases} \tag{5.32}$$

With the αs and βs expressed by (5.32) and (5.31) in terms of the σs, it remains to compute $\sigma_{k,\ell}$. This can be done recursively, using the recurrence (0.11) for the π_k and (5.28) (with k replaced by ℓ) for the p_ℓ:

$$\begin{aligned} \sigma_{k,\ell} &= \int_{\mathbb{R}} [(t-\alpha_{k-1})\pi_{k-1}(t) - \beta_{k-1}\pi_{k-2}(t)] p_\ell(t)\,\mathrm{d}\lambda(t) \\ &= \int_{\mathbb{R}} \pi_{k-1}(t)[p_{\ell+1}(t) + a_\ell p_\ell(t) + b_\ell p_{\ell-1}(t)]\,\mathrm{d}\lambda(t) \\ &\qquad -\alpha_{k-1}\sigma_{k-1,\ell} - \beta_{k-1}\sigma_{k-2,\ell} \\ &= \sigma_{k-1,\ell+1} - (\alpha_{k-1} - a_\ell)\sigma_{k-1,\ell} - \beta_{k-1}\sigma_{k-2,\ell} + b_\ell \sigma_{k-1,\ell-1}. \end{aligned}$$

The algorithm is now complete: to compute α_k, β_k for $k = 0, 1, \ldots, n-1$, one first initializes

$$\begin{aligned} &\sigma_{-1,\ell} = 0, \qquad \ell = 1, 2, \ldots, 2n-2, \\ &\sigma_{0,\ell} = m_\ell, \qquad \ell = 0, 1, \ldots, 2n-1, \\ &\alpha_0(\mathrm{d}\lambda) = a_0 + \frac{m_1}{m_0}, \qquad \beta_0(\mathrm{d}\lambda) = m_0, \end{aligned} \tag{5.33}$$

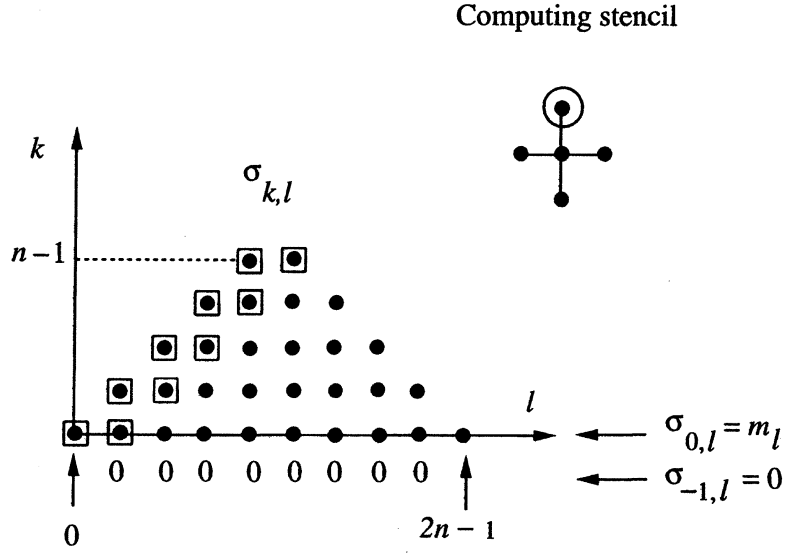

Fig. 3. The modified Chebyshev algorithm, schematically

and then continues, for $k = 1, 2, \ldots, n-1$, with

$$\begin{aligned} \sigma_{k,\ell} &= \sigma_{k-1,\ell+1} - (\alpha_{k-1} - a_\ell)\sigma_{k-1,\ell} - \beta_{k-1}\sigma_{k-2,\ell} + b_\ell \sigma_{k-1,\ell-1}, \\ &\qquad \ell = k, k+1, \ldots, 2n-k-1, \\ \alpha_k(\mathrm{d}\lambda) &= a_k + \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \qquad \beta_k(\mathrm{d}\lambda) = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}} \end{aligned} \tag{5.34}$$

Given the first $2n$ modified moments $m_0, m_1, \ldots, m_{2n-1}$ and the first $2n-1$ coefficients $a_0, a_1, \ldots, a_{2n-2}$ and $b_0, b_1, \ldots, b_{2n-2}$, this generates the first n coefficients $\alpha_0, \alpha_1, \ldots, \alpha_{n-1}$ and $\beta_0, \beta_1, \ldots, \beta_{n-1}$ via a trapezoidal array of auxiliary quantities $\sigma_{k,\ell}$ depicted schematically (for $n = 5$) in Fig. 3. The computing stencil in Fig. 3 indicates the location of the five entries in the array that are involved in the relation (5.34). The circled entry in the stencil is the one the algorithm computes in terms of the other four. The entries in boxes are used to compute the α_k and β_k. The complexity of the algorithm is clearly $\mathcal{O}(n^2)$.

It is interesting to observe that in the special case of a discrete measure $\mathrm{d}\lambda_N$ and ordinary moments (that is, $a_k = b_k = 0$), algorithm (5.34) was already known to Chebyshev (1859). We therefore call (5.34) the *modified Chebyshev algorithm*. The modified moments required can sometimes be computed in closed form or by a judicious application of recurrence formulae, or else can be approximated by a suitable discretization, similarly as in Section 6.1 in another context.

We remark that by virtue of (5.30), the algorithm (5.34) also provides the normalization constants $\sigma_{k,k} = (\pi_k, \pi_k)_{\mathrm{d}\lambda}$.

Table 1. *Errors in the α_ks and β_ks*

k	err α_k	err β_k
2	4.2×10^{-13}	7.6×10^{-13}
5	4.2×10^{-9}	1.2×10^{-10}
8	4.3×10^{-6}	3.8×10^{-6}
11	1.3×10^{0}	3.2×10^{-1}

5.3. An example

We illustrate the advantage of modified over classical moments in the case of the measure

$$d\lambda_\sigma(t) = t^\sigma \ln(1/t)\, dt \qquad \text{on } [0,1], \qquad \sigma > -1. \tag{5.35}$$

We expect this advantage to be rather noticeable here, since, as was already observed in Section 5.1.2, the map $\tilde{G}_n$: $\tilde{m} \mapsto \gamma$ based on (normalized) Legendre moments is quite well conditioned in this case, even for large n, in contrast to the map G_n: $\mu \mapsto \gamma$, which rapidly becomes ill conditioned as n increases (*cf.* Section 5.1.1).

The classical moments for $d\lambda_\sigma$ are simple enough,

$$\mu_k(d\lambda_\sigma) = \frac{1}{\sigma + 1 + k}, \qquad k = 0, 1, 2, \dots, \tag{5.36}$$

whereas the modified moments with respect to the Legendre polynomials on $[0,1]$ (that is, $a_k = \frac{1}{2}$ for $k \geq 0$ and $b_0 = 1$, $b_k = (4(4 - k^{-2}))^{-1}$ for $k \geq 1$ in (5.28)) are more complicated, but still easy to compute:

$$\frac{(2k)!}{k!^2}\, m_k(d\lambda_\sigma) = \begin{cases} (-1)^{k-\sigma}\, \frac{\sigma!^2 (k-\sigma-1)!}{(k+\sigma+1)!}, & 0 \leq \sigma < k, \qquad \sigma \in \mathbb{N}, \\ \frac{1}{\sigma+1} \left\{ \frac{1}{\sigma+1} + \sum_{r=1}^{k} \left(\frac{1}{\sigma+1+r} - \frac{1}{\sigma+1-r} \right) \right\} \prod_{r=1}^{k} \frac{\sigma+1-r}{\sigma+1+r}, & \text{otherwise.} \end{cases} \tag{5.37}$$

Applying the modified Chebyshev algorithm in single precision (machine precision $\approx 7 \times 10^{-15}$) for the case $\sigma = 0$, using the ordinary moments (5.36) (that is, $a_k = b_k = 0$), one obtains the recursion coefficients α_k, β_k with relative errors shown in Table 1. As can be seen, the accuracy deteriorates rapidly, there being no significance left by the time $k = 11$. In contrast, the use of modified moments (5.37) allows us to compute the first 100 (*sic*) recursion coefficients to an accuracy of at least 12 decimal digits.

Unfortunately, such a dramatic improvement in accuracy is not always realizable. In particular, for measures $d\lambda$ with unbounded support, even the modified version of Chebyshev's algorithm, as already mentioned, must be

expected to become quite susceptible to error growth. It all depends on the condition of the underlying (nonlinear) map $\tilde{G}_n$.

Notes to Section 5

The numerical condition of the classical moment map $G_n : \mu \mapsto \gamma$ was studied in Gautschi (1968); the lower bound (5.15) for the condition number rephrases one of the basic results of Gautschi (1968). For the growth of the condition number of the Hilbert matrix, mentioned at the end of Section 5.1.1, see Todd (1954). Although the explicit expressions (5.2) for the recursion coefficients are extremely sensitive to rounding errors, with the use of high-precision arithmetic they can be applied to validate the accuracy of Gaussian quadrature formulae; see Gautschi (1983) for an example.

The idea of using modified moments to generate orthogonal polynomials was first advanced by Sack and Donovan (1969, 1971/2), who developed an algorithm similar to the one in (5.34). The latter was derived by Wheeler (1974) independently of the work of Chebyshev (1859), where the same algorithm was obtained in the case of discrete measures and classical moments. Another algorithm, based on the Cholesky decomposition of a Gram matrix, is given in Gautschi (1970), but is not competitive with the modified Chebyshev algorithm, since it has complexity $\mathcal{O}(n^3)$. The reference Gautschi (1970), however, contains the first analysis of the condition of the underlying moment map, using the L_1-norm for vectors and matrices. The analysis given in Section 5.1.2, based on the more convenient Frobenius norm, is taken from Gautschi (1982a), where (in Section 3.1) one also finds the use of more refined condition numbers based on relative errors. The example of the Maxwell distribution (5.27) is taken from Gautschi (1991c); other illustrations of the basic formula (5.24) for the condition of the map $\tilde{G}_n$ can be found in Gautschi (1984c) and Gautschi (1985). The properties (5.26) of the function g_n in (5.25) suggest the distinction between 'strong' and 'weak' Gaussian nodes, the former being more likely than the latter to develop severe ill conditioning. For this, and an application to Jacobi polynomials, see Gautschi (1986a). The example at the end of Section 5.1.2 is taken from Wheeler (1984) and Gautschi (1984a); see also Gautschi (1985, Example 4.3) for further details. For the example in Section 5.3, *cf.* Gautschi (1994, Example 3.2).

6. Discretization methods

These methods, as the name implies, involve a preliminary discretization of the given measure $\mathrm{d}\lambda$, that is, one approximates $\mathrm{d}\lambda$ by a discrete N-point Dirac measure,

$$\mathrm{d}\lambda(t) \approx \mathrm{d}\lambda_N(t) := \sum_{k=1}^{N} w_k \delta(t - t_k)\,\mathrm{d}t. \tag{6.1}$$

This is often done by a suitable quadrature formula (more on this in Section 6.1):

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) \approx \sum_{k=1}^{N} w_k p(t_k) =: \int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_N(t). \tag{6.2}$$

The desired recursion coefficients are then approximated by

$$\left.\begin{aligned} \alpha_k(\mathrm{d}\lambda) &\approx \alpha_k(\mathrm{d}\lambda_N) \\ \beta_k(\mathrm{d}\lambda) &\approx \beta_k(\mathrm{d}\lambda_N) \end{aligned}\right\} \qquad k = 0, 1, \ldots, n-1. \tag{6.3}$$

Assuming $\mathrm{d}\lambda$ is a positive measure, and $w_k > 0$ in (6.1), one can show that for any fixed k,

$$\left.\begin{aligned} \alpha_k(\mathrm{d}\lambda_N) &\longrightarrow \alpha_k(\mathrm{d}\lambda) \\ \beta_k(\mathrm{d}\lambda_N) &\longrightarrow \beta_k(\mathrm{d}\lambda) \end{aligned}\right\} \qquad \text{as } N \to \infty, \tag{6.4}$$

provided the discretization process (6.2) has the property that

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda_N(t) \to \int_{\mathbb{R}} p(t)\,\mathrm{d}\lambda(t) \qquad \text{as } N \to \infty \tag{6.5}$$

for any polynomial p. Thus, by choosing a quadrature rule in (6.2) that is convergent for polynomials, we can obtain the coefficients α_k, β_k, $0 \le k \le n-1$, to any desired accuracy, by selecting N sufficiently large. More precisely, one selects a sequence $N_1 < N_2 < N_3 < \cdots$ of integers N (for a specific choice, see Gautschi 1994, Equation (4.16)) and iterates until

$$\max_{0 \le k \le n-1} \left| \frac{\beta_k(\mathrm{d}\lambda_{N_{i+1}}) - \beta_k(\mathrm{d}\lambda_{N_i})}{\beta_k(\mathrm{d}\lambda_{N_{i+1}})} \right| \le \varepsilon,$$

where ε is a preassigned error tolerance. The convergence criterion is based on the relative errors in the β-coefficients, which is possible because the β_k are known to be positive. The α-coefficients are expected to converge at a similar speed (at least in the sense of absolute errors), as their definition is similar to that of the β_k (*cf.* (0.12)).

In Section 6.1 we indicate some possible ways of discretizing the measure $\mathrm{d}\lambda$. Once the discrete measure is at hand, it remains to compute its first n recursion coefficients, that is, the approximations on the right of (6.3). We will discuss two methods in Sections 6.2 and 6.3.

6.1. Discretization of the measure

Suppose the measure $\mathrm{d}\lambda$ has the form

$$\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t \qquad \text{on } [a, b], \tag{6.6}$$

where $[a, b]$ is a finite or infinite interval and w an appropriate weight function. The first step, in general, is the decomposition of $[a, b]$ into a finite number

of (possibly overlapping) subintervals,

$$[a,b] = \bigcup_{i=1}^{m} [a_i, b_i] \qquad (m \geq 1), \tag{6.7}$$

and to rewrite integrals such as those on the left of (6.2) as

$$\int_{\mathbb{R}} p(t)w(t)\,\mathrm{d}t = \sum_{i=1}^{m} \int_{a_i}^{b_i} p(t)w_i(t)\,\mathrm{d}t, \tag{6.8}$$

where w_i is an appropriate weight function on $[a_i, b_i]$. For example, the weight function w may be the sum $w = w_1 + w_2$ of two weight functions on $[a,b]$ that we wish to treat individually. In that case, one would take $[a_1,b_1] = [a_2,b_2] = [a,b]$ and associate w_1 with $[a_1,b_1]$ and w_2 with $[a_2,b_2]$. Alternatively, we may simply want to use a composite quadrature rule to approximate the integral, in which case (6.7) is a partition of $[a,b]$ and $w_i(t) = w(t)$ for each i. Still another example is a weight function w which is already supported on a union of disjoint intervals; in this case, (6.7) would be the same union, or possibly a refined union where some of the subintervals are further partitioned.

However (6.7) and (6.8) are constructed, the desired discretization (6.2) is now obtained by approximating each integral on the right of (6.8) by an appropriate quadrature rule,

$$\int_{a_i}^{b_i} p(t)w_i(t)\,\mathrm{d}t \approx Q_i p, \qquad Q_i p = \sum_{r=1}^{N_i} w_{r,i}\, p(t_{r,i}), \tag{6.9}$$

for example a Gaussian rule for the weight function w_i. This yields

$$\int_{\mathbb{R}} p(t)w(t)\,\mathrm{d}t \approx \sum_{i=1}^{m} \sum_{r=1}^{N_i} w_{r,i}\, p(t_{r,i}), \tag{6.10}$$

a formula of the type (6.2) with $N = \sum_{i=1}^{m} N_i$.

There is enough flexibility in this approach – choosing the subdivision (6.7), the local weight functions w_i in (6.8), and the quadrature rules in (6.9) – to come up with an effective scheme of discretization, that is, one that not only converges in the sense of (6.5), but converges reasonably fast. Further variations, of course, are possible. In particular, it is straightforward to adapt the approach to deal with measures containing, in addition to an absolutely continuous component (6.6), a discrete point spectrum, say

$$\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t + \sum_{j} \omega_j \delta(t - \tau_j)\,\mathrm{d}t. \tag{6.11}$$

One only has to add $\sum_j \omega_j p(\tau_j)$ to (6.10).

Example 6.1. A good example of the kind of discretization indicated above is furnished by the measure

$$d\lambda(t) = t^\mu K_0(t)\,dt \qquad \text{on } [0,\infty), \qquad \mu > -1, \tag{6.12}$$

where K_0 is the modified Bessel function.

It is important, here, that one find a discretization that does justice to the special properties of the weight function $w(t) = t^\mu K_0(t)$, in particular its behaviour for small and large t. For the factor K_0, this behaviour can be described by

$$K_0(t) = \begin{cases} R(t) + I_0(t)\ln(1/t), & 0 < t \le 1, \\ t^{-1/2}e^{-t}S(t), & 1 \le t < \infty, \end{cases} \tag{6.13}$$

where R, S are well-behaved smooth functions, and I_0 is the 'regular' modified Bessel function. All three functions can be accurately evaluated on their respective intervals by rational approximations (Russon and Blair 1969). Therefore,

$$\begin{aligned} \int_0^\infty p(t)\,d\lambda(t) = \int_0^1 t^\mu [R(t)p(t)]\,dt + \int_0^1 t^\mu \ln(1/t)[I_0(t)p(t)]\,dt \\ + \int_1^\infty e^{-t}[t^{\mu-1/2}S(t)p(t)]\,dt. \end{aligned} \tag{6.14}$$

This suggests a decomposition (6.7) with $m = 3$, namely $[0,\infty) = [0,1] \cup [0,1] \cup [1,\infty)$, weight functions $w_1(t) = t^\mu$, $w_2(t) = t^\mu \ln(1/t)$ and $w_3(t) = e^{-t}$, and for Q_i the corresponding Gaussian quadrature rules, after the last integral in (6.14) has been rewritten as

$$\int_1^\infty e^{-t}[t^{\mu-1/2}S(t)p(t)]\,dt = e^{-1}\int_0^\infty e^{-t}[(1+t)^{\mu-1/2}S(1+t)p(1+t)]\,dt.$$

The first and last Gauss formulae are classical – Gauss–Jacobi and Gauss–Laguerre – and are easily generated by the method of Section 4.1. The second is nonclassical, but can be generated by the same method, once the recursion coefficients for the respective orthogonal polynomials have been generated by the modified Chebyshev algorithm, as discussed in Sections 5.2 and 5.3.

Example 6.2. We call *generalized Jacobi measure* a measure of the form

$$d\lambda(t) = \varphi(t)(1-t)^\alpha(1+t)^\beta \prod_{i=2}^m |t - a_i|^{\gamma_i}, \qquad t \in (-1,1), \tag{6.15}$$

where φ is a smooth function, $m \ge 2$, $-1 < a_2 < \cdots < a_m < 1$, and

$$\gamma_1 = \beta > -1; \qquad \gamma_i > -1, \qquad i = 2,\dots,m; \qquad \gamma_{m+1} = \alpha > -1. \tag{6.16}$$

Here, the natural decomposition is

$$[-1,1] = \bigcup_{i=1}^m [a_i, b_i], \quad a_1 = -1, \quad b_i = a_{i+1}, \quad a_{m+1} = 1,$$

and the appropriate weight function w_i on $[a_i, b_i]$ is the Jacobi weight with parameters γ_i, γ_{i+1}, transformed to the interval $[a_i, b_i]$. One then obtains a formula similar to (6.8), except that on the right, $p(t)$ has to be replaced by

$$p(t)\varphi(t) \prod_{j=1, j\neq i, j\neq i+1}^{m+1} |t - a_j|^{\gamma_j}, \qquad a_i \leq t \leq b_i.$$

This function is free of singularities in $[a_i, b_i]$, so that its Gauss–Jacobi quadrature with weight function w_i will converge – and reasonably fast at that, unless one of the a_j is very close to either a_i or b_i (and γ_j not an integer).

It may not always be possible to come up with natural discretizations as in these examples. In that case, one may try to apply a standard quadrature rule to each integral on the right of (6.8), paying no special attention to the weight function w_i and treat it as part of the integrand. Since w_i may have singularities at the endpoints of $[a_i, b_i]$, it is imperative that an open quadrature formula be used; stability considerations furthermore favour Chebyshev nodes, and convergence considerations an interpolatory formula. Taking the same number of nodes for each Q_i, we are thus led to choose, on the canonical interval $[-1, 1]$, the N^F-point *Fejér rule*, that is, the interpolatory quadrature rule

$$\int_{-1}^{1} f(t)\,\mathrm{d}t \approx Q_{N^F} f, \qquad Q_{N^F} f = \sum_{r=1}^{N^F} w_r^F f(t_r^F), \tag{6.17}$$

where $t_r^F = \cos((2r-1)\pi/2N^F)$ are the Chebyshev points. The weights are expressible in trigonometric form as

$$w_r^F = \frac{2}{N^F}\left(1 - 2\sum_{s=1}^{\lfloor N^F/2 \rfloor} \frac{\cos(2s\theta_r^F)}{4s^2 - 1}\right), \qquad t_r^F = \cos\theta_r^F, \tag{6.18}$$

and are known to be all positive (Fejér 1933). Furthermore, the rule converges as $N^F \to \infty$, even in the presence of singularities, provided they occur at the endpoints and are monotone and integrable (Gautschi 1967). The rule (6.17) is now applied to each integral on the right of (6.8) by transforming the interval $[-1, 1]$ to $[a_i, b_i]$ via some monotone function ϕ_i (a linear function if $[a_i, b_i]$ is finite) and letting $f(t) = p(t)w_i(t)$:

$$\begin{aligned}\int_{a_i}^{b_i} p(t)w_i(t)\,\mathrm{d}t &= \int_{-1}^{1} p(\phi_i(\tau))w_i(\phi_i(\tau))\phi_i'(\tau)\,\mathrm{d}\tau \\ &\approx \sum_{r=1}^{N^F} w_r^F w_i(\phi_i(t_r^F))\phi_i'(t_r^F)\cdot p(\phi_i(t_r^F)).\end{aligned}$$

Thus, in effect, we take in (6.9)

$$t_{r,i} = \phi_i(t_r^F), \qquad w_{r,i} = w_r^F w_i(\phi_i(t_r^F))\phi_i'(t_r^F), \qquad i = 1, 2, \ldots, m. \tag{6.19}$$

Suitable functions ϕ_i are $\phi_i(t) = (1+t)/(1-t)$ if the interval $[a_i, b_i]$ is half-infinite, say of the form $[0, \infty)$, and similarly for intervals $[a, \infty)$ and $(-\infty, b]$, and $\phi_i(t) = t/(1-t^2)$ if $[a_i, b_i] = (-\infty, \infty)$.

6.2. Orthogonal reduction method

Assuming now that a discrete measure (6.1) has been constructed, with (positive) weights w_k and abscissae t_k, we denote by $\sqrt{w}$ the column vector whose components are $\sqrt{w_k}$, and by D_t the diagonal matrix with the t_k on the diagonal. Since for any function p,

$$\int_{\mathbb{R}} p(t)\, \mathrm{d}\lambda_N(t) = \sum_{k=1}^{N} w_k p(t_k) \tag{6.20}$$

(*cf.* (6.2)), we may interpret (6.20) as a 'Gauss formula' for the measure $\mathrm{d}\lambda_N$. From (4.15) it then follows that there exists an orthogonal matrix $Q_1 \in \mathbb{R}^{N\times N}$ such that

$$\begin{bmatrix} 1 & 0^T \\ 0 & Q_1^T \end{bmatrix} \begin{bmatrix} 1 & \sqrt{w}^T \\ \sqrt{w} & D_t \end{bmatrix} \begin{bmatrix} 1 & 0^T \\ 0 & Q_1 \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{\beta_0(\mathrm{d}\lambda_N)}\, e_1^T \\ \sqrt{\beta_0(\mathrm{d}\lambda_N)}\, e_1 & J_N(\mathrm{d}\lambda_N) \end{bmatrix}, \tag{6.21}$$

where $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^N$ is the first coordinate vector and $J_N(\mathrm{d}\lambda_N)$ the Jacobi matrix of order N for the measure $\mathrm{d}\lambda_N$ (*cf.* (4.4)). It is the latter that we wish to obtain.

Observe that (6.21) has the form

$$Q^T A Q = T, \tag{6.22}$$

where all matrices are $(N+1)\times(N+1)$, Q is orthogonal and T symmetric tridiagonal with positive elements on the side diagonals. It is then well known (see, for instance, Parlett 1980, p. 113) that Q and T in (6.22) are uniquely determined by A and the first column of Q. Since the latter in (6.21) is e_1, and the former $\begin{bmatrix} 1 & \sqrt{w}^T \\ \sqrt{w} & D_t \end{bmatrix}$, we see that knowledge of w and D_t, that is, of $\mathrm{d}\lambda_N$, uniquely determines the desired $J_N(\mathrm{d}\lambda_N)$ and $\beta_0(\mathrm{d}\lambda_N)$ by the orthogonal similarity transformation (6.21). A method that accomplishes this transformation is *Lanczos's algorithm.* There are various versions of this algorithm, a particularly elegant one consisting of a sequence of elementary orthogonal similarity transformations of Givens type designed to successively push the elements bordering the diagonal matrix D_t in (6.21) towards the diagonal. It is not necessary to carry the transformation to completion; it can be terminated once the submatrix $J_n(\mathrm{d}\lambda_N)$ has been produced, which is all that is needed. Also, in spite of the square roots of the weights appearing

on the left of (6.21), it is not required in the resulting algorithm that all weights be of the same (positive) sign, since only their squares enter into the algorithm.

6.3. The Stieltjes procedure

This is based on the explicit formulae (see (0.12))

$$\alpha_k(\mathrm{d}\lambda) = \frac{(t\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}, \qquad k = 0, 1, 2, \ldots,$$
$$\beta_0(\mathrm{d}\lambda) = (\pi_0, \pi_0)_{\mathrm{d}\lambda}, \qquad \beta_k(\mathrm{d}\lambda) = \frac{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_{k-1}, \pi_{k-1})_{\mathrm{d}\lambda}}, \qquad k = 1, 2, 3, \ldots, \tag{6.23}$$

where $\pi_k(\cdot) = \pi_k(\cdot\,; \mathrm{d}\lambda)$. One applies (6.23) for $\mathrm{d}\lambda = \mathrm{d}\lambda_N$ in tandem with the basic recurrence relation (see (0.11))

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0, 1, 2, \ldots,$$
$$\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1. \tag{6.24}$$

Note that all inner products in (6.23) are finite sums when $\mathrm{d}\lambda = \mathrm{d}\lambda_N$, so that they are easily computed once the π_k are known. Since $\pi_0 = 1$, we can thus compute α_0, β_0 from (6.23). Having obtained α_0, β_0, we then use (6.24) with $k = 0$ to compute π_1 for all $\{t_1, \ldots, t_N\}$ to obtain the values of π_1 needed to reapply (6.23) with $k = 1$. This yields α_1, β_1, which in turn can be used in (6.24) to obtain the values of π_2 needed to return to (6.23) for computing α_2, β_2. In this way, alternating between (6.23) and (6.24), we can 'bootstrap' ourselves up to any desired order of the recursion coefficients. The procedure is now commonly referred to as the *Stieltjes procedure.*

Although the recurrence relation (6.24) may develop the phenomenon of pseudostability mentioned at the end of Section 0.2, as k approaches N, this normally causes no problem for the Stieltjes procedure since the maximum order $n-1$ desired for the recursion coefficients α_k, β_k is usually much smaller than the integer N eventually needed for convergence in (6.4). The onset of pseudostability is thus avoided. On the other hand, suitable scaling of the weights w_k may be required to stay clear of overflow or underflow. No such problems occur with the Lanczos method, which, moreover, has been observed to be typically about twice as fast as the Stieltjes procedure. For these reasons, one normally prefers orthogonal reduction methods over the Stieltjes procedure.

Notes to Section 6

6.1. The idea of discretizing the measure to approximate the recursion coefficients, and the use of Fejér's quadrature rule (6.17) in this context, goes back to Gautschi (1968). The convergence property (6.4), (6.5) is proved in Gautschi (1968, Theorem 4). The idea has been further developed along the lines of Section 6.1 in Gautschi

(1982a) and is implemented in the computer routine `mcdis` of Gautschi (1994). Example 6.1 is taken from Gautschi (1982a, Example 4.10) and is of interest in the asymptotic approximation of oscillatory integral transforms (Wong 1982).

6.2, 6.3. A Lanczos-type algorithm of the type mentioned at the end of Section 6.2 can be found in Gragg and Harrod (1984) and is used in the routine `lancz` of Gautschi (1994). The bootstrap procedure of Section 6.3 was briefly mentioned by Stieltjes (1884) and also forms the basis of the procedures in Forsythe (1957). For the phenomenon of pseudostability mentioned at the end of Section 6.3, see Gautschi (1993a) and Gautschi (1996b).

7. Modification algorithms

The idea of (and need for) looking at orthogonal polynomials relative to modified measures goes back to Christoffel (1858), who multiplied the measure $d\lambda$ by a polynomial $u(t) = \prod_{\lambda=1}^{\ell}(t-u_\lambda)$, where all u_λ are outside the support interval (the smallest interval containing $\operatorname{supp}(d\lambda)$); he represented the polynomial $u(t)\pi_n(t; u\,d\lambda)$ in determinantal form as a linear combination of $\pi_n(t; d\lambda), \ldots, \pi_{n+\ell}(t; d\lambda)$. This is now known as *Christoffel's theorem.* More recently, Uvarov (1959, 1969) extended Christoffel's result to measures multiplied by a rational function $u(t)/v(t)$, where $v(t) = \prod_{\mu=1}^{m}(t-v_\mu)$, expressing $u(t)\pi_n(t; (u/v)\,d\lambda)$ again in determinantal form as a linear combination of $\pi_{n-m}(t; d\lambda), \ldots, \pi_{n+\ell}(t; d\lambda)$ if $m \le n$, and of $\pi_0(t; d\lambda), \ldots, \pi_{n+\ell}(t; d\lambda)$ if $m > n$. We have called this (Gautschi 1982*b*) the *generalized Christoffel theorem.*

While these theorems are mathematically elegant, they do not lend themselves easily to computational purposes. What is more useful is trying to compute the recursion coefficients $\alpha_k(d\hat{\lambda})$, $\beta_k(d\hat{\lambda})$ for the modified measure $d\hat{\lambda} = (u/v)\,d\lambda$ in terms of those for $d\lambda$, which we assume are known. This need not be accomplished all at once, but can be carried out in elementary steps: multiply or divide by one linear complex factor $t-z$ at a time, or else, if we prefer to compute in the real domain, multiply or divide by either a linear real factor $t-x$, or a quadratic real factor $(t-x)^2+y^2$. Thus, the problem we wish to consider is the following. Given the recursion coefficients $\alpha_k(d\lambda)$, $\beta_k(d\lambda)$ for the measure $d\lambda$, compute the recursion coefficients $\alpha_k(d\hat{\lambda})$, $\beta_k\,d(\hat{\lambda})$ for the measures $d\hat{\lambda} = u\,d\lambda$ and $d\hat{\lambda} = d\lambda/v$, where $u(t)$ and $v(t)$ are elementary real factors of the type $t-x$ or $(t-x)^2+y^2$, $x \in \mathbb{R}$, $y \in \mathbb{R}$.

We begin in Section 7.1 with the theory of quasi-definite measures and kernel polynomials, which lies at the heart of modification algorithms for linear and quadratic factors. The latter are discussed in Section 7.2. In Section 7.3 we develop algorithms for linear and quadratic divisors. The division algorithms, finally, are applied in Section 7.4 to construct the rational Gauss quadrature formulae that were discussed in Section 3.1.

7.1. Quasi-definite measures and kernel polynomials

It is convenient, in this subsection, to allow $d\lambda$ to be any real or complex-valued measure on $\mathbb{R}$ having finite moments of all orders,

$$\mu_r = \mu_r(d\lambda) = \int_{\mathbb{R}} t^r \, d\lambda(t), \qquad r = 0, 1, 2, \ldots . \tag{7.1}$$

The measure $d\lambda$ is called *quasi-definite* if all Hankel determinants D_n in the moments are nonzero, that is,

$$D_n = \det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \cdots & \cdots & \cdots & \cdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} \end{bmatrix} \neq 0, \qquad n = 1, 2, 3, \ldots . \tag{7.2}$$

If $d\lambda$ is quasi-definite, there exists a unique system $\{\pi_k\}_{k=0}^{\infty}$ of (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot\,; d\lambda)$ relative to the measure $d\lambda$, which satisfy the three-term recurrence relation (0.11) with coefficients $\alpha_k = \alpha_k(d\lambda)$, $\beta_k = \beta_k(d\lambda)$ that are now complex-valued in general, but with $\beta_k \neq 0$. The measure $d\lambda$ is called *positive definite* if $\int_{\mathbb{R}} p(t)\, d\lambda(t) > 0$ for every polynomial $p(t) \not\equiv 0$ that is nonnegative on $\operatorname{supp}(d\lambda)$. Equivalently, $d\lambda$ is positive definite if all moments (7.1) are real and $D_n > 0$ for all $n \geq 1$.

For arbitrary $z \in \mathbb{C}$, and for $\alpha_k = \alpha_k(d\lambda)$, $\beta_k = \beta_k(d\lambda)$, $\beta_0 = 0$, let

$$\left.\begin{aligned} \alpha_k &= z + q_k + e_{k-1} \\ \beta_k &= e_{k-1} q_{k-1} \end{aligned}\right\} \qquad k = 0, 1, 2, \ldots \,; e_{-1} = q_{-1} = 0. \tag{7.3}$$

Lemma 1 Let $d\lambda$ be quasi-definite and $\pi_k(\cdot) = \pi_k(\cdot\,; d\lambda)$.

(a) If $\pi_n(z) \neq 0$ for all $n = 1, 2, 3, \ldots$, then the relations (7.3) uniquely determine q_0, e_0, q_1, $e_1, \ldots$ in this order, and

$$q_k = -\frac{\pi_{k+1}(z)}{\pi_k(z)}, \qquad k = 0, 1, 2, \ldots . \tag{7.4}$$

(b) If $\pi_{\ell+1}(z) = 0$ for some $\ell \geq 0$, and $\pi_k(z) \neq 0$ for all $k \leq \ell$, then q_k, e_k are uniquely determined by (7.3) for $k < \ell$, while $q_\ell = 0$ and e_ℓ is undefined.

Proof. (a) The quantities q_0, e_0, q_1, $e_1, \ldots$ are uniquely defined if and only if $q_k \neq 0$ for all $k \geq 0$. It suffices, therefore, to prove (7.4). For $k = 0$, this follows from the first relation in (7.3) with $k = 0$:

$$q_0 = \alpha_0 - z = -(z - \alpha_0) = -\frac{\pi_1(z)}{\pi_0(z)} .$$

Proceeding by induction, assume (7.4) true for $k - 1$. Then, by (7.3),

$$q_k = \alpha_k - z - e_{k-1} = \alpha_k - z - \frac{\beta_k}{q_{k-1}} = \alpha_k - z + \beta_k \frac{\pi_{k-1}(z)}{\pi_k(z)} ,$$

hence

$$q_k = -\frac{1}{\pi_k(z)}\{(z-\alpha_k)\pi_k(z) - \beta_k\pi_{k-1}(z)\} = -\frac{\pi_{k+1}(z)}{\pi_k(z)},$$

where the recurrence relation (0.11) has been used in the last step.

(b) The argument in the proof of (a) establishes (7.4) for all $k \leq \ell$, from which the assertion follows immediately. □

Consider now

$$d\hat{\lambda}(t) = (t-z)\,d\lambda(t), \qquad z \in \mathbb{C}.$$

If $d\lambda$ is quasi-definite, and z satisfies the assumption of Lemma 1(a), then $d\hat{\lambda}$ is also quasi-definite (Chihara 1978, Chapter I, Theorem 7.1), and hence gives rise to a sequence of (monic) orthogonal polynomials $\hat{\pi}_k(\cdot\,;z) = \pi_k(\cdot\,; d\hat{\lambda})$, $k = 0, 1, 2, \ldots$. These are called the *kernel polynomials.* They are given explicitly in terms of the polynomials $\pi_k(\cdot) = \pi_k(\cdot\,; d\lambda)$ by

$$\hat{\pi}_n(t;z) = \frac{1}{t-z}\left[\pi_{n+1}(t) - \frac{\pi_{n+1}(z)}{\pi_n(z)}\,\pi_n(t)\right], \qquad k = 0, 1, 2, \ldots, \tag{7.5}$$

as is readily verified.

Let $\hat{\alpha}_k = \alpha_k(d\hat{\lambda})$, $\hat{\beta}_k = \beta_k(d\hat{\lambda})$ be the recursion coefficients for the kernel polynomials $\hat{\pi}_k(\cdot) = \hat{\pi}_k(\cdot\,;z)$,

$$\begin{aligned} \hat{\pi}_{k+1}(t) &= (t-\hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k\hat{\pi}_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \\ \hat{\pi}_{-1}(t) &= 0, \qquad \hat{\pi}_0(t) = 1, \end{aligned} \tag{7.6}$$

where the dependence on z has been suppressed. The following theorem shows how the coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ can be generated in terms of the quantities q_k, e_k of Lemma 1.

Theorem 7 Let $d\lambda$ be quasi-definite and $z \in \mathbb{C}$ be such that $\pi_n(z; d\lambda) \neq 0$ for all n. Let q_k, e_k, be the quantities uniquely determined by (7.3). Then

$$\left.\begin{aligned} \hat{\alpha}_k &= z + q_k + e_k \\ \hat{\beta}_k &= q_k e_{k-1} \end{aligned}\right\} \qquad k = 0, 1, 2, \ldots . \tag{7.7}$$

In (7.7), $\hat{\beta}_0$ receives the value zero; it could be assigned any other convenient value such as the customary $\hat{\beta}_0 = \int_{\mathbb{R}} d\hat{\lambda}(t)$. In that case, $\hat{\beta}_0 = \int_{\mathbb{R}}(t-z)\,d\lambda(t) = \int_{\mathbb{R}}(t-\alpha_0+\alpha_0-z)\,d\lambda(t) = (\alpha_0-z)\beta_0$, since $t-\alpha_0 = \pi_1(t; d\lambda)$ and $\int_{\mathbb{R}} \pi_1(t)\,d\lambda(t) = 0$.

Proof of Theorem 7. By (7.5) and (7.4) we can write

$$\hat{\pi}_k(t) = \frac{1}{t-z}[\pi_{k+1}(t) + q_k\pi_k(t)], \tag{7.8}$$

or, solved for π_{k+1},

$$\pi_{k+1}(t) = (t-z)\hat{\pi}_k(t) - q_k\pi_k(t), \qquad k = 0, 1, 2, \ldots . \tag{7.9}$$

The three-term recurrence relation for the $\{\pi_k\}$, with the coefficients α_k, β_k written in the form (7.3), yields

$$\pi_{k+1}(t) = (t-z)\pi_k(t) - (q_k + e_{k-1})\pi_k(t) - e_{k-1}q_{k-1}\pi_{k-1}(t),$$

from which

$$\frac{\pi_{k+1}(t) + q_k\pi_k(t)}{t-z} = \pi_k(t) - e_{k-1}\,\frac{\pi_k(t) + q_{k-1}\pi_{k-1}(t)}{t-z},$$

or, by (7.8),

$$\hat{\pi}_k(t) = \pi_k(t) - e_{k-1}\hat{\pi}_{k-1}(t), \qquad k = 0, 1, 2, \ldots . \tag{7.10}$$

Replacing k by $k+1$ in (7.10) and applying first (7.9), and then again (7.10), we get

$$\begin{aligned}\hat{\pi}_{k+1}(t) &= \pi_{k+1}(t) - e_k\hat{\pi}_k(t)\\ &= (t-z)\hat{\pi}_k(t) - q_k\pi_k(t) - e_k\hat{\pi}_k(t)\\ &= (t-z)\hat{\pi}_k(t) - q_k[\hat{\pi}_k(t) + e_{k-1}\hat{\pi}_{k-1}(t)] - e_k\hat{\pi}_k(t),\end{aligned}$$

that is,

$$\hat{\pi}_{k+1}(t) = (t - z - q_k - e_k)\hat{\pi}_k(t) - q_k e_{k-1}\hat{\pi}_{k-1}(t), \qquad k = 0, 1, 2, \ldots . \tag{7.11}$$

The assertion (7.7) now follows by comparing (7.11) with (7.6). □

7.2. Linear and quadratic factors

We assume from now on that $d\lambda$ is a positive measure. The support of $d\lambda$ may extend to infinity at one end, when dealing with linear factors, but will be arbitrary otherwise.

Consider first modification by a linear factor,

$$d\hat{\lambda}(t) = (t-x)\,d\lambda(t), \qquad x \in \mathbb{R}\backslash I_{\text{supp}}(d\lambda),$$

where, as indicated, x is any real number outside the 'support interval' $I_{\text{supp}}(d\lambda)$ of $d\lambda$, that is, outside the smallest interval containing the support of $d\lambda$. Then $d\hat{\lambda}$ is positive definite if x is to the left of this interval, and negative definite otherwise. In either case, $\pi_n(x; d\lambda) \neq 0$ for all n, since the zeros of π_n are known to lie in the support interval. Theorem 7, therefore, applies with $z = x$ and, together with the remark immediately after Theorem 7, and (7.3), produces the following algorithm for calculating the first

n recursion coefficients of $\{\hat{\pi}_k\}$ from those of $\{\pi_k\}$:

$$\left.\begin{aligned} e_{-1} &= 0 \\ q_k &= \alpha_k - e_{k-1} - x \\ \hat{\beta}_k &= q_k \cdot \begin{cases} \beta_0 & \text{if } k = 0 \\ e_{k-1} & \text{if } k > 0 \end{cases} \\ e_k &= \beta_{k+1}/q_k \\ \hat{\alpha}_k &= x + q_k + e_k \end{aligned}\right\} \qquad k = 0, 1, \ldots, n-1. \tag{7.12}$$

Note that we need β_n in addition to α_k, β_k, $k = 0, 1, \ldots, n-1$, to obtain the first n recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$, $k = 0, 1, \ldots, n-1$. Numerical experience seems to indicate that the nonlinear recursion (7.12) is quite stable. In cases where the coefficients $\hat{\alpha}_k$ tend rapidly to zero, it is true that they can be obtained only to full absolute accuracy, not relative accuracy. This, however, should not impair the accuracy in the recursive computation of $\hat{\pi}_k$ by (7.6).

There is a similar, but more complicated, algorithm for modification by a quadratic factor,

$$\mathrm{d}\hat{\lambda}(t) = ((t-x)^2 + y^2)\,\mathrm{d}\lambda(t), \qquad x \in \mathbb{R}, \qquad y > 0, \tag{7.13}$$

which can be obtained by two successive applications of linear (complex) factors $t - z$ and $t - \bar{z}$, where $z = x + \mathrm{i}y$. A particularly elegant algorithm is known when $y = 0$ in (7.13). In terms of the Jacobi matrices of $\mathrm{d}\lambda$ and $\mathrm{d}\hat{\lambda}$, it consists in applying one QR step with the shift x: if

$$\begin{aligned} &J_{n+1}(\mathrm{d}\lambda) - xI_{n+1} = QR, \\ &\qquad Q \text{ orthogonal, } R \text{ upper triangular, } \operatorname{diag} R \geq 0, \end{aligned} \tag{7.14}$$

then

$$J_n(\mathrm{d}\hat{\lambda}) = (RQ + xI_{n+1})_{n\times n}. \tag{7.15}$$

Thus, having completed the QR step applied to the Jacobi matrix of order $n+1$ for the measure $\mathrm{d}\lambda$, one discards the last row and last column to obtain the Jacobi matrix of order n for the modified measure $\mathrm{d}\hat{\lambda}$. This algorithm, too, appears to be quite stable.

7.3. Linear and quadratic divisors

Consider first division by a linear divisor,

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t-x}, \qquad x \in \mathbb{R}\backslash I_{\text{supp}}(\mathrm{d}\lambda), \tag{7.16}$$

where x is assumed real, outside the support interval of $\mathrm{d}\lambda$. Here again, there exists a nonlinear algorithm of the type (7.12) (indeed, a reversal thereof), but it is quite unstable unless x is very close to the support interval of $\mathrm{d}\lambda$. Although such values of x are not without interest in applications, we shall not develop the algorithm here and refer instead to Gautschi (1982b).

For other values of x, and particularly for measures with bounded support (*cf.* the remark at the end of Section 5.3), we recommend applying the modified Chebyshev algorithm, using the orthogonal polynomials $p_k(\cdot) = \pi_k(\cdot; \mathrm{d}\lambda)$ as the polynomial system defining the modified moments, that is, letting

$$m_k = \int_{\mathbb{R}} \pi_k(t; \mathrm{d}\lambda) \frac{\mathrm{d}\lambda(t)}{t - x}, \qquad k = 0, 1, 2, \ldots . \tag{7.17}$$

We shall assume again that the recursion coefficients $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$ are known. Under mild assumptions on the measure $\mathrm{d}\lambda$ (for instance, if $I_{\text{supp}}(\mathrm{d}\lambda)$ is a finite interval), the sequence $\{m_k\}$ is a minimal solution of the basic recurrence relation

$$\begin{aligned} &y_{k+1} = (x - \alpha_k)y_k - \beta_k y_{k-1}, \qquad k = 0, 1, 2, \ldots, \\ &y_{-1} = -1, \end{aligned} \tag{7.18}$$

where $\alpha_k = \alpha_k(\mathrm{d}\lambda)$, $\beta_k = \beta_k(\mathrm{d}\lambda)$. Its first $N + 1$ members can then be computed by the following algorithm: select $\nu > N$ and recur backwards by means of

$$r_\nu^{(\nu)} = 0, \qquad r_{k-1}^{(\nu)} = \frac{\beta_k}{x - \alpha_k - r_k^{(\nu)}}, \qquad k = \nu, \nu - 1, \ldots, 0. \tag{7.19}$$

Then compute

$$m_{-1}^{(\nu)} = -1, \qquad m_k^{(\nu)} = r_{k-1}^{(\nu)} m_{k-1}^{(\nu)}, \qquad k = 0, 1, \ldots, N. \tag{7.20}$$

The algorithm converges in the sense that

$$m_k = \lim_{\nu \to \infty} m_k^{(\nu)}. \tag{7.21}$$

Thus, applying (7.19) and (7.20) for ν sufficiently large, we can compute m_k to any desired accuracy.

A similar algorithm works for division by a quadratic divisor, say

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{(t - x)^2 + y^2}, \qquad x \in \mathbb{R}, \qquad y > 0, \tag{7.22}$$

if one notes that

$$\frac{1}{(t - x)^2 + y^2} = \frac{1}{2\,\mathrm{i}y}\left(\frac{1}{t - z} - \frac{1}{t - \bar{z}}\right), \qquad z = x + \mathrm{i}y,$$

hence

$$m_k = \int_{\mathbb{R}} \pi_k(t; \mathrm{d}\lambda) \frac{\mathrm{d}\lambda(t)}{(t - x)^2 + y^2} = \frac{\operatorname{Im} f_k(z)}{\operatorname{Im} z}, \tag{7.23}$$

where

$$f_k(z) = \int_{\mathbb{R}} \pi_k(t; \mathrm{d}\lambda) \frac{\mathrm{d}\lambda(t)}{t - z}. \tag{7.24}$$

This again is a minimal solution of (7.18), where x is to be replaced by z,

and therefore the same algorithm applies as in (7.19)–(7.20) with x replaced by z.

7.4. Application to rational Gauss quadrature

We have seen in Section 3.1 that the construction of rational Gauss-type quadrature rules requires the computation of (ordinary) Gaussian quadrature formulae relative to a measure that involves division by a polynomial. These can be generated by the eigenvalue techniques discussed in Section 4.1, once the recursion coefficients of the required orthogonal polynomials have been obtained. This in turn can be accomplished by methods discussed in Sections 7.2 and 7.3.

We will assume in the rational quadrature rule (3.5) that the divisor polynomial ω_m is positive on the support interval of $d\lambda$.

The problem, therefore, is to generate the first n recursion coefficients $\hat{\alpha}_k = \alpha_k(d\hat{\lambda})$, $\hat{\beta}_k = \beta_k(d\hat{\lambda})$, $k = 0, 1, \ldots, n-1$, for the modified measure

$$d\hat{\lambda}(t) = \frac{d\lambda(t)}{\omega_m(t)}, \tag{7.25}$$

assuming the coefficients known for $d\lambda$. Here, ω_m is a polynomial of degree m,

$$\omega_m(t) = \prod_{\mu=1}^{M} (1 + \zeta_\mu t)^{s_\mu}, \qquad \sum_{\mu=1}^{M} s_\mu = m, \tag{7.26}$$

with ζ_μ distinct real or complex numbers such that ω_m is positive on the support interval of $d\lambda$.

A possible solution of the problem is based on the following observation. Suppose $d\Lambda_N$ is a discrete N-point measure, say

$$\int_{\mathbb{R}} p(t)\, d\Lambda_N(t) = \sum_{k=1}^{N} W_k p(T_k), \tag{7.27}$$

with coefficients W_k not necessarily all positive, and suppose further that it provides a quadrature formula for the measure $d\hat{\lambda}$ having degree of exactness $2n-1$, that is,

$$\int_{\mathbb{R}} p(t)\, d\hat{\lambda}(t) = \sum_{k=1}^{N} W_k p(T_k), \qquad \text{all } p \in \mathbb{P}_{2n-1}, \qquad d\hat{\lambda} = \frac{d\lambda}{\omega_m}. \tag{7.28}$$

Then the first n recursion coefficients for $d\hat{\lambda}$ are identical with those for $d\Lambda_N$:

$$\begin{aligned} \alpha_k(d\hat{\lambda}) &= \alpha_k(d\Lambda_N), \\ \beta_k(d\hat{\lambda}) &= \beta_k(d\Lambda_N), \end{aligned} \qquad k = 0, 1, \ldots, n-1. \tag{7.29}$$

This follows immediately from the inner product representation (0.12) of the

coefficients on the left of (7.29), since all inner products are integrals (with respect to $\mathrm{d}\hat{\lambda}$) over polynomials of degree $\leq 2n-1$ and are thus integrated exactly by the formula (7.28). To generate the coefficients on the right of (7.29), we can now apply either the Stieltjes procedure of Section 6.3 or the Lanczos method (of Section 6.2); for the latter, see the remark at the end of Section 6.2.

It remains to show how a formula of the type (7.28) can be constructed. We first look at the simplest case where the polynomial ω_m in (7.26) has all $s_\mu = 1$ (hence $M = m$) and $\zeta_\mu = \xi_\mu$ are all real. Expanding its reciprocal into partial fractions,

$$\frac{1}{\omega_m(t)} = \frac{1}{\prod_{\nu=1}^m (1+\xi_\nu t)} = \sum_{\nu=1}^m \frac{c_\nu}{t+(1/\xi_\nu)} ,$$

where

$$c_\nu = \frac{\xi_\nu^{m-2}}{\prod_{\substack{\mu=1 \\ \mu\neq\nu}}^m (\xi_\nu - \xi_\mu)} , \qquad \nu = 1,2,\ldots,m,$$

we then have

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\hat{\lambda}(t) = \sum_{\nu=1}^m \int_{\mathbb{R}} p(t)\,\frac{c_\nu\,\mathrm{d}\lambda(t)}{t+(1/\xi_\nu)} . \tag{7.30}$$

Each integral on the right now involves modification of the measure $\mathrm{d}\lambda$ by a linear divisor. The first n recursion coefficients of the modified measure can therefore be obtained by the procedure of Section 7.3 (using the modified Chebyshev algorithm), which then enables us to compute the respective n-point Gauss formula

$$\int_{\mathbb{R}} p(t)\,\frac{c_\nu\,\mathrm{d}\lambda(t)}{t+(1/\xi_\nu)} = \sum_{r=1}^n w_r^{(\nu)} p(t_r^{(\nu)}), \qquad p \in \mathbb{P}_{2n-1}, \tag{7.31}$$

by the techniques of Section 4.1. Inserting (7.31) in (7.30) then yields

$$\int_{\mathbb{R}} p(t)\,\mathrm{d}\hat{\lambda} = \sum_{\nu=1}^m \sum_{r=1}^n w_r^{(\nu)} p(t_r^{(\nu)}), \qquad p \in \mathbb{P}_{2n-1},$$

the desired quadrature formula (7.28), with $N = mn$ and

$$\begin{aligned} T_{(\nu-1)n+r} &= t_r^{(\nu)}, \\ W_{(\nu-1)n+r} &= w_r^{(\nu)}, \end{aligned} \qquad \nu = 1,2,\ldots,m; \qquad r = 1,2,\ldots,n. \tag{7.32}$$

Analogous procedures apply to other polynomials ω_m, for example to those for which the ζ_μ occur in $m/2$ pairs of conjugate complex numbers: $\zeta_\nu = \xi_\nu + \mathrm{i}\eta_\nu$, $\zeta_{\nu+m/2} = \bar{\zeta}_\nu$, $\nu = 1,2,\ldots,m/2$, where $\xi_\nu \in \mathbb{R}$, $\eta_\nu > 0$, and m is even.

An elementary computation then yields the partial fraction decomposition

$$\frac{1}{\omega_m(t)} = \sum_{\nu=1}^{m/2} \frac{c_\nu + d_\nu t}{\left(t + \frac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2 + \left(\frac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2}, \qquad t \in \mathbb{R}, \tag{7.33}$$

where

$$c_\nu = \frac{1}{\eta_\nu}\left(\frac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\operatorname{Im} p_\nu + \frac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\operatorname{Re} p_\nu\right),$$
$$d_\nu = \frac{1}{\eta_\nu}\operatorname{Im} p_\nu$$

and

$$p_\nu = \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} \frac{(\xi_\nu + i\eta_\nu)^2}{(\xi_\nu - \xi_\mu)^2 - (\eta_\nu^2 - \eta_\mu^2) + 2i\eta_\nu(\xi_\nu - \xi_\mu)},$$

with $p_1 = 1$ if $m = 2$. One can proceed as before, except that the modification of the measure $d\lambda$ now involves a quadratic divisor (see (7.33)) and, if $d_\nu \neq 0$, in addition a linear factor. Thus, not only the methods of Section 7.3, but also those of Section 7.2 come into play.

The procedures described here, since they rely on the modified Chebyshev algorithm to execute the division algorithm of Section 7.3, work best if the support of $d\lambda$ is a finite interval. For measures with unbounded support, methods based on discretization (see Section 6.1) will be more effective, but possibly also more expensive.

Notes to Section 7

7.1. A good reference for the theory of quasi-definite measures and kernel polynomials is Chihara (1978, Chapter I). Lemma 1 and Theorem 7 are from Gautschi (1982b). Kernel polynomials also play an important role in numerical linear algebra in connection with iterative methods for solving linear algebraic systems and eigenvalue problems; for these applications, see Stiefel (1958). The proof of Theorem 7 indeed follows closely an argumentation used in Stiefel (1958), but does not require the assumption of a positive definite measure.

7.2. The algorithm (7.12) for modification by a linear factor is due to Galant (1971); an extension to quadratic factors (7.13) is given in Gautschi (1982b). The procedure (7.14), (7.15) based on QR methodology is due to Kautsky and Golub (1983). See also Buhmann and Iserles (1992) for an alternative proof.

7.3, 7.4. The treatment of linear and quadratic divisors follows Gautschi (1981b), where further details, in particular regarding the recursion algorithm (7.19), (7.20), can be found. For other, algebraic methods and a plausibility argument for the instability noted at the beginning of Section 7.3, see Galant (1992). The application to rational Gauss quadrature is taken from Gautschi (1993b).

8. Orthogonal polynomials of Sobolev type

As already mentioned in Section 2.2, the computation of orthogonal polynomials in the Sobolev space H_s of (2.21), involving the inner product

$$(u, v)_{H_s} = \sum_{\sigma=0}^{s} \int_{\mathbb{R}} u^{(\sigma)}(t) v^{(\sigma)}(t)\, \mathrm{d}\lambda_\sigma(t), \tag{8.1}$$

is complicated by the lack of symmetry of this inner product with respect to multiplication by t (see (2.26)). This means that we can no longer expect a three-term recurrence relation to hold, or even a recurrence relation of constant order. On the other hand, it is certainly true, as for any sequence of monic polynomials whose degrees increase by 1 from one member to the next, that

$$\pi_{k+1}(t) = t\pi_k(t) - \sum_{j=0}^{k} \beta_j^k \pi_{k-j}(t), \qquad k = 0, 1, 2, \dots, \tag{8.2}$$

for suitable coefficients β_j^k. We may thus pose the problem of computing $\{\beta_j^k\}_{0 \le j \le k}$ for $k = 0, 1, \dots, n-1$, which will allow us to generate the first $n+1$ polynomials $\pi_0, \pi_1, \dots, \pi_n$ by (8.2). Moreover, the zeros of π_n are computable as eigenvalues of the $n \times n$ Hessenberg matrix

$$B_n = \begin{bmatrix} \beta_0^0 & \beta_1^1 & \beta_2^2 & \cdots & \beta_{n-2}^{n-2} & \beta_{n-1}^{n-1} \\ 1 & \beta_0^1 & \beta_1^2 & \cdots & \beta_{n-3}^{n-2} & \beta_{n-2}^{n-1} \\ 0 & 1 & \beta_0^2 & \cdots & \beta_{n-4}^{n-2} & \beta_{n-3}^{n-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \beta_0^{n-2} & \beta_1^{n-1} \\ 0 & 0 & 0 & \cdots & 1 & \beta_0^{n-1} \end{bmatrix}. \tag{8.3}$$

In Section 8.1 we briefly describe how moment information can be used to develop a 'modified Chebyshev algorithm' for Sobolev orthogonal polynomials, and in Section 8.2 show how Stieltjes's idea can be adapted for the same purpose. Special inner products (8.1) of Sobolev type sometimes lead to simpler recurrence relations. An instance of this is described in Section 8.3.

8.1. Algorithm based on moment information

In analogy to (5.5), we define modified moments for all $s+1$ measures $\mathrm{d}\lambda_\sigma$, but for simplicity use the same system of polynomials $\{p_k\}$ for each,

$$m_k^{(\sigma)} = \int_{\mathbb{R}} p_k(t)\, \mathrm{d}\lambda_\sigma(t), \qquad k = 0, 1, 2, \dots; \qquad \sigma = 0, 1, \dots, s. \tag{8.4}$$

As in Section 5.2, we assume these polynomials to satisfy a three-term recurrence relation

$$\begin{aligned} &p_{-1}(t) = 0, \qquad p_0(t) = 1, \\ &p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \end{aligned} \tag{8.5}$$

where the coefficients a_k, b_k are given real numbers. The objective is, for given $n \geq 1$, to compute the coefficients $\{\beta_j^k\}_{0 \leq j \leq k}$ in (8.2) for $k = 0, 1, \ldots, n-1$, using the recursion coefficients a_j, b_j, $0 \leq j \leq 2n-2$ in (8.5) and the modified moments $m_j^{(0)}$, $0 \leq j \leq 2n-1$, and $m_j^{(\sigma)}$, $0 \leq j \leq 2n-2$ (if $n \geq 2$), $\sigma = 1, 2, \ldots, s$.

It is possible to accomplish this task with the help of an algorithm that resembles the modified Chebyshev algorithm of Section 5.2. Like the latter, it uses 'mixed moments' $\sigma_{k,\ell} = (\pi_k, \pi_\ell)_{H_s}$, but now relative to the Sobolev inner product in H_s. These, in turn, require for their computation 'mixed derivative moments' $\mu_{k,\ell,\sigma}^{(i,j)} = (\pi_k^{(i)}, p_\ell^{(j)})_{\mathrm{d}\lambda_\sigma}$, $\sigma = 1, \ldots, s$; $i, j \leq \sigma$, relative to the individual inner products $(u, v)_{\mathrm{d}\lambda_\sigma} = \int_{\mathbb{R}} u(t)v(t)\,\mathrm{d}\lambda_\sigma(t)$, $\sigma \geq 1$. Accordingly, there will be a tableau containing the mixed moments $\sigma_{k,\ell}$, very much like the tableau in Fig. 3, and for each i, j and σ another auxiliary tableau containing the mixed derivative moments, which has a similar trapezoidal shape, but with height $n-2$ instead of $n-1$. Each quantity in these tableaux is computed recursively in terms of the three nearest quantities on the next lower level, and in terms of all quantities vertically below. The initialization of these tableaux calls for the modified moments (8.4), since $\sigma_{0,\ell} = m_\ell^{(0)}$ and $\mu_{0,\ell,\sigma}^{(0,0)} = m_\ell^{(\sigma)}$, $\sigma \geq 1$, but the complete initialization of all the quantities $\mu_{0,\ell,\sigma}^{(i,j)}$ is a rather involved process. Once the tableau for the $\sigma_{k,\ell}$ has been completed, one obtains first

$$\beta_0^0 = \frac{\sigma_{0,1}}{\sigma_{0,0}} + a_0,$$

and then, successively, for $k = 1, 2, \ldots, n-1$,

$$\begin{aligned} \beta_0^k &= \tfrac{\sigma_{k,k+1}}{\sigma_{k,k}} + a_k - \tfrac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \\ \beta_{k-j}^k &= \tfrac{\sigma_{j,k+1}}{\sigma_{j,j}} + a_k \tfrac{\sigma_{j,k}}{\sigma_{j,j}} + b_k \tfrac{\sigma_{j,k-1}}{\sigma_{j,j}} - \tfrac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1} \beta_{\ell-j}^\ell \tfrac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}, \\ &\qquad j = k-1, k-2, \ldots, 1 \text{ (if } k \geq 2), \\ \beta_k^k &= \tfrac{\sigma_{0,k+1}}{\sigma_{0,0}} + a_k \tfrac{\sigma_{0,k}}{\sigma_{0,0}} + b_k \tfrac{\sigma_{0,k-1}}{\sigma_{0,0}} - \sum_{\ell=0}^{k-1} \beta_\ell^\ell \tfrac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}, \end{aligned}$$

where a_k , b_k are the coefficients in (8.5).

The algorithm is considerably more complicated than the modified Chebyshev algorithm of Section 5.2 – its complexity, indeed, is $\mathcal{O}(n^3)$ rather than $\mathcal{O}(n^2)$ – but this seems to reflect an inherently higher level of difficulty.

8.2. Stieltjes-type algorithm

The procedure sketched in Section 8.1 employs only *rational* operations on the data, which is one of the reasons why the resulting algorithm is so complicated. Allowing also *algebraic* operations (that is, solving algebraic equations) permits a simpler and more transparent (though not necessarily more efficient) approach. Basically, one expresses $-\beta_j^k$ in (8.2) as the Fourier–Sobolev coefficients of $\pi_{k+1} - t\pi_k(t)$, that is,

$$\beta_j^k = \frac{(t\pi_k, \pi_{k-j})_{H_s}}{\| \pi_{k-j} \|_{H_s}^2}, \qquad j = 0, 1, \ldots, k, \tag{8.6}$$

and evaluates the inner products in both numerator and denominator by numerical integration. If $k \leq n-1$, then all inner products involve polynomials of degree less than $2n$, and hence can be computed exactly by n-point Gaussian quadrature rules relative to the measures $\mathrm{d}\lambda_\sigma$. It is in the generation of these Gaussian rules where algebraic processes are required. The polynomials intervening in (8.6), and their derivatives, are computed recursively by (8.2) and its differentiated version, employing the coefficients β_j^k already computed. Thus, initially, (see (0.12))

$$\beta_0^0 = \frac{(t,1)_{\mathrm{d}\lambda_0}}{(1,1)_{\mathrm{d}\lambda_0}} = \alpha_0(\mathrm{d}\lambda_0),$$

which allows us to obtain π_1 by (8.2). In turn, this allows us to compute $\{\beta_j^1\}_{0\leq j\leq 1}$ by (8.6), and hence, via (8.2), to obtain π_2. Continuing in this manner yields the following 'bootstrapping' procedure:

$$\beta_0^0 \overset{(8.2)}{\mapsto} \pi_1 \overset{(8.6)}{\mapsto} \{\beta_j^1\}_{0\leq j\leq 1} \overset{(8.2)}{\mapsto} \pi_2 \overset{(8.6)}{\mapsto} \cdots \overset{(8.6)}{\mapsto} \{\beta_j^{n-1}\}_{0\leq j\leq n-1} \overset{(8.2)}{\mapsto} \pi_n.$$

8.3. Special inner products

While symmetry with respect to multiplication by t in general does not hold for the inner product (8.1), a more general symmetry property may hold, namely

$$(hu, v)_{H_s} = (u, hv)_{H_s}, \tag{8.7}$$

where h is a polynomial of degree ≥ 1. This, however, implies, as is shown in Evans, Littlejohn, Marcellán, Markett and Ronveaux (1995), that all measures $\mathrm{d}\lambda_\sigma$, $\sigma \geq 1$, must be of Dirac type. On the other hand, there then exists a $(2m+1)$-term recurrence relation of the form

$$h(t)\pi_k(t; H_s) = \sum_{j=k-m}^{k+m} \omega_{kj}\pi_j(t; H_s), \tag{8.8}$$

where m is the smallest degree among polynomials h satisfying (8.7) and h in (8.8) is a polynomial of that minimum degree.

If, for example,

$$(u,v)_{H_s} = \int_{\mathbb{R}} u(t)v(t)\,\mathrm{d}\lambda(t) + u^{(s)}(c)v^{(s)}(c), \tag{8.9}$$

where $\mathrm{d}\lambda$ is a positive measure, s an integer ≥ 1, and $c \in \mathbb{R}$, then clearly

$$h(t) = (t-c)^{s+1} \tag{8.10}$$

satisfies (8.7) and is a polynomial of minimum degree $m = s+1$ in (8.8). In this case,

$$\pi_k(\cdot; H_s) = \pi_k(\cdot; \mathrm{d}\lambda), \qquad k = 0, 1, \ldots, s, \tag{8.11}$$

as follows easily from (8.9). Moreover, there is an alternative expansion of the polynomial on the left of (8.8), namely

$$h(t)\pi_k(t; H_s) = \sum_{j=k-m}^{k+m} \theta_{kj}\pi_j(t; \mathrm{d}\lambda), \tag{8.12}$$

where h is as in (8.10) and $m = s+1$. The coefficients in (8.8), as well as those in (8.12), can be computed with some effort, but the resulting procedure appears to be quite robust.

The two expansions above, together with (8.11), suggest the following two methods for computing the Sobolev-type orthogonal polynomials belonging to the inner product (8.9). In Method I, one computes π_{k+s+1} by solving (8.8) for π_{k+s+1}, noting that $\omega_{k,k+s+1} = 1$ (since the π_k are monic). Thus,

$$\pi_{k+s+1}(t; H_s) = (t-c)^{s+1}\pi_k(t; H_s) - \sum_{j=k-s-1}^{k+s} \omega_{kj}\pi_j(t; H_s), \qquad k = 0, 1, 2, \ldots, \tag{8.13}$$

where (8.11) is used on the right, when appropriate, and where $\omega_{kj} = 0$ if $j < 0$. In Method II, one computes π_k directly from (8.12),

$$\pi_k(t; H_s) = \frac{1}{(t-c)^{s+1}} \sum_{j=k-s-1}^{k+s+1} \theta_{kj}\pi_j(t; \mathrm{d}\lambda), \tag{8.14}$$

where again $\theta_{kj} = 0$ if $j < 0$, and this time the polynomials $\pi_j(\cdot; \mathrm{d}\lambda)$ on the right are generated by the basic three-term recurrence relation. Method I, curiously enough, may develop huge errors at a certain distance from c, either on one, or both, sides of c. Apparently, there is consistent cancellation at work, but the inherent reasons for this are not known. Some caution in the use of Method I is therefore indicated. Method II is more reliable, except in the immediate neighbourhood of $t = c$ (where it is safe to use Method I).

Notes to Section 8

8.1. A more detailed description and derivation of the moment-based procedure for generating Sobolev orthogonal polynomials can be found in Gautschi and Zhang (1995, Section 2). Section 3 of the same reference reports on numerical experience with this procedure and on attempts to locate the zeros of various orthogonal polynomials of Sobolev type. A sensitivity analysis with respect to small perturbations in the moments (8.4), where $s = 1$, is given in Zhang (1994).

8.2. For measures $d\lambda_\sigma$ in (8.1) that consist of an absolutely continuous measure with a discrete measure superimposed on it, the Stieltjes procedure is described more fully, for the case $s = 1$, and sketched for the general case $s \geq 1$, in Gautschi and Zhang (1995, Section 4).

8.3. Complete algorithmic details for, as well as experience with, the procedure of generating (by Methods I and II) the Sobolev-type orthogonal polynomials associated with the special inner product (8.9) are given in Gautschi (1996a). Much of this work is based on algebraic groundwork laid in Marcellán and Ronveaux (1990).

9. Software

A software package, called ORTHPOL, has been written, that implements all the procedures discussed above and a few others; see Gautschi (1994). Here is a brief description of the principal components of the package.

`recur`	generates the recursion coefficients for the classical orthogonal polynomials (of Legendre, Chebyshev, Jacobi, Laguerre and Hermite)
`cheb`	implements the modified Chebyshev algorithm (see Section 5.2)
`sti`	implements the Stieltjes procedure for discrete measures (see Section 6.3)
`lancz`	implements Lanczos's algorithm for discrete measures (see Section 6.2)
`mcdis`	implements the discretization procedure sketched in Section 6.1
`mccheb`	implements a version of the modified Chebyshev algorithm (not described in this article) that uses approximate values of the modified moments obtained by a discretization process similar to the one used in Section 6.1
`chri`	implements the nonlinear modification algorithms of Section 7, as well as modification by a QR step (see Section 7.2)
`gchri`	implements the modified moment procedure for linear and quadratic divisors (see Section 7.3)
`gauss`	generates Gauss quadrature formulae via eigenvalues and eigenvectors of the Jacobi matrix (see Section 4.1)
`radau`	generates Gauss–Radau formulae (see Section 4.2)
`lob`	generates Gauss–Lobatto formulae (see Section 4.3)

Numerical experience reported in this article and elsewhere is based on the use of one or a combination of these routines. Routines for rational Gauss quadrature rules and Sobolev orthogonal polynomials have also been written, but are not yet ready for publication.

Notes to Section 9

Historically, the first major effort of computing Gauss quadrature rules on electronic computers was made in the mid- and late 1950s. Davis and Rabinowitz (1956) computed Gauss–Legendre rules with up to 48 points to an accuracy of 20–21 decimal digits, and went up to 96-point rules in Davis and Rabinowitz (1958). Gauss–Laguerre rules were computed by Rabinowitz and Weiss (1959), and Gauss–Lobatto rules by Rabinowitz (1960). For a summary, as of 1981, of the major tables of Gaussian rules and computer programs for generating them, see Gautschi (1981a, Section 5.4). More recent software that includes also Gauss–Kronrod rules and other

quadrature methods can be found in Piessens, de Doncker-Kapenga, Überhuber and Kahaner (1983); see also NAG (1991).

The software package in Gautschi (1994) is the first that includes routines for generating Gauss-type formulae and orthogonal polynomials not only for classical but also for essentially arbitrary measures. The package is public domain, and can be received via e-mail by sending the following message to netlib@netlib.org:

send 726 from toms

Alternatively, one can access the package via a WWW browser, using the following URL:

http://www.netlib.org/toms/726

The routines `recur` and `gauss` were instrumental in computations assisting de Branges in his famous proof of the Bieberbach conjecture (Gautschi 1986*b*).

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16.8. [151] "On the computation of special Sobolev-type orthogonal polynomials"

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On the computation of special Sobolev-type orthogonal polynomials*

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Dedicated, in friendship, to Ted Rivlin on his 70th birthday

The concern here is with polynomials, considered previously by Marcellán and Ronveaux and others, which are orthogonal with respect to an ordinary inner product on the real line involving a positive measure, superimposed by a one-point (atomic) inner product involving a derivative of fixed order. The support point of the atomic component of the inner product can be located anywhere on the real axis. Two recursive schemes are developed which, in combination, allow one to compute these orthogonal polynomials, assuming that those relative to the nonatomic component of the inner product are available. The methods are illustrated in the case of Hermite, Laguerre and Legendre measures and are used to explore numerically the zeros of the respective Sobolev-type orthogonal polynomials.

Keywords: Orthogonal polynomials of Sobolev type, recurrence relations, computational algorithm, zeros.

Subject classification: 33C45, 65D20.

1. Introduction

There is a growing literature on orthogonal polynomials of Sobolev type, i.e., polynomials orthogonal with respect to an inner product involving derivative values in addition to function values. A large part of this work is concerned with analytic and algebraic properties of these polynomials. Computational aspects have been systematically discussed only recently in [7], where the inner product considered is a bilinear functional involving derivatives up to order $s \geq 1$ with arbitrary positive measures associated with each. Here we discuss a rather special inner product, already considered in [9], that involves functions with an arbitrary positive measure, and a derivative of fixed order with a one-point atomic measure. We combine algebraic properties known from [9] with algorithmic ideas to arrive at computational methods that can be used to generate the resulting orthogonal polynomials numerically. Ordinary orthogonal polynomials that will be needed in this context are assumed to be computable by methods previously discussed (see, e.g.,

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[4–6]). We also comment on computational experience with our algorithms, and use them to explore the zeros of the respective polynomials.

To keep the paper self-contained, some of the fomulae needed from [9] will be rederived from first principles.

2. Statement of the problem

Given a positive measure $d\lambda$ on $\mathbb{R}$ having finite moments of all orders and being supported on a set of infinitely many points, we define the inner products

$$(f,g) = \int_{\mathbb{R}} f(x)g(x)d\lambda(x), \tag{2.1}$$

$$[f,g] = (f,g) + f^{(r)}(c)g^{(r)}(c), \qquad r \geq 1, \qquad c \in \mathbb{R}. \tag{2.2}$$

Throughout the paper, f and g are always real polynomials. Since both inner products are positive definite, there exist orthogonal polynomials with respect to each. Those orthogonal with respect to (2.1) are denoted by p_k, the others (orthogonal with respect to (2.2)) by q_k. Both are assumed monic for each $k \geq 0$.

We have set the coefficient of the derivative term in (2.2) arbitrarily equal to 1. If it were different, say ω^{-1} for some $\omega > 0$, then the resulting orthogonal polynomials q_k could be obtained from ours simply by changing $d\lambda$ to $\omega d\lambda$, which in the procedures below implies only one single change, namely replacing β_0 (in (2.8)) by $\omega\beta_0$. Therefore, we may as well take $\omega = 1$.

A fundamental property of the inner products (2.1), (2.2), which will be used repeatedly, is the fact that the factor $c_r(\cdot) = (\cdot - c)^{r+1}$ can be transferred from one term of the inner product to the other without affecting the value of the inner product (see also [3] for a deeper reason for this):

$$[c_r f, g] = [f, c_r g] = (f, c_r g) = (c_r f, g), \qquad c_r(\cdot) = (\cdot - c)^{r+1}. \tag{2.3}$$

This has two immediate consequences: If $(x-c)^{r+1}q_k(x)$ is expanded in the q-polynomials, then except for normalization, the expansion coefficients are $[(\cdot - c)^{r+1}q_k, q_j] = [q_k, (\cdot - c)^{r+1}q_j]$, which vanishes if $j + r + 1 < k$. Thus,

$$(x-c)^{r+1}q_k(x) = \sum_{j=k-r-1}^{k+r+1} \omega_{kj} q_j(x), \qquad \omega_{kj} = \frac{[(\cdot - c)^{r+1}q_k, q_j]}{|||q_j|||^2}, \tag{2.4}$$

where $|||q_j|||^2 = [q_j, q_j]$. Note that $\omega_{k,k+r+1} = 1$, since the q's are monic. In the summation of (2.4) and in similar summations below, it is always understood that coefficients with negative second index are zero – in this case, $\omega_{kj} = 0$ if $j < 0$.

Likewise, in the expansion of the left-hand side of (2.4) in the polynomials p_j, we have $((\cdot - c)^{r+1}q_k, p_j) = [q_k, (\cdot - c)^{r+1}p_j] = 0$ if $j + r + 1 < k$, and thus

$$(x-c)^{r+1}q_k(x) = \sum_{j=k-r-1}^{k+r+1} \theta_{kj} p_j(x), \qquad \theta_{kj} = \frac{((\cdot - c)^{r+1}q_k, p_j)}{\|p_j\|^2}, \tag{2.5}$$

where $\|p_j\|^2 = (p_j, p_j)$. Here also, $\theta_{k,k+r+1} = 1$.

Both (2.4) and (2.5), once the coefficients are known, lend themselves for the calculation of q_k. Note, first of all, that

$$q_k = p_k, \qquad k = 0, 1, \ldots, r, \tag{2.6}$$

which can be computed recursively by (2.8) below. With these as starting values, (2.4) can then be used to compute $q_{r+1}, q_{r+2}, \ldots$ by

$$q_{k+r+1}(x) = (x-c)^{r+1} q_k(x) - \sum_{j=k-r-1}^{k+r} \omega_{kj} q_j(x), \qquad k = 0, 1, 2, \ldots. \tag{2.7}$$

In (2.5), on the other hand, one computes the p_j on the right recursively by the well-known three-term recurrence relation

$$\begin{aligned} p_{s+1}(x) &= (x-\alpha_s)p_s(x) - \beta_s p_{s-1}(x), \qquad s = 0, 1, 2, \ldots, \\ p_0(x) &= 1, \qquad p_{-1}(x) = 0, \end{aligned} \tag{2.8}$$

where the coefficients $\alpha_s = \alpha_s(d\lambda)$, $\beta_s = \beta_s(d\lambda)$ are uniquely determined by $d\lambda$ and by convention $\beta_0 = \int_{\mathbb{R}} d\lambda(x)$. If $k \le r$, one conveniently uses (2.6); otherwise, the summation in (2.5) is completed and the result divided by $(x-c)^{r+1}$. We call the first method (based on (2.4)) *Method I*, and the second (based on (2.5)) *Method II*.

The matrices $\Omega = [\omega_{kj}]$, $\Theta = [\theta_{kj}]$ of the coefficients in (2.4) and (2.5) are banded matrices. By defining

$$\bar{\omega}_{kj} = \omega_{k,k+j}, \qquad \bar{\theta}_{kj} = \theta_{k,k+j}, \qquad -r-1 \le j \le r+1, \tag{2.9}$$

we can store these coefficients in rectangular matrices

$$\overline{\Omega} = [\bar{\omega}_{kj}] \in \mathbb{R}^{n\times(2r+3)}, \qquad \overline{\Theta} = [\bar{\theta}_{kj}] \in \mathbb{R}^{n\times(2r+3)}, \tag{2.10}$$

assuming that the index k runs from 0 to $n-1$. This allows us to compute q_0, $q_1, \ldots, q_{n+r}$ by Method I, and $q_0, q_1, \ldots, q_{n-1}$ by Method II.

We can now state the problem we wish to consider.

Problem

Given $r \ge 1$, $c \in \mathbb{R}$, $n \ge 1$, and given the coefficients $\alpha_s = \alpha_s(d\lambda)$, $\beta_s = \beta_s(d\lambda)$, $s = 0, 1, \ldots, n+2r+1$, in (2.8), compute the matrices $\overline{\Omega}$, $\overline{\Theta}$ of (2.10).

It turns out that the computation of Ω (resp. $\overline{\Omega}$) requires the matrix Θ (resp. $\overline{\Theta}$), so that both matrices will be available and we are free to use either of the two methods above to compute the desired polynomials.

3. Computational algorithm

3.1. *Computation of the* ω_{kj}

From (2.4), using (2.3) and (2.5), we have

$$|||q_j|||^2 \omega_{kj} = [(\cdot - c)^{r+1} q_k, q_j] = ((\cdot - c)^{r+1} q_k, q_j)$$

$$= \left(\sum_{\ell=k-r-1}^{k+r+1} \theta_{k\ell} p_\ell, q_j \right) = \sum_{\ell=k-r-1}^{k+r+1} \theta_{k\ell}(p_\ell, q_j).$$

We now expand q_j in the polynomials p_ℓ,

$$q_j(x) = \sum_{\ell=0}^{j} \beta_{j\ell} p_\ell(x), \qquad \beta_{jj} = 1, \tag{3.1}$$

and use orthogonality of the p's to obtain

$$\begin{aligned} |||q_j|||^2 \omega_{kj} &= \sum_{\ell=k-r-1}^{k+r+1} \theta_{k\ell} \sum_{m=0}^{j} \beta_{jm}(p_\ell, p_m) \\ &= \sum_{\ell=k-r-1}^{k+r+1} \theta_{k\ell}\beta_{j\ell}||p_\ell||^2 \\ &= \sum_{\ell=k-r-1}^{j} \theta_{k\ell}\beta_{j\ell}||p_\ell||^2, \qquad k-r-1 \le j \le k+r+1, \end{aligned}$$

since $\beta_{j\ell} = 0$ if $\ell > j$. Thus, separating out the term with $\ell = j$ gives

$$\omega_{kj} = \theta_{kj} \frac{||p_j||^2}{|||q_j|||^2} + \sum_{\ell=k-r-1}^{j-1} \theta_{k\ell}\beta_{j\ell} \frac{||p_\ell||^2}{|||q_j|||^2}, \qquad k-r-1 \le j \le k+r+1. \tag{3.2}$$

To compute the β's, note from (3.1) that

$$\beta_{j\ell}||p_\ell||^2 = (q_j, p_\ell) = [q_j, p_\ell] - q_j^{(r)}(c)p_\ell^{(r)}(c),$$

hence, for $\ell < j$, by orthogonality of the q's,

$$\beta_{j\ell}||p_\ell||^2 = -q_j^{(r)}(c)p_\ell^{(r)}(c), \qquad \ell < j. \tag{3.3}$$

We need to compute $q_j^{(r)}(c)$. By (3.1), (3.3) we have

$$q_j(x) = p_j(x) - q_j^{(r)}(c) \sum_{\ell=0}^{j-1} \frac{p_\ell^{(r)}(c)}{||p_\ell||^2} p_\ell(x),$$

which, differentiated r times and evaluated at $x = c$, gives

$$q_j^{(r)}(c) = p_j^{(r)}(c) - q_j^{(r)}(c) \sum_{\ell=0}^{j-1} \frac{[p_\ell^{(r)}(c)]^2}{||p_\ell||^2}. \tag{3.4}$$

Define

$$\lambda_{-1} = \lambda_0 = 1, \qquad \lambda_h = 1 + \sum_{\ell=0}^{h} \frac{[p_\ell^{(r)}(c)]^2}{||p_\ell||^2}, \qquad h = 1, 2, 3, \ldots. \tag{3.5}$$

(Note that $\lambda_h = 1$ for $h < r$.) Then, by (3.4),

$$q_j^{(r)}(c) = p_j^{(r)}(c) - q_j^{(r)}(c)(\lambda_{j-1} - 1),$$

that is,

$$q_j^{(r)}(c) = \frac{p_j^{(r)}(c)}{\lambda_{j-1}}, \qquad j = 0, 1, 2, \ldots. \tag{3.6}$$

Thus, from (3.3),

$$\beta_{j\ell} = -\frac{p_j^{(r)}(c)p_\ell^{(r)}(c)}{\lambda_{j-1}\|p_\ell\|^2}, \qquad \ell < j; \qquad \beta_{jj} = 1. \tag{3.7}$$

Next we compute the norm of q_j in (3.2). Since q_j and p_j are both monic, we have $[q_j, q_j] = [q_j, p_j]$, hence, by the definition of the inner product, and (3.6),

$$|||q_j|||^2 = (q_j, p_j) + q_j^{(r)}(c)p_j^{(r)}(c) = (p_j, p_j) + \frac{[p_j^{(r)}(c)]^2}{\lambda_{j-1}}.$$

Since, by (3.5),

$$\lambda_j = \lambda_{j-1} + \frac{[p_j^{(r)}(c)]^2}{\|p_j\|^2},$$

we can write

$$|||q_j|||^2 = \|p_j\|^2 + \frac{\lambda_j - \lambda_{j-1}}{\lambda_{j-1}}\|p_j\|^2,$$

which gives

$$|||q_j|||^2 = \frac{\lambda_j}{\lambda_{j-1}}\|p_j\|^2. \tag{3.8}$$

Substituting (3.7) and (3.8) in (3.2) now yields

$$\omega_{kj} = \frac{\lambda_{j-1}}{\lambda_j}\theta_{kj} - \frac{p_j^{(r)}(c)}{\lambda_j\|p_j\|^2}\sum_{\ell=k-r-1}^{j-1}\theta_{k\ell}p_\ell^{(r)}(c), \qquad k-r-1 \le j \le k+r+1. \tag{3.9}$$

Up to this point, the algebraic development followed the one in [9]. It remains to compute the $\theta_{k\ell}$.

3.2. *Computation of the* θ_{kj}

From (2.5), using (3.1), we have

$$\begin{aligned}\theta_{kj}\|p_j\|^2 &= ((\cdot - c)^{r+1}q_k, p_j) \\ &= \left((\cdot - c)^{r+1}\sum_{\ell=0}^{k}\beta_{k\ell}p_\ell, p_j\right) = \sum_{\ell=0}^{k}\beta_{k\ell}((\cdot - c)^{r+1}p_\ell, p_j) \\ &= \sum_{\ell=0}^{k}\beta_{k\ell}\gamma_{\ell j}^{(r+1)}, \qquad k-r-1 \le j \le k+r+1,\end{aligned} \tag{3.10}$$

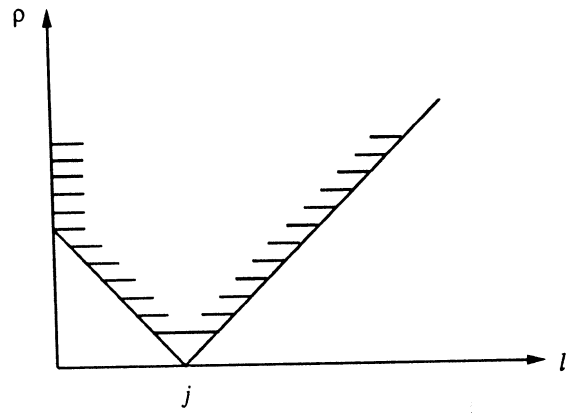

Figure 1. Region in which $\gamma_{\ell j}^{(\rho)}$ is nonzero.

where we define

$$\gamma_{\ell j}^{(\rho)} := \int_{\mathbb{R}} (x-c)^{\rho} p_\ell(x) p_j(x) d\lambda(x), \qquad \rho = 0, 1, \ldots, r+1. \tag{3.11}$$

We note that

$$\begin{aligned} \gamma_{\ell j}^{(\rho)} &= \|p_j\|^2 \qquad \text{if } \rho + \ell = j, \\ \gamma_{\ell j}^{(\rho)} &= \|p_\ell\|^2 \qquad \text{if } \rho + j = \ell, \\ \gamma_{\ell j}^{(\rho)} &= 0 \qquad \text{if } \rho + \ell < j \text{ or } \rho + j < \ell. \end{aligned} \tag{3.12}$$

Thus, for fixed $j \geq 0$, in the (ℓ, ρ)-plane, the γ's are nonzero only in the shaded region of figure 1. On the left slanted boundary, the γ's are constant equal to $\|p_j\|^2$, and on the right slanted boundary, they are equal to $\|p_\ell\|^2$, $\ell = j, j+1, \ldots$. From these boundary values, all remaining values can be determined recursively as follows:

$$\begin{aligned} \gamma_{\ell j}^{(\rho+1)} &= \int_{\mathbb{R}} (x-c)^{\rho+1} p_\ell(x) p_j(x) d\lambda(x) \\ &= \int_{\mathbb{R}} (x-c) \cdot (x-c)^{\rho} p_\ell(x) p_j(x) d\lambda(x) \\ &= \int_{\mathbb{R}} (x-c)^{\rho} \cdot x p_\ell(x) p_j(x) d\lambda(x) - c \int_{\mathbb{R}} (x-c)^{\rho} p_\ell(x) p_j(x) d\lambda(x) \\ &= \int_{\mathbb{R}} (x-c)^{\rho} \{p_{\ell+1}(x) + \alpha_\ell p_\ell(x) + \beta_\ell p_{\ell-1}(x)\} p_j(x) d\lambda(x) - c\gamma_{\ell j}^{(\rho)}, \end{aligned}$$

that is,

$$\gamma_{\ell j}^{(\rho+1)} = \gamma_{\ell+1, j}^{(\rho)} + (\alpha_\ell - c)\gamma_{\ell j}^{(\rho)} + \beta_\ell \gamma_{\ell-1, j}^{(\rho)}, \qquad \rho = 0, 1, \ldots, r. \tag{3.13}$$

This allows us to generate the desired quantities row by row, starting at the lower tip of the shaded domain in figure 1 and, for the quantities on the vertical boundary

(when $\ell = 0$), using $\gamma_{-1,j}^{(\rho)} = 0$ in (3.13). With the γ's so generated, we get from (3.10)

$$\theta_{kj} = \frac{1}{\|p_j\|^2} \sum_{\ell=0}^{k} \beta_{k\ell} \gamma_{\ell j}^{(r+1)}, \qquad k - r - 1 \le j \le k + r + 1, \tag{3.14}$$

with the β's as in (3.7). By the last relation in (3.12) the terms in (3.14) with $\ell < j - r - 1$ and $\ell > j + r + 1$ (if present) are actually zero.

3.3. *Summary of the computational algorithm*

As previously mentioned, we assume that the coefficients $\alpha_s(d\lambda)$, $\beta_s(d\lambda)$ in the recurrence formula (2.8) for the orthogonal polynomials p_j have already been computed by known techniques. We need them up to $s = n + 2r + 1$ in order to implement (3.13) for all $j \le n + r$. It is convenient, then, to first precompute certain basic quantities that are needed in the formula (3.9) for ω_{kj} and in (3.14) for θ_{kj}. These are:

(i) the rth derivative values $p_0^{(r)}(c), p_1^{(r)}(c), \ldots, p_{n+r}^{(r)}(c)$. These are readily computed by the successively differentiated recurrence relation (2.8) evaluated at $x = c$.

(ii) The squared norms $\|p_0\|^2, \|p_1\|^2, \ldots, \|p_{n+r}\|^2$. They are immediately obtained from

$$\|p_j\|^2 = \beta_0 \beta_1 \cdots \beta_j, \qquad j = 0, 1, \ldots, n + r.$$

(iii) The constants $\lambda_{-1}, \lambda_0, \lambda_1, \ldots, \lambda_{n+r}$. These are straightforwardly computed from the quantities obtained in (i) and (ii).

In terms of these precomputed quantities, one next computes the elements $\bar{\theta}_{kj}$ of the matrix $\overline{\Theta}$ in (2.10), using (3.14), suitably rewritten, and (3.7):

$$\bar{\theta}_{kj} = \frac{1}{\|p_{k+j}\|^2} \left(\gamma_{k,k+j}^{(r+1)} - \frac{p_k^{(r)}(c)}{\lambda_{k-1}} \sum_{\ell=0}^{k-1} \frac{p_\ell^{(r)}(c)}{\|p_\ell\|^2} \gamma_{\ell,k+j}^{(r+1)} \right), \qquad -r - 1 \le j \le r + 1. \tag{3.15}$$

Here, the γ's are generated as described in section 3.2, and there is little point in checking which of these are zero in the summation on the right, since everything (including the zero elements) has been precomputed. Finally, the elements $\bar{\omega}_{kj}$ of the matrix $\overline{\Omega}$ in (2.10) are computed by (3.9), suitably rewritten:

$$\bar{\omega}_{kj} = \frac{\lambda_{k+j-1}}{\lambda_{k+j}} \bar{\theta}_{kj} - \frac{p_{k+j}^{(r)}(c)}{\lambda_{k+j} \|p_{k+j}\|^2} \sum_{\ell=-r-1}^{j-1} \bar{\theta}_{k\ell} p_{k+\ell}^{(r)}(c), \qquad -r - 1 \le j \le r + 1, \tag{3.16}$$

being careful to start the summation with $\ell = -k$ if $k \le r + 1$, and with $\ell = -r - 1$ otherwise, provided $\ell \le j - 1$. As mentioned earlier, the quantities on the left of both (3.15) and (3.16) are zero if $j < 0$.

The desired polynomials can then be computed either by (Method I)

$$q_{k+r+1}(x) = (x - c)^{r+1} q_k(x) - \sum_{j=-r-1}^{r} \bar{\omega}_{kj} q_{k+j}(x), \qquad k = 0, 1, 2, \ldots, n - 1, \tag{3.17}$$

or by (Method II)

$$q_k(x) = (x-c)^{-(r+1)} \sum_{j=-r-1}^{r+1} \bar{\theta}_{kj} p_{k+j}(x), \qquad k = r+1, r+2, \ldots, n-1, \tag{3.18}$$

recalling that $q_k = p_k$ for $0 \le k \le r$.

4. Examples

Before we consider the numerical performance of the algorithms of section 3, we observe, in section 4.1, some elementary symmetry properties of the polynomials q_k when the measure $d\lambda$ in (2.1) and its support are symmetric with respect to the origin. In the remaining subsections, evidence is provided for the numerical robustness of the algorithms for generating the recursion matrices $\overline{\Omega}$ and $\overline{\Theta}$ of (2.10). In addition, the two methods of section 2 for evaluating the polynomials q_k are compared with regard to their accuracy. Here, surprising numerical difficulties are uncovered in the cases of the Hermite and Laguerre measure, as well as for measures supported on a finite interval. Finally, we explore by numerical computation properties of the zeros of the respective polynomials.

All numerical results reported in sections 4.2–4.4 were obtained on a SUN SPARC station IPX in double precision ($\approx 1.1 \times 10^{-16}$); quadruple precision ($\approx .96 \times 10^{-34}$) was used to ascertain the accuracy of the double-precision results.

4.1. *Symmetric measures*

We assume in this subsection that the support of $d\lambda$ – bounded or unbounded – is symmetric with respect to the origin and $d\lambda(-x) = d\lambda(x)$. We denote the orthogonal polynomials q_k belonging to the inner product (2.2) more precisely by $q_k(\cdot) = q_k(\cdot\,; c\,; d\lambda)$ and the inner product (2.2) by $[\cdot,\cdot](c)$. (There is no need to indicate the dependence on r.)

The first symmetry property is

$$q_k(x; -c; d\lambda) = (-1)^k q_k(-x; c; d\lambda) \qquad (d\lambda \text{ symmetric}). \tag{4.1}$$

This is easily shown by defining $\bar{q}_k(x) := (-1)^k q_k(-x; c; d\lambda)$ and observing that, for $k \neq \ell$,

$$\begin{aligned}
[\bar{q}_k, \bar{q}_\ell](-c) &= \int_{\mathbb{R}} (-1)^{k+\ell} q_k(-x; c; d\lambda) q_\ell(-x; c; d\lambda) d\lambda(x) + (-1)^{k+\ell} q_k^{(r)}(c) q_\ell^{(r)}(c) \\
&= (-1)^{k+\ell} \left\{ \int_{\mathbb{R}} q_k(t; c; d\lambda) q_\ell(t; c; d\lambda) d\lambda(t) + q_k^{(r)}(c) q_\ell^{(r)}(c) \right\} \\
&= 0,
\end{aligned}$$

by the orthogonality of the q's. Since the $\bar{q}$'s are monic, the assertion (4.1) then follows by the uniqueness of the orthogonal polynomials.

Table 1
Accuracy of the ω- and θ-coefficients.

c	r	err $\bar{\omega}$	k	j	err $\bar{\theta}$	k	j
0.0	1	.46(−15)	3	−2	.31(−15)	3	−2
	2	.35(−15)	11	−3	.27(−15)	4	−3
	3	.47(−15)	53	−4	.40(−15)	53	−4
	4	.59(−15)	28	−5	.59(−15)	28	−5
1.0	1	.39(−15)	67	0	.27(−15)	69	−2
	2	.43(−15)	51	−1	.32(−15)	3	−3
	3	.52(−15)	32	−3	.38(−15)	45	−3
	4	.89(−15)	12	5	.92(−15)	10	−5
5.0	1	.49(−15)	8	−2	.41(−15)	12	−2
	2	.20(−14)	9	3	.66(−15)	15	−3
	3	.56(−14)	13	4	.23(−14)	15	−4
	4	.11(−13)	19	5	.55(−14)	28	−5
10.0	1	.16(−14)	33	2	.69(−15)	56	−2
	2	.27(−14)	23	3	.15(−14)	25	−3
	3	.62(−14)	49	4	.25(−14)	50	−4
	4	.16(−13)	52	5	.66(−14)	57	−5

The practical implication of (4.1) is that in the case of symmetry we can restrict ourselves to *nonnegative* parameters c.

The next property is the special case $c = 0$ of (4.1), that is,

$$(-1)^k q_k(-x; 0; d\lambda) = q_k(x; 0; d\lambda) \qquad (d\lambda \text{ symmetric}). \tag{4.2}$$

Thus, when $c = 0$, then q_k is even or odd depending on the parity of k, regardless of the value of r. Since, in particular, $q_k^{(r)}(0) = 0$ if either k is even and r odd, or k is odd and r even, it follows from (2.1), (2.2) that

$$q_k(x) \equiv p_k(x) \qquad \text{if } k \text{ and } r \text{ have different parity} \qquad (c = 0). \tag{4.3}$$

4.2. *Hermite measure*

This is the case (2.1), (2.2) with $d\lambda(x) = e^{-x^2}dx$ on $\mathbb{R}$, which has already been considered analytically (for $c = 0$ and $r = 1$) in [9]. Here we deal with this example from the numerical point of view (also for $c \neq 0$ and $r > 1$).

We first determine the accuracy with which the $\bar{\omega}$- and $\bar{\theta}$-coefficients can be obtained by the algorithms of section 3. We do this by comparing double-precision with quadruple-precision results. (In single precision, overflow occurred in equation (3.5) when $c = 10$ and $n \geq 18$.) The maximum relative errors (in the double-precision values) that we observed are listed in table 1 for $n = 80$ (in (2.10)), $r = 1(1)4$, and selected values of c. The columns headed "k" and "j" indicate for which k and j the maximum error in $\bar{\omega}_{kj}$ resp. $\bar{\theta}_{kj}$ is attained; here, k and j vary over the integers 0 to $n-1$ ($=79$) and $-(r+1)$ to $r+1$, respectively. As can be seen, the coefficients are obtained quite accurately, suggesting a high degree of

robustness of the computational methods when the exponent range in machine arithmetic is adequately large.

To our surprise, the same cannot be said about the two methods (Methods I and II) for evaluating the polynomials q_k, especially not about the first. When $c = 0$ and and $r = 1$, both methods perform reasonably well, with the obvious exception (because of division by x^2 in (3.18)) of the second method in the immediate neighborhood of $x = 0$. Even Method I suffers a bit in accuracy near the origin, the maximum relative error (in q_k, $0 \le k \le n-1$) being about 10^{-14} when $n = 20$, and about 10^{-12} when $n = 80$. For $r > 1$, however, Method I develops huge relative errors on both sides away from the origin, where, for $n = 80$, the error is 100% or more in the $|x|$-range from about 4 to 10. When $n = 20$, the error peaks at levels of about 10^{-9}–10^{-11} for $r = 2$, 3 and 4. Further examination revealed that the recursion (3.17), in these ranges of x, is subject to persistent doses of cancellation errors. Sufficiently far away from the origin, at about $|x| = 25$, the error drops down to a more reasonable level of 10^{-14}. In contrast, Method II exhibits relative errors which gradually decrease on either side of the origin, becoming, when $n = 80$, smaller than about 10^{-12} for $|x|$ exceeding approximately 0.3, 1.5, 1.75, 2.5 for $r = 1, 2, 3, 4$, respectively; when $n = 20$, these numbers are somewhat smaller.

The difficulties with Method I persist for values $c \neq 0$ of the parameter c, especially on the left [right] side of $x = c$ when c is positive [negative] (cf. (4.1) for symmetry), but also, for awhile, on the other side of c. The magnitude of the errors indeed is consistently larger than for $c = 0$,

Unless $c = 0$ and $r = 1$, it is cautious, therefore, to use Method I only in a small interval around $x = c$ (the length of which should be chosen in dependence of c, r and the maximum degree of the desired q_k's), and use Method II outside that interval. We have done so in all computations relating to the zeros of q_k.

To look for zeros of q_k, we scanned the real axis (in practice, the interval $[-15, 15]$) for sign changes in q_k, taking a sufficiently small step (the length of the interval divided by some "irregular" integer like 1537 to avoid hitting exactly the origin). After a sign change has been discovered, the corresponding zero was computed by Newton's method. In this way we were usually able to determine a full set of k real zeros, or $k-2$, if there is a pair of conjugate complex zeros. Occasionally, the interval $[-15, 15]$ had to be enlarged to accommodate an exceptionally large zero. (This occurred, e.g., for $c = 5$, $r = 3$, when q_4 has the zero 19.36544 ..., or for $c = 5$, $r = 4$, in which case q_5 vanishes at 24.96544...) Also, on one occasion, the scanning had to be refined to detect two zeros located very closely together (the zeros 4.98794 ... , 5.01128... when $c = 5$ and $r = 1$). In view of the numerical difficulties described above, the computations were done in both double and quadruple precision, and the largest relative error in the trial values of q_k as well as in the zeros of q_k was carefully monitored to provide confidence in the empirical results below.

We begin with the simplest case $c = 0$, where the q_k's are alternately equal to (monic) Hermite polynomials (cf. (4.3)). Thus, every other of the polynomials q_k

has a complete set of real distinct zeros. This does not rule out, however, that those "inbetween" (which for $r = 1$ were identified in [9] as linear combinations of Hermite and generalized Hermite polynomials) could deviate from this pattern. We found that this does not happen when $r = 1$, i.e., in this case *all* polynomials q_k appear to have a complete set of real distinct zeros. This was verified numerically up to degree $n = 80$ and was in fact proved in [2, proposition 4.4], not only for the Hermite measure but also for general symmetric measures. Nevertheless, the zeros of q_k do not, in general, interlace with those of q_{k+1}; exceptions occur as early as $k = 4$. Interlacing occurs, however, between the zeros of q_k and p_k [2, proposition 4.6].

When $r = 2$, it was found that the "inbetween polynomials" q_k (i.e., for k even ≥ 4) are consistently short of 2 real zeros, and thus (by (4.2)) must have a pair of conjugate complex zeros on the imaginary axis. This was verified numerically up to $n = 40$; the complex zeros were seen to move along the imaginary axis down toward the real axis as k increases (from $k = 6$ on). An analogous situation was found to prevail for $r > 2$ (specifically, $r = 3$ and $r = 4$). See also theorem 8 in [1] for more general symmetric measures.

When $c \neq 0$, we found that $q_k(\,\cdot\,; c, d\lambda)$ either has exactly k real distinct zeros, or $k - 2$ and a pair of conjugate complex zeros. (For $r = 1$, this is true for general positive measures $d\lambda$; see, e.g., [12].) When $c = 1$ and $c = 5$, and for $1 \leq r \leq 4$, the occurrence of complex zeros and their values are documented in table 2 for the range $1 \leq k \leq 40$. All zeros (real and complex) were computed to 25 decimal digits, but only two digits are shown in table 2. For values of k with $1 \leq k \leq 40$ that do not appear in table 2, there exists a complete set of k real distinct zeros. Note how a larger value of c pushes the complex zeros further to the right.

Table 2
Complex zeros of $q_k(\,\cdot\,; c; d\lambda)$, $1 \leq k \leq 40$, for $d\lambda(x) = e^{-x^2}dx$ on $\mathbb{R}$ and $1 \leq r \leq 4$, $c = 1$, and $c = 5$.

c	k	$r = 1$ zeros	k	$r = 2$ zeros	k	$r = 3$ zeros	k	$r = 4$ zeros
1	5	$1.49 \pm .35i$	6	$1.80 \pm .60i$	7	$2.10 \pm .80i$	8	$2.41 \pm .97i$
	10	$1.42 \pm .25i$	8	$.71 \pm .38i$	9	$.61 \pm .55i$	10	$.50 \pm .80i$
	12	$1.15 \pm .25i$	11	$1.66 \pm .39i$	12	$1.87 \pm .50i$	13	$2.07 \pm .62i$
	17	$1.38 \pm .14i$	13	$1.09 \pm .44i$	14	$1.15 \pm .67i$	15	$1.19 \pm .88i$
	19	$1.24 \pm .22i$	15	$.72 \pm .27i$	16	$.57 \pm .38i$	17	$.48 \pm .51i$
			18	$1.59 \pm .22i$	19	$1.77 \pm .26i$	20	$1.94 \pm .31i$
			20	$1.32 \pm .32i$				
5	21	$5.16 \pm .18i$	22	$5.31 \pm .26i$	23	$5.46 \pm .33i$	24	$5.61 \pm .39i$
	25	$5.05 \pm .13i$	26	$5.18 \pm .20i$	24	$5.74 \pm .10i$	25	$5.91 \pm .16i$
	26	$5.31 \pm .04i$	27	$5.47 \pm .16i$	27	$5.28 \pm .26i$	28	$5.37 \pm .30i$
	29	$5.08 \pm .15i$	30	$5.19 \pm .22i$	28	$5.63 \pm .22i$	29	$5.79 \pm .27i$
	33	$5.18 \pm .15i$	31	$5.47 \pm .08i$	31	$5.29 \pm .27i$	32	$5.36 \pm .33i$
	36	$5.06 \pm .13i$	34	$5.31 \pm .23i$	32	$5.63 \pm .14i$	33	$5.79 \pm .18i$
	40	$5.23 \pm .10i$	37	$5.15 \pm .19i$	35	$5.43 \pm .30i$	36	$5.55 \pm .37i$
			38	$5.44 \pm .07i$	38	$5.21 \pm .23i$	39	$5.21 \pm .30i$
			40	$5.08 \pm .05i$	39	$5.58 \pm .12i$	40	$5.73 \pm .15i$

4.3. *Laguerre measure*

This is the case (2.1), (2.2) with $d\lambda(x) = e^{-x}dx$ on $\mathbb{R}_+$. Our experience with the algorithms of section 3 is similar to the one described in section 4.2 for the Hermite measure. The matrices $\overline{\Omega}$ and $\overline{\Theta}$ (again for $1 \leq r \leq 4$) are obtained to an accuracy close to machine precision when $n < 70$. For $n = 70$, we observed overflow in the double-precision evaluation (exponent range $\approx [-308, 308]$) of θ_{kj} by (3.14).

The two methods for evaluating the polynomials q_k were compared for values of n up to $n = 40$. It was found that Method I always develops huge errors (even in the case $c = 0, r = 1$) when x is sufficiently far to the right of c. This happens regardless of whether $c \geq 0$ or $c < 0$. As before, Method II must be avoided in a neighborhood of $x = c$ whose length depends on c, r and n. Method I is superior to Method II for most $x \leq c$, and we recommend its use in this range.

We followed the same approach as in section 4.2 to explore the zeros of q_k. Computations in the range $1 \leq k \leq 20$, and for $c = 0, -1, -5, 1 \leq r \leq 4$, led us to conjecture that $q_k(\,\cdot\,; c; d\lambda)$ for $c \leq 0$ has exactly k distinct real zeros, all positive except one, when $k > r$, which is negative. For $r = 1$, this has been proven in [8] for $c = 0$, and in [10] for $c \leq 0$, also for more general measures $d\lambda$. The general result for $r \geq 1$ has been proven in [11] (cf. theorems 4.2 and 4.5).

For $c > 0$, we found the occurrence not only of negative zeros, but also of complex zeros. A summary for $c = 1$ and $c = 5$ is provided in table 3. For values of $k \leq 20$ not contained in table 3, all zeros are distinct and positive. Again, the zeros were computed to 25 decimal places, but only 2 digits are shown in table 3. It appears, similarly as in the Hermite case, that when $c > 0$ the polynomial $q_k(\,\cdot\,; c; d\lambda)$ has either a set of k distinct real zeros (with one possibly nonpositive) or exactly $k - 2$ positive zeros and a pair of conjugate complex zeros. The latter again move to the right with increasing c.

4.4. *Legendre measure*

We now consider (2.1), (2.2) with $d\lambda(x) = dx$ on $[-1, 1]$. Being again a symmetric measure, it exhibits similar numerical properties as the Hermite measure in section 4.2. We used $n = 40$ for our numerical comparisons, and $n = 20$ for the exploration of the zeros. When $n = 40$, the matrices $\overline{\Omega}$ and $\overline{\Theta}$, as before, were obtained to an accuracy close to machine precision. Methods I and II are both quite accurate for $c = 0$ and $r = 1$, with a small interval (of length 0.1, say) excepted for Method II. When $r > 1$, Method I develops significant "bulges" of errors in the $|x|$-range from approx. 0.5 to 1.5, in contrast to Method II, which remains accurate there. Method II, therefore, should always be employed, with the exception noted above. When $c > 0$ (even in the case $r = 1$), the error buildup in Method I is intolerable in certain intervals located to the left of c. (For negative c, observe (4.1).) We recommend its use only for $x \geq c - \varepsilon$, where ε is a small positive number to be selected in dependence on c, r and n. For all other x-values, Method II should be used.

Table 3
Nonpositive and complex zeros of $q_k(\cdot\,; c; d\lambda)$, $1 \le k \le 20$, for $d\lambda(x) = e^{-x}dx$ on $\mathbb{R}_+$ and $r = 1(1)4$, $c = 1$, and $c = 5$.

c	k	$r=1$ zeros	k	$r=2$ zeros	k	$r=3$ zeros	k	$r=4$ zeros
1	6	$1.86 \pm .30i$	3	0.00	4	$-.91$	5	-2.86
	7	$1.29 \pm .06i$	4	$-.24$	5	-1.97	6	-4.94
	16	$1.57 \pm .27i$	5	$-.03$	6	-1.19	7	-3.23
	17	$1.33 \pm .32i$	10	$1.52 \pm .74i$	7	$-.61$	8	-2.10
	18	$1.12 \pm .18i$	11	$.78 \pm .73i$	8	$-.24$	9	-1.38
	19	$.71 \pm .13i$	12	$.48 \pm .39i$	9	$-.03$	10	$-.88$
	20	$.61 \pm .10i$	13	$.26 \pm .16i$	14	$2.06 \pm .77i$	11	$-.52$
			14	$.21 \pm .05i$	15	$1.10 \pm 1.04i$	12	$-.26$
					16	$.48 \pm .76i$	13	$-.08$
					17	$.26 \pm .45i$	19	$2.27 \pm .77i$
					18	$.17 \pm .23i$	20	$1.24 \pm 1.17i$
					19	$.13 \pm .12i$		
					20	$.13 \pm .04i$		
5	4	$6.48 \pm 1.47i$	6	$5.99 \pm 1.36i$	5	$4.72 \pm .40i$	6	$11.22 \pm 2.41i$
	7	$6.29 \pm 1.23i$	9	$7.53 \pm 1.69i$	7	$10.90 \pm .95i$	9	$11.73 \pm 1.53i$
	11	$6.14 \pm .99i$	10	$4.21 \pm .97i$	8	$4.56 \pm 2.14i$	10	$4.04 \pm 2.94i$
	12	$5.05 \pm .29i$	13	$7.78 \pm .44i$	11	$9.21 \pm 1.21i$	14	$7.18 \pm 3.04i$
	16	$6.00 \pm .81i$	14	$5.81 \pm 1.35i$	12	$5.00 \pm 2.23i$	15	$3.43 \pm 1.72i$
	17	$5.16 \pm .52i$	15	$4.11 \pm .67i$	13	$3.10 \pm .30i$	19	$8.56 \pm 1.14i$
			19	$6.69 \pm 1.04i$	16	$8.22 \pm 1.02i$	20	$5.24 \pm 2.46i$
			20	$4.93 \pm 1.12i$	17	$5.34 \pm 2.00i$		
					18	$3.59 \pm .79i$		

As far as the zeros are concerned, we have a situation similar to the one for the Hermite and Laguerre measures. Computations for $c = 1, 2, 5$ and $1 \le r \le 4$ suggest that for $c \ge 1$ there is always a complete set of real zeros, all in the interior of $[-1, 1]$ except for one that is larger than 1 whenever $k > r$. (For $c \le -1$, use (4.1).)

Table 4
Complex zeros of $q_k(\cdot\,; c; d\lambda)$, $1 \le k \le 20$, for $d\lambda(x) = dx$ on $[-1, 1]$ and $1 \le r \le 4$, $c = .5$.

c	k	$r=1$ zeros	k	$r=2$ zeros	k	$r=3$ zeros	k	$r=4$ zeros
0.5	5	$.79 \pm .12i$	6	$.70 \pm .28i$	7	$.43 \pm .44i$	8	$.002 \pm .30i$
	8	$.68 \pm .10i$	9	$.54 \pm .23i$	8	$.94 \pm .42i$	9	$.98 \pm .10i$
	11	$.63 \pm .08i$	12	$.50 \pm .18i$	10	$.28 \pm .24i$	12	$.78 \pm .20i$
	14	$.60 \pm .06i$	15	$.48 \pm .14i$	11	$.81 \pm .05i$	15	$.66 \pm .21i$
	17	$.58 \pm .05i$	18	$.48 \pm .12i$	13	$.30 \pm .15i$	18	$.59 \pm .20i$
	20	$.57 \pm .05i$			14	$.71 \pm .06i$		
					16	$.32 \pm .10i$		
					17	$.67 \pm .08i$		
					19	$.35 \pm .07i$		

For $r = 1$, this is proved in [10], and for general $r \geq 1$ can be deduced by an affine transformation of variables from the results in [11, §4].

When $c = 0, r = 2, 3, 4$, we observed, like in the Hermite case, that the inbetween polynomials have real distinct zeros in $(-1, 1)$, except for a pair of purely imaginary zeros moving toward the real axis as the degree increases. We suspect this remains true for all $r \geq 2$.

The "difficult" case is $-1 < c < 1, c \neq 0$, when complex zeros off the imaginary axis make their entrance. We illustrate this in table 4 for the case $c = 0.5$.

For a detailed discussion of the location of real and complex zeros of $q_k(\,\cdot\,; c; d\lambda)$ in the case $r = 1$, we refer to [12].

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Zeros and Critical Points of Sobolev Orthogonal Polynomials

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Using potential theoretic methods we study the asymptotic distribution of zeros and critical points of Sobolev orthogonal polynomials, i.e., polynomials orthogonal with respect to an inner product involving derivatives. Under general assumptions it is shown that the critical points have a canonical asymptotic limit distribution supported on the real line. In certain cases the zeros themselves have the same asymptotic limit distribution, while in other cases we can only ascertain that the support of a limit distribution lies within a specified set in the complex plane. One of our tools, which is of independent interest, is a new result on zero distributions of asymptotically extremal polynomials. Our results are illustrated by numerical computations for the case of two disjoint intervals. We also describe the numerical methods that were used.

1. INTRODUCTION AND STATEMENT OF MAIN RESULTS

We consider a Sobolev inner product

$$\langle f, g\rangle = \int f(t)\, g(t)\, d\mu_0(t) + \int f'(t)\, g'(t)\, d\mu_1(t), \tag{1.1}$$

where μ_0 and μ_1 are compactly supported positive measures on the real line with finite total mass. We put

$$\Sigma_0 := \operatorname{supp}(\mu_0), \qquad \Sigma_1 := \operatorname{supp}(\mu_1), \qquad \Sigma := \Sigma_0 \cup \Sigma_1. \tag{1.2}$$

If, as we assume, μ_0 has infinite support, there exists a unique sequence of monic polynomials π_n, $\deg \pi_n = n$, which is orthogonal with respect to the

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inner product (1.1). These Sobolev orthogonal polynomials have properties that clearly distinguish them from ordinary orthogonal polynomials, most notably by the fact that some or many of the zeros of π_n may be outside the convex hull of Σ, or even off the real line; cf. [1, 9]. In recent papers many results on zeros of special classes of Sobolev orthogonal polynomials were obtained. We refer to the surveys [8, 10].

Asymptotic properties of Sobolev orthogonal polynomials were obtained by López, Marcellán, and Van Assche [7]. These authors considered a general class of inner products, including inner products (1.1) with discrete measure μ_1.

In the present paper, we study the asymptotic behavior of zeros and critical points of orthogonal polynomials in a continuous Sobolev space, i.e., when both μ_0 and μ_1 are nondiscrete measures. Our results will be stated in terms of weak* convergence of measures. We associate with a polynomial P of exact degree n its normalized zero distribution,

$$\nu(P) := \frac{1}{n} \sum_{j=1}^{n} \delta_{z_j}, \tag{1.3}$$

where $z_1, \ldots, z_n$ are the zeros of P counted according to their multiplicities. A sequence of polynomials $\{P_n\}_{n=1}^{\infty}$, $\deg P_n = n$, is said to have asymptotic zero distribution μ if μ is a probability measure on $\bar{\mathbf{C}}$ and

$$\lim_{n \to \infty} \int f \, d\nu(P_n) = \int f \, d\mu \tag{1.4}$$

for every continuous function f on $\bar{\mathbf{C}}$. That is, their normalized zero distributions converge in the weak* sense to μ.

Asymptotic zero distributions for orthogonal polynomials with respect to an ordinary inner product

$$\langle f, g \rangle = \int f(t)\, g(t)\, d\mu(t), \qquad \Sigma := \operatorname{supp}(\mu) \subset \mathbf{R}, \tag{1.5}$$

have been studied by many authors. The most comprehensive account can be found in the monograph of Stahl and Totik [13]. They introduce a class **Reg** of regular measures. One of their results is that for $\mu \in \mathbf{Reg}$, the orthogonal polynomials p_n for the inner product (1.5) have regular asymptotic zero distribution. This means that

$$\lim_{n \to \infty} \nu(p_n) = \omega_{\Sigma},$$

where ω_Σ is the equilibrium measure of Σ; see [13, Theorem 3.6.1]. In case $\Sigma = \operatorname{supp}(\mu)$ is regular with respect to the Dirichlet problem in $\mathbf{C}\backslash\Sigma$, the measure μ belongs to **Reg** if and only if

$$\lim_{n\to\infty}\left(\frac{\|P_n\|_\Sigma}{\|P_n\|_{L^2(\mu)}}\right)^{1/n}=1 \tag{1.6}$$

for every sequence of polynomials $\{P_n\}_{n=1}^{\infty}$, $\deg P_n \leqslant n$, $P_n \not\equiv 0$. Here and in the following we use $\|\cdot\|_\Sigma$ to denote the supremum norm on Σ. Regularity of a measure indicates that it is sufficiently dense on its support. For example, it is enough that μ has a density which is positive almost everywhere on Σ. See [13, Chap. 4] for this and other criteria for regularity of μ.

Motivated by these facts, we make the following assumptions on the measures μ_0 and μ_1 in (1.1). Recall that $\Sigma_j = \operatorname{supp}(\mu_j)$, $j=0, 1$.

Assumption A. For $j=0, 1$, the set Σ_j is compact and regular for the Dirichlet problem in $\bar{\mathbf{C}}\backslash\Sigma_j$.

Assumption B. The measures μ_0 and μ_1 belong to the class **Reg**.

Our first result concerns the asymptotic zero distribution for the derivatives π_n' of the Sobolev orthogonal polynomials.

THEOREM 1. *Let μ_0 and μ_1 be measures on the real line satisfying Assumptions* A *and* B. *Let $\{\pi_n\}$ be the sequence of monic orthogonal polynomials for the inner product* (1.1). *Then*

$$\lim_{n\to\infty} \nu(\pi_n') = \omega_\Sigma,$$

where $\Sigma = \operatorname{supp}(\mu_0) \cup \operatorname{supp}(\mu_1)$ and ω_Σ is the equilibrium measure of Σ.

Thus the sequence of derivatives $\{\pi_n'\}$ has regular asymptotic zero distribution. Note, however, that this does not imply that the zeros of π_n' are all real. In fact, we do not even know if the zeros remain uniformly bounded. In our computations we found in all cases that the zeros of π_n' are real, see Section 2. While we have no reason to believe that this is true in general, we feel confident about the following conjecture.

Conjecture 1. Under the same conditions as in Theorem 1, let U be an arbitrary open set containing the convex hull of Σ. Then there is an n_0 such that for every $n \geqslant n_0$, all zeros of π_n' are in U.

To discuss the zeros of the Sobolev orthogonal polynomials π_n themselves, we need to introduce some more notation. Set

$$\Omega := \overline{\mathbf{C}} \setminus \Sigma,$$

and let $g_\Omega(z; \infty)$ be the Green function for Ω with pole at infinity; see [12, 13]. For $r > 0$, we denote by V_r the union of those components of $\{z \in \mathbf{C}: g_\Omega(z; \infty) < r\}$ having empty intersection with Σ_0, and we put

$$V := \bigcup_{r>0} V_r.$$

Finally, we put

$$K := \partial V \cup (\Sigma \setminus V).$$

THEOREM 2. *Let μ_0 and μ_1 be measures on the real line satisfying Assumptions* A *and* B. *Let $\{\pi_n\}$ be the sequence of monic orthogonal polynomials for the inner product* (1.1). *Let ν be a weak* limit of a subsequence of $\{\nu(\pi_n)\}$. Then*

(a) $\operatorname{supp}(\nu) \subset \bar{V} \cup \Sigma$,

(b) *the balayage of ν onto K is equal to the balayage of ω_Σ onto K.*

See [13] for the notion of balayage of a measure onto a compact set.

The information on the zeros of π_n we get from Theorem 2 is less precise than the information on the critical points from Theorem 1. In particular, it does not follow that the full sequence $\{\nu(\pi_n)\}$ converges. However, in some cases we can say more.

COROLLARY 3. *Under the same conditions as in Theorem* 2, *let ν be a weak* limit of a subsequence of $\{\nu(\pi_n)\}$. If $K = \Sigma$ (e.g., if $\Sigma_1 \subseteq \Sigma_0$), then $\nu = \omega_\Sigma$. In this case the full sequence $\{\nu(\pi_n)\}$ converges to ω_Σ.*

Corollary 3 follows immediately from Theorem 2. In our numerical examples, see Sections 2.3–2.4, we found that for n up to 50, part of the zeros of π_n are still pretty far outside K. But we conjecture that they do not accumulate outside of $\bar{V}$ and the convex hull of Σ.

Conjecture 2. Under the same conditions as in Theorem 2, let U be an arbitrary open set containing $\bar{V}$ and the convex hull of Σ. Then there is an n_0 such that for every $n \geqslant n_0$, all zeros of π_n are in U.

Conjecture 2 actually follows from Conjecture 1.

The rest of this paper is organized as follows. We first present numerical results on zeros and critical points for several special cases, where Σ consists of two disjoint intervals. The numerical methods we used are discussed

in Section 6. The proofs of the theorems are in Sections 3–5. They depend essentially on results on zero distributions of asymptotically minimal polynomials obtained by Blatt, Saff, and Simkani [2] and Mhaskar and Saff [11]. For the proof of Theorem 2 we need an extension of these results, which will be presented as Theorem 5 in Section 3. In Section 4 we give the proof of Theorem 1 and in Section 5 the proof of Theorem 2.

2. TWO DISJOINT INTERVALS: NUMERICAL RESULTS

In this section we present numerical calculations to illustrate our results. The methods used are described in Section 6.

We consider the case where Σ consists of two disjoint intervals of equal length. We choose

$$\Sigma = [-1, -\tfrac{1}{2}] \cup [\tfrac{1}{2}, 1].$$

With λ_+ the Lebesgue measure restricted to $[\frac{1}{2}, 1]$ and λ_- the Lebesgue measure restricted to $[-1, -\frac{1}{2}]$, we distinguish the following four cases:

Case A: $\mu_0 = \mu_1 = \lambda_+ + \lambda_-$;

Case B: $\mu_0 = \lambda_+ + \lambda_-$, $\mu_1 = \lambda_-$;

Case C: $\mu_0 = \lambda_+$, $\mu_1 = \lambda_+ + \lambda_-$;

Case D: $\mu_0 = \lambda_+$, $\mu_1 = \lambda_-$.

In all four cases, we know from Theorem 1 that the asymptotic zero distribution for the derivatives is equal to ω_Σ. In Cases A and B we have $\Sigma_1 \subseteq \Sigma_0$. Thus, it follows from Corollary 3 that in these two cases the asymptotic zero distribution for the Sobolev orthogonal polynomials is also equal to ω_Σ. This is confirmed by our calculations.

2.1. *Case A*: $\mu_0 = \mu_1 = \lambda_+ + \lambda_-$ (*Table I*)

In our calculations for $n = 1(1)25(5)50$ we found complex zeros of π_n only for $n = 5$, 7, and 9. All zeros of π_n' were found to be simple, real, and in the interval $(-1, 1)$.

2.2. *Case B*: $\mu_0 = \lambda_+ + \lambda_-$, $\mu_1 = \lambda_-$ (*Table II*)

Again, most of the zeros are real. Only for $n = 4$ and 6 did we find complex zeros of π_n. The zeros of π_n' are all simple, real, and in $(-1, 1)$. (Calculations for the same n as in Case A.)

The situation is different in Cases C and D. In these cases the set K of Theorem 2 may be described as follows. The Green function $g_\Omega(z; \infty)$ of $\Omega = \bar{\mathbb{C}} \setminus \Sigma$ has one level set $\{z: g_\Omega(z; \infty) = r_c\}$ consisting of a figure eight.

TABLE I

Zeros of π_n and π_n', $n=5$, 10, in Case A

	Zeros of π_n	Zeros of π_n'
$n=5$	$-0.93646854 - 0.20876772i$	-0.88534979
	$-0.93646854 + 0.20876772i$	-0.46499783
	0.0	0.46499783
	$0.93646854 - 0.20876772i$	0.88534979
	$0.93646854 + 0.20876772i$	
$n=10$	-1.00052723	-0.97497028
	-0.93567713	-0.87345927
	-0.80269592	-0.71474572
	-0.62612019	-0.55444777
	-0.50181795	0.0
	0.50181795	0.55444777
	0.62612019	0.71474572
	0.80269592	0.87345927
	0.93567713	0.97497028
	1.00052723	

TABLE II

Zeros of π_n and π_n', $n=5$, 10, in Case B

	Zeros of π_n	Zeros of π_n'
$n=5$	-1.01982013	-0.91709404
	-0.74396812	-0.64370369
	-0.55435292	0.14139821
	0.61214903	0.78137665
	0.90846355	
$n=10$	-1.00290062	-0.97911875
	-0.93891943	-0.89422735
	-0.84280403	-0.75923516
	-0.66396367	-0.61066220
	-0.55481204	-0.51231989
	-0.48324766	0.16014304
	0.55639877	0.62971341
	0.71942191	0.80459125
	0.87676555	0.93865007
	0.97576614	

For symmetry reasons, this is the level set containing 0. The set K consists of two parts. It is the union of $[\frac{1}{2}, 1]$ with that part of the figure eight that encircles $[-1, -\frac{1}{2}]$.

2.3. *Case C*: $\mu_0 = \lambda_+$, $\mu_1 = \lambda_+ + \lambda_-$ (*Table III*)

In our calculations for $n = 1(1)25(5)50$ all zeros of π_n' were found to be simple, real, and in $(-1, 1)$. All zeros of π_n are real only for $n = 1$, 2, 3, 4, 6, 8, and 10. All complex zeros have a negative real part and they are encircling $[-1, -\frac{1}{2}]$. Furthermore, we noted some peculiarities in the behavior of the complex zeros. For odd n, the complex zeros are outside

TABLE III

Zeros of π_n and π_n', $n = 5$, 10, 15, in Case C

	Zeros of π_n	Zeros of π_n'
$n=5$	$-1.13970225 - 0.44661459i$	-0.90932823
	$-1.13970225 + 0.44661459i$	-0.62403037
	0.50779290	0.62478703
	0.76816794	0.90887919
	1.00382819	
$n=10$	-0.98774277	-0.97498555
	-0.95967689	-0.87349586
	-0.77454092	-0.71478191
	-0.65462781	-0.55436421
	-0.48961896	0.00056691
	0.50181827	0.55445253
	0.62612626	0.71475358
	0.80270124	0.87346371
	0.93567933	0.97497123
	1.00052715	
$n=15$	-1.20729028	-0.99008732
	$-1.11842498 - 0.23762201i$	-0.94869995
	$-1.11842498 + 0.23762201i$	-0.87812479
	$-0.86567461 - 0.41291713i$	-0.78542939
	$-0.86567461 + 0.41291713i$	-0.68199701
	$-0.48045299 - 0.45544118i$	-0.58497964
	$-0.48045299 + 0.45544118i$	-0.51762420
	0.50000295	0.51762967
	0.54387032	0.58499199
	0.63049097	0.68200314
	0.73428763	0.78542581
	0.83481287	0.87811753
	0.91801959	0.94869496
	0.97492010	0.99008612
	0.99999844	

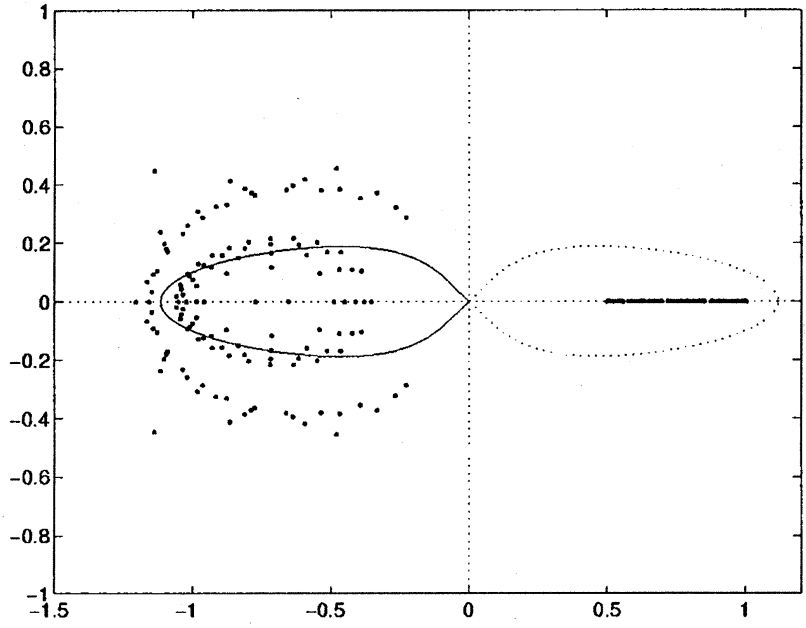

FIG. 1. Plot of the zeros of π_n, $n = 5(5)50$, in Case C.

the set K, while for even n, they are initially inside, but eventually some cross over to the outside. It seems likely that for odd n, the zeros tend to K from the outside but the convergence is very slow. For even n, there might be a different limit distribution, although it is conceivable that also for even n, the zeros accumulate on K. It is also remarkable that the zeros

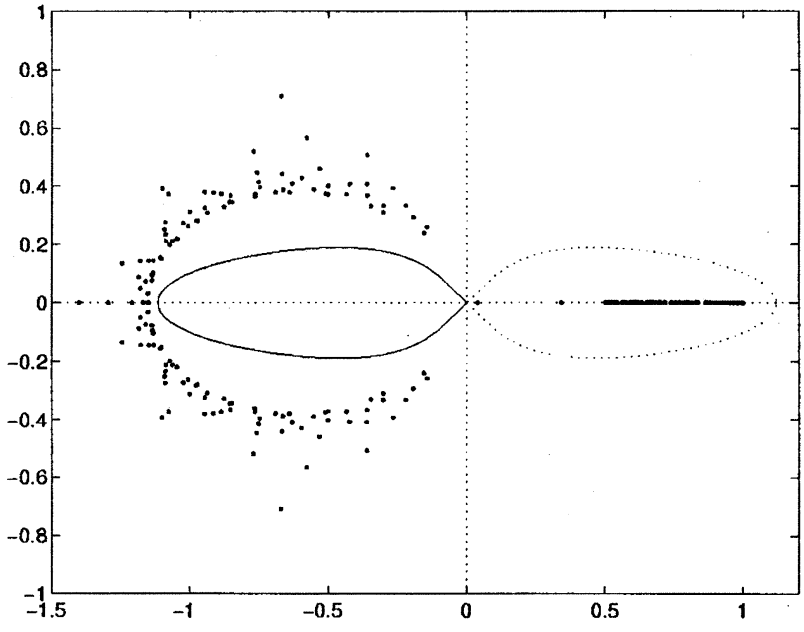

FIG. 2. Plot of the zeros of π_n, $n = 5(5)50$, in Case D.

of π_n' are very close to being symmetric around 0. We have no explanations for these phenomena.

Figure 1 depicts the zeros of π_n, $n=5(5)50$, along with that part of K that encircles $[-1, -\frac{1}{2}]$.

2.4. *Case D*: $\mu_0=\lambda_+$, $\mu_1=\lambda_-$ (*Table IV*)

We found complex zeros of π_n for all n, except $n=1$, 2, and 3. Again, all the zeros of π_n' are simple, real, and in $(-1, 1)$.

In contrast to Case C, we found no zeros of π_n inside the curve K (except for $n=3$). This is illustrated in Fig. 2 with the plots of the zeros of π_n, $n=5(5)50$. Note that the zeros are pretty far from K.

TABLE IV

Zeros of π_n and π_n', $n=5$, 10, 15, in Case D

	Zeros of π_n	Zeros of π_n'
$n=5$	-1.40237979	-0.91931357
	$-0.67193855 - 0.70835815i$	-0.64605904
	$-0.67193855 + 0.70835815i$	-0.18436141
	0.62935932	0.78712860
	0.91364079	
$n=10$	-1.29703537	-0.98088476
	$-1.10126374 - 0.39294199i$	-0.90316848
	$-1.10126374 + 0.39294199i$	-0.77960092
	$-0.57893971 - 0.56595190i$	-0.63989830
	$-0.57893971 + 0.56595190i$	-0.53049964
	0.51468739	0.55298588
	0.60589851	0.68147141
	0.75300437	0.83024743
	0.89081502	0.94619968
	0.97842844	
$n=15$	$-1.24663987 - 0.13488685i$	-0.99138203
	$-1.24663987 + 0.13488685i$	-0.95536746
	$-1.07914072 - 0.37346724i$	-0.89378004
	$-1.07914072 + 0.37346724i$	-0.81229432
	$-0.77108509 - 0.51962021i$	-0.71962499
	$-0.77108509 + 0.51962021i$	-0.62805945
	$-0.36124445 - 0.50773392i$	-0.55324965
	$-0.36124445 + 0.50773392i$	-0.50975247
	0.51791298	0.54446702
	0.58620377	0.63199538
	0.68402014	0.73630329
	0.78755144	0.83660513
	0.87969723	0.91913536
	0.94947423	0.97530045
	0.99024926	

2.5. *Another Choice for λ_+ and λ_-*

We also experimented with λ_+ the measure $|t|\,(t^2-\frac{1}{4})^{-1/2}(1-t^2)^{-1/2}$ restricted to $[\frac{1}{2}, 1]$ and λ_- the same measure restricted to $[-1, -\frac{1}{2}]$. The results, on the whole, are very similar to those for the Lebesgue measure. The differences noted were that complex zeros of π_n occur also for $n=11$ and 13 in Case A, and for $n=8$ in Case B. In Case C, all zeros of π_n are real only for $n=1$, 2, 3, 4, 6, and 8.

3. AN AUXILIARY RESULT ON ASYMPTOTICALLY MINIMAL POLYNOMIALS

A major tool in the proof of Theorem 1 is a well-known result on zero distributions of polynomials, which we state below for the case of a set $E \subset \mathbf{R}$. Here and in the following, $\mathrm{cap}(E)$ denotes the logarithmic capacity of E; see, e.g., [12, 13].

LEMMA 4. *Let $E \subset \mathbf{R}$ be compact with $\mathrm{cap}(E) > 0$ and let $\{p_n\}$ be a sequence of monic polynomials, $\deg p_n = n$, such that*

$$\limsup_{n\to\infty} \|p_n\|_E^{1/n} \leqslant \mathrm{cap}(E). \tag{3.1}$$

Then

$$\lim_{n\to\infty} \nu(p_n) = \omega_E. \tag{3.2}$$

Proof. See the paper of Blatt, Saff, and Simkani [2]. ∎

Monic polynomials satisfying (3.1) are called asymptotically minimal polynomials, since every monic polynomial p_n of degree n satisfies

$$\|p_n\|_E^{1/n} \geqslant \mathrm{cap}(E).$$

Hence, if (3.1) holds, we have in fact equality.

A weighted analogue of this theorem was obtained by Mhaskar and Saff [11]. To prove Theorem 2, we will need a slightly stronger result, which may be of independent interest. To state it, we recall the situation of [11]. Assume $E \subset \mathbf{C}$ is a closed set. A function $w: E \to [0, \infty)$ is an admissible weight if

(a) w is upper semicontinuous;

(b) the set $\{z \in E: w(z) > 0\}$ has positive capacity;

(c) if E is unbounded, then $|z|\, w(z) \to 0$ as $|z| \to \infty$, $z \in E$.

Associated with an admissible weight w is a unique positive unit measure μ_w and a unique constant F_w such that

$$U^{\mu_w}(z) - \log w(z) = F_w \qquad \text{q.e. on } \operatorname{supp}(\mu_w),$$
$$U^{\mu_w}(z) - \log w(z) \geqslant F_w \qquad \text{q.e. on } E. \tag{3.3}$$

Here, U^μ denotes the logarithmic potential of the measure μ,

$$U^\mu(z) := \int \log \frac{1}{|z-t|}\, d\mu(t),$$

and q.e. means quasi-everywhere, that is, except for a set of zero capacity.

In the following theorem we use S_w to denote the support of μ_w, $Pc(S_w)$ denotes the polynomial convex hull of S_w, $D_w = \bar{\mathbf{C}} \backslash Pc(S_w)$ denotes the unbounded component of $\bar{\mathbf{C}} \backslash S_w$, and ∂D_w denotes the boundary of D_w (also known as the outer boundary of S_w).

THEOREM 5. *Let w be an admissible weight on the closed set $E \subset \mathbf{C}$. Let $\{p_n\}_{n=1}^{\infty}$ be a sequence of monic polynomials, $\deg p_n = n$, such that for q.e. $z \in \partial D_w$,*

$$\limsup_{n \to \infty} [w(z)\, |p_n(z)|^{1/n}] \leqslant \exp(-F_w). \tag{3.4}$$

Then for every closed $A \subset D_w$,

$$\lim_{n \to \infty} \nu(p_n)(A) = 0. \tag{3.5}$$

Furthermore, if ν is the weak limit of a subsequence of $\{\nu(p_n)\}$, then $\operatorname{supp}(\nu^*) \subset Pc(S_w)$ and the balayage of ν^* onto ∂D_w is equal to the balayage of μ_w onto ∂D_w.*

In [11] the same result was obtained from the stronger assumption

$$\limsup_{n \to \infty} \|w^n p_n\|_{\partial D_w}^{1/n} \leqslant \exp(-F_w).$$

Proof. In terms of potentials, the relation (3.4) is

$$F_w + \log w(z) \leqslant \liminf_{n \to \infty} U^{\nu(p_n)}(z), \qquad \text{q.e. } z \in \partial D_w,$$

and in view of (3.3) this implies

$$U^{\mu_w}(z) \leqslant \liminf_{n \to \infty} U^{\nu(p_n)}(z), \qquad \text{q.e. } z \in \partial D_w. \tag{3.6}$$

Let ν_n be the balayage of $\nu(p_n)$ onto $Pc(S_w)$. Then

$$U^{\nu_n}(z) = U^{\nu(p_n)}(z) + c_n, \qquad \text{q.e. } z \in Pc(S_w), \tag{3.7}$$

with a constant c_n given by (see [13, Appendix VII])

$$c_n = \int g_{D_w}(z; \infty)\, d\nu(p_n)(z) \geqslant 0. \tag{3.8}$$

Let ν be the weak* limit of a subsequence of $\{\nu_n\}$, say $\nu_n \to \nu$ as $n \to \infty$, $n \in \Lambda$, where Λ is a subsequence of the natural numbers. Then $\operatorname{supp}(\nu) \subset Pc(S_w)$, and by the lower envelope theorem [13, Appendix III]

$$U^{\nu}(z) = \liminf_{n \to \infty,\, n \in \Lambda} U^{\nu_n}(z), \qquad \text{q.e. } z \in \mathbf{C}.$$

Combining this with (3.7), (3.8), and (3.6), we find for q.e. $z \in \partial D_w$:

$$\begin{aligned} U^{\nu}(z) &= \liminf_{n \to \infty,\, n \in \Lambda} U^{\nu_n}(z) = \liminf_{n \to \infty,\, n \in \Lambda} [U^{\nu(p_n)}(z) + c_n] \\ &\geqslant \liminf_{n \to \infty,\, n \in \Lambda} U^{\nu(p_n)}(z) \geqslant U^{\mu_w}(z). \end{aligned} \tag{3.9}$$

Since $U^{\nu} - U^{\mu_w}$ is harmonic in D_w and zero at infinity, the minimum principle and (3.9) give that $U^{\nu}(z) = U^{\mu_w}(z)$ for $z \in D_w$, and therefore,

$$U^{\nu}(z) = U^{\mu_w}(z), \qquad \text{q.e. } z \in \partial D_w.$$

Consequently, equality holds in every inequality in (3.9) for q.e. $z \in \partial D_w$. Then it follows that $\liminf_{n \in \Lambda} c_n = 0$. Since this holds for every subsequence $\Lambda \subset \mathbf{N}$ for which $\{\nu_n\}_{n \in \Lambda}$ converges, we obtain

$$\lim_{n \to \infty} c_n = 0. \tag{3.10}$$

Since for a closed set $A \subset D_w$ there exists a constant $C > 0$ such that $g_{D_w}(z; \infty) \geqslant C$ for $z \in A$, it follows from (3.8) and (3.10) that

$$\lim_{n \to \infty} \nu(p_n)(A) = 0.$$

This proves (3.5).

To prove the rest of the theorem, let ν^* be the weak* limit of a subsequence of $\{\nu(p_n)\}$; say Λ is a subsequence of the natural numbers such that $\nu(p_n) \to \nu^*$ as $n \to \infty$, $n \in \Lambda$. Having (3.5), we see that ν^* is supported on $Pc(S_w)$. Define

$$A := \{z \in D_w : \operatorname{dist}(z, S_w) \geqslant 1\}.$$

Let $\zeta_{j,n}$, $j=1, ..., n$, be the zeros of p_n counted according to multiplicity, and put

$$r_n(z) := \prod_{\zeta_{j,n} \in A} (z-\zeta_{j,n}), \qquad q_n(z) := \frac{p_n(z)}{r_n(z)} = \prod_{\zeta_{j,n} \notin A} (z-\zeta_{j,n}).$$

Then, because of (3.5),

$$\deg q_n = n(1-\delta_n), \qquad \delta_n \to 0, \tag{3.11}$$

and the sequence $\{\nu(q_n)\}_{n \in \Lambda}$ converges to ν^* in the weak* sense. Since the measures $\nu(q_n)$ are supported on a fixed compact set, the lower envelope theorem can be applied. It gives

$$U^{\nu^*}(z) = \liminf_{n \to \infty, n \in \Lambda} U^{\nu(q_n)}(z), \qquad \text{q.e. } z \in \mathbf{C}. \tag{3.12}$$

Next, since $r_n(z) \geqslant 1$ for $z \in S_w$, we have for $z \in S_w$

$$U^{\nu(p_n)}(z) = (1-\delta_n)\, U^{\nu(q_n)}(z) - \delta_n \log |r_n(z)| \leqslant (1-\delta_n)\, U^{\nu(q_n)}(z);$$

hence, by (3.11), (3.12),

$$\begin{aligned} \liminf_{n \to \infty, n \in \Lambda} U^{\nu(p_n)}(z) &\leqslant \liminf_{n \to \infty, n \in \Lambda} [(1-\delta_n)\, U^{\nu(q_n)}(z)] \\ &= U^{\nu^*}(z), \qquad \text{q.e. } z \in S_w. \end{aligned}$$

Combining this with (3.6), we obtain

$$U^{\mu_w}(z) \leqslant U^{\nu^*}(z), \qquad \text{q.e. } z \in \partial D_w.$$

In the same way as before, cf. (3.9), this implies equality for q.e. $z \in \partial D_w$. Now the equality of the balayages of ν^* and μ_w onto ∂D_w follows from the uniqueness of balayage. This completes the proof of Theorem 5. ∎

4. PROOF OF THEOREM 1

We start with a lemma which will also be useful for the proof of Theorem 2.

LEMMA 6. *Let μ_0 and μ_1 be measures satisfying Assumptions A and B. Let π_n be the sequence of monic orthogonal polynomials with respect to* (1.1). *Then we have*

$$\limsup_{n \to \infty} \|\pi_n\|_{\Sigma_0}^{1/n} \leqslant \operatorname{cap}(\Sigma) \tag{4.1}$$

and

$$\limsup_{n\to\infty} \|\pi_n'\|_\Sigma^{1/n} \leqslant \operatorname{cap}(\Sigma). \tag{4.2}$$

Proof. Let $\|\cdot\|_H$ denote the norm associated with the inner product (1.1),

$$\|f\|_H^2 = \|f\|_{L^2(\mu_0)}^2 + \|f'\|_{L^2(\mu_1)}^2.$$

We first prove that

$$\limsup_{n\to\infty} \|\pi_n\|_H^{1/n} \leqslant \operatorname{cap}(\Sigma). \tag{4.3}$$

Let T_n be the monic Chebyshev polynomial of degree n for Σ. That is, $\|T_n\|_\Sigma \leqslant \|P_n\|_\Sigma$ for all monic polynomials P_n of degree n. It is well known that

$$\lim_{n\to\infty} \|T_n\|_\Sigma^{1/n} = \operatorname{cap}(\Sigma). \tag{4.4}$$

From the regularity of Σ_1 (see Assumption A) it is easy to see (using the continuity of the Green function, the Bernstein–Walsh lemma and Cauchy's formula) that the Markov constants for Σ_1 have subexponential growth. This means that there exist constants M_n with $\lim_{n\to\infty} M_n^{1/n} = 1$ such that

$$\|P_n'\|_{\Sigma_1} \leqslant M_n \|P_n\|_{\Sigma_1}, \qquad \deg P_n \leqslant n. \tag{4.5}$$

Then, for certain constants c_1, c_2,

$$\begin{aligned} \|T_n\|_H^2 = \|T_n\|_{L_2(\mu_0)}^2 + \|T_n'\|_{L_2(\mu_1)}^2 &\leqslant c_1 \|T_n\|_{\Sigma_0}^2 + c_2 \|T_n'\|_{\Sigma_1}^2 \\ &\leqslant c_1 \|T_n\|_{\Sigma_0}^2 + c_2 M_n^2 \|T_n\|_{\Sigma_1}^2 \leqslant (c_1 + c_2 M_n^2) \|T_n\|_\Sigma^2. \end{aligned} \tag{4.6}$$

Using (4.4), (4.6), and $M_n^{1/n} \to 1$, we find

$$\limsup_{n\to\infty} \|T_n\|_H^{1/n} \leqslant \operatorname{cap}(\Sigma).$$

Since π_n minimizes the Sobolev norm among all monic polynomials of degree n, we have $\|\pi_n\|_H \leqslant \|T_n\|_H$ for all n, and (4.3) follows.

Now, because $\mu_0 \in \mathbf{Reg}$, we have by (1.6),

$$\lim_{n\to\infty} \left(\frac{\|\pi_n\|_{\Sigma_0}}{\|\pi_n\|_{L^2(\mu_0)}} \right)^{1/n} = 1. \tag{4.7}$$

Since $\|\pi_n\|_{L^2(\mu_0)} \leqslant \|\pi_n\|_H$, we get (4.1) from (4.3) and (4.7).

Next, using the regularity of Σ_0, we find that the Markov constants for Σ_0 grow subexponentially. Thus,

$$\limsup_{n\to\infty}\left(\frac{\|\pi_n'\|_{\Sigma_0}}{\|\pi_n\|_{\Sigma_0}}\right)^{1/n}\leqslant 1.$$

Hence, from (4.1),

$$\limsup_{n\to\infty}\|\pi_n'\|_{\Sigma_0}^{1/n}\leqslant\limsup_{n\to\infty}\|\pi_n\|_{\Sigma_0}^{1/n}\leqslant\operatorname{cap}(\Sigma). \tag{4.8}$$

Further, we get from $\mu_1\in\mathbf{Reg}$ and (1.6)

$$\limsup_{n\to\infty}\left(\frac{\|\pi_n'\|_{\Sigma_1}}{\|\pi_n'\|_{L^2(\mu_1)}}\right)^{1/n}\leqslant 1. \tag{4.9}$$

Since $\|\pi_n'\|_{L^2(\mu_1)}\leqslant\|\pi_n\|_H$, (4.3) and (4.9) give

$$\limsup_{n\to\infty}\|\pi_n'\|_{\Sigma_1}^{1/n}\leqslant\operatorname{cap}(\Sigma). \tag{4.10}$$

Combining (4.8) and (4.10), we obtain (4.2). ∎

Remark. Actually, we have equality in (4.1) and (4.2), and we can replace the lim sup's by lim's, but this will not be used in the proof. It is straightforward to see that equality holds in (4.2); cf. the discussion after Lemma 4. Since Σ_0 has positive capacity, it then also follows that

$$\lim_{n\to\infty}\|\pi_n'\|_{\Sigma_0}^{1/n}=\operatorname{cap}(\Sigma).$$

Using (4.8), we obtain equality in (4.1) as well.

Proof of Theorem 1. The theorem follows immediately from Lemma 4 and (4.2). ∎

5. PROOF OF THEOREM 2

Recall the definitions of Ω, V, V_r, and K from Section 1. The significance of the set V is described in the following lemma.

LEMMA 7. *Let $z\in\mathbf{C}$. Then $z\notin V$ if and only if for every $r>g_\Omega(z;\infty)$, there is a differentiable path $\gamma\colon[0,1]\to\mathbf{C}$ such that*

(a) $\gamma(0)\in\Sigma_0$,

(b) $\gamma(1)=z$,

(c) $g_\Omega(\gamma(t);\infty)<r$ *for all* $t\in[0,1]$.

Proof. If $z \in V$, then $z \in V_r$ for some $r > g_\Omega(z; \infty)$. From the definition of V_r it follows that the connected component of $\{\zeta: g_\Omega(\zeta; \infty) < r\}$ containing z does not contain a point of Σ_0. Hence there is no path satisfying (a), (b), and (c).

On the other hand, if $z \notin V$ and $r > g_\Omega(z; \infty)$, then $z \notin V_r$. Thus the connected component of $\{\zeta: g_\Omega(\zeta; \infty) < r\}$ does contain a point of Σ. Consequently, there is a path satisfying (a), (b), and (c). ∎

This allows us to estimate $|\pi_n(z)|$ for z outside V.

LEMMA 8. *For every* $z \in \mathbf{C} \setminus V$,

$$\limsup_{n \to \infty} |\pi_n(z)|^{1/n} \leqslant \operatorname{cap}(\Sigma)\, e^{g_\Omega(z; \infty)}. \tag{5.1}$$

Proof. Let $z \in \mathbf{C} \setminus V$ and $r > g_\Omega(z; \infty)$. By Lemma 7 there is a differentiable path $\gamma: [0, 1] \to \mathbf{C}$ satisfying (a), (b), and (c) of Lemma 7. By the Bernstein–Walsh lemma we have

$$|\pi_n'(\zeta)| \leqslant \|\pi_n'\|_\Sigma\, e^{n g_\Omega(\zeta; \infty)}, \qquad \zeta \in \mathbf{C}.$$

Using this and the properties of γ, we find

$$|\pi_n(z)| \leqslant |\pi_n(\gamma(0))| + \left| \int_\gamma \pi_n'(\zeta)\, d\zeta \right| \leqslant \|\pi_n\|_{\Sigma_0} + L(\gamma)\, \|\pi_n'\|_\Sigma\, e^{nr},$$

where $L(\gamma)$ denotes the length of γ. Then, by (4.1) and (4.2),

$$\limsup_{n \to \infty} |\pi_n(z)|^{1/n} \leqslant \operatorname{cap}(\Sigma)\, e^r.$$

Since $r > g_\Omega(z; \infty)$ can be chosen arbitrarily close to $g_\Omega(z; \infty)$, (5.1) follows. ∎

Proof of Theorem 2. Define

$$w(z) := \exp(-g_\Omega(z; \infty)), \qquad z \in K.$$

Let $\hat{\omega}$ be the balayage of ω_Σ onto K. Since $\Sigma \subset Pc(K)$, we have

$$U^{\hat{\omega}}(z) = U^{\omega_\Sigma}(z), \qquad z \in K.$$

We also have

$$U^{\omega_\Sigma}(z) + g_\Omega(z; \infty) = -\log \operatorname{cap}(\Sigma), \qquad z \in \mathbf{C},$$

so that

$$U^{\hat{\omega}}(z) - \log w(z) = -\log \operatorname{cap}(\Sigma), \qquad z \in K.$$

Thus, by (3.3),

$$\mu_w = \hat{\omega}, \qquad F_w = -\log \operatorname{cap}(\Sigma).$$

Because of (5.1) we can apply Theorem 5, and Theorem 2 follows. ∎

6. COMPUTATIONAL METHODS

There are two general procedures for calculating Sobolev orthogonal polynomials: the modified Chebyshev algorithm [6, Section 2] and the Stieltjes algorithm [6, Section 4]. Both generate the coefficients β_j^k in the recursion

$$\pi_{k+1}(t) = t\pi_k(t) - \sum_{j=0}^{k} \beta_j^k \pi_{k-j}(t), \qquad k = 0, 1, 2, \ldots, \tag{6.1}$$

for the respective polynomials π_k. Being interested in the polynomials up to (and including) degree n, we need the coefficients $\{\beta_j^k\}_{0 \leqslant j \leqslant k}$ for $k = 0, 1, \ldots, n-1$.

6.1. *Modified Chebyshev Algorithm*

This computes the desired coefficients $\{\beta_j^k\}$ from "modified moments"

$$\begin{aligned} v_j^{(0)} &= \int p_j(t)\, d\mu_0(t), \qquad 0 \leqslant j \leqslant 2n-1, \\ v_j^{(1)} &= \int p_j(t)\, d\mu_1(t), \qquad 0 \leqslant j \leqslant 2n-2 \quad (\text{if } n \geqslant 2), \end{aligned} \tag{6.2}$$

where $\{p_j\}$ is a given set of polynomials, with p_j monic of degree j. "Ordinary moments" correspond to $p_j(t) = t^j$, but are numerically unsatisfactory. A better choice are modified moments corresponding to a set $\{p_j\}$ of orthogonal polynomials, $p_j(\cdot) = p_j(\cdot\,; \lambda)$, relative to some suitable measure λ on $\mathbf{R}$. These are known to satisfy a three-term recurrence relation,

$$\begin{aligned} &p_{k+1}(t) = (t - a_k)\, p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \\ &p_0(t) = 1, \qquad p_{-1}(t) = 0, \end{aligned} \tag{6.3}$$

with coefficients $a_k = a_k(\lambda)$, $b_k = b_k(\lambda)$ depending on λ. We need the coefficients $\{a_j\}$, $\{b_j\}$ for $0 \leqslant j \leqslant 2n-2$.

In the context of the Sobolev orthogonal polynomials of Section 2, a natural choice of λ, and one that was found to work well, is $\lambda = \lambda_+ + \lambda_-$. By the orthogonality of the p_j we then have

$$\int_{-1}^{-1/2} p_j(t)\, d\lambda_-(t) + \int_{1/2}^{1} p_j(t)\, d\lambda_+(t) = 0, \qquad j \geqslant 1,$$

so that

$$\int_{-1}^{-1/2} p_j(t)\, d\lambda_-(t) = -\int_{1/2}^{1} p_j(t)\, d\lambda_+(t). \tag{6.4}$$

Since, by symmetry, $p_j(-t) = (-1)^j p_j(t)$, the change of variables $t = -\tau$ in (6.4) yields

$$\int_{1/2}^{1} p_j(t)\, d\lambda_+(t) = 0 \qquad \text{if } j \text{ is even } \geqslant 2. \tag{6.5}$$

Let

$$I_j = \int_{1/2}^{1} p_j(t)\, d\lambda_+(t), \qquad 0 \leqslant j \leqslant 2n-1, \tag{6.6}$$

so that $I_j = 0$ if $j \geqslant 2$ is even. We then have, in Case A,

$$v_j^{(0)} = v_j^{(1)} = 2\delta_{j,0} I_0, \qquad j = 0, 1, 2, \ldots, \tag{6.7}$$

where $\delta_{j,0}$ is the Kronecker delta. Similarly, in Case B,

$$v_j^{(0)} = 2\delta_{j,0} I_0, \qquad v_j^{(1)} = \begin{cases} I_0, & j = 0, \\ -I_j, & j \text{ odd}, \\ 0, & \text{otherwise}, \end{cases} \tag{6.8}$$

in Case C:

$$v_j^{(0)} = \begin{Bmatrix} I_j, & j = 0 \text{ or } j \text{ odd}, \\ 0, & \text{otherwise}, \end{Bmatrix}, \qquad v_j^{(1)} = 2\delta_{j,0} I_0, \tag{6.9}$$

and in Case D:

$$v_j^{(0)} = \begin{Bmatrix} I_j, & j = 0 \text{ or } j \text{ odd}, \\ 0, & \text{otherwise}, \end{Bmatrix}, \quad v_0^{(1)} = I_0, \quad v_j^{(1)} = -v_j^{(0)}, \quad j \geqslant 1. \tag{6.10}$$

In Sections 2.1–2.4 we have that λ_+ and λ_- are Lebesgue measure supported on $[\frac{1}{2}, 1]$ and $[-1, -\frac{1}{2}]$, respectively. Here, $I_0 = \frac{1}{2}$. The coefficients $a_j(\lambda)$, $b_j(\lambda)$ in (6.3) can be computed very accurately by known procedures of Stieltjes or Lanczos type (cf. [3, Example 4.7; 5, Section 4.3]), whereupon the integrals I_j in (6.6) can be computed (exactly) by (6.3) and n-point Gauss–Legendre quadrature.

In Section 2.5, λ_+ and λ_- are equal to the measure $|t|\,(t^2-\frac{1}{4})^{-1/2}\times(1-t^2)^{-1/2}$ supported on $[\frac{1}{2}, 1]$ and $[-1, -\frac{1}{2}]$, respectively. Here, $I_0 = \frac{1}{2}\pi$. The coefficients $a_j(\lambda)$, $b_j(\lambda)$ are known explicitly (cf. [4, Section 5.1]):

$$\begin{aligned} &a_j = 0, && 0 \leqslant j \leqslant 2n-2, \\ &b_0 = \pi, && b_1 = \tfrac{5}{8}, \\ &b_j = \frac{1}{16}\begin{cases} 9\dfrac{1+3^{j-2}}{1+3^j}, & j \text{ even}, \\ \dfrac{1+3^{j+1}}{1+3^{j-1}}, & j \text{ odd}, \end{cases} && j = 2, 3, \ldots, 2n-2. \end{aligned} \tag{6.11}$$

The integrals I_j can no longer be computed exactly by numerical quadrature, but can be approximated by N-point Gauss–Chebyshev quadrature with N sufficiently large. Indeed, if in

$$I_j = \int_{1/2}^{1} p_j(t)\, t(t^2-\tfrac{1}{4})^{-1/2}\,(1-t^2)^{-1/2}\,dt$$

one makes the change of variables $t^2 = (1+3s)/4$, one gets

$$I_j = \tfrac{1}{2}\int_0^1 p_j(\tfrac{1}{2}\sqrt{1+3s})\, s^{-1/2}(1-s)^{-1/2}\,ds,$$

or, transforming to the interval $[-1, 1]$,

$$I_j = \frac{1}{2}\int_{-1}^{1} p_j\left(\frac{1}{2\sqrt{2}}\sqrt{5+3x}\right)(1-x^2)^{-1/2}\,dx. \tag{6.12}$$

Gauss–Chebyshev quadrature applied to the integral in (6.12) converges fast.

6.2. *Stieltjes Algorithm*

Here the coefficients $\{\beta_j^k\}$ are computed as Fourier–Sobolev coefficients

$$\beta_j^k = \frac{(t\pi_k, \pi_{k-j})_H}{\|\pi_{k-j}\|_H^2}, \qquad j = 0, 1, \ldots, k, \tag{6.13}$$

where appropriate quadrature rules are used to compute the inner products in (6.13). The coefficients β_j^k and polynomials π_m intervening in (6.13) are computed simultaneously, the polynomials recursively by (6.1) using the coefficients β_j^k already obtained. The choice of quadrature rules is particularly simple in the case of Lebesgue measures. Indeed, for $k \leqslant n-1$, the integrands in (6.13) are polynomials of degree $\leqslant 2n-1$, so that n-point Gauss–Legendre rules on the respective intervals $[-1, -\frac{1}{2}]$ and $[\frac{1}{2}, 1]$ will do the job. In the other example, one has to integrate numerically as described above in connection with I_j.

6.3. *Zeros*

The zeros of π_n (including the complex ones, if any) can be conveniently computed as eigenvalues of the Hessenberg matrix (cf. [6, Section 1])

$$B_n = \begin{bmatrix} \beta_0^0 & \beta_1^1 & \beta_2^2 & \cdots & \beta_{n-2}^{n-2} & \beta_{n-1}^{n-1} \\ 1 & \beta_0^1 & \beta_1^2 & \cdots & \beta_{n-3}^{n-2} & \beta_{n-2}^{n-1} \\ 0 & 1 & \beta_0^2 & \cdots & \beta_{n-4}^{n-2} & \beta_{n-3}^{n-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \beta_0^{n-2} & \beta_1^{n-1} \\ 0 & 0 & 0 & \cdots & 1 & \beta_0^{n-1} \end{bmatrix}. \tag{6.14}$$

To compute all real zeros of π_n and π_n', we scanned a suitable interval (typically, $[-1.6, 1.6]$) for sign changes in π_n and π_n' and used the midpoints of the smallest intervals found on which π_n (resp. π_n') changes sign as initial approximations to Newton's method.

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Computing polynomials orthogonal with respect to densely oscillating and exponentially decaying weight functions and related integrals

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Abstract

Software (in Matlab) is developed for computing variable-precision recurrence coefficients for orthogonal polynomials with respect to the weight functions $1+\sin(1/t)$, $1+\cos(1/t)$, $e^{-1/t}$ on $[0, 1]$, as well as $e^{-1/t-t}$ on $[0, \infty]$ and e^{-1/t^2-t^2} on $[-\infty, \infty]$. Numerical examples are given involving Gauss quadrature relative to these weight functions.

Keywords: Orthogonal polynomials; Densely oscillating weight functions; Exponentially decaying weight functions; Gaussian quadrature

1. Introduction

The availability of constructive methods and related software for orthogonal polynomials makes it possible to numerically generate such polynomials relative to weight functions of ever increasing complexity. This is illustrated here in the case of weight functions on [0, 1], such as $1 + \sin(1/t)$ or $1 + \cos(1/t)$, that are densely oscillating near the origin, and weight functions decaying exponentially fast near the origin, such as $e^{-1/t}$ on [0, 1], none of which is in the Szegö class. We also consider the weight function $e^{-1/t-t}$ on $[0, \infty]$ and e^{-1/t^2-t^2} on $[-\infty, \infty]$. In all these cases, the moments of the weight function

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are expressible in terms of special functions (sine, cosine, and exponential integrals and modified Bessel functions), which can all be evaluated to arbitrary precision. With the moments at hand, an algorithm due to Chebyshev can be applied to compute the recurrence coefficients for the orthogonal polynomials from the given moments. Although there is a great deal of ill-conditioning involved in this approach, it can be surmounted by symbolic computation and variable-precision arithmetic as supplied, e.g., by the current release of Matlab.

A number of Matlab routines are developed for computing the recurrence coefficients of the desired orthogonal polynomials to arbitrary precision, and files are produced containing the first 40 of the coefficients to 34 decimal digits. All Matlab routines and files referenced in this paper are downloadable individually from the web site

`http://www.cs.purdue.edu/archives/2002/wxg/codes/`

containing the Matlab package `OPQ` and the relevant collection `OWF`. Numerical examples involving integration of weighted integrals by Gaussian quadrature are provided illustrating the power and effectiveness of the software.

2. Densely oscillating trigonometric weight functions

2.1. *The weight function* $w(t) = 1 + \sin(1/t)$ *on* $[0, 1]$

Constructing orthogonal polynomials relative to this weight function is a challenging task, given the densely oscillating behavior of w near the origin. The only approach that seems feasible is one based on the moments of w; indeed, the Chebyshev algorithm (cf. [2, Section 2.1.7]) generates the three-term recurrence relation for the (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; w)$ from the moments

$$\mu_k = \int_0^1 t^k [1 + \sin(1/t)]\,\mathrm{d}t, \quad k = 0, 1, 2, \ldots. \tag{1}$$

In view of the well-known ill-conditioning of this approach [2, Section 2.1.4], it can only succeed if high-precision arithmetic is used. We propose to invoke the symbolic/variable-precision capabilities of Matlab 6, Release 12, for this purpose.

To compute the moments (1), we first consider the "core moments" $\mu_k^0 = \int_0^1 t^k \sin(1/t)\,\mathrm{d}t$. By the change of variable $t \mapsto 1/t$, one has

$$\mu_k^0 = \int_1^\infty t^{-(k+2)} \sin t\,\mathrm{d}t,$$

and two integrations by part will show that μ_k^0 satisfies the recurrence relation

$$\mu_{k+1}^0 = \frac{1}{k+2}\left[\frac{1}{k+1}(\cos 1 - \mu_{k-1}^0) + \sin 1\right], \quad k = 0, 1, 2, \ldots. \tag{2}$$

Here,

$$\mu_{-1}^0 = \int_1^\infty \frac{\sin t}{t}\,\mathrm{d}t = \frac{\pi}{2} - \mathrm{Si}(1), \quad \mu_0^0 = \int_1^\infty \frac{\sin t}{t^2}\,\mathrm{d}t = \sin 1 - \mathrm{Ci}(1), \tag{3}$$

where Si and Ci are the sine and cosine integrals, respectively (cf. [1, Eqs. (5.2.1 and 5.2.2)]). In terms of the core moments μ_k^0, the actual moments μ_k are simply

$$\mu_k = \frac{1}{k+1} + \mu_k^0, \quad k = 0, 1, 2, \ldots . \tag{4}$$

The Chebyshev algorithm now takes the first $2n$ moments μ_k, $k=0, 1, \ldots, 2n-1$, and from them produces the first n recurrence coefficients α_k, β_k, $k = 0, 1, \ldots, n-1$, in the three-term recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, \ldots, n-1,$$
$$\pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \tag{5}$$

for the orthogonal polynomials π_k. This is implemented in the Matlab routine `schebyshev.m`, a symbolic version of the `OPQ` routine `chebyshev.m`. The Matlab script below uses this routine with `d`-decimal-digit arithmetic to generate the first `N` recurrence coefficients in (5).

```
% S RSIN0 Symbolic/variable-precision recurrence coefficients
%    for the weight function w(x)=1+sin(1/x) on [0,1]
%
syms mom ab
digits(d); dig=d;
mom(1)='sin(1)-Ci(1)';
mom(2)='(Si(1)-pi/2+sin(1)+cos(1))/2';
for k=3:2*N
    mom(k)=(('cos(1)'-mom(k-2))/(k-1)+'sin(1)')/k;
end
for k=1:2*N
    mom(k)=mom(k)+1/k;
end
ab=schebyshev(dig,N,mom);
```

How much precision is needed to obtain 34 good decimal digits for the first $N=40$ recurrence coefficients? Using $d = 70$ in the above routine, one obtains

$$\alpha_{39} = .510028114107\underline{742}\ldots,$$
$$\beta_{39} = .609363829421\underline{165}\ldots(-1).$$

Comparing this with 95-digit computation, one observes agreement to only the first 12 digits; the digits underlined are therefore in error. As k is decreased down from 39, the results for α_k, β_k gradually become more accurate. This behavior is typical for the ill-conditioning of the underlying moment map, which here, in the worst case, causes a loss of $70-12=58$ digits. To obtain 34 good digits for all results, one thus expects to need about 92-digit computation. It is found that 95- and 100-digit computation indeed yield results which agree to at least 37 digits. Rounded to 34 digits, the results are stored in the file `absin0`; a few beginning and final entries of the file are displayed below to 16 digits. Note that the αs are hovering around $\frac{1}{2}$ and the βs around $\frac{1}{16}$, the limit values that would be attained if the weight function were in the

Szegö class.

```
ab =
[ .5841029561609566,  1.504067061906928]
[ .4634474607770499,  .7094822535096882e-1]
[ .4977629714178322,  .7892077774694954e-1]
[ .5356590088623750,  .5547885019105795e-1]
[ .4669144430825117,  .6259489484316939e-1]
[ .4951204560106238,  .7262419731845188e-1]
       ... ...               ... ...
[ .5109646577717308,  .5919672749794708e-1]
[ .4919346767523436,  .6218164541801303e-1]
[ .4973070307106440,  .6494413841533854e-1]
[ .5100281141083978,  .6093638294208964e-1]
```

Some of the early coefficients α_k, β_k were checked (successfully) by a quadruple-precision Fortran program.

Example 1.1. Compute the integral $\int_0^1 f(t)\sin(1/t)\,\mathrm{d}t$, where $f(t) = \tan((\frac{1}{2}\pi - \delta)t)$, $\delta = .1$.

We use

$$\int_0^1 f(t)\sin(1/t)\,\mathrm{d}t = \int_0^1 f(t)[1+\sin(1/t)]\,\mathrm{d}t - \int_0^1 f(t)\,\mathrm{d}t \tag{6}$$

and apply to the first integral on the right Gaussian quadrature relative to the weight function w and to the second Gauss–Legendre quadrature on [0, 1]. This is carried out in the following script:

```
% INTSIN0 Integration relative to the weight function
%    w(t) = sin(1/t)
%
f1 = '%5.0f %21.13e %21.13e %21.13e\n';
fprintf('\n')
disp('    n    n-point Gauss')
load -ascii absin0;
ab = absin0; abl = r_jacobi01(40);
delta = .1;
for n = 4:4:36
    xwl = gauss(n,abl); xw = gauss(n,ab);
    intl = sum(xwl(:,2).*tan((pi/2-delta).*xwl(:,1)));
    ints = sum(xw(:,2).*tan((pi/2-delta).*xw(:,1)));
    int = ints-intl;
    fprintf(f1,n,int)
end
```

Table 1
Results for Example 1.1

```
>> intsin0
 n      n-point Gauss
 4      1.2716655036125e+00
 8      1.2957389942560e+00
12      1.2961790099686e+00
16      1.2961860624657e+00
20      1.2961861691603e+00
24      1.2961861708344e+00
28      1.2961861708631e+00
32      1.2961861708636e+00
36      1.2961861708636e+00
```

The output of the script is shown in Table 1.

There is practically no cancellation occurring when computing the difference of the two integrals on the right of (6).

Convergence is seen to be relatively fast (it is faster for $\delta = .3$ or $\delta = .5$), but is the limit correct? Seeing some other quadrature scheme yielding similar, albeit less accurate, results would give us more confidence in the limit value of Table 1. We tried the N-point Gauss–Legendre rule on [0, 1] for large values of N, applied directly to the integral on the left of (6), and found

```
N      N-point GL
200    1.29623...e+00
400    1.29614...e+00
600    1.29621...e+00
800    1.29617...e+00
1000   1.29619...e+00
```

The first four digits are the same as in Table 1 and are established rather quickly (relatively speaking). Evidently they correspond to the part of the integral away from zero. The difficult behavior of the integrand very close to zero causes the remaining digits to converge very hesitantly. Nevertheless, the correctness of the limit in Table 1 seems to be beyond doubt.

2.2. *The weight function* $w(t) = 1 + \cos(1/t)$ *on* [0, 1]

Analogously to Section 2.1, we define

$$\mu_k = \int_0^1 t^k [1 + \cos(1/t)]\,\mathrm{d}t, \quad k = 0, 1, 2, \ldots, \tag{7}$$

and $\mu_k^0 = \int_0^1 t^k \cos(1/t)\,\mathrm{d}t$, and find for μ_k^0 the recurrence relation

$$\mu_{k+1}^0 = \frac{1}{k+2}\left[\cos 1 - \frac{1}{k+1}(\sin 1 + \mu_{k-1}^0)\right], \quad k = 0, 1, 2, \ldots, \tag{8}$$

with

$$\mu_{-1}^0 = -\mathrm{Ci}(1), \quad \mu_0^0 = \cos 1 + \mathrm{Si}(1) - \frac{\pi}{2}. \tag{9}$$

This yields μ_k as in (4) and gives rise to a routine `sr_cos0.m` similar to `sr_sin0.m`. The first $N = 40$ recurrence coefficients can again be obtained to 34 decimal digits using 95- resp. 100-digit arithmetic; they are stored in the file `abcos0`. The first six and last four, rounded to 16 digits, are shown below.

```
ab =
[ .5658844678158393,  .9155890494404261]
[ .4366405849780814,  .1027346437337914]
[ .5796274186498604,  .5270964252517353e-1]
[ .4239578421345528,  .6199408887322155e-1]
[ .5354625727005339,  .7671995359431511e-1]
[ .5373660897782133,  .4556076502616208e-1]
       ... ...               ... ...
[ .5186905674873959,  .6081660814714736e-1]
[ .5003375738978038,  .5901663246762277e-1]
[ .4979767366985249,  .6422084071680227e-1]
[ .4970744762251129,  .6172998651366585e-1]
```

Example 1.2. Compute $\int_0^1 f(t)\sin(1/t+t)\,\mathrm{d}t$.

We write

$$\int_0^1 f(t)\sin(1/t+t)\,\mathrm{d}t = \int_0^1 f(t)\cos t\,[1+\sin(1/t)]\,\mathrm{d}t + \int_0^1 f(t)\sin t\,[1+\cos(1/t)]\,\mathrm{d}t - \int_0^1 f(t)(\cos t+\sin t)\,\mathrm{d}t \tag{10}$$

and use Gaussian quadrature relative to the weight functions $1+\sin(1/t)$ and $1+\cos(1/t)$ for the first two integrals, and Gauss–Legendre quadrature on [0, 1] for the last. The Matlab script below implements this for $f(t) = \mathrm{e}^{-t}$.

```
% INTSIN01 Integration relative to the weight function
%    w(t) = sin(1/t+t)
%
f1 = '%5.0f %21.13e\n';
fprintf('\n')
disp('    n    n-point Gauss')
load -ascii absin0; abs = absin0;
load -ascii abcos0; abc = abcos0;
abl = r_jacobi01(40);
for n = 1:7
    xwl = gauss(n,abl); xws = gauss(n,abs); xwc = gauss(n,abc);
    intl = sum(xwl(:,2).*exp(-xwl(:,1)).*(cos(xwl(:,1))...
      +sin(xwl(:,1))));
    ints = sum(xws(:,2).*exp(-xws(:,1)).*cos(xws(:,1)));
    intc = sum(xwc(:,2).*exp(-xwc(:,1)).*sin(xwc(:,1)));
    int = ints+intc-intl;
    fprintf(f1,n,int)
end
```

Table 2
Results for Example 1.2 when $f(t) = e^{-t}$

```
>> intsin01
n       n-point Gauss
1       1.5532688394788e-01
2       1.5896667464309e-01
3       1.5875741460598e-01
4       1.5875671404065e-01
5       1.5875671541036e-01
6       1.5875671541391e-01
7       1.5875671541391e-01
```

The results are shown in Table 2.

Gauss–Legendre quadrature applied directly to the integral on the left of (10), with $N = 200{:}\,200{:}\,1000$ points, manages to confirm only the first two digits, but enough to have confidence in the rapidly converging sequence of approximations displayed in Table 2.

3. Rapidly decaying exponential weight functions

Replacing the trigonometric functions in Sections 2.1 and 2.2 by the exponential function yields rapidly decaying exponential weight functions.

3.1. The weight function $w(t) = \exp(-1/t)$ on $[0, 1]$

Proceeding as in Section 2, we start from the moments

$$\mu_k = \int_0^1 t^k e^{-1/t}\, dt, \quad k = 0, 1, 2, \ldots, \tag{11}$$

and use the Chebyshev algorithm in high precision to generate the recurrence coefficients of the desired orthogonal polynomials $\pi_k(\cdot; w)$. By a change of variable, we have

$$\mu_k = \int_1^\infty t^{-(k+2)} e^{-t}\, dt = E_{k+2}(1), \tag{12}$$

where E_n is the exponential integral (cf. [1, Eq. (5.1.4)]), which can be computed recursively [1, Eq. (5.1.14)], giving

$$\mu_{k+1} = \frac{1}{k+2}(e^{-1} - \mu_k), \quad k = 0, 1, 2, \ldots,$$
$$\mu_0 = E_2(1). \tag{13}$$

Table 3
Results for Example 3.1

```
>> intexp0
 n      n-point Gauss
 2      8.1262554100479e-02
 4      8.1255735149253e-02
 6      8.1255733983155e-02
 8      8.1255733982820e-02
10      8.1255733982819e-02
12      8.1255733982819e-02
```

This is incorporated in the routine `sr_exp0.m`, as shown below:

```
% S REXP0 Symbolic/variable-precision recurrence coefficients
%    for the weight function w(x)=exp(-1/x) on [0,1]
%
syms mom ab
digits(d); dig=d;
mom(1)=vpa('Ei(2,1)',d);
for k=2:2*N
    mom(k)=('exp(-1)'-mom(k-1))/k;
end
ab=schebyshev(dig,N,mom);
```

For $N = 40$, the choice $d = 70$ yields results correct to 9 or more decimal digits, corresponding to a loss of as much as 61 digits. With $d = 95$ and $d = 100$, therefore, we can again secure 34 correct decimals. The respective results are stored in the file `abexp0`.

Example 3.1. Compute $\int_0^1 \ln(1+t)\mathrm{e}^{-1/t}\,\mathrm{d}t$.

The routine `sr_exp0.m` is used, in conjunction with the routine `gauss.m`, to generate Gaussian quadrature rules for the weight function $\exp(-1/t)$, which, applied to the integral of Example 3.1, produce results as shown in Table 3.

The same limit value is obtained by 102-point Gauss–Laguerre quadrature of $\mathrm{e}^{-1}(1+t)^{-2}\log(1+(1+t)^{-1})$; see the routine `intexp0.m`.

3.2. *The weight function* $w(t) = \exp(-1/t - t)$ *on* $[0, \infty]$

Here, the moments of w are expressible in terms of the modified Bessel functions according to [3, Eq. (3.471.9)]

$$\mu_k = \int_0^\infty t^k \mathrm{e}^{-(1/t+t)}\,\mathrm{d}t = 2K_{k+1}(2), \quad k = 0, 1, 2, \ldots . \tag{14}$$

This can be computed recursively as follows (cf. [1, Eq. (9.6.26)]):

$$\mu_{k+1} = (k+1)\mu_k + \mu_{k-1}, \quad k = 0, 1, 2, \ldots,$$

$$\mu_{-1} = 2K_0(2), \quad \mu_0 = 2K_1(2), \tag{15}$$

and gives rise to the routine `sr_exp0inf.m`:

```
% S REXP0INF Symbolic/variable-precision recurrence
%    coefficients for the weight function
%    w(x) = exp(-1/x-x) on [0,inf]
%
syms mom ab
digits(d); dig = d;
mom(1) = vpa('2*BesselK(1,2)',dig);
mom(2) = mom(1)+vpa('2*BesselK(0,2)',dig);
for k = 3:2*N
   mom(k) = (k-1)*mom(k-1)+mom(k-2);
end
ab = schebyshev(dig,N,mom);
```

In the case $N = 40$, $d = 70$, the loss of accuracy is at most 36 digits, leaving us with about 34 correct digits. This is confirmed by running `sr_exp0inf` with $d = 75$ and $d = 80$, the results of which agree to at least 38 digits. The file `abexp0inf` is provided with 34-digit values of the desired recurrence coefficients. The beginning and end of the file, rounded to 16 decimals, are shown below:

```
ab =
[ 1.814307758763789,  .2797317636330449]
[ 3.647885050815283,  1.336902874017094]
[ 5.563608408242503,  4.576187502809998]
[ 7.510248881089434,  9.776110045536486]
[ 9.472385776425876,  16.95364518291704]
[ 11.44360258233455,  26.11622048172850]
       ... ...              ... ...
[ 73.23900952424970,  1300.294223771922]
[ 75.23687505008481,  1373.374066736622]
[ 77.23481475899122,  1448.453190623454]
[ 79.23282425676095,  1525.531620678047]
```

Example 3.2. Compute $\int_0^\infty J_0(t)\mathrm{e}^{-1/t-t}\,\mathrm{d}t$.

Gauss quadrature relative to the weight function $w(t) = \exp(-1/t - t)$ yields results as shown in Table 4.

In contrast, Gauss–Laguerre quadrature of $J_0(t)\mathrm{e}^{-1/t}$ requires $N = 1000$ points only to get 11-digit accuracy. Such is the debilitating effect of the strong decay of $\mathrm{e}^{-1/t}$ as $t \downarrow 0$. On the other hand,

Table 4
Results for Example 3.2

```
>> intexp0inf
 n      n-point Gauss
 4      1.1162402700893e-01
 8      1.1153340191221e-01
12      1.1153288987809e-01
16      1.1153289176609e-01
20      1.1153289176207e-01
24      1.1153289176207e-01
```

writing

$$\int_0^\infty J_0(t)\mathrm{e}^{-1/t-t}\,\mathrm{d}t = \int_0^1 [J_0(t)\mathrm{e}^{-t}]\mathrm{e}^{-1/t}\,\mathrm{d}t + \mathrm{e}^{-1}\int_0^\infty [J_0(1+t)\mathrm{e}^{-1/(1+t)}]\mathrm{e}^{-t}\,\mathrm{d}t$$

and evaluating the first integral on the right by n-point Gauss quadrature with respect to the weight function $\mathrm{e}^{-1/t}$ (cf. Section 3.1) and the second by n-point Gauss–Laguerre quadrature yields also 11-digit accuracy, but already with $N = 40$. Nevertheless, this requires two different, more slowly convergent, quadrature routines, compared to just one in the solution given in Example 3.2. The slowdown is actually caused by the Gauss–Laguerre quadrature of the second integral. See the routine `intexp0inf.m`.

3.3. The weight function $\exp(-1/t^2 - t^2)$ *on* $[-\infty, \infty]$

Similarly as in Section 3.2, one can express the moments in terms of modified Bessel functions: all moments of odd order are zero, while those of even order are

$$\mu_{2k} = 2K_{k+1/2}(2), \quad k = 0, 1, 2, \ldots, \tag{16}$$

and can be computed recursively by

$$\mu_{2k+2} = (k + \tfrac{1}{2})\mu_{2k} + \mu_{2k-2}, \quad k = 0, 1, 2, \ldots,$$

$$\mu_{-2} = \mu_0 = 2K_{1/2}(2). \tag{17}$$

This is done in the routine `sr_expminfpinf.m`:

```
% S REXPMINFPINF Symbolic/variable-precision recurrence
%    coefficients for the weight function
%    w(x) = exp(-1/x^2-x^2) on [-inf,inf]
%
syms mom ab
digits(d); dig = d;
mom(2:2:2*N) = vpa(0,dig);
mom(1) = vpa('2*BesselK(1/2,2)',dig);
mom(3) = 3*mom(1)/2;
for k = 3:2*N
    mom(2*k-1) = (k-3/2)*mom(2*k-3)+mom(2*k-5);
end
ab = schebyshev(dig,N,mom);
```

Ill-conditioning of the moment map here is considerably less severe than in the case of the weight function $\exp(-1/t - t)$, a phenomenon similar to one observed for Laguerre vs Hermite weight functions (see [2, Tables 2.2 and 2.3]). Comparing the results of `sr_expminfpinf.m` for $d = 50$ with those for $d = 55$ reveals a loss of at most 17 digits as compared to 36 digits in the case of `sr_exp0inf.m` (cf. Section 3.2). The choices $d = 55$ and $d = 60$ produce results that agree to at least 38 digits. They are stored in the file `abexpminfpinf` to 34 digits and, rounded to 16 digits, are partially displayed below.

```
ab =
[0, .2398755439361229]
[0, 1.500000000000000]
[0, .6666666666666667]
[0, 2.583333333333333]
[0, 1.475806451612903]
[0, 3.659439450026441]
 ...       ...
[0, 16.49963635631090]
[0, 20.31604933808658]
[0, 17.46711169129393]
[0, 21.34281282504185]
```

Table 5
Results for Example 3.3

```
>> intexpminfpinf
 n      n-point Gauss
 2      1.5040374279876e-01
 4      1.1308193957943e-01
 6      1.1342796227803e-01
 8      1.1342695840745e-01
10      1.1342695981592e-01
12      1.1342695981475e-01
14      1.1342695981475e-01
```

Example 3.3. Compute $\int_{-\infty}^{\infty} \mathrm{e}^{-t} \cos t \, \mathrm{e}^{-1/t^2 - t^2} \, \mathrm{d}t$.

Table 5 illustrates the use of Gauss quadrature relative to the weight function $w(t) = \exp(-1/t^2 - t^2)\,\mathrm{d}t$.

In stark contrast, 1000-point Gauss–Hermite quadrature of $\mathrm{e}^{-t-1/t^2} \cos t$ yields only 8 correct digits; see the routine `intexpminfpinf.m`.

References

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16.11. [195] "Variable-precision recurrence coefficients for nonstandard orthogonal polynomials"

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ORIGINAL RESEARCH

Variable-precision recurrence coefficients for nonstandard orthogonal polynomials

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Abstract A symbolic/variable-precision procedure is described (and implemented in Matlab) that generates an arbitrary number `N` of recurrence coefficients for orthogonal polynomials to any given precision `nofdig`. The only requirement is the availability of a variable-precision routine for computing the first 2`N` moments of the underlying weight function to any precision `dig` > `nofdig`. The procedure is applied to Freud, Bose–Einstein, and Fermi–Dirac orthogonal polynomials.

Keywords Variable-precision recurrence coefficients · Symbolic Chebyshev algorithm · Freud orthogonal polynomials · Bose–Einstein orthogonal polynomials · Fermi–Dirac oerthogonal polynomials

Mathematics Subject Classifications (2000) 3304 · 33C47

1 Introduction

The availability of symbolic/variable-precision software for orthogonal polynomials (for software in *Mathematica*, see the package `OrthogonalPolynomials` in [1]; for software in *Matlab*, the package `SOPQ` at http://www.cs.purdue.edu/archives/2002/wxg/codes) makes it possible to generate the respective recurrence coefficients to arbitrary precision also in nonstandard cases where they are not known explicitly. The basic vehicle is the Chebyshev

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algorithm, which allows us to compute the recurrence coefficients from the moments of the underlying weight function. Thus, all that is required is a procedure for evaluating the moments in variable-precision arithmetic. Since, as is well known, the problem of computing recurrence coefficients from moments is highly unstable, it will be necessary to employ high-precision computation to overcome the instability.

We illustrate this capability for a variety of weight functions, thereby, in part, extending existing software and tables to an arbitrary number of recurrence coefficients and arbitrary precision.

In Section 2 the basic algorithm is described. It uses the symbolic Matlab program[1] `schebyshev.m` implementing the Chebyshev algorithm and requires a symbolic routine `mom`*name*`.m` that generates the necessary moments. In the subsequent sections, the algorithm is applied to a variety of orthogonal polynomials, including Freud polynomials, Bose–Einstein polynomials, and Fermi–Dirac polynomials, corresponding, respectively, to weight functions $w(x) = |x|^\alpha \exp(-|x|^\beta)$ on $\mathbb{R}$ $(\alpha > -1,\ \beta > 0)$, $w(x) = [x/(e^x - 1)]^r$, $w(x) = [1/(e^x + 1)]^r$ on $\mathbb{R}_+$ $(r = 1, 2, 3, \ldots)$.

2 Basic algorithm

Suppose we are given a (nonnegative) weight function w on some interval (a, b), $-\infty \le a < b \le \infty$, defining a set of (monic) orthogonal polynomials π_k, $k = 0, 1, 2, \ldots$, where

$$\begin{aligned} \pi_{k+1}(x) &= (x - \alpha_k)\pi_k(x) - \beta_k \pi_{k-1}(x), \\ &\qquad k = 0, 1, 2, \ldots, \\ \pi_0(x) &= 1, \quad \pi_{-1}(x) = 0 \end{aligned} \tag{1}$$

is the three-term recurrence relation satisfied by the polynomials π_k. Here, $\alpha_k = \alpha_k(w)$, $\beta_k = \beta_k(w)$ are certain constants depending on the weight function w, where $\alpha_k \in \mathbb{R}$, $\beta_k > 0$, and β_0, though arbitrary, is defined by $\beta_0 = \int_a^b w(x)\mathrm{d}x$. Our objective is to compute the first `N` of these coefficients to an accuracy of `nofdig` decimal places. To do so in Matlab, we store these coefficients in an `N` × 2 array `ab`, where the first column of `ab` contains $\alpha_0, \alpha_1, \ldots, \alpha_{N-1}$, and the second column $\beta_0, \beta_1, \ldots, \beta_{N-1}$ (cf. [3, §2.1]).

In principle, these coefficients can be computed from the first 2`N` moments

$$\mu_k = \int_a^b x^k w(x)\mathrm{d}x, \quad k = 0, 1, \ldots 2N - 1, \tag{2}$$

[1] All Matlab routines referred to in this paper can be downloaded from the Purdue web site mentioned at the beginning of this section.

of w by means of the Chebyshev algorithm (cf. [3, §2.2], where $a_k = b_k = 0$, all k). Because of the severe ill-conditioning of the map from the 2N moments μ_k to the 2N recurrence coefficients $\alpha_k, \beta_k, 0 \le k \le N-1$, the desired accuracy of nofdig decimal digits can be achieved only if the computation is carried out in a precision considerably higher than nofdig. We determine this required precision iteratively by starting with a precision of dig0=nofdig decimal digits and increasing it in steps of dd = 10 digits until the desired accuracy of nofdig digits is achieved. (The choice dd = 10 was arrived at by experimentation as being reasonably efficient, but can easily be changed if deemed necessary.)

The procedure requires two variable-precision algorithms, the first one for computing the 2N moments μ_k in dig-digit arithmetic, and the second one implementing the Chebyshev algorithm in the same precision of dig decimal digits. If the given weight function w depends on parameters, then so does the first routine,

$$\text{mom} = \text{mom}\textit{name}(\text{dig}, \text{N}, \ldots), \tag{3}$$

where *name* is the name for the orthogonal polynomials in question, and the three dots indicate the list of parameters. The second routine is the symbolic Chebyshev algorithm (cf. Section 1),

$$\text{ab} = \text{schebyshev}(\text{dig}, \text{N}, \text{mom}). \tag{4}$$

The details of the iterative procedure can be gathered from the following Matlab function.

```
% SR_name  This computes the first N recurrence
% coefficients α_k, β_k, k = 0,1,...,N-1, to an
% accuracy of nofdig digits for the system of
% orthogonal polynomials named name. The output
% variable ab is the N×2 array of the nofdig-digit
% recurrence coefficients, and dig is the number
% of digits required to achieve the target
% precision of nofdig decimal places.
%
function [ab,dig]=sr_name(N,...,nofdig)
syms mom ab ab0 ab1
dd=10; dig0=nofdig;
i=dig0-dd;
maxerr=1;
while maxerr>.5*10^(-nofdig)
   i=i+dd; dig=i;
   mom=momname(dig,N,...);
   if i==dig0
      ab0=schebyshev(dig,N,mom);
```

```
        else
            ab1=schebyshev(dig,N,mom);
            serr=vpa(abs(ab1-ab0),dig);
            err=subs(serr);
            maxerr=max(max(err));
            ab0=ab1;
        end
    end
    ab=vpa(ab1,nofdig);
```

The procedure is essentially the same for any particular system of orthogonal polynomials and requires only the specification of the routine mom*name*. Still, there are instances where instead of an absolute error criterion, a relative one may be preferable, either for the α-coefficients, or the β-coefficients, or both. If, for example, we want to control the absolute error in the α-coefficients and the relative error in the β-coefficients, we let the statement defining `serr` be followed by

$$\texttt{serr(:, 2)} = \texttt{vpa(abs((ab1(:, 2)} - \texttt{ab0(:, 2))./ab1(:, 2)), dig).} \tag{5}$$

Similarly for other combinations of absolute and relative error. In the special case of symmetric weight functions, where all $\alpha_k = 0$, to control the relative error of the β-coefficients, it suffices to define `serr` by the right-hand side of (5).

3 Freud and half-range Hermite polynomials

Freud orthogonal polynomials are associated with the weight function

$$w(x) = |x|^{\alpha} \exp(-|x|^{\beta}), \quad x \in \mathbb{R},\ \alpha > -1,\ \beta > 0. \tag{6}$$

Its moments are easily found to be

$$\mu_k = \begin{cases} 0 & \text{if } k \text{ is odd,} \\ \dfrac{2}{\beta}\,\Gamma\left(\dfrac{k+\alpha+1}{\beta}\right) & \text{if } k \text{ is even.} \end{cases} \tag{7}$$

The `dig`-digit routine mom*freud*.m, therefore, looks as follows.

```
% MOMFREUD
%
function mom=momfreud(dig,N,alpha,beta)
digits(dig);
for k=1:2*N
    if rem(k,2)==0
        mom(k)=0;
```

```
    else
       mom(k)=vpa(2*gamma(vpa((k+alpha)/beta))/beta);
    end
end
```

Since w is symmetric, all $\alpha_k = 0$. The special case $\beta = 2$, giving rise to generalized Hermite polynomials, may serve as a test example, since the recurrence coefficients are known to be $\beta_0 = \Gamma((\alpha+1)/2)$, $\beta_k = (k + \varepsilon_k\alpha)/2$, where $\varepsilon_k = 0$ if k is even, and $\varepsilon_k = 1$ if k is odd. Running `sr_freud(N,alpha,beta,nofdig)` with `N` $= 100$, `alpha` $= \pm 1/2$, `beta` $=$ 2, and `nofdig` $= 40$, indeed passed the test.

The routine was then applied to generate the first `N` $= 100$ recurrence coefficients β_k for the Freud weight (6) with $\alpha = 0$, $\beta = 4{:}2{:}10$, calling for `nofdig`=32 digit accuracy. The results can be found in the files `coefffreud4–10` on the web site http://www.cs.purdue.edu/archives/2001/wxg/tables. In the case $\beta = 4$, they are in complete agreement with results obtained with *Mathematica* by A. Cvetković and G. V. Milovanović, using a different method (the nonlinear recurrence relation in [7]). Each case took about 30 min. to run on a Sun Ultra 5 workstation and required as much as 112-digit calculations.

As a matter of curiosity, when $\beta = 6$, we observed that $\beta_1 = \beta_2$. Generally, however, the β_k slowly increase monotonically (except for the first few). In fact, for $\beta \geq 2$, the following asymptotic result holds (cf. [6, eq (1.10)], adapted to our notations, which differ from those in [6]),

$$\beta_k = \frac{1}{4}(\gamma k)^{2/\beta} + O(k^{2/\beta-2}), \quad k \to \infty, \tag{8}$$

where

$$\gamma = \frac{\Gamma(\beta/2)\Gamma(1/2)}{\Gamma((\beta+1)/2)}. \tag{9}$$

Our computations, moreover, suggest that

$$\frac{4\beta_k}{(\gamma k)^{2/\beta}} \downarrow 1 \quad \text{for } k \geq k_0(\beta), \tag{10}$$

where $k_0(\beta)$ is relatively small (equal to $5, 6, 4, 4$ for respectively $\beta = 4, 6, 8, 10$).

A weight function somewhat related to Freud's is the half-range Hermite weight function

$$w(x) = \exp(-x^2), \quad x \in \mathbb{R}_+, \tag{11}$$

whose moments are given by

$$\mu_k = \frac{1}{2}\Gamma\left(\frac{k+1}{2}\right), \quad k = 0, 1, 2, \ldots, 2\mathtt{N}-1, \tag{12}$$

and evaluated to dig decimal places by the routine mom*halfrangehermite*.m:

```
% MOMHALFRANGEHERMITE
%
function mom=momhalfrangehermite(dig,N)
digits(dig);
for k=1:2*N
   mom(k)=vpa(gamma(vpa(k/2))/2);
end
```

The first 100 recurrence coefficients are generated by the routine sr_*halfrangehermite*(N,nofdig) to nofdig = 32 decimal places and stored in the file coeffhalfrangehermite of the web site indicated above. They agree (except for occasional last-digit discrepancies of one unit) with all 25-digit values produced by other methods and stored in the OPQ file abhrhermite (cf. [2, Example 2.31]).

4 Bose–Einstein polynomials

Polynomials orthogonal with respect to the weight function

$$\left(\frac{x}{e^{\omega x}-1}\right)^r \quad \text{on } \mathbb{R}_+,\ \omega > 0,\ r \in \mathbb{N}_+$$

we call Bose–Einstein polynomials since for $r = 1$ the weight function in statistical mechanics defines a Bose–Einstein distribution. For the purpose of computing their recurrence coefficients, it suffices to consider the special case $\omega = 1$, since the α-coefficients in this special case, if divided by ω, and the β-coefficients divided by ω^2, yield the recurrence coefficients in the general case $\omega > 0$. So let the weight function be

$$w(x) = \left(\frac{x}{e^x-1}\right)^r \quad \text{on } \mathbb{R}_+,\ r \in \mathbb{N}_+. \tag{13}$$

The moments of w,

$$\mu_k^{(r)} = \int_0^\infty \frac{x^{k+r}}{(e^x-1)^r}\,dx, \quad k = 0, 1, 2, \ldots, 2\mathtt{N}-1, \tag{14}$$

are known explicitly when $r = 1$,

$$\mu_k^{(1)} = \Gamma(k+2)\zeta(k+2) \tag{15}$$

(cf. [5, eq 3.411.1]). To obtain the moments for any fixed $r > 1$, we observe that for $\rho > 1$,

$$\begin{aligned}\mu_{k+1}^{(\rho-1)} &= \int_0^\infty \frac{x^{k+\rho}}{(e^x-1)^{\rho-1}}\,dx = \int_0^\infty \frac{x^{k+\rho}}{(e^x-1)^\rho}\,[e^x-1]dx \\ &= \int_0^\infty \frac{x^{k+\rho}}{(e^x-1)^\rho}\,e^x dx - \mu_k^{(\rho)},\end{aligned}$$

that is,

$$\mu_k^{(\rho)} = \int_0^\infty \frac{x^{k+\rho}}{(e^x-1)^\rho} e^x \mathrm{d}x - \mu_{k+1}^{(\rho-1)}.$$

The integral on the right can be evaluated using integration by parts,

$$\begin{aligned}\int_0^\infty \frac{x^{k+\rho}}{(e^x-1)^\rho} e^x \mathrm{d}x &= -\frac{1}{\rho-1}\int_0^\infty x^{k+\rho}\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{1}{(e^x-1)^{\rho-1}}\right\}\mathrm{d}x \\ &= -\frac{1}{\rho-1}\left\{\frac{x^{k+\rho}}{(e^x-1)^{\rho-1}}\Big|_0^\infty - (k+\rho)\int_0^\infty \frac{x^{k+\rho-1}}{(e^x-1)^{\rho-1}}\mathrm{d}x\right\} \\ &= -\frac{1}{\rho-1}\left\{-(k+\rho)\mu_k^{(\rho-1)}\right\}.\end{aligned}$$

Therefore,

$$\mu_k^{(\rho)} = \frac{k+\rho}{\rho-1}\mu_k^{(\rho-1)} - \mu_{k+1}^{(\rho-1)}. \tag{16}$$

Since the moments $\mu_k^{(1)}$ are known by (15), the relation (16) allows us to compute from the first $2\mathtt{N}+r$ of them recursively (in ρ) all the desired moments in (14). For example, with $\rho = 2$, we find $\mu_k^{(2)} = (k+2)\mu_k^{(1)} - \mu_{k+1}^{(1)}$, hence, by (15), $\mu_k^{(2)} = \Gamma(k+3)[\zeta(k+2) - \zeta(k+3)]$, which is a known result (cf. [5, eq 3.423.1]).

The following routine mom*boseeinstein*.m implements the above procedure in dig-digit arithmetic.

```
% MOMBOSEEINSTEIN
%
function mom=momboseeinstein(dig,N,r)
digits(dig);
for k=1:2*N+r
   m(k,1)=gamma(vpa(k+1))*zeta(vpa(k+1));
   if r==1 & k<=2*N
      mom(k)=m(k,1);
   end
end
if r>1
   for rho=2:r
      for k=1:2*N+r-rho
         m(k,rho)=vpa(((k+rho-1)/(rho-1))*m(k,rho-1)...
            -m(k+1,rho-1));
```

```
            if rho==r
               mom(k)=m(k,rho);
            end
         end
      end
   end
```

In the corresponding procedure `sr_boseeinstein(N,r,nofdig)`, it is advisable to use the relative error criterion, both for the α- and β-coefficients (cf. the final paragraph in Section 2). When run with `N` $= 100$, `r` $= 1$ and 2, `nofdig` $= 32$, it reproduced the first 40 recurrence coefficients in Table 1 and Table 2 of [4, Appendix 1], with almost perfect agreement in all 25 decimal digits given there, the exceptions being occasional discrepancies of one unit in the last decimal place. The running times on a Sun Ultra 5 workstation, for $r = 1:4$, were respectively about 52, 72, 86, and 102 min., and the required precisions 142, 182, 212, and 242 digits. The results, along with those for `r` $= 3$ and 4, are posted in the files `coeffboseeinstein1–4` on the web site given in Section 3.

5 Fermi–Dirac polynomials

We call Fermi–Dirac polynomials those that are orthogonal with respect to the weight function

$$\left(\frac{1}{e^{\omega x}+1}\right)^r \quad \text{on } \mathbb{R}_+,\ \omega > 0,\ r \in \mathbb{N}_+$$

since, for $r = 1$, it defines in statistical mechanics a Fermi–Dirac distribution. As explained in Section 4, it suffices to deal with the case $\omega = 1$,

$$w(x) = \left(\frac{1}{e^x+1}\right)^r \quad \text{on } R_+,\ r \in \mathbb{N}_+. \tag{17}$$

To compute the moments

$$\mu_k^{(r)} = \int_0^\infty \frac{x^k}{(e^x+1)^r}\,\mathrm{d}x, \quad k = 0, 1, \ldots, 2\mathtt{N}-1, \tag{18}$$

of w, for fixed $r \geq 1$, we first observe that

$$\begin{aligned}\mu_0^{(1)} &= \int_0^\infty \frac{\mathrm{d}x}{e^x+1} = \int_1^\infty \frac{\mathrm{d}t}{t(t+1)} = \lim_{u\to\infty}\int_1^u \left(\frac{1}{t}-\frac{1}{t+1}\right)\mathrm{d}t \\ &= \lim_{u\to\infty}\left(\ln\frac{u}{u+1}+\ln 2\right) = \ln 2,\end{aligned} \tag{19}$$

and, for $k > 0$,

$$\mu_k^{(1)} = (1-2^{-k})\Gamma(k+1)\zeta(k+1), \quad k = 1, 2, \ldots, 2\mathtt{N}-1 \tag{20}$$

(cf. [5, eq 3.411.3]). Furthermore,

$$\mu_k^{(\rho+1)} - \mu_k^{(\rho)} = \int_0^\infty \frac{x^k}{(e^x+1)^{\rho+1}}[1-(e^x+1)]\mathrm{d}x$$
$$= -\int_0^\infty x^k \frac{e^x}{(e^x+1)^{\rho+1}}\,\mathrm{d}x = \frac{1}{\rho}\int_0^\infty x^k \frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{1}{(e^x+1)^\rho}\right\}\mathrm{d}x, \tag{21}$$

and using integration by parts,

$$\mu_k^{(\rho+1)} = \mu_k^{(\rho)} - \begin{cases} \dfrac{1}{\rho\cdot 2^\rho} & \text{if } k=0, \\ \dfrac{k}{\rho}\mu_{k-1}^{(\rho)} & \text{if } k>0. \end{cases} \tag{22}$$

The Eq. 22 with $k=0$, in combination with (19), allows us to compute

$$\mu_0^{(\rho)} \quad \text{for} \quad \rho = 1,2,\ldots,r, \tag{23}$$

which, in particular, gives us the zero-order moment $\mu_0^{(r)}$. Next, (20) can be used to compute

$$\mu_k^{(1)} \quad \text{for} \quad k = 1,2,\ldots,2\mathtt{N}-1, \tag{24}$$

which, if $r=1$, gives us the remaining higher-order moments. If $r>1$, we use (23) and (24) as initial values to compute from (22), successively for $k=1,2,\ldots,2\mathtt{N}-1$, the quantities $\mu_k^{(\rho)}$ for $\rho=2,3,\ldots,r$, which yields the higher-order moments $\mu_k^{(r)}$, $k=1,2,\ldots,2\mathtt{N}-1$.

The procedure outlined above is implemented in the following `dig`-digit routine mom*fermidirac*.m.

```
% MOMFERMIDIRAC
%
function mom=momfermidirac(dig,N,r)
digits(dig);
m(1,1)=vpa('log(2)');
if r==1
   mom(1)=m(1,1);
else
   for rho=1:r-1
      m(1,rho+1)=vpa((m(1,rho)-1/(rho*(2^rho))));
   end
   mom(1)=m(1,r);
end
```

```
for k=2:2*N
    m(k,1)=vpa((1-2^(1-k))*gamma(vpa(k))*zeta(vpa(k)));
    if r==1
        mom(k)=m(k,1);
    end
end
if r>1
    for k=2:2*N
        for rho=1:r-1
            m(k,rho+1)=vpa(m(k,rho)-(k-1)*m(k-1,rho)/rho);
        end
        mom(k)=m(k,r);
    end
end
```

The procedure `sr_fermidirac(N,r,nofdig)` (with relative error control in both the α- and β-coefficients) was run with `N` $= 100$, `r` $= 1:4$ and `nofdig`$=$ 32. The results, obtained with an effort comparable to the one in the case of Bose–Einstein coefficients, are stored in the files `coeffermidirac1`–`4` on the web site mentioned in Section 3. In the process, Tables 3–4 in [4] of the first 40 recurrence coefficients for $r = 1$ and 2 were checked and found to be correct in all 25 decimal digits given there.

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ORIGINAL PAPER

Sub-range Jacobi polynomials

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Abstract Orthogonal polynomials relative to the Jacobi weight function, but orthogonal on a strict subinterval of $[-1, 1]$, are studied, in particular with regard to their numerical computation. Related Gaussian quadrature rules are also considered.

Keywords Sub-range Jacobi polynomials · Computation of recurrence coefficients and special Gaussian quadrature rules

Mathematics Subject Classifications (2010) 33C47 · 65D20

1 Introduction

Let $w \not\equiv 1$ be one of the classical weight functions for orthogonal polynomials and I the associated interval of orthogonality. Given a strict subinterval $I_0 \subset I$, polynomials orthogonal on I_0 relative to w are here called *sub-range orthogonal polynomials* relative to w. Examples of such polynomials, occurring in physics and statistics, are the half-range Hermite polynomials orthogonal on $\mathbb{R}_+$ relative to the weight function $w(t) = e^{-t^2}$ (cf. [6, Examples 2.31 and 2.41], [5, Section 2.2(iii)]), the finite-range Hermite polynomials orthogonal with respect to the same weight function, but on $[-c, c]$ or $[0, c]$ $(c > 0)$, the latter being known as Maxwell's distribution, and the finite-range Laguerre polynomials orthogonal relative to the weight function $w(t) = e^{-t}$ on $[0, c]$ (cf. [5, Section 2.2,(iv)]).

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Recently, in connection with subperiodic trigonometric quadrature, Da Fies and Vianello [1] used sub-range Chebyshev polynomials orthogonal with respect to the weight function $w(t) = (1 - t^2)^{-1/2}$ on the interval $[-c, c]$, where $c = \sin(\omega/2)$, $0 < \omega < \pi$, and applied them to construct interesting Gaussian product formulae for integration over circular and annular sectors, circular zones, and circular lenses; see also [2]. In their computations they apply the modified Chebyshev algorithm (cf. [6, Section 2.1.7]) with Chebyshev moments of the weight function $(1 - c^2t^2)^{-1/2}$ on $[-1, 1]$; see [1, Section 2.1]. This work is specifically tailored to Chebyshev weight functions and rests heavily on the ability to accurately compute the modified moments—a nontrivial task. A more general, and at the same time simpler, approach is via discretization methods (cf. [6, Section 2.2.2]), which are used here to compute not only sub-range Chebyshev, but arbitrary sub-range Jacobi polynomials. The same method, in principle, can be applied to any weight function w.

2 Sub-range Jacobi polynomials and related Gaussian quadratures

Let

$$w(x) = (1 - x)^\alpha (1 + x)^\beta, \quad \alpha > -1, \ \beta > -1, \tag{2.1}$$

be the Jacobi weight function on $I = [-1, 1]$, and let the subinterval be $I_0 = [-c, c]$, $0 < c < 1$. Denote the corresponding (monic) sub-range Jacobi polynomials by $\pi_k(x)$, so that

$$\int_{-c}^{c} \pi_k(x)\pi_\ell(x)w(x)dx = 0 \quad \text{if } k \neq \ell.$$

Define

$$p_k(t) = \frac{1}{c^k}\pi_k(ct), \quad k = 0, 1, 2, \ldots . \tag{2.2}$$

These are monic polynomials satisfying the orthogonality relation

$$\int_{-1}^{1} p_k(t)p_\ell(t)w(ct)dt = 0 \quad \text{if } k \neq \ell, \tag{2.3}$$

and therefore satisfy a three-term recurrence relation

$$\begin{aligned} p_{k+1}(t) &= (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ p_0(t) &= 1, \quad p_{-1}(t) = 0, \end{aligned} \tag{2.4}$$

where by convention, $b_0 = \int_{-1}^{1} w(ct)dt$. The coefficients a_k, b_k (which depend on c) can easily be computed by the "general-purpose" discretization method described in [6, Section 2.2.2], using the software package OPQ[1] (for details,

[1]The package OPQ can be accessed at OPQ.html of the website http://www.cs.purdue.edu/archives/2002/wxg/codes, and all Matlab routines referenced in this paper at SRJAC of the same website.

see Section 3). Once they have been computed, the recurrence coefficients α_k, β_k of the sub-range Jacobi polynomials can be obtained by putting $t = x/c$ in (2.4) and multiplying through by c^{k+1}. In view of (2.2), i.e., $c^k p_k(x/c) = \pi_k(x)$, one gets

$$\alpha_k = ca_k, \quad k \geq 0; \quad \beta_k = c^2 b_k, \quad k \geq 1. \tag{2.5}$$

Furthermore, by convention, $\beta_0 = \int_{-c}^{c} w(x)dx = c\int_{-1}^{1} w(ct)dt$, so that

$$\beta_0 = cb_0. \tag{2.6}$$

The first n recurrence coefficients a_k, b_k in (2.4) allow us to generate the n-point Gauss formula

$$\int_{-1}^{1} f(t)w(ct)dt = \sum_{k=1}^{n} w_k(c) f(t_k(c)), \quad f \in \mathbb{P}_{2n-1}, \tag{2.7}$$

using the `OPQ` routine `gauss.m`. As c varies from 0 to 1, (2.7) describes a continuous transition from the Gauss–Legendre to the Gauss–Jacobi rule.

The same approach can be used to deal with asymmetric subintervals I_0, say, $I_0 = [-1, c]$, where $0 < c < 1$. Instead of the simple transformation $x = ct$, used in (2.2), one must use

$$x = x(t; c) := \frac{1}{2}(1 + c)t - \frac{1}{2}(1 - c), \quad -1 \leq t \leq 1.$$

The polynomials

$$p_k(t) = \frac{1}{\left[\frac{1}{2}(1 + c)\right]^k} \pi_k(x(t; c)), \quad k = 0, 1, 2, \ldots, \tag{2.8}$$

are then orthogonal on $[-1, 1]$ with respect to the weight function $w(x(t; c))$. If (2.4) is again their recurrence relation, with $b_0 = \int_{-1}^{1} w(x(t; c))dt = [\frac{1}{2}(1 + c)]^{-1} \int_{-1}^{c} w(x)dx$, we get for the recurrence coeficients α_k, β_k of the sub-range Jacobi polynomials

$$\alpha_k = a_k - \frac{1}{2}(1 - c), \quad k \geq 0; \quad \beta_k = \left[\frac{1}{2}(1 + c)\right]^2 b_k, \quad k \geq 1, \tag{2.9}$$

and $\beta_0 = \int_{-1}^{c} w(x)dx = \frac{1}{2}(1 + c)b_0$.

For $c = 0$, we have

$$w(x(t; 0)) = 2^{-(\alpha+\beta)}(3 - t)^{\alpha}(1 + t)^{\beta}, \tag{2.10}$$

so that

$$\int_{-1}^{1} f(t)w(x(t; c))dt = \sum_{k=1}^{n} w_k(c) f(t_k(c)), \quad f \in \mathbb{P}_{2n-1}, \tag{2.11}$$

now represents a continuous transition from the Gauss formula for the weight function (2.10) (when $c = 0$) to the Gauss–Jacobi formula (when $c = 1$).

3 Computational algorithms

The basic computational problem consists in computing, for any given integer n, the first n recursion coefficients a_k, b_k, $k = 0, 1, 2, \ldots, n-1$, in (2.4). We propose to do this by (what in [4] is termed) *Stieltjes's procedure*, more precisely, by an appropriately discretized Stieltjes procedure.

If

$$(p, q) = \int_{-1}^{1} p(t)q(t)v(t; c)dt \tag{3.1}$$

is the underlying inner product (where $v(t; c) = w(ct)$ in the case of (2.3), and $v(t; c) = w(x(t; c))$ in the case of (2.8)), Stieltjes's procedure uses classical formulae for the recurrence coefficients a_k, b_k in terms of this inner product, in combination with the three-term recurrence relation (2.4) itself, to progressively generate the desired coefficients, starting with a_0, b_0 (cf. [6, Section 2.2.3.1]). It uses the inner product (3.1) only for p and q polynomials of progressively increasing degrees.

In the case $v(t; c) = w(ct)$, the integrand in (3.1) is a C^∞ function and thus amenable to numerical quadrature. As already suggested in [4], Fejér quadrature is quite suitable for this purpose and gives rise to the discrete inner product

$$(p, q)_N = \sum_{k=1}^{N} w_k^F w\left(ct_k^F\right) \cdot p\left(t_k^F\right) q\left(t_k^F\right), \tag{3.2}$$

where t_k^F, w_k^F are the nodes and weights of he N-point Fejér rule, that is, the interpolatory quadrature rule based on the N Chebyshev points $t_k^F = \cos\left(\frac{2k-1}{2N}\pi\right)$, $k = 1, 2, \ldots, N$. The *discretized Stieltjes procedure* is simply Stieltjes's procedure in which (3.1) is replaced by (3.2). This produces certain approximations, $a_{k,N}$, $b_{k,N}$, $k = 0, 1, \ldots, n-1$, of the desired recursion coefficients. Since Fejér's rule is interpolatory and positive, the procedure converges in the sense

$$a_{k,N} \to a_k, \quad b_{k,N} \to b_k, \quad k = 0, 1, \ldots, n-1, \quad \text{as } N \to \infty. \tag{3.3}$$

The discretized Stieltjes procedure is implemented in the `OPQ` routine `mcdis.m` (multiple-component discretization), which allows for the interval of integration to be decomposed into any number of subintervals prior to

discretization. In the present case, the one-component procedure suffices, i.e., Fejér's rules can be applied to the whole interval $[-1, 1]$. The Matlab routine that implements this procedure in the case of the sub-range Jacobi polynomials is `r_subjacobi.m` and is called by

$$\texttt{[ab, Ncap] = r\_subjacobi(n, eps0, c, alpha, beta).} \tag{3.4}$$

Here, the input parameters are `n`—the number n of desired recursion coefficients, `eps0`—the desired relative accuracy, `alpha, beta`—the Jacobi parameters α, β, and `c`—the parameter c. The output is the $n \times 2$ array `ab` containing in the first column the n coefficients $\{a_k\}_{k=0}^{n-1}$ and in the second column $\{b_k\}_{k=0}^{n-1}$. The (optional) output parameter `Ncap` is a value of N in (3.3) that achieves the accuracy `eps0`.

In the case $v(t; c) = w(x(t; c))$, the matter is a little bit more complicated, since

$$v(t; c) = \left[\frac{1}{2}(1+c)\right]^{\alpha+\beta} \left(\frac{3-c}{1+c} - t\right)^{\alpha} (1+t)^{\beta}, \quad -1 < t < 1, \tag{3.5}$$

and the last factor has an algebraic singularity at $t = -1$ if β is not an integer. This calls for a two-component discretization, splitting the integral in (3.1) into two parts, one extended from -1 to 0, the other from 0 to 1. To discretize the second part, we can again apply the Fejér rule (transformed to the interval $[0, 1]$). For the first part (disregarding for the moment the constant factor) we must use Gauss–Jacobi quadrature on $[0, 1]$ by writing

$$\int_{-1}^{0} p(t)q(t) \left(\frac{3-c}{1+c} - t\right)^{\alpha} (1+t)^{\beta} dt = \int_{0}^{1} p(-x)q(-x) \left(\frac{3-c}{1+c} + x\right)^{\alpha} (1-x)^{\beta} dx$$

and applying to the second integral the Gauss–Jacobi rule on $[0, 1]$ with Jacobi parameters β and 0 (and obvious notation):

$$\begin{aligned} &\int_{0}^{1} p(-x)q(-x) \left(\frac{3-c}{1+c} + x\right)^{\alpha} (1-x)^{\beta} dx \\ &\quad \approx \sum_{k=1}^{N} w_k^{GJ} p\left(-x_k^{GJ}\right) q\left(-x_k^{GJ}\right) \left(\frac{3-c}{1+c} + x_k^{GJ}\right)^{\alpha}. \end{aligned}$$

Multiplying this by the constant factor in (3.5) and adding the result to the N-point Fejér discretization of the second part,

$$\left[\frac{1}{4}(1+c)\right]^{\alpha+\beta} \sum_{k=1}^{N} \frac{1}{2} w_k^F p\left(\frac{1}{2}\left(t_k^F + 1\right)\right) q\left(\frac{1}{2}\left(t_k^F + 1\right)\right) \left(\frac{5-3c}{1+c} - t_k^F\right)^{\alpha} \left(3 + t_k^F\right)^{\beta},$$

will give the appropriate discrete inner product $(p, q)_N$. The routine `r_subjacobi0`, analogous to the routine (3.4), implements the discretized Stieltjes procedure in this case.

4 Numerical results

We first illustrate the transition from Gauss–Legendre to Gauss–Jacobi quadrature in (2.7). We take $n = 20$ and $\alpha = \beta = -1/2$, and for 100 equally-spaced values of c between 0 and 1 compute and plot the nodes and weights of the n-point Gauss formula (2.7) as functions of c. The results, produced by the routine `transG.m`, are shown in Fig. 1. It can be seen that the nodes are more or less constant, while the weights grow monotonically from the Legendre weights to the (constant) Chebyshev weights $w_k = \pi/n = .15707\ldots$, $k = 1, 2, \ldots, n$. Because of symmetry there are only $n/2 = 10$ curves in Fig. 1b. Figure 2 shows the analogous results for $\alpha = -\beta = -1/2$. Here, each Legendre weight (for $c = 0$) splits into a pair of distinct weights as c moves away from zero, one monotonically decreasing, the other monotonically increasing.

The analogous transitions for the Gauss formulae (2.11) are depicted in Figs. 3 and 4, which are produced by the same routine `transG.m`.

We next illustrate the "circle theorem" for Gauss (and other) quadratures, first enunciated by Davis and Rabinowitz [3] and later extended in [7]. According to this theorem, the nodes and weights of (2.7) and (2.11) satisfy

$$\frac{nw_k}{\pi w(ct_k)} \sim \sqrt{1 - t_k^2} \text{ resp. } \frac{nw_k}{\pi w(x(t_k; c))} \sim \sqrt{1 - t_k^2} \quad \text{as } n \to \infty \tag{4.1}$$

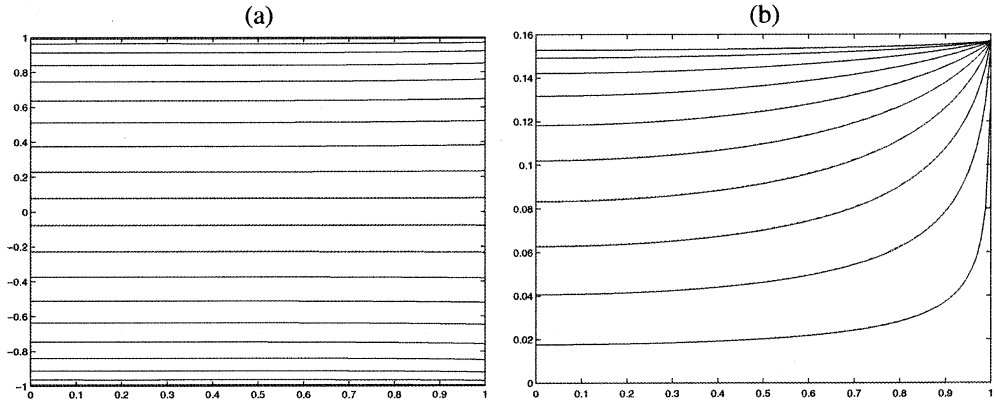

Fig. 1 Nodes (**a**) and weights (**b**) of (2.7) for $0 < c < 1$ when $\alpha = \beta = -1/2$

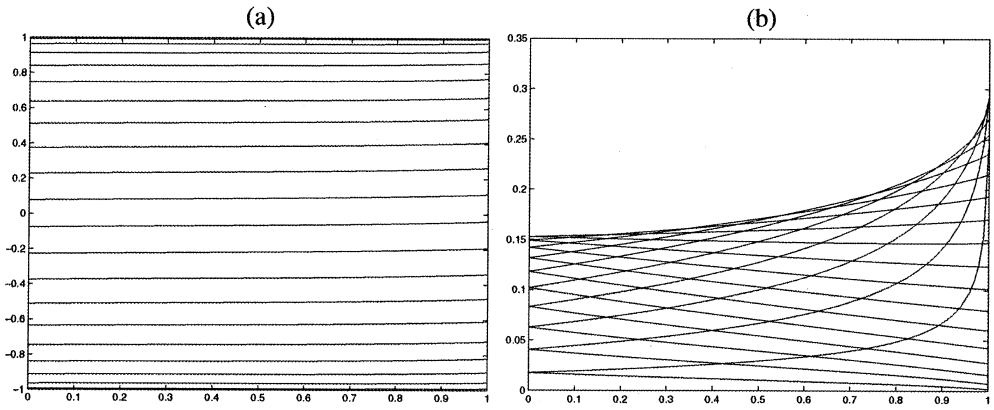

Fig. 2 Nodes (**a**) and weights (**b**) of (2.7) for $0 < c < 1$ when $\alpha = -\beta = -1/2$

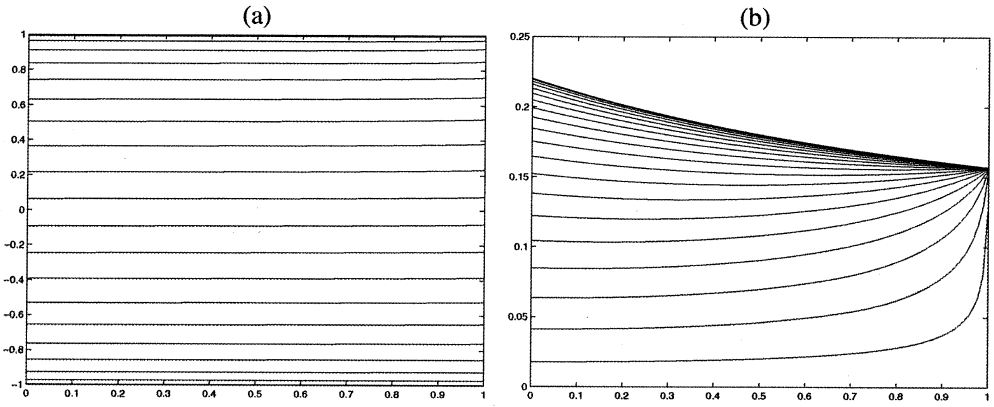

Fig. 3 Nodes (**a**) and weights (**b**) of (2.11) for $0 < c < 1$ when $\alpha = \beta = -1/2$

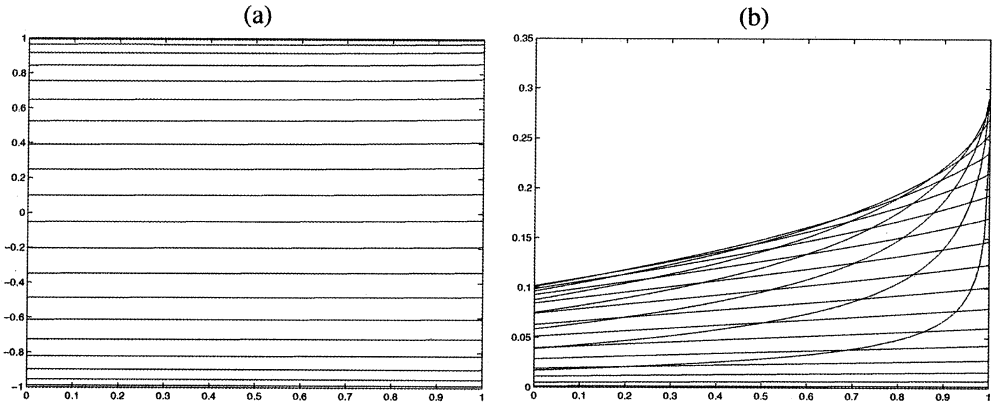

Fig. 4 Nodes (**a**) and weights (**b**) of (2.11) for $0 < c < 1$ when $\alpha = -\beta = -1/2$

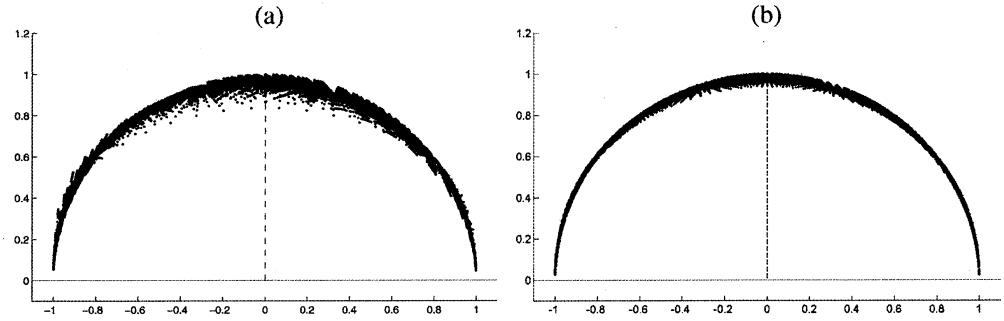

Fig. 5 The circle theorem for sub-range Jacobi weight functions

for all nodes t_k that lie in any compact subinterval of $[-1, 1]$. In Fig. 5, the quantities on the far left in (4.1) for the Gauss formula (2.7) are plotted against the nodes t_k for all α, β in the set $\mathcal{D} = \{\alpha, \beta = [-.9, -.7, -.5, -.3, -.1, 0, .1, .3, .5, .7, .9, 1.5, 3, 6], \beta \geq \alpha\}$, and $c = .1 : .1 : .9$, for $n = 20 : 5 : 40$ in (a), and for $n = 60 : 5 : 80$ in (b). The routine producing these graphs is `circle_thm.m`. For the Gauss formula (2.11) the results, as expected, are practically identical.

In the case of sub-range Chebyshev polynomials (cf. Section 1), we have checked our method against the one used in [1] for $c = \sin(\omega/2)$, $\omega = \pi/2, 9\pi/10, 99\pi/100$, and $n = 5 : 5 : 20$, $30 : 10 : 100$, 200, 300, and found excellent agreement; see `testFV.m`.

We also checked the performance of our routine `r_subjacobi.m` on sub-range Jacobi polynomials with $\alpha, \beta \in \mathcal{D}$. For the values of n and c shown in Table 1, we list Ncap, the maximum values of N over all $(\alpha, \beta) \in \mathcal{D}$ that yield a relative accuracy of `eps0` $= .5 \times 10^{-12}$. These values are by no means sharp, since convergence is checked in increments of N that become larger as N increases. Table 1 was produced by the routine `runsubjac.m`. Similar, often more favorable, results are obtained for the routine `r_subjacobi0`.

Table 1 Convergence behavior of the discretized Stieltjes procedure

$n = 10$		$n = 55$		$n = 100$		$n = 200$		$n = 300$	
c	Ncap	c	Ncap	c	Ncap	c	Ncap	c	Ncap
.100	41	.100	221	.100	401	.100	801	.100	1201
.500	51	.500	221	.500	401	.500	801	.500	1201
.900	91	.900	221	.900	401	.900	801	.900	1201
.990	231	.990	386	.990	501	.990	801	.990	1201
.999	591	.999	606	.999	901	.999	1001	.999	1501

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ORIGINAL PAPER

Repeated modifications of orthogonal polynomials by linear divisors

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Abstract Algorithms are developed for computing the coefficients in the three-term recurrence relation of repeatedly modified orthogonal polynomials, the modifications involving division of the orthogonality measure by a linear function with real or complex coefficient. The respective Gaussian quadrature rules can be used to account for simple or multiple poles that may be present in the integrand. Several examples are given to illustrate this.

Keywords Modification algorithms for orthogonal polynomials · Gaussian quadrature of functions having poles

Mathematics Subject Classifications (2010) 33C47 · 65D30

1 Introduction

There are well-known algorithms that generate the recurrence coefficients of orthogonal polynomials relative to a (positive) measure $d\lambda$ multiplied, or divided, by a (positive) linear or quadratic function, in terms of the recurrence coefficients of the original orthogonal polynomials relative to the measure $d\lambda$. These are called *modification algorithms* (see, e.g., [2, §2.4]). Since they are derived entirely on the basis of the existence of a three-term recurrence relation for orthogonal polynomials, and such recurrence relations hold also (barring the possibility of breakdowns) for formal orthogonal polynomials (see, e.g., [1, §2.2]) that are orthogonal with respect to a nondefinite, for example complex-valued, inner product, the same modification algorithms are

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also valid if the multiplier or divisor is a complex-valued linear function (i.e., involves a complex coefficient). There is no need, then, to consider separately positive quadratic multipliers or divisors, since they can be obtained by a succession of two modifications, one by a complex linear function, and the other by the conjugate complex thereof.

We are thus interested in algorithms for *repeated* modifications. In this regard, repeated linear divisors are conceptionally simpler, and in practice also more important, than repeated linear multipliers, inasmuch as they allow us to generate, say n pairs, of recurrence coefficients for the modified measure from the same number of recurrence coefficients of the original measure. Repeated linear multipliers, nevertheless, have been used in an algorithm for generating "induced" orthogonal polynomials; cf. [3].

We here confine ourselves to modification algorithms involving repeated linear divisors, both real and complex. In Sections 2 and 3 we develop appropriate algorithms, and in Section 4 provide a number of examples.

2 Repeated modification algorithm for distinct linear divisors

We begin by recalling the modification algorithm involving one linear divisor. Let $\{\pi_n\}$ be a set of (monic) polynomials orthogonal with respect to a positive measure $d\lambda$. As is well known, they satisfy a three-term recurrence relation

$$\begin{aligned} \pi_{k+1}(t) &= (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2, \dots, \\ \pi_0(t) &= 1, \quad \pi_{-1}(t) = 0, \end{aligned} \tag{2.1}$$

with coefficients $\alpha_k \in \mathbb{R}$ and $\beta_k > 0$, where by convention $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$. Let $\{\hat{\pi}_n\}$ be the set of (monic) polynomials orthogonal with respect to the measure $d\lambda(t)/(t-z)$, where z is a constant, real or complex, outside the support of $d\lambda$. In the case of complex z, the resulting polynomials $\{\hat{\pi}_n\}$ are formal orthogonal polynomials. If $\hat{\alpha}_k$, $\hat{\beta}_k$ are the recurrence coefficients of $\{\hat{\pi}_n\}$, then we have the following algorithm (cf. [2, Algorithm 2.8]).

Algorithm 1 (modification by a linear divisor $t - z$)

Initialization:

$$\hat{\alpha}_0 = \alpha_0 + r_0, \quad \hat{\beta}_0 = -\rho_0(z). \tag{2.2}$$

Continuation (*if* $n > 1$): *for* $k = 1, 2, \dots, n-1$, *do*

$$\begin{aligned} \hat{\alpha}_k &= \alpha_k + r_k - r_{k-1}, \\ \hat{\beta}_k &= \beta_{k-1} r_{k-1}/r_{k-2}. \end{aligned} \tag{2.3}$$

Here, ρ_k are the Cauchy integrals,

$$\rho_k(z) = \int_{\mathbb{R}} \frac{\pi_k(t)}{z-t}\, d\lambda(t), \quad k = 0, 1, 2, \dots; \quad \rho_{-1}(z) = 1, \tag{2.4}$$

and

$$r_n = r_n(z) := \frac{\rho_{n+1}(z)}{\rho_n(z)}, \quad n = -1, 0, 1, 2, \ldots, \tag{2.5}$$

which can be generated either recursively, if z is close to the support of $d\lambda$, by

$$\begin{aligned} r_k &= z - \alpha_k - \beta_k / r_{k-1}, \quad k = 0, 1, 2, \ldots, \\ r_{-1} &= \rho_0(z), \end{aligned} \tag{2.6}$$

or otherwise by a continued fraction algorithm (cf. [2, §2.3.2]), based on the fact that $\{\rho_k(z)\}$ is the minimal solution of (2.1) (where t is replaced by z) satisfying $\rho_{-1}(z) = 1$. The algorithm is implemented in the `OPQ` routine `chri4.m`,[1] which uses the continued fraction algorithm if the input parameter `iopt` is equal to 1, and the recurrence relation (2.6) otherwise. For reasons explained later, we will here ignore option 1 of the algorithm.

Our objective is to generate the (recurrence coefficients of the) polynomials $\{p_n\}$ orthogonal with repect to the modified measure

$$d\ell(t) = \frac{d\lambda(t)}{(t - z_1)(t - z_2) \cdots (t - z_m)}, \tag{2.7}$$

where $z_1, z_2, \ldots, z_m$ are distinct real or complex numbers outside the support of $d\lambda$. It seems natural to try applying Algorithm 1 repeatedly, in fact m times: first, the measure $d\lambda$ is modified by the linear divisor $t - z_1$. Algorithm 1 then produces the recurrence coefficients for $d\lambda_1(t) = d\lambda(t)/(t - z_1)$ in terms of those (assumed known) for $d\lambda$. Next, the measure $d\lambda_1$ is modified, again using Algorithm 1, dividing by $t - z_2$. This yields $d\lambda_2(t) = d\lambda_1(t)/(t - z_2)$ and its recurrence coefficients. Continuing in this manner, we eventually obtain the recurrence coefficients of (2.7).

This may look straightforward except for an important issue so far glossed over: what do we use for the input parameter $\rho_0(z)$ in Algorithm 1 in each of these applications? To discuss this, let

$$d\lambda_\mu(t) = \frac{1}{t - z_\mu} d\lambda_{\mu-1}(t), \quad \mu = 1, 2, \ldots, m, \tag{2.8}$$

where $d\lambda_0(t) = d\lambda(t)$. Evidently,

$$d\lambda_\mu(t) = \frac{1}{t - z_\mu} \frac{1}{t - z_{\mu-1}} \cdots \frac{1}{t - z_1} d\lambda(t), \tag{2.9}$$

and the input parameter $\rho_0^{[\mu]}$ for the μth modification must be taken to be

$$\rho_0^{[\mu]} = \int_{\mathbb{R}} \frac{1}{z_\mu - t} d\lambda_{\mu-1}(t),$$

[1]The package `OPQ` can be accessed at `OPQ.html` of the website http://www.cs.purdue.edu/archives/2002/wxg/codes, and all Matlab routines referenced in this paper at `RMOP` of the same website.

that is, by (2.9),

$$\rho_0^{[\mu]} = (-1)^{\mu-1} \int_{\mathbb{R}} \frac{d\lambda(t)}{(z_\mu - t)(z_{\mu-1} - t)\cdots(z_1 - t)}, \quad \mu = 1, 2, \ldots, m.$$

Now,

$$\frac{1}{(z_\mu - t)(z_{\mu-1} - t)\cdots(z_1 - t)} = \frac{c_\mu^{[\mu]}}{z_\mu - t} + \frac{c_{\mu-1}^{[\mu]}}{z_{\mu-1} - t} + \cdots + \frac{c_1^{[\mu]}}{z_1 - t},$$

where

$$c_\nu^{[\mu]} = \frac{1}{\prod_{k=1:k\neq\nu}^{\mu}(z_k - z_\nu)}, \quad \nu = 1, 2, \ldots, \mu, \ \mu > 1; \ \ c_1^{[1]} = 1.$$

Therefore,

$$\rho_0^{[\mu]} = (-1)^{\mu-1} \sum_{\nu=1}^{\mu} c_\nu^{[\mu]} \int_{\mathbb{R}} \frac{d\lambda(t)}{z_\nu - t} = (-1)^{\mu-1} \sum_{\nu=1}^{\mu} c_\nu^{[\mu]} \rho_0(z_\nu), \tag{2.10}$$

where $\rho_0(z)$ is the Cauchy integral (2.4) with $k = 0$.

This completes the description of the repeated modification algorithm. To formulate it, we denote the recurrence coefficients of the (monic) orthogonal polynomials for the measure $d\lambda_\mu$ by $\alpha_k^{[\mu]}, \beta_k^{[\mu]}$.

Algorithm 2 (repeated modification by m linear divisors)

For $\mu = 1, 2, \ldots, m$

apply Algorithm 1 with z replaced by z_μ and $\rho_0(z)$ replaced by $\rho_0^{[\mu]}$ of (2.10) (in both (2.2) and (2.6)) to update the recurrence coefficients from $\alpha_k = \alpha_k^{[\mu-1]}, \beta_k = \beta_k^{[\mu-1]}$ to $\hat{\alpha}_k = \alpha_k^{[\mu]}, \hat{\beta}_k = \beta_k^{[\mu]}, k = 0, 1, \ldots, n-1$.

The desired recurrence coefficients for $d\ell$ are $\alpha_k^{[m]}$ and $\beta_k^{[m]}, k = 0, 1, \ldots, n-1$.

Algorithm 2 is implemented in the Matlab routine `mod_md.m` (modification by multiple divisors).

The conceptional simplicity of Algorithm 1, and thus also of Algorithm 2, comes at a price: the basic recurrence relation in (2.6), used for the various values $z = z_\mu$, is unstable, since the Cauchy integrals involved in (2.5), as was already mentioned, are a minimal solution of the basic three-term recurrence relation. It is also known that the severity of instability increases as the z_μ move away from the support of $d\lambda$, and weakens as they approach the support. If the number n of recurrence coefficients desired is large, however, even weak instability may eventually lead to loss of accuracy.

One could of course take recourse to the continued fraction algorithm alluded to earlier, but this would destroy the basic simplicity of the algorithm and also raises issues of convergence, which may be slow for z_μ close to the support of $d\lambda$. For this reason we stick with our simpler approach based on the recurrence (2.6) and deal with its possible instability by running Algorithm 2 in variable-precision arithmetic, using the symbolic capabilities of Matlab. As a matter of fact, we developed an algorithm that for given $d\lambda$, n, and

$z_1, z_2, \ldots, z_m$ will tell us how much precision is needed to obtain all recurrence coefficients $\alpha_k^{[m]}$, $\beta_k^{[m]}$, $k = 0, 1, 2, \ldots, n-1$, to a preassigned accuracy (either absolute or relative, as appropriate). Once obtained in higher precision, the $\alpha_k^{[m]}$, $\beta_k^{[m]}$ can then be converted to standard Matlab double precision for any further computations with them.

3 Repeated modification algorithm for the same linear divisor

We are now interested in the modified measure (2.7) in which $z_k = z$ has the same value (outside the support of $d\lambda$) for all $k = 1, 2, \ldots, m$,

$$d\ell(t) = \frac{d\lambda(t)}{(t-z)^m}. \tag{3.1}$$

If z is complex, we want to continue with the same modification where z is replaced by $\overline{z}$, to obtain

$$d\tilde{\ell}(t) = \frac{d\ell(t)}{(t-\overline{z})^m} = \frac{d\lambda(t)}{|t-z|^{2m}}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2}$$

We proceed as in Section 2, first letting

$$d\lambda_\mu(t) = \frac{1}{t-z}\, d\lambda_{\mu-1}, \quad \mu = 1, 2, \ldots, m; \quad d\lambda_0(t) = d\lambda(t),$$

that is,

$$d\lambda_\mu(t) = \frac{1}{(t-z)^\mu}\, d\lambda(t), \quad \mu = 1, 2, \ldots, m. \tag{3.3}$$

The input parameter for the μth modification (division by $t-z$) in Algorithm 1 then is

$$\rho_0^{[\mu]} = \int_{\mathbb{R}} \frac{1}{z-t}\, d\lambda_{\mu-1}(t) = (-1)^{\mu-1} \int_{\mathbb{R}} \frac{d\lambda(t)}{(z-t)^\mu}.$$

If we let

$$\rho_{0,\mu}(z) = \int_{\mathbb{R}} \frac{d\lambda(t)}{(z-t)^\mu}, \tag{3.4}$$

we have

$$\rho_0^{[\mu]} = (-1)^{\mu-1} \rho_{0,\mu}(z), \quad \mu = 1, 2, \ldots, m, \tag{3.5}$$

hence Algorithm 3 on the following page.

If z is real, we are done. If not, we need to continue with m further modifications involving divisions by $t - \overline{z}$. For this, we let

$$d\tilde{\lambda}_\mu(t) = \frac{1}{t-\overline{z}}\, d\tilde{\lambda}_{\mu-1}(t),$$

that is,

$$d\tilde{\lambda}_\mu(t) = \frac{1}{(t-\overline{z})^\mu}\, d\tilde{\lambda}_0(t), \quad \mu = 1, 2, \ldots, m, \tag{3.6}$$

Algorithm 3 (m-times repeated modification by the linear divisor $t - z$)

For $\mu = 1, 2, \ldots, m$

apply Algorithm 1 with $\rho_0(z)$ replaced by $\rho_0^{[\mu]}$ of (3.5) (in both (2.2) and (2.6)) to update the recurrence coefficients from $\alpha_k = \alpha_k^{[\mu-1]}$, $\beta_k = \beta_k^{[\mu-1]}$ to $\hat{\alpha}_k = \alpha_k^{[\mu]}$, $\hat{\beta}_k = \beta_k^{[\mu]}$, $k = 0, 1, \ldots, n-1$.

The desired recurrence coefficients for $d\ell$ in (3.1) are $\alpha_k^{[m]}$ and $\beta_k^{[m]}$, $k = 0, 1, \ldots, n-1$.

where

$$d\tilde{\lambda}_0(t) = d\lambda_m(t) = \frac{1}{(t-z)^m}\, d\lambda(t).$$

The input parameter $\tilde{\rho}_0^{[\mu]}$ for the μth modification (division by $t - \overline{z}$) in Algorithm 1 now is

$$\tilde{\rho}_0^{[\mu]} = \int_{\mathbb{R}} \frac{1}{\overline{z} - t}\, d\tilde{\lambda}_{\mu-1}(t) = (-1)^{\mu-1} \int_{\mathbb{R}} \frac{d\tilde{\lambda}_0(t)}{(\overline{z} - t)^{\mu}},$$

that is,

$$\tilde{\rho}_0^{[\mu]} = (-1)^{m+\mu-1} \int_{\mathbb{R}} \frac{d\lambda(t)}{(\overline{z} - t)^{\mu}(z - t)^m}, \quad \mu = 1, 2, \ldots, m. \tag{3.7}$$

Now let

$$\frac{1}{(\overline{z} - t)^{\mu}(z - t)^m} = \sum_{\nu=1}^{\mu} \frac{c_{\nu}^{[\mu]}}{(\overline{z} - t)^{\nu}} + \sum_{\kappa=1}^{m} \frac{c_{\mu+\kappa}^{[\mu]}}{(z - t)^{\kappa}}, \quad \mu = 1, 2, \ldots, m, \tag{3.8}$$

be the partial fraction decomposition of the integrand in (3.7). Then

$$\tilde{\rho}_0^{[\mu]} = (-1)^{m+\mu-1} \left(\sum_{\nu=1}^{\mu} c_{\nu}^{[\mu]} \rho_{0,\nu}(\overline{z}) + \sum_{\kappa=1}^{m} c_{\mu+\kappa}^{[\mu]} \rho_{0,\kappa}(z) \right), \quad \mu = 1, 2, \ldots, m. \tag{3.9}$$

Hence we have the continuation of Algorithm 3 as follows.

Algorithm $\tilde{3}$ (continuing Algorithm 3 with m-times repeated modification by the linear divisor $t - \overline{z}$)

For $\mu = 1, 2, \ldots, m$

apply Algorithm 1 with z replaced by $\overline{z}$ and $\rho_0(z)$ replaced by $\tilde{\rho}_0^{[\mu]}$ of (3.9) (in both (2.2) and (2.6)) to update the recurrence coefficients from $\alpha_k = \tilde{\alpha}_k^{[\mu-1]}$, $\beta_k = \tilde{\beta}_k^{[\mu-1]}$ to $\hat{\alpha}_k = \tilde{\alpha}_k^{[\mu]}$, $\hat{\beta}_k = \tilde{\beta}_k^{[\mu]}$, $k = 0, 1, \ldots, n-1$, where $\tilde{\alpha}_k^{[0]} = \alpha_k^{[m]}$, $\tilde{\beta}_k^{[0]} = \beta_k^{[m]}$.

The desired recurrence coefficients for $d\tilde{\ell}$ in (3.2) are $\tilde{\alpha}_k^{[m]}$ and $\tilde{\beta}_k^{[m]}$, $k = 0, 1, \ldots, n-1$.

This completes our procedure in the case of complex z. It requires the partial fraction decomposition (3.8), which can be obtained as follows. Multiplying (3.8) by $(\overline{z}-t)^{\mu}$ gives

$$\frac{1}{(z-t)^m} = c_1^{[\mu]}(\overline{z}-t)^{\mu-1} + \cdots + c_{\mu-1}^{[\mu]}(\overline{z}-t) + c_{\mu}^{[\mu]} + O((\overline{z}-t)^{\mu}). \tag{3.10}$$

Putting $t=\overline{z}$ in (3.10) and letting $y = \operatorname{Im} z$ yields

$$c_{\mu}^{[\mu]} = \frac{1}{(2\mathrm{i}y)^m}.$$

Subtracting $c_{\mu}^{[\mu]}$ on both sides of (3.10), dividing by $\overline{z}-t$, and letting $t \to \overline{z}$ (using the rule of Bernoulli–l'Hôpital) gives

$$c_{\mu-1}^{[\mu]} = \left.\frac{\frac{d}{dt}(z-t)^{-m}}{\frac{d}{dt}(\overline{z}-t)}\right|_{t=\overline{z}} = -\frac{m}{(2\mathrm{i}y)^{m+1}}.$$

Continuing in this manner, subtracting from (3.10) the terms already obtained, dividing by successively higher powers of $\overline{z}-t$, and going to the limit $t \to \overline{z}$ gives

$$c_{\mu-k}^{[\mu]} = \left.\frac{\frac{d^k}{dt^k}(z-t)^{-m}}{\frac{d^k}{dt^k}(\overline{z}-t)^k}\right|_{t=\overline{z}} = (-1)^k\binom{m+k-1}{k}\frac{1}{(2\mathrm{i}y)^{m+k}}, \quad k=0,1,\ldots,\mu-1.$$

Thus,

$$c_{\nu}^{[\mu]} = (-1)^{\mu-\nu}\binom{m+\mu-\nu-1}{m-1}\frac{1}{(2\mathrm{i}y)^{m+\mu-\nu}}, \quad \nu=1,2,\ldots,\mu. \tag{3.11}$$

Analogously, one finds

$$c_{\mu+\kappa}^{[\mu]} = (-1)^{\mu}\binom{\mu+m-\kappa-1}{\mu-1}\frac{1}{(2\mathrm{i}y)^{\mu+m-\kappa}}, \quad \kappa=1,2,\ldots,m. \tag{3.12}$$

In particular,

$$c_{\mu+\kappa}^{[\mu]} = (-1)^{\kappa}\frac{\binom{m-1}{\kappa-1}}{\binom{\mu-1}{\kappa-1}}c_{\kappa}^{[\mu]}, \quad \kappa=1,2,\ldots,\mu, \tag{3.13}$$

As can be seen, the coefficients in (3.8) depend only on the imaginary part y of z.

4 Examples

Example 1 Compute the integral (of interest in quantum chemistry calculations)

$$I(\beta) = \int_0^1 \frac{\sinh(\beta t)}{1+\cosh(\beta t)}\frac{dt}{\sqrt{1-t}}, \quad \beta > 0. \tag{4.1}$$

When β is small or only moderately large, this is easily evaluated by Gauss–Jacobi quadrature on $[0, 1]$ with Jacobi parameters $-1/2$ and 0. For larger values of β, the evaluation becomes increasingly more difficult because of the poles of the integrand, which are located at the odd multiples of $\pm i\pi/\beta$ and thus approach the lower limit of integration as $\beta \to \infty$. This suggests to "remove" the first k pairs of poles by multiplying the integrand by $\prod_{r=1}^{k}[t^2 + ((2r-1)\pi/\beta)^2]$ and consequently dividing the measure $d\lambda(t) = dt/\sqrt{1-t}$ by the same function. We are led to the measure

$$d\lambda_m(t) = \frac{d\lambda(t)}{\prod_{\mu=1}^{m}(t - z_\mu)}, \quad m = 2k,$$

where

$$z_{2r-1} = (2r-1)i\pi/\beta, \quad z_{2r} = \overline{z}_{2r-1}, \quad r = 1, 2, \ldots, k,$$

which is precisely of the form (2.7). Thus, we use Algorithm 2 (in variable-precision arithmetic) to generate the recurrence coefficients of the orthogonal polynomials relative to $d\lambda_m$ and then the corresponding Gaussian quadrature rules by the standard Golub–Welsch algorithm to integrate

$$I(\beta) = \int_0^1 \prod_{\mu=1}^{m}(t - z_\mu)\, \frac{\sinh(\beta t)}{1 + \cosh(\beta t)}\, d\lambda_m(t). \tag{4.2}$$

To carry out Algorithm 2, we need the Cauchy integral

$$\rho_0(z) = \int_0^1 \frac{1}{z - t}\, \frac{dt}{\sqrt{1-t}}.$$

This is easily evaluated by a change of variables, $t = 1 - \tau^2$, which yields

$$\rho_0(z) = 2\int_0^1 \frac{d\tau}{z - 1 + \tau^2} = \frac{2}{z-1}\int_0^1 \frac{d\tau}{1 + \left(\frac{\tau}{\sqrt{z-1}}\right)^2} = \frac{2}{\sqrt{z-1}}\int_0^{1/\sqrt{z-1}} \frac{dx}{1+x^2},$$

that is,

$$\rho_0(z) = \frac{2}{\sqrt{z-1}} \arctan \frac{1}{\sqrt{z-1}}. \tag{4.3}$$

It is instructive to plot the integrand of (4.2) for, say, $m = 0 : 2 : 8$, where $m = 0$ and $d\lambda_0 = d\lambda$ correspond to (4.1). The graphs, for $\beta = 50$, are shown in Fig. 1. It can be seen that the graph y for $m = 0$ exhibits a boundary layer phenomenon near the origin and thereafter is practically constant equal to 1. For the other values of m the graphs look almost polynomial, like $y = t^m$.

The routine `Example1.m` applies Algorithm 2 (in 28-digit arithmetic, as determined by the routine `test_precision1.m`) and subsequent n-point Gaussian quadrature ($n = 20$) to the integral in (4.2), with $\beta = 100, 200, 400$. The results are displayed in Table 1. The improvement of the results with increasing m may not be spectacular; it is slow and steady. This is because *all* poles tend to zero as $\beta \to \infty$.

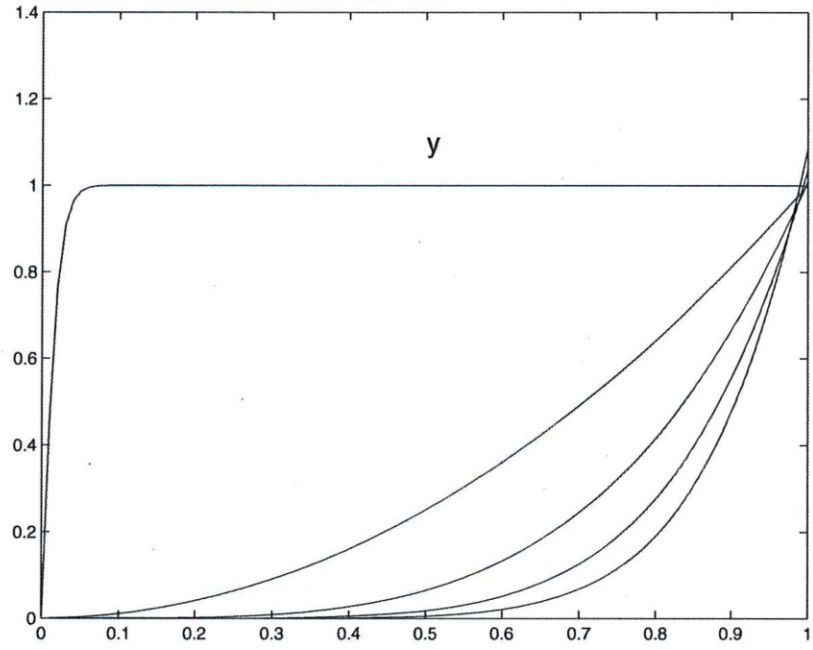

Fig. 1 The integrand of (4.2) with $\beta = 50$ for $m = 0, 2, \ldots, 8$

Example 2 Compute the integral

$$I(\beta, c) = \int_0^1 \frac{\sinh(\beta t)}{1 + \cosh(\beta t)} \frac{1}{t - c} \frac{dt}{\sqrt{1 - t}}, \quad \beta > 0, \ c > 1. \tag{4.4}$$

This is the same as Example 1, but with one more pole added, at $t = c$. This one causes problems when c approaches the upper limit of integration. But we can proceed as in Example 1, letting $z_1 = c$, $z_2 = i\pi/\beta$, $z_3 = \overline{z}_2$, etc. The results (multiplied by -1), using 28-point quadrature (n=28), are shown in Table 2 for the same values of β, and for $c = 1.01, 1.001, 1.0001$. They are produced by the routine `Example2.m`.

In both Examples 1 and 2 the results are qualitatively very much alike.

Table 1 20-point quadrature results for (4.2)

m	$\beta = 100$	$\beta = 200$	$\beta = 400$
0	1.98606...	1.9929...	1.9964...
2	1.986053423...	1.9930478...	1.996527...
4	1.986053420515	1.993047793...	1.99652913...
6	1.986053420520	1.99304779517...	1.996529104...
8	1.986053420520	1.993047795217	1.996529102571

Table 2 28-point quadrature results for (4.4)

c	m	$\beta = 100$	$\beta = 200$	$\beta = 400$
1.01	0	29.4077...	29.414...	29.418...
	1	29.40857820...	29.41563...	29.41906...
	3	29.408578255093	29.415629132...	29.41910684...
	5	29.408578255090	29.415629130283	29.419106791...
	7	29.408578255090	29.415629130287	29.41910679240...
	9	29.408578255090	29.415629130287	29.419106792418
1.001	0	91.9...	91.9...	91.9...
	1	97.33244644...	97.339567...	97.34302...
	3	97.332446495151	97.339561938...	97.3430712...
	5	97.332446495148	97.339561936201	97.343071148...
	7	97.332446495148	97.339561936206	97.34307114923...
	9	97.332446495148	97.339561936206	97.343071149311
1.0001	0	158.7...	158.7...	158.7...
	1	312.14521668...	312.15234...	312.15580...
	3	312.145216744523	312.152338709...	312.15585116...
	5	312.145216744520	312.152338707265	312.155851105...
	7	312.145216744521	312.152338707269	312.15585110697...
	9	312.145216744518	312.152338707271	312.155851106987

Example 3 Evaluate (cf. also [4])

$$I_r = \int_0^\infty f(t)\varepsilon_r(t)dt, \quad \varepsilon_r(t) = \left(\frac{t}{e^t - 1}\right)^r, \tag{4.5}$$

for a given (well-behaved) function f.

The function $\varepsilon_1(t)$ (known to physicists as Bose–Einstein distribution and to mathematicians as the generating function of the Bernoulli numbers) has also infinitely many poles (at $z_\nu = \pm 2\nu\pi i$, $\nu = 1, 2, 3, \ldots$), but they are now at fixed distances from the real line.

The approach taken in [4] for doing the integration in (4.5) is to account for the totality of these poles by treating the function $\varepsilon_r(t)$ as a weight function and generating the corresponding orthogonal polynomials by a discretized Stieltjes procedure, and then the Gauss formulae in the usual way from these orthogonal polynomials. It may be interesting to see how successive removal of the poles closest to the real line compares with the all-inclusive approach taken in [4].

We write

$$I_r = \int_0^\infty f(t)\left(\frac{t}{1-e^{-t}}\right)^r \cdot e^{-rt}dt = \frac{1}{r}\int_0^\infty f(t/r)\left(\frac{t/r}{1-e^{-t/r}}\right)^r e^{-t}dt, \quad (4.6)$$

and thus take $d\lambda(t) = e^{-t}dt$ to be the Laguerre measure. The Cauchy integral required is

$$\rho_0(z) = \int_0^\infty \frac{e^{-t}}{z-t}dt = -e^{-z}\int_{-z}^\infty \frac{e^{-u}}{u}du,$$

that is,

$$\rho_0(z) = -e^{-z}E_1(-z) = e^{-z}\mathrm{Ei}(z), \quad (4.7)$$

where E_1 and Ei are the exponential integrals. (Variable-precision evaluation of exponential integrals for complex arguments is currently not available in Matlab, but can be achieved by using the `MuPAD` engine within the Matlab Symbolic Math Toolbox.)

Since the poles closest to the real line are at least a distance of 2π away from the real axis, the demand on Algorithm 2 for high precision is now greater than in the previous examples. According to the routine `test_precision3.m`, the number (in multiples of 4) of digits required to obtain the first n recurrence coefficients for m linear divisors to an accuracy of $\frac{1}{2}10^{-15}$ is shown in Table 3 (for $r = 1$). For $r = 1$ and $r = 2$, and $f(t) = e^{-t}$, the integral (4.5) is explicitly known in terms of the zeta and generalized zeta function,

$$I_1 = \zeta(2) - 1 = \frac{\pi^2}{6} - 1 = .6449340668482264\ldots,$$
$$I_2 = 2[\zeta(2,2) - 2\zeta(3,2)] = \frac{\pi^2}{3} + 2 - 4\zeta(3) = .4816405210580763\ldots.$$

The routine `Example3.m` applies Algorithm 2 (in 28-digit arithmetic) and subsequent Gaussian quadrature to evaluate I_1 and I_2 with $m = 0, 2, 4$. The absolute errors observed are shown in Table 4. This is to be compared with the case $m = \infty$ (when ε_r is treated as a weight function), the errors of which are shown in Table 5. Rather surprisingly, already the case $m = 2$ does better than $m = \infty$, both in the case $r = 1$ and $r = 2$, there being one exception in the latter case (when $n = 12$). It may be noted that when $r = 2$ the poles are of order 2, and Algorithm 2 removes only simple poles; see, however, Example 5.

Table 3 Precision (number of digits) required for Algorithm 2

n	$m = 2$	$m = 4$	$m = 6$	$m = 8$
10	20	24	24	28
25	24	32	32	40
50	32	40	40	52
80	36	48	48	68

Table 4 n-point quadrature errors for the integral (4.5) with $f(t) = e^{-t}$

	$r=1$			$r=2$		
n	$m=0$	$m=2$	$m=4$	$m=0$	$m=2$	$m=4$
2	1.01 (–04)	1.36 (–03)	1.51 (–03)	1.41 (–04)	9.49 (–05)	7.94 (–05)
4	1.28 (–05)	8.20 (–07)	5.12 (–08)	2.37 (–06)	4.70 (–07)	3.10 (–07)
6	6.23 (–08)	6.07 (–10)	3.06 (–10)	2.92 (–08)	1.49 (–09)	6.68 (–10)
8	9.48 (–08)	3.33 (–11)	9.65 (–13)	6.58 (–10)	8.54 (–13)	6.90 (–12)
10	1.43 (–08)	9.70 (–13)	1.44 (–15)	2.92 (–11)	6.16 (–15)	2.44 (–13)
12	7.53 (–10)	4.44 (–16)	0.00 (+00)	1.91 (–12)	2.84 (–14)	2.61 (–15)

Example 4 (Szegö–Bernstein measure)

$$d\lambda_m(t) = \frac{1}{(c_1^2 - t^2)(c_2^2 - t^2)\cdots(c_{m/2}^2 - t^2)} \frac{dt}{\sqrt{1-t^2}}, \quad -1 < t < 1,$$
$$m \text{ even}, \ c_k > 1, \ k = 1, 2, \ldots, m/2. \tag{4.8}$$

This is a special case of a Szegö–Bernstein measure, for which, when $n > m/2$, the orthogonal polynomials π_n of degree n are explicitly known [6, Theorem 2.6]. Here we use Algorithm 2 to generate the array `ab` of recurrence coefficients for $\{\pi_n\}$. Note that (4.8), except for sign, is (2.7) with $d\lambda(t) = dt/\sqrt{1-t^2}$ and $z_k = c_{\lfloor (k+1)/2 \rfloor}$, $z_{k+1} = -c_{\lfloor (k+1)/2 \rfloor}$, $k = 1, 3, \ldots, m-1$. The respective Cauchy integral is (cf. [5, 3.613.1 for $n = 0$])

$$\rho_0(c) = \int_{-1}^{1} \frac{1}{c-t} \frac{dt}{\sqrt{1-t^2}} = \int_0^{\pi} \frac{d\theta}{c - \cos\theta} = \operatorname{sgn}(c) \frac{\pi}{\sqrt{c^2-1}}. \tag{4.9}$$

The routine `Example4.m` computes the 30×2-array `ab` in 52-digit arithmetic for $c_k = 1 + 1/k$, $k = 1, 2, \ldots, m/2$, and $m = 2, 4, \ldots, 48$. All α-coefficients, of course, are zero, whereas the β_k are all equal to 1/4 when $k > 1 + m/2$, reflecting what was said in the introductory sentence above. Not

Table 5 Quadrature errors for the integral (4.5) when $m = \infty$

n	$r=1$	$r=2$
2	5.34 (–02)	7.74 (–03)
4	1.34 (–03)	3.39 (–05)
6	2.62 (–05)	1.07 (–07)
8	4.56 (–07)	2.88 (–10)
10	7.39 (–09)	7.04 (–13)
12	1.15 (–10)	1.50 (–15)

Table 6 Selected β-coefficients for $d\lambda_m$ with real c_k

m	$\beta_{1+m/2}$	m	$\beta_{1+m/2}$
4	.2526187518831068	28	.2500000105993838
8	.2501334100968554	32	.2500000025371004
12	.2500122983685047	36	.2500000006601609
16	.2500015886586432	40	.2500000001842993
20	.2500002570365245	44	.2500000000546533
24	.2500000489998413	48	.2500000000170815

unexpectedly, the β_k, before they become 1/4, approach this number (in an oscillating manner). In Table 6, we display $\beta_{1+m/2}$, the last β_k not equal to 1/4, for $m = 4 : 4 : 48$.

If all factors in (4.8) involving the c_k have a plus sign instead of the minus sign, the c_k must be taken in complex conjugate pairs. An example in point, also implemented by `Example4.m`, is $c_k = \pm i/k$, $k = 1, 2, \ldots, m/2$, for which the analogue of Table 6 is shown in Table 7. The approach of the β_k to 1/4 is now much slower, first increasing and then briefly decreasing monotonically.

Example 5 We return to Example 3, evaluating (cf. (4.6))

$$I_r = \frac{1}{r}\int_0^\infty f(t/r)\left(\frac{t/r}{1-e^{-t/r}}\right)^r d\lambda(t), \quad d\lambda(t) = e^{-t}dt,$$

for $f(t) = e^{-t}$, and $r = 2, 3, 4$.

Noting that the second factor of the integrand has poles of order r at $z = \pm r \cdot 2\pi i$, we apply Algorithms 3 and $\tilde{3}$ with $m = r$ to remove both poles in their entirety, computing the (recurrence coefficients for the) orthogonal polynomials associated with the measure

$$d\lambda_r(t) = \frac{d\lambda(t)}{[t^2 + (2\pi r)^2]^r}$$

Table 7 Selected β-coefficients for $d\lambda_m$ with complex c_k

m	$\beta_{1+m/2}$	m	$\beta_{1+m/2}$
4	.2722827635216653	28	.2532299127159494
8	.2612647900497343	32	.2528263844392646
12	.2575258651139427	36	.2525124702616266
16	.2556486476924788	40	.2522613060125720
20	.2545204983065458	44	.2520557884307700
24	.2537677987514944	48	.2518845115641227

Table 8 n-point quadrature results for (4.10)

r	n	I_r	r	I_r	r	I_r
2	2	.48160...	3	.38579...	4	.32221...
	4	.481640525...		.385766867...		.322239558...
	6	.48164052111...		.385766859955...		.322239565840...
	8	.481640521058022		.385766859951251		.322239565842369
	10	.481640521058074		.385766859951252		.322239565842370
	12	.481640521058076		.385766859951252		.322239565842371

and applying Gaussian quadrature for this measure to the integral in

$$I_r = \frac{1}{r}\int_0^\infty [t^2 + (2\pi r)^2]^r f(t/r)\left(\frac{t/r}{1-e^{-t/r}}\right)^r d\lambda_r(t). \tag{4.10}$$

This requires the integral (cf. (3.4))

$$\rho_{0,\mu}(z) = \int_0^\infty \frac{e^{-t}}{(z-t)^\mu}\,dt = -z^{1-\mu}e^{-z}E_\mu(-z)$$

in order to evaluate (cf. (3.5))

$$\rho_0^{[\mu]} = (-1)^{\mu-1}\rho_{0,\mu}(z) = (-1)^\mu z^{1-\mu}e^{-z}E_\mu(-z)$$

in Algorithm 3, and (cf. (3.9))

$$\tilde{\rho}_0^{[\mu]} = (-1)^{r+\mu}\left(e^{-\overline{z}}\sum_{\nu=1}^{\mu} c_\nu^{[\mu]}\overline{z}^{1-\nu}E_\nu(-\overline{z}) + e^{-z}\sum_{\kappa=1}^{r} c_{\mu+\kappa}^{[\mu]}z^{1-\kappa}E_\kappa(-z)\right)$$

in Algorithm $\tilde{3}$.

The procedure is implemented in the Matlab routine `Example5.m`. Run for $r = 2, 3, 4$, it produces the results shown in Table 8. The errors for $r = 2$ are somewhat smaller than those observed in Example 3 (cf. the column headed $r = 2, m = 2$ in Table 4), and convergence is remarkably fast.

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ORIGINAL PAPER

Neutralizing nearby singularities in numerical quadrature

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Abstract A method of "neutralization" is presented that significantly weakens, if not eliminates, a singularity close to, but outside, the interval of integration. The effectiveness of the method is illustrated by a number of examples.

Keywords Gaussian quadrature · nearby singularities

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1 Introduction

There are various known methods for numerically evaluating definite integrals in the presence of a pole outside, but near, the interval of integration. One is to simply remove the pole by multiplying the integrand by an appropriate linear or higher-degree factor and adjusting the measure of integration accordingly, and then use Gaussian quadrature with respect to the adjusted measure (see [2]). Unfortunately, other types of singularities, for example algebraic or logarithmic singularities, cannot be removed in this manner. In fact, there are no general methods known to the author that deal with such "nonpolar" singularities located very closely to the interval of integration. Here we propose a method of *neutralizing* such singularities, i.e., of weakening their harmful effect on convergence by multiplying the integrand by a factor vanishing to a high order at the location of the singularity, adjusting the measure of integration accordingly, and then continuing with Gaussian quadrature. While this does not remove the singularity, it makes the modified integrand more regular in the sense of having more continuous derivatives at the location of the singularity.

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Although generally applicable, the method requires high-precision values of certain Cauchy-type integrals relative to the original measure of integration. This limits the applicability of the method to relatively simple measures of integration.

In Section 2, the method is described in more detail. Examples are given in Section 3.

2 The method of neutralization

We are interested in computing an integral

$$I = \int_{\mathbb{R}} \omega(t) f(t) \mathrm{d}\lambda(t), \tag{2.1}$$

where $\mathrm{d}\lambda$ is a given measure supported on a finite or infinite interval, f is a well-behaved function defined on this interval, and $\omega(t)$ a function having a singularity other than a pole at the (real or complex) point z outside, but possibly close to, the support of $\mathrm{d}\lambda$. If z is complex, we assume that $\overline{z}$ is also a singular point of ω.

If z is real (and therefore $\mathrm{supp}(\mathrm{d}\lambda)$ not equal to all of $\mathbb{R}$), we "neutralize" the singularity by multiplying and dividing by $(t-z)^m$, where m is a suitable, perhaps large, positive integer. That is,

$$I = \int_{\mathbb{R}} (t-z)^m \omega(t) f(t) \frac{\mathrm{d}\lambda(t)}{(t-z)^m}, \quad z \in \mathbb{R} \backslash \mathrm{supp}(\mathrm{d}\lambda). \tag{2.2}$$

Then we use Gaussian quadrature relative to the modified measure

$$\mathrm{d}\lambda_m(t) = \frac{\mathrm{d}\lambda(t)}{(t-z)^m}. \tag{2.3}$$

We may proceed similarly for nonreal $z \in \mathbb{C}$, first multiplying and dividing by $[(t-z)(t-\overline{z})]^m = |t-z|^{2m}$,

$$I = \int_{\mathbb{R}} |t-z|^{2m} \omega(t) f(t) \frac{\mathrm{d}\lambda(t)}{|t-z|^{2m}}, \quad z \in \mathbb{C} \backslash \mathbb{R}, \tag{2.4}$$

and then applying Gaussian quadrature relative to the measure

$$\mathrm{d}\tilde{\lambda}_m(t) = \frac{\mathrm{d}\lambda(t)}{|t-z|^{2m}}. \tag{2.5}$$

Since Gaussian quadrature requires orthogonal polynomials, what is called for, technically, are algorithms that, given the orthogonal polynomials with respect to the measure $\mathrm{d}\lambda$, generate orthogonal polynomials with respect to the measures $\mathrm{d}\lambda_m$ and $\mathrm{d}\tilde{\lambda}_m$. Such algorithms have recently been developed in [2], where Algorithm 3 of [2, §3] solves the problem for the measure (2.3), and Algorithm 3 followed by Algorithm $\tilde{3}$ of [2, §3] solves the problem for the measure (2.5). Both algorithms depend critically on the ability to calculate Cauchy-type integrals

$$\rho_{0,\mu}(z) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{(z-t)^\mu}, \quad \mu = 1, 2, \ldots, m, \tag{2.6}$$

to high accuracy.

Table 1 The number of digits required to obtain results to full machine precision

N	$m = 10$	$m = 20$	$m = 30$	$m = 40$	$m = 50$
10	24	24	28	32	36
20	24	28	36	40	44
30	24	28	36	40	52
40	24	28	36	40	52
50	24	28	36	40	52

The algorithms also require variable-precision calculation to overcome instabilities in parts of the algorithms. Given z, m, and the desired degree N of the orthogonal polynomial, Matlab routines[1] are available that tell us how many digits are required in Algorithm 3 resp. $\tilde{3}$ to get answers to full machine precision or to any given precision; cf. Examples 1, 3 and 4–6.

3 Examples

Example 1 The integral (2.1) with $\omega(t) = (t - z)^{\alpha}$, $z < 0$, $\alpha > -1$, and $\mathrm{d}\lambda(t) = \mathrm{d}t$ on $[0, 1]$.

Here, the integrals (2.6) are simply

$$\rho_{0,\mu}(z) = \int_0^1 \frac{\mathrm{d}t}{(z-t)^{\mu}} = \begin{cases} -\ln(1 - 1/z) & \text{if } \mu = 1, \\ \dfrac{1}{\mu - 1} z^{1-\mu}[(1 - 1/z)^{1-\mu} - 1] & \text{if } \mu > 1. \end{cases} \tag{3.1}$$

For illustration we take $\alpha = -1/2$, $z = -1/1000$. Then, according to the routine `test_precision_mod14.m`, one needs the number of digits (in multiples of 4) shown in Table 1 to obtain to full machine precision `eps=.5e-16` the first N recurrence coefficients for the desired orthogonal polynomials.

To test our method, we first let $f(t) \equiv 1$, in which case $I = 1.93775419692\,1554\ldots$. When $N = 50$, a bit of experimentation shows that a reasonable choice of m to be used in (2.2) is $m = 24$. The absolute errors in the n-point quadrature results (obtained in 28-digit arithmetic by the routine `neutral_Ex1.m` in combination with the proper selection in `rho01_mu.m`) are as shown in Table 2. It can be seen that the speed-up in convergence, when $m = 24$, is quite striking, although for small n the results are more accurate when $m = 0$.

The integer m may be viewed as the "dosage" of neutralization. Table 3 (generated in 52-digit arithmetic if $m > 24$) shows that overdosing is relatively harmless, whereas underdosing eventually (for large n) becomes counterproductive, as expected. If only low accuracy is needed, however, neutralizing the singularity is not

[1] These, and all other Matlab routines referenced (or implied) in this paper are accessible on the website http://www.cs.purdue.edu/archives/2002/wxg/codes/NEUTRAL.html.

Table 2 n-point Gaussian quadrature errors for (2.2) with $f(t) \equiv 1$

n	Error ($m = 0$)	Error ($m = 24$)
10	3.535(−2)	1.684(+00)
20	6.960(−3)	2.865(−07)
30	1.634(−3)	1.575(−10)
40	4.054(−4)	5.902(−13)
50	1.033(−4)	8.882(−16)

necessarily advisable since its benefit is high accuracy, which materializes only when n becomes sufficiently large.

We next show in Table 4 results (also obtained in 28-digit arithmetic using `neutral_Ex1.m`) analogous to those in Table 2 when $f(t) = \cos(\frac{\pi}{2}t)$.

The singularity does not have to be algebraic, as in Example 1. The case of a logarithmically singular factor, $\omega(t) = \ln(1/(t - z))$, with the same value of z and the same function f, is demonstrated in the next example.

Example 2 The integral (2.1) with $\omega(t) = \ln(1/(t - z))$, $z = -1/1000$, $f(t) = \cos(\frac{\pi}{2}t)$ and $d\lambda(t) = dt$ on $[0, 1]$.

The results, obtained by the routine `neutral_Ex2.m` (in combination with `rho01_mu.m`), very similar in quality to those in Table 4, are shown in Table 5.

Example 3 The integral (2.1) with $\omega(t) = (t^2 + y^2)^\alpha$, $y > 0$, and $d\lambda(t) = dt$ on $[0, 1]$.

The Cauchy-type integral (2.6) required for this example is the same as the one in Examples 1 and 2; see (3.1). We can write $\omega(t) = |t - z|^{2\alpha}$ with $z = iy$. For the purpose of illustration, we take $\alpha = -1/2$ and $z = i/1000$. The routine `test_precision_mod3.m` then provides the number of digits, shown in Table 6, that are required to obtain results to full machine precision.

Our method involves (2.4) with $z = iy$, $y = 1/000$, hence the Algorithms 3 and $\tilde{3}$ of [2, §3]. Run in 32-digit arithmetic, with $f(t) = 1$, $m = 12$, they produce results as shown in Table 7; see the routine `neutral_Ex3.m`.

Example 4 Same as Example 1 with $f(t) = \cos(\frac{\pi}{2}t)$, but $d\lambda(t) = dt/\sqrt{1 - t}$.

Table 3 n-point Gaussian quadrature errors for (2.2) with $f(t) \equiv 1$ in dependence of the neutralization dosage

n	$m = 6$	$m = 12$	$m = 18$	$m = 24$	$m = 30$	$m = 36$	$m = 42$
10	4.91(−04)	4.60(−04)	1.02(−02)	1.68(+00)	1.83(+00)	1.87(+00)	1.89(+00)
20	5.96(−06)	4.67(−07)	1.91(−07)	2.87(−07)	1.72(−06)	8.73(−05)	9.63(−01)
30	2.36(−07)	4.89(−09)	5.13(−10)	1.58(−10)	1.18(−10)	2.04(−10)	8.75(−10)
40	1.54(−08)	1.20(−10)	5.01(−12)	5.90(−13)	1.50(−13)	8.15(−14)	8.35(−14)
50	1.34(−09)	4.73(−12)	1.01(−13)	8.88(−16)	8.66(−15)	2.00(−15)	1.24(−14)

Table 4 n-point Gaussian quadrature results for (2.2) with $\omega(t) = (t - z)^{-1/2}$, $z = -1/1000$, and $f(t) = \cos(\frac{\pi}{2}t)$

n	$I\ (m = 0)$	$I\ (m = 24)$
10	1.46...	0.2...
20	1.490...	1.4979166...
30	1.496...	1.4979169811...
40	1.4975...	1.4979169812729...
50	1.49781...	1.49791698127350

Table 5 n-point Gaussian quadrature results for (2.2) with $\omega(t) = \ln(1/(t - z))$, $z = -1/1000$, and $f(t) = \cos(\frac{\pi}{2}t)$

n	$I\ (m = 0)$	$I\ (m = 24)$
10	0.861...	0.1...
20	0.8648...	0.8653020...
30	0.86522...	0.86530226833...
40	0.86528...	0.8653022684101...
50	0.865298...	0.865302268410424

Table 6 The number of digits required to obtain results to full machine precision

N	$m = 10$	$m = 12$	$m = 14$	$m = 16$	$m = 18$
20	24	28	28	32	32
40	24	28	28	32	36
60	24	28	28	32	36
80	28	28	32	32	36
100	28	32	32	36	40

Table 7 n-point Gaussian quadrature results for (2.4) with $\omega(t) = (t^2 + y^2)^{-1/2}$, $y = 1/1000$, $f(t) \equiv 1$, and $d\lambda(t) = dt$

n	$I\ (m = 0)$	$I\ (m = 12)$
20	7.0...	7.6009027092...
40	7.65...	7.60090270952...
60	7.606...	7.6009027095407...
80	7.5993...	7.60090270954194...
100	7.60088...	7.600902709542003

The Cauchy-type integral (2.6) now is

$$\rho_{0,\mu}(z) = \int_0^1 \frac{1}{(z-t)^\mu} \frac{\mathrm{d}t}{\sqrt{1-t}},$$

which, by the change of variables $t = 1 - (1-z)\tau^2$, becomes

$$\rho_{0,\mu}(z) = \frac{2(-1)^\mu}{(1-z)^{\mu-1/2}} R_\mu\left(\frac{1}{\sqrt{1-z}}\right), \tag{3.2}$$

where

$$R_\mu(v) = \int_0^v \frac{\mathrm{d}t}{(1-t^2)^\mu}.$$

As is well known from calculus (or see [3, 2.143.2 and 2.149.2]), we have

$$R_1(v) = \frac{1}{2} \ln \frac{1+v}{1-v},$$
$$R_{k+1}(v) = \left(1 - \frac{1}{2k}\right) R_k(v) + \frac{v}{2k(1-v^2)^k}, \quad k = 1, 2, \ldots \mu - 1. \tag{3.3}$$

The number of digits required to obtain answers to machine precision, according to `test_precision_mod14.m`, is similar to those shown in Table 1, although larger by four units in several cases. Results produced by the routine `neutral_Ex4.m` (in combination with `rho01_mu.m`) in 32-digit arithmetic are shown in the first three columns of Table 8.

The routine `test_precision_mod14.m` also allows us to estimate the accuracy attainable if the number of digits in the arithmetic is prescribed. Thus, if we let this number be 16 (Matlab double precision), we can expect to still get about 11-digit accuracy by choosing $m = 10$. (Much larger values of m reduce the attainable accuracy.) This is confirmed by running the routine `neutral_Ex4.m` with `dig` $= 16$ and $m = 10$, producing the results shown in the last column of Table 8.

Example 5 Same as Example 1, but with $\mathrm{d}\lambda(t) = e^{-t}\mathrm{d}t$ on $\mathbb{R}_+$.

In this example, the required Cauchy-type integral (2.6) is

$$\rho_{0,\mu}(z) = \int_0^\infty \frac{e^{-t}\mathrm{d}t}{(z-t)^\mu} = -z^{1-\mu}e^{-z}E_\mu(-z), \tag{3.4}$$

where $E_\mu(z) = \int_1^\infty e^{-zt}\mathrm{d}t/t^\mu$ is the μth exponential integral. This can be computed to arbitrary precision by using the `MuPAD` engine within the Matlab Symbolic Math Toolbox.

Table 8 n-point Gaussian quadrature results for (2.2) with $\omega(t) = (t-z)^{-1/2}$, $z = -1/1000$, $f(t) = \cos(\frac{\pi}{2}t)$, and $\mathrm{d}\lambda(t) = \mathrm{d}t/\sqrt{1-t}$

n	I ($m = 0$)	I ($m = 24$)	I ($m = 10$)
10	1.792...	0.2...	1.8290...
20	1.822...	1.8294765...	1.8294758...
30	1.827...	1.8294768551...	1.82947683...
40	1.8290...	1.8294768553640...	1.8294768548...
50	1.82937...	1.829476855364679	1.82947685533...

Table 9 n-point Gaussian quadrature errors for (2.2) with $\omega(t) = (t - z)^{-1/2}$, $z = -1/1000$, $f(t) \equiv 1$, and $d\lambda(t) = e^{-t}dt$

	Error					
n	$m = 0$	$m = 10$	$m = 20$	$m = 30$	$m = 40$	$m = 50$
40	8.373(−02)	2.603(−04)	2.064(−05)	4.197(−06)	1.632(−06)	1.354(−06)
80	4.747(−02)	3.698(−05)	1.206(−06)	1.012(−07)	1.458(−08)	3.090(−09)
120	3.246(−02)	1.059(−05)	2.088(−07)	1.121(−08)	1.048(−09)	1.428(−10)
160	2.410(−02)	4.102(−06)	5.606(−08)	2.205(−09)	1.545(−10)	1.591(−11)
200	1.876(−02)	1.887(−06)	1.926(−08)	5.942(−10)	3.338(−11)	2.770(−12)

Table 10 n-point Gaussian quadrature results for (2.2) with $\omega(t) = (t - z)^{-1/2}$, $z = -1/1000$, $f(t) = \arctan(t)$, and $d\lambda(t) = e^{-t}dt$

n	I $(m = 0)$	I $(m = 50)$
40	0.6282...	0.6277897...
80	0.6279...	0.6277892428...
120	0.62787...	0.6277892424...
160	0.62784...	0.627789242439...
200	0.62782...	0.62778924243796

For illustration, we take again $\alpha = -1/2$ and $z = -1/1000$. The routine `test_precision_mod5.m` then tells us that 48-digit arithmetic should be sufficient to obtain to full machine precision the first 200 recurrence coefficients for the orthogonal polynomials relative to the measure (2.3) with m as large as 50. Letting first $f(t) \equiv 1$, in which case the integral (2.1) can be expressed explicitly as $I = e^{-z}\Gamma(\alpha + 1, -z) = 1.710939457503026$ in terms of the incomplete gamma function, our procedure of neutralization, implemented in 48-digit arithmetic by the routine `neutral_Ex5.m` (in combination with `rho01_mu.m`), yields errors as shown in Table 9. Thus, with 200 quadrature points we are gaining about ten decimal places by choosing $m = 50$ instead of $m = 0$.

Running the same routine (with $m = 50$ and appropriate small changes) for $f(t) = \arctan(t)$ yields the results shown in Table 10.

Example 6 The integral (2.1) with $\omega(t) = (t^2 + y^2)^\alpha$, $y > 0$, $\alpha > -1$, and $d\lambda(t) = e^{-t}dt$ on $\mathbb{R}_+$.

We begin with $f(t) \equiv 1$, in which case the integral (2.1) is known to be (cf. [3, 3.387.7][2])

$$I = \int_0^\infty (t^2 + y^2)^\alpha e^{-t}dt = \frac{\sqrt{\pi}}{2}(2y)^{\alpha+1/2}\Gamma(\alpha + 1)\left[\mathrm{H}_{\alpha+1/2}(y) - Y_{\alpha+1/2}(y)\right],$$

[2]There is a misprint in the formula of this reference: $N_{\nu-1/2}(u, \mu)$ should read $N_{\nu-1/2}(u\mu)$, where $N_{\nu-1/2}$ is the same as $Y_{\nu-1/2}$.

Table 11 n-point Gaussian quadrature results and errors for (2.4) with $\omega(t) = |t - \mathrm{i}/10|^{2\alpha}$, $f(t) \equiv 1$, and $\mathrm{d}\lambda(t) = e^{-t}\mathrm{d}t$

α	n	$I \approx$	Error
−0.75	20	5.35784566...	1.694(−09)
	40	5.3578456588019...	9.868(−13)
	60	5.3578456588009...	2.043(−14)
	80	5.357845658801011	6.217(−15)
−0.50	20	2.50986537127...	1.945(−11)
	40	2.5098653712915...	6.626(−13)
	60	2.50986537129212...	5.507(−14)
	80	2.509865371292172	3.997(−15)
−0.25	20	1.409483808...	1.571(−09)
	40	1.4094838104039...	8.276(−13)
	60	1.40948381040479...	2.598(−14)
	80	1.409483810404821	4.441(−16)
0.25	20	0.906236938...	1.878(−09)
	40	0.9062369367739...	2.883(−13)
	60	0.906236936773654	2.220(−16)
	80	0.906236936773654	5.551(−16)
0.50	20	1.014902776624...	4.039(−13)
	40	1.01490277662516...	1.532(−14)
	60	1.014902776625171	3.997(−15)
	80	1.014902776625174	1.554(−15)
0.75	20	1.340431153...	2.915(−09)
	40	1.3404311566536...	1.665(−13)
	60	1.340431156653803	3.109(−15)
	80	1.340431156653805	1.776(−15)

where H_ν is the Struve function (cf. [1, Ch. 12]) and Y_ν the Bessel function of the second kind.

Here we use (2.4) with $z = \mathrm{i}y$. The required Cauchy-type integral (2.6) for this example has already been used in Example 5 (see (3.4)). Taking $y = 1/10$ and applying Algorithms 3 and $\tilde{3}$ of [2, §3] in 28-digit arithmetic (as determined by the routine `test_precision_mod6.m`) with $m = 12$, which is about optimal, we get the results shown in Table 11. They are produced by the routine `neutral_Ex6.m` in combination with `rho01_mu.m` and `struve.m`.

Table 12 n-point Gaussian quadrature results for (2.4) with $\omega(t) = |t - \mathrm{i}/10|^{-1/2}$, $f(t) = J_0(t)$, and $\mathrm{d}\lambda(t) = e^{-t}\mathrm{d}t$

n	I $(m = 0)$	I $(m = 12)$
20	1.195...	1.18776706...
40	1.18789...	1.1877669740463...
60	1.1875...	1.187766974047072...
80	1.18770...	1.187766974047098...

We next let $f(t) = J_0(t)$, the Bessel function of the first kind, and display results for $\alpha = -1/4$, also obtained by the routine `neutral_Ex6.m`, in Table 12.

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17

Papers on Orthogonal Polynomials on the Semicircle

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Polynomials Orthogonal on the Semicircle*

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Complex polynomials $\{\pi_k\}$, $\pi_k(z)=z^k+\cdots$, orthogonal with respect to the complex-valued inner product $(f, g)=\int_0^\pi f(e^{i\theta})g(e^{i\theta})d\theta$ are studied. By direct calculation of moment determinants it is shown that these polynomials exist uniquely. The three-term recurrence relation satisfied by these polynomials is obtained explicitly as well as their relationship with Legendre polynomials. It is shown that the zeros of π_n are all simple and are located in the interior of the upper unit half disc, distributed symmetrically with respect to the imaginary axis. They can be (and have been) computed as eigenvalues of a real nonsymmetric tridiagonal matrix. A linear second-order differential equation is obtained for $\pi_n(z)$ which has regular singular points at $z=1, -1, \infty$ (like Legendre's equation) and an additional regular singular point on the negative imaginary axis. Applications are discussed involving Gauss–Christoffel quadrature over the semicircle, numerical differentiation, and the computation of Cauchy principal value integrals.

1. INTRODUCTION

We study orthogonal polynomials relative to the inner product

$$(f, g)=\int_\Gamma (iz)^{-1} f(z)g(z)\,dz, \tag{1.1}$$

where Γ is the semicircle $\Gamma=\{z\in\mathbb{C}: z=e^{i\theta}, 0\leqslant\theta\leqslant\pi\}$. Alternatively,

$$(f, g)=\int_0^\pi f(e^{i\theta})g(e^{i\theta})d\theta. \tag{1.1'}$$

Note that the second factor g is not conjugated, so that the inner product is not Hermitian. Nevertheless, the orthogonal polynomials can be viewed

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as being orthogonal with respect to the (complex-valued) moment functional

$$\mathscr{L}z^k = \mu_k, \qquad \mu_k = \int_0^\pi e^{ik\theta}d\theta = \begin{cases} \pi, & k = 0, \\ 2i/k, & k \text{ odd}, \\ 0, & k \text{ even}, k \neq 0. \end{cases} \tag{1.2}$$

This moment functional is shown to be quasi-definite; it therefore generates a unique system of (monic, complex) polynomials $\{\pi_k\}$ satisfying

$$\begin{aligned} &\deg \pi_k = k, && k = 0, 1, 2, \ldots, \\ &(\pi_k, \pi_l) = 0 && \text{if } k \neq l, \\ &\neq 0 && \text{if } k = l. \end{aligned} \tag{1.3}$$

It turns out, moreover, that $(\pi_k, \pi_k) > 0$ for $k = 0, 1, 2, \ldots$. Orthogonality could not be achieved if Γ were the complete circle, since in that case $(f, g) = 2\pi f(0)g(0)$. One could consider, however, arbitrary circular arcs. Also, weight functions other than the constant weight function in (1.1′) can be studied. Some results in this direction, involving Gegenbauer type weight functions, indeed have already been obtained, but they are not yet sufficiently complete for presentation at this time.

The paper is organized as follows. In Section 2 we develop preliminary material on moment determinants which is used to establish quasi-definiteness of the moment functional (1.2). Section 3 develops the three-term recurrence relation for the orthogonal polynomials and Section 4 their connection with Legendre polynomials. In Section 5 we discuss the zeros of the orthogonal polynomial π_n and show, in particular, that all are contained in the open half disc $D_+ = \{z \in \mathbb{C}: |z| < 1, \operatorname{Im} z > 0\}$. A second-order linear differential equation for π_n is obtained in Section 6. Section 7 deals with Gauss–Christoffel quadrature formulae for integration over the semicircle, which are applied to numerical differentiation and, in Section 8, to compute Cauchy principal value integrals.

2. Preliminaries on Moment Determinants

The purpose of this section is to evaluate the determinants

$$\Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{vmatrix}, \qquad \Delta_n' = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-2} & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n-1} & \mu_{n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-3} & \mu_{2n-1} \end{vmatrix}, \tag{2.1}$$

where μ_k are the moments defined in (1.2). We first express these determinants in terms of the Hilbert-type determinants

$$H_0 = 1, \qquad H_m = \det\left[\frac{1}{2i+2j-3}\right]_{i,j=1}^{m},$$
$$H'_0 = 1, \qquad H'_m = \det\left[\frac{1}{2i+2j-1}\right]_{i,j=1}^{m}, \tag{2.2}$$

$m = 1, 2, 3, \ldots$.

LEMMA 2.1. *We have*

$$\Delta_n = 2^n H_{n/2}^2,\ n \text{ (even)} \geqslant 2; \qquad \Delta_n = 2^{n-1}\pi H'^2_{(n-1)/2},\ n \text{ (odd)} \geqslant 1. \tag{2.3}$$

Proof. Let first n be even. By (1.2) and (2.1), after removing a factor $2i$ from each even-numbered row and column, we have

$$\Delta_n = (-1)^{n/2}\, 2^n \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & 0 & \frac{1}{n-1} \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & \frac{1}{n-1} & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & 0 & \frac{1}{n+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \cdots & 0 & \frac{1}{2n-3} \\ \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \frac{1}{n+3} & \cdots & \frac{1}{2n-3} & 0 \end{vmatrix}, \qquad n \text{ even}. \tag{2.4}$$

Using Laplace expansion by columns numbered $1, 3, \ldots, n-1$, one finds that only one non-zero contribution results, namely from the minor and cominor pair

$$\begin{pmatrix} 2 & 4 & 6 & \cdots & n \\ 1 & 3 & 5 & \cdots & n-1 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 3 & 5 & \cdots & n-1 \\ 2 & 4 & 6 & \cdots & n \end{pmatrix}. \tag{2.5}$$

Since the moment matrix is symmetric, and the sign associated with the pair (2.5) is $(-1)^{n^2/4}$, one immediately obtains the first relation in (2.3).

To prove the second relation, for n odd, we use Laplace expansion by columns 1, 3,..., n in

$$\Delta_n = (-1)^{(n-1)/2}\, 2^{n-1} \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & \frac{1}{n-2} & 0 \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & 0 & \frac{1}{n} \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & \frac{1}{n} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ \frac{1}{n-2} & 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & \cdots & 0 & \frac{1}{2n-3} \\ 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & 0 & \cdots & \frac{1}{2n-3} & 0 \end{vmatrix}, \quad n \text{ odd.} \blacksquare \tag{2.6}$$

LEMMA 2.2. *We have*

$$\begin{aligned} \Delta_n' &= 2^{n-1} i\pi H_{n/2}' H_{(n-2)/2}', && n \text{ (even)} \geqslant 2, \\ &= 2^n i H_{(n+1)/2} H_{(n-1)/2}, && n \text{ (odd)} \geqslant 1. \end{aligned} \tag{2.7}$$

Proof. If n is even, then

$$\Delta_n' = (-1)^{(n-2)/2}\, 2^{n-1} i \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & \frac{1}{n-3} & 0 & 0 \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & 0 & \frac{1}{n-1} & \frac{1}{n+1} \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & \frac{1}{n-1} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \cdots & \frac{1}{2n-5} & 0 & 0 \\ \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \frac{1}{n+3} & \cdots & 0 & \frac{1}{2n-3} & \frac{1}{2n-1} \end{vmatrix}, \quad n \text{ even.} \tag{2.8}$$

Laplace expansion by columns $1, 3, 5, \ldots, n-1, n$ results in a single non-vanishing term, namely

$$\begin{pmatrix} 1 & 2 & 4 & \cdots & n-2 & n \\ 1 & 3 & 5 & \cdots & n-1 & n \end{pmatrix} \times \begin{pmatrix} 3 & 5 & 7 & \cdots & n-1 \\ 2 & 4 & 6 & \cdots & n-2 \end{pmatrix},$$

with sign $1+1+3+5+\cdots+(n-1)=(n^2+4)/4$, from which the first relation in (2.7) follows readily. The second relation follows similarly, using Laplace expansion by columns $2, 4, \ldots, n-1, n$ in

$$\Delta_n' = (-1)^{(n-1)/2} 2^n i \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & 0 & \frac{1}{n-2} & \frac{1}{n} \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & \frac{1}{n-2} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & 0 & \frac{1}{n} & \frac{1}{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ \frac{1}{n-2} & 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & \cdots & \frac{1}{2n-5} & 0 & 0 \\ 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & 0 & \cdots & 0 & \frac{1}{2n-3} & \frac{1}{2n-1} \end{vmatrix}, \quad n \text{ odd.} \quad \blacksquare \tag{2.9}$$

In order to evaluate the determinants in (2.2), we use Cauchy's formula (Muir [11, p. 345])

$$\det\left[\frac{1}{a_i+b_j}\right]_{i,j=1}^{m} = \frac{\prod_{i>j=1}^{m}(a_i-a_j)(b_i-b_j)}{\prod_{i,j=1}^{m}(a_i+b_j)}. \tag{2.10}$$

LEMMA 2.3. *We have*

$$H_m = \frac{2^{2m^2-m}\prod_{k=1}^{2m-1} k! \prod_{k=1}^{m-1}(2k)!}{\prod_{k=1}^{m}(2m+2k-2)!}, \qquad m=1, 2, 3, \ldots, \tag{2.11}$$

$$H_m' = \frac{2^{2m^2-m}\prod_{k=1}^{2m} k! \prod_{k=1}^{m}(2k)!}{m!^2 \prod_{k=1}^{m}(2m+2k)!}, \qquad m=1, 2, 3, \ldots. \tag{2.12}$$

Proof. Use (2.10) with $a_i=2i$, $b_j=2j-3$, and simplify, to get (2.11). Similarly, (2.12) follows from (2.10) with $a_i=2i$, $b_j=2j-1$. ∎

Combining Lemmas 2.1 and 2.3 yields

LEMMA 2.4. *We have*

$$\Delta_n = 2^{(n-1)^2}\pi \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n-1)/2} (2k)!^2}{((n-1)/2)!^4 \prod_{k=1}^{(n-1)/2} (n+2k-1)!^2}, \qquad n \text{ (odd)} \geqslant 1, \tag{2.13}$$

$$\Delta_n = 2^{n^2} \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n/2)-1} (2k)!^2}{\prod_{k=1}^{n/2} (n+2k-2)!^2}, \qquad n \text{ (even)} \geqslant 2. \tag{2.14}$$

Combining Lemmas 2.2 and 2.3 yields

LEMMA 2.5. *We have*

$$\Delta'_n = 2^{n^2} i \frac{\prod_{k=1}^{n-2} k!^2 \prod_{k=1}^{(n-1)/2} (2k)!^2}{(2n-1) \prod_{k=1}^{(n-1)/2} (n+2k-1)!^2}, \qquad n \text{ (odd)} \geqslant 1, \tag{2.15}$$

$$\Delta'_n = 2^{n^2-2n-1} i\pi \frac{n^2}{2n-1} \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n/2)-1} (2k)!^2}{(n/2)!^4 \prod_{k=1}^{(n/2)-1} (n+2k)!^2}, \qquad n \text{ (even)} \geqslant 2. \tag{2.16}$$

3. RECURRENCE RELATION

We note, first of all, from Lemma 2.4, that $\Delta_n > 0$, all $n \geqslant 1$, and therefore, in particular, that the moment sequence (1.2) is quasi-definite (cf., e.g., Chihara [2, Chap. 1, Definition 3.2]). The orthogonal polynomials (1.3) therefore exist uniquely, and $(\pi_k, \pi_k) = \Delta_{k+1}/\Delta_k > 0$ (Chihara [2, Chap. 1, Theorems 3.1 and 3.2]). Moreover, the following theorem holds.

THEOREM 3.1. *The (monic, complex) polynomials* $\{\pi_k\}$ *orthogonal with respect to the inner product* (1.1) *satisfy the recurrence relation*

$$\begin{aligned} &\pi_{k+1}(z) = (z - i\alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z), \qquad k = 0, 1, 2, \ldots, \\ &\pi_{-1}(z) = 0, \qquad \pi_0(z) = 1, \end{aligned} \tag{3.1}$$

where

$$\alpha_0 = \theta_0, \qquad \alpha_k = \theta_k - \theta_{k-1}, \qquad \beta_k = \theta_{k-1}^2, \qquad k \geqslant 1, \tag{3.2}$$

and θ_k *is given by*

$$\theta_k = \frac{2}{2k+1} \left[\frac{\Gamma((k+2)/2)}{\Gamma((k+1)/2)} \right]^2, \qquad k \geqslant 0. \tag{3.3}$$

Proof. The fact that the polynomials $\{\pi_k\}$ satisfy a three-term recurrence relation (3.1) follows from the property $(zf, g) = (f, zg)$ of the inner product (1.1) (cf. Gautschi [6, Theorem 2]). It is well-known that

$$\beta_k = \frac{\Delta_{k-1}\Delta_{k+1}}{\Delta_k^2}, \qquad k \geq 1, \tag{3.4}$$

from which the last relation in (3.2) follows via Lemma 2.4 by an elementary (but lengthy) computation. Likewise,

$$i\alpha_k = \frac{\Delta_{k+1}'}{\Delta_{k+1}} - \frac{\Delta_k'}{\Delta_k}, \qquad k \geq 0$$

(where $\Delta_0' = 0$), from which the first two relations in (3.2) follow via Lemmas 2.4 and 2.5. ∎

Using Stirling's formula in (3.3), one finds from (3.2)

$$\alpha_k \to 0, \qquad \beta_k \to \tfrac{1}{4} \qquad \text{as } k \to \infty,$$

just like in Szegö's theory for orthogonal polynomials on the interval $[-1, 1]$ (Szegö [14, Eqs. (12.7.4) and (12.7.6)]).

From (3.1) and (3.2) it follows easily that $-i\theta_{k-1}$ is the coefficient of z^{k-1} in π_k,

$$\pi_k(z) = z^k - i\theta_{k-1}z^{k-1} + \cdots, \qquad k \geq 1. \tag{3.5}$$

Furthermore, $\|\pi_k\|^2 = \pi\beta_1\beta_2\cdots\beta_k = \pi(\theta_0\theta_1\cdots\theta_{k-1})^2$, by (3.2), and hence, by (3.3),

$$\|\pi_k\| = \frac{1}{\sqrt{\pi}} 2^{2k} \frac{k![\Gamma((k+1)/2)]^2}{(2k)!}, \qquad k \geq 0. \tag{3.6}$$

4. Connection with Legendre Polynomials

The polynomial π_n in (1.3) is simply related to the (monic) Legendre polynomials. We have, in fact,

Theorem 4.1. *Let $\{\hat{P}_k\}$ denote the sequence of monic Legendre polynomials. Then the representation*

$$\pi_n(z) = \hat{P}_n(z) - i\theta_{n-1}\hat{P}_{n-1}(z), \qquad n \geq 1, \tag{4.1}$$

holds, where θ_k is given by (3.3).

Proof. Let $\hat{h}_k = \int_{-1}^{1} [\hat{P}_k(z)]^2 dz$. Then

$$\pi_n(z) = \gamma_0 \hat{P}_0(z) + \gamma_1 \hat{P}_1(z) + \cdots + \gamma_n \hat{P}_n(z),$$

where

$$\hat{h}_k \gamma_k = \int_{-1}^{1} \pi_n(z) \hat{P}_k(z)\, dz = -\int_0^{\pi} \pi_n(e^{i\theta}) \hat{P}_k(e^{i\theta}) i e^{i\theta} d\theta,$$

the second equality following from Cauchy's theorem. Since $z\hat{P}_k(z)$ is a linear combination of $\pi_0(z), \pi_1(z), \ldots, \pi_{k+1}(z)$, the orthogonality relations (1.3) yield $\gamma_0 = \gamma_1 = \cdots = \gamma_{n-2} = 0$. Clearly, $\gamma_n = 1$, while, in view of (3.5),

$$\hat{h}_{n-1} \gamma_{n-1} = \int_{-1}^{1} (z^n - i\theta_{n-1} z^{n-1} + \cdots) \hat{P}_{n-1}(z) dz$$

$$= \int_{-1}^{1} z^n \hat{P}_{n-1}(z) dz - i\theta_{n-1} \hat{h}_{n-1}.$$

Here the second integral vanishes, the integrand being an odd function, and so $\gamma_{n-1} = -i\theta_{n-1}$. ∎

5. The Zeros of $\pi_n(z)$

We begin with a simple symmetry property.

THEOREM 5.1. *If $\zeta \in \mathbb{C}$ is a zero of the polynomial π_n, then so is $-\bar{\zeta}$. The zeros of π_n are thus located symmetrically with respect to the imaginary axis.*

Proof. Denote by $\bar{\pi}_n$ the polynomial obtained from π_n by conjugating all coefficients,

$$\bar{\pi}_n(z) = \overline{\pi_n(\bar{z})}.$$

Equation (4.1) then shows that

$$\pi_n(-z) = (-1)^n \bar{\pi}_n(z). \tag{5.1}$$

Therefore, if ζ is a zero of π_n, there follows

$$0 = \pi_n(\zeta) = (-1)^n \bar{\pi}_n(-\zeta) = (-1)^n \overline{\pi_n(-\bar{\zeta})},$$

hence $\pi_n(-\bar{\zeta}) = 0$. ∎

We show next that all zeros of π_n lie in the upper unit half disc.

THEOREM 5.2. *All zeros of the polynomial* π_n *are contained in* $D_+ = \{z \in \mathbb{C}: |z| < 1 \text{ and } \operatorname{Im} z > 0\}$.

Proof. We first apply Rouché's theorem to show that all zeros of π_n lie in the open unit disc $D = \{z \in \mathbb{C}: |z| < 1\}$. Consider

$$Q_n(z) = \frac{\hat{P}_n(z)}{\hat{P}_{n-1}(z)}, \qquad z \in \partial D.$$

We are seeking lower bounds q_n (not depending on z) of $|Q_n(z)|$ for $z \in \partial D$,

$$|Q_n(z)| \geqslant q_n, \qquad z \in \partial D.$$

From the recurrence relation for the (monic) Legendre polynomials

$$\hat{P}_n(z) = z\hat{P}_{n-1}(z) - \frac{1}{4-(n-1)^{-2}}\hat{P}_{n-2}(z),$$

we find

$$Q_n(z) = z - \frac{1}{4-(n-1)^{-2}}\frac{1}{Q_{n-1}(z)}. \tag{5.2}$$

Since $Q_1(z) = z$, we clearly have $q_1 = 1$. Furthermore, (5.2) shows that we can take

$$q_1 = 1, \qquad q_n = 1 - \frac{1}{4-(n-1)^{-2}}\frac{1}{q_{n-1}}, \qquad n \geqslant 2.$$

It is readily seen by induction that

$$q_n = \frac{n}{2n-1}, \qquad n \geqslant 1.$$

Therefore, $|\hat{P}_n(z)| \geqslant (n/(2n-1))|\hat{P}_{n-1}(z)|$ on ∂D, and thus

$$|\hat{P}_n(z)| \geqslant \frac{n}{2n-1}\frac{1}{\theta_{n-1}}|\theta_{n-1}\hat{P}_{n-1}(z)|, \qquad z \in \partial D,$$

where θ_k is given in (3.3). Now,

$$\frac{n}{2n-1}\frac{1}{\theta_{n-1}} = \frac{2}{n}\left[\Gamma\left(\frac{n}{2}+1\right)\Big/\Gamma\left(\frac{n+1}{2}\right)\right]^2,$$

and using a refinement of Gautschi's inequality for the gamma function,

$$\frac{\Gamma(x+1)}{\Gamma(x+s)} > (x+\tfrac{1}{2}s)^{1-s}, \qquad x > 0,\ 0 < s < 1,$$

due to Kershaw [10], with $x=n/2$, $s=\frac{1}{2}$, one finds

$$\frac{n}{2n-1}\frac{1}{\theta_{n-1}}>\frac{2n+1}{2n}>1. \tag{5.3}$$

Consequently, $|\hat{P}_n(z)|>|\theta_{n-1}\hat{P}_{n-1}(z)|$ on ∂D, and therefore by Rouché's theorem, applied to (4.1), all zeros of π_n lie in D.

To complete the proof of Theorem 5.2 we use in (4.1) a result of Giroux [8, Corollary 3], according to which all zeros of π_n either lie in the half strip $\operatorname{Im} z\geqslant 0$, $-\xi_n\leqslant \operatorname{Re} z\leqslant \xi_n$, or in the conjugate half strip, where ξ_n is the largest zero of the Legendre polynomial P_n. Since by (3.5) the sum of the zeros has positive imaginary part, it is the upper half strip that applies. It remains to show that all zeros of π_n are nonreal. If there were a zero $\zeta=x\in\mathbb{R}$, then indeed $\hat{P}_{n-1}(x)\neq 0$, since otherwise, by (4.1), we would have the contradiction $\hat{P}_n(x)=\hat{P}_{n-1}(x)=0$. The same equation (4.1) then implies $i\theta_{n-1}=\hat{P}_n(x)/\hat{P}_{n-1}(x)$, which is plainly impossible. ∎

Remarks. (1) We have proved, more precisely, that all zeros of π_n are contained in the region $\{z\in\mathbb{C}: |z|<1\}\cap\{z\in\mathbb{C}: \operatorname{Im} z>0, -\xi_n\leqslant \operatorname{Re} z\leqslant\xi_n\}$, where ξ_n is the largest zero of the Legendre polynomial P_n.

(2) The fact that all zeros of π_n lie in the closure of D follows also from a result of Specht [13, Satz 7*], applied to (4.1), and Kershaw's inequality used above. We feel, however, that our proof has independent interest.

THEOREM 5.3. *All zeros of π_n are simple.*

Proof. Let ζ be a zero of π_n, hence, by (4.1),

$$\hat{P}_n(\zeta)=i\theta_{n-1}\hat{P}_{n-1}(\zeta).$$

We prove that $\pi_n'(\zeta)\neq 0$.

Using the recurrence relations

$$\hat{P}_{k+1}(z)=z\hat{P}_k(z)-\frac{k^2}{4k^2-1}\hat{P}_{k-1}(z) \tag{5.4}$$

and

$$(1-z^2)\,\hat{P}_k'(z)=(k+1)\,z\hat{P}_k(z)-(2k+1)\,\hat{P}_{k+1}(z) \tag{5.5}$$

in

$$\pi_n'(\zeta)=\hat{P}_n'(\zeta)-i\theta_{n-1}\hat{P}_{n-1}'(\zeta)=\frac{1}{\hat{P}_{n-1}(\zeta)}\left[\hat{P}_n'(\zeta)\hat{P}_{n-1}(\zeta)-\hat{P}_n(\zeta)\hat{P}_{n-1}'(\zeta)\right]$$

yields, after a little computation,

$$\pi_n'(\zeta)=\frac{1}{(1-\zeta^2)\hat{P}_{n-1}(\zeta)}\left[\frac{n^2}{2n-1}\hat{P}_{n-1}^2(\zeta)+(2n-1)\hat{P}_n^2(\zeta)-2n\zeta\hat{P}_n(\zeta)\hat{P}_{n-1}(\zeta)\right]$$
$$=\frac{\hat{P}_{n-1}(\zeta)}{(1-\zeta^2)\,(2n-1)}\left[n^2-(2n-1)^2\theta_{n-1}^2-2n(2n-1)\zeta\theta_{n-1}i\right].$$

Letting $\zeta=\alpha+i\beta$, the expression in brackets becomes

$$n^2-(2n-1)^2\theta_{n-1}^2+2n(2n-1)\beta\theta_{n-1}-2n(2n-1)\alpha\theta_{n-1}i,$$

which, by virtue of $\beta>0$ and (5.3), is clearly nonzero. ∎

The zeros ζ_ν of π_n may be computed as eigenvalues of the Jacobi matrix

$$J_n=\begin{bmatrix} i\alpha_0 & \theta_0 & & & 0 \\ \theta_0 & i\alpha_1 & \theta_1 & & \\ & \theta_1 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ 0 & & & \theta_{n-2} & i\alpha_{n-1} \end{bmatrix}. \tag{5.6}$$

By a similarity transformation with the diagonal matrix $D_n=\operatorname{diag}(1, i, i^2, i^3, 1, i,\ldots)\in\mathbb{R}^{n\times n}$ these can be seen to equal $\zeta_\nu=i\eta_\nu$, where η_ν are the eigenvalues of the real nonsymmetric tridiagonal matrix

$$-iD_n^{-1}J_nD_n=\begin{bmatrix} \alpha_0 & \theta_0 & & & 0 \\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ 0 & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix}. \tag{5.7}$$

Using the EISPACK routine HQR [12, p. 240], we computed all zeros of π_n for selected values of n up to $n=73$. Figure 1 shows those with nonnegative real parts for $n=2(1)11$, as well as those with smallest, and next to smallest, positive real parts for $n=12, 16, 24, 40, 72$ and those with smallest positive real parts for $n=13, 17, 25, 41, 73$.

Figure 1, together with the facts that $\pi_1(z)=z-(2i/\pi)$ and $\pi_3(z)=z^3-(8i/5\pi)z^2-(3/5)z+(8i/15\pi)$, suggests that the imaginary part of every zero of π_n is $\leqslant 2/\pi$, if $n\geqslant 1$, and $\leqslant .315076\ldots$, the unique positive root of $t^3-(8/5\pi)t^2+(3/5)t-(8/15\pi)=0$, if $n\geqslant 2$.

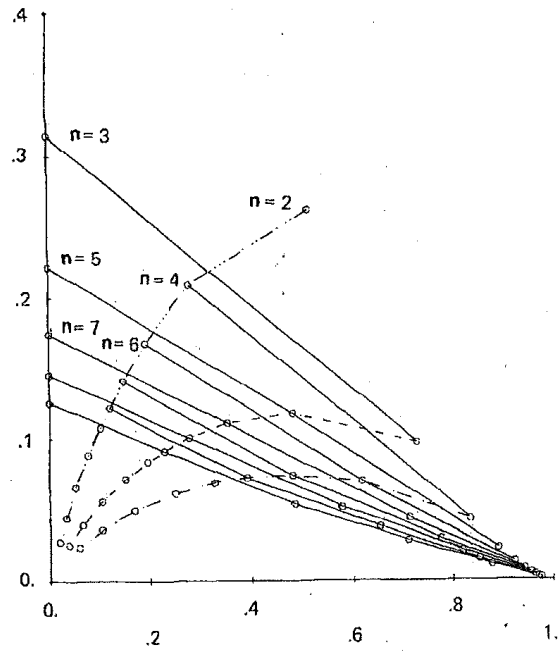

FIGURE 1

6. DIFFERENTIAL EQUATION

Like the Legendre polynomial P_n, the polynomial π_n satisfies a second-order linear differential equation with regular singular points at $1, -1, \infty$. There is, however, an additional regular singular point on the negative imaginary axis which moves as a function of n.

THEOREM 6.1. *The polynomial $\pi_n(z)$ satisfies the differential equation*

$$\begin{aligned}(1-z^2)\,&[n^2-(2n-1)^2\theta_{n-1}^2-2n(2n-1)zi\theta_{n-1}]\pi_n''(z)\\ &-2[(n^2-(2n-1)^2\theta_{n-1}^2)z-n(2n-1)(z^2+1)i\theta_{n-1}]\pi_n'(z)\\ &+n[(n+1)n^2-(n-1)(2n-1)^2\theta_{n-1}^2-2(2n-1)n^2zi\theta_{n-1}]\pi_n(z)=0,\end{aligned} \tag{6.1}$$

where θ_k is given by (3.3).

Proof[1]. Let $u=\hat{P}_{n-1}(z)$ and $v=(2n-1)\pi_n(z)$, and define

$$\omega(z)=(z-1)^{(n/2)-(n-1/2)i\theta_{n-1}}(z+1)^{(n/2)+(n-1/2)i\theta_{n-1}}, \tag{6.2}$$

[1] The authors are indebted to Professor F. Calogero for the reference Ahmed and Bruschi [1], where similar proof techniques are employed.

where we assume, for the moment, that $z \in D_+ = \{z \in \mathbb{C}: |z| < 1$ and $\operatorname{Im} z > 0\}$ and where fractional and imaginary powers denote principal branches. An elementary calculation, using (5.5) and (4.1), will show that

$$(z^2-1)[\omega(z)u]' = \omega(z)v, \tag{6.3}$$

where the prime denotes differentiation with respect to z. There follows

$$u = \frac{1}{\omega}\int \frac{\omega}{z^2-1} v\,dz,$$

$$u' = \left(\frac{1}{\omega}\right)' \int \frac{\omega}{z^2-1} v\,dz + \frac{1}{z^2-1} v,$$

$$u'' = \left(\frac{1}{\omega}\right)'' \int \frac{\omega}{z^2-1} v\,dz + \left(\frac{1}{\omega}\right)' \frac{\omega}{z^2-1} v + \left(\frac{1}{z^2-1}\right)' v + \frac{1}{z^2-1} v'.$$

Inserting this into Legendre's differential equation

$$(z^2-1)u'' + 2zu' - n(n-1)u = 0,$$

and simplifying, yields

$$v' - \frac{\omega'}{\omega} v + \left[\left((z^2-1)\left(\frac{1}{\omega}\right)'\right)' - \frac{n(n-1)}{\omega}\right] \int \frac{\omega}{z^2-1} v\,dz = 0. \tag{6.4}$$

Noting by (6.2) that

$$-\frac{\omega'}{\omega} = \frac{-nz + (2n-1)i\theta_{n-1}}{z^2-1} =: a(z),$$

$$\left((z^2-1)\left(\frac{1}{\omega}\right)'\right)' - \frac{n(n-1)}{\omega} = \frac{1}{\omega}\frac{n^2 - (2n-1)^2\theta_{n-1}^2 - 2n(2n-1)zi\theta_{n-1}}{z^2-1}$$

$$=: b(z), \tag{6.5}$$

one obtains from (6.4)

$$\frac{1}{b(z)} v' + \frac{a(z)}{b(z)} v + \int \frac{\omega}{z^2-1} v\,dz = 0.$$

Differentiating this with respect to z and multiplying the result by $-[n^2 - (2n-1)^2\theta_{n-1}^2 - 2n(2n-1)zi\theta_{n-1}]^2/\omega(z)$ yields, after some lengthy, but elementary computation, the desired differential equation (6.1). By the permanence principle, the restriction imposed on z can now be lifted. ∎

We remark that the differential equation (6.1) has four regular singular points, one each at $1, -1$, and ∞, and an additional one at $z_0 = -[n^2 - (2n-1)^2\theta_{n-1}^2]i/[2n(2n-1)\theta_{n-1}]$. In view of (5.3), z_0 is located on the negative imaginary axis; it approaches the origin monotonically as n increases. Since by Theorem 5.2 the zeros of π_n are contained in D_+, and therefore are regular points of the differential equation (6.1), it follows again that they must all be simple.

7. Gauss–Christoffel Quadrature over the Semicircle

The orthogonal polynomials $\pi_n(z)$ can be used in the usual way (see, e.g., Gautschi [7, Section 1.3]) to construct a Gauss–Christoffel quadrature rule

$$\int_0^\pi g(e^{i\theta})d\theta = \sum_{\nu=1}^{n} \sigma_\nu g(\zeta_\nu) + R_n(g), \qquad R_n(\mathbf{P}_{2n-1}) = 0, \tag{7.1}$$

for integrals over the semicircle. Indeed, the nodes $\zeta_\nu = \zeta_\nu^{(n)}$ are precisely the zeros of $\pi_n(z)$, whereas the weights $\sigma_\nu = \sigma_\nu^{(n)}$ can be obtained by an adaptation of the procedure of Golub and Welsch [9]. Letting $\tilde{\pi}_k(z) = \pi_k(z)/\|\pi_k\|$ denote the normalized orthogonal polynomials and

$$\tilde{\pi}(z) = [\tilde{\pi}_0(z), \tilde{\pi}_1(z), \ldots, \tilde{\pi}_{n-1}(z)]^T$$

the vector of the first n of them, it is easily seen that

$$J_n\tilde{\pi}(\zeta_\nu) = \zeta_\nu\tilde{\pi}(\zeta_\nu),$$

where J_n is the Jacobi matrix in (5.6). The nodes ζ_ν are therefore the eigenvalues of J_n and $\tilde{\pi}(\zeta_\nu)$ the corresponding eigenvectors. Defining

$$p(z) = D_n^{-1}\tilde{\pi}(z), \tag{7.2}$$

where, as before, $D_n = \operatorname{diag}(1, i, i^2, i^3, 1, i, \ldots)$, one finds

$$[-iD_n^{-1}J_nD_n]p(\zeta_\nu) = \eta_\nu p(\zeta_\nu), \tag{7.3}$$

i.e., $p(\zeta_\nu)$ is an eigenvector of the real matrix (5.7) corresponding to the eigenvalue $\eta_\nu = -i\zeta_\nu$. Denote by V_n the matrix of the eigenvectors of (5.7), each normalized so that the first component is equal to 1. Then

$$V_n = [v_1, v_2, \ldots, v_n], \qquad v_\nu = \sqrt{\pi}p(\zeta_\nu). \tag{7.4}$$

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Now substituting in (7.1) for g in turn all components of the vector $p(z)$ in (7.2) yields

$$\sqrt{\pi}e_1 = \frac{1}{\sqrt{\pi}} V_n \sigma, \qquad \sigma = [\sigma_1, \sigma_2, \ldots, \sigma_n]^T,$$

where e_1 is the first coordinate vector. Therefore,

$$V_n \sigma = \pi e_1. \tag{7.5}$$

The weights σ_ν in (7.1) can thus be found by solving the linear system of equations (7.5). Using the EISPACK routine HQR2 [12, p. 248] to compute the matrix V_n, and the LINPACK routines CGECO and CGESL [4, Chap. 1] to solve the system (7.5), we observed estimates of the condition number (furnished by CGECO) which were only moderately large. For example, cond $V_n = 20.5, 73.3, 184.9$ for $n = 10, 20, 40$, respectively. It thus appears that the system (7.5) is reasonably well conditioned.

Since the matrix in (7.3) is real, the nonreal eigenvalues η_ν occur in conjugate complex pairs (see also Theorem 5.1). One has, moreover, the following theorem.

THEOREM 7.1. *If η_ν is real, so is σ_ν. If $\eta_{\nu+1} = \bar{\eta}_\nu$ is complex, then $\sigma_{\nu+1} = \bar{\sigma}_\nu$.*

Proof. Assume first that n is odd, and for simplicity, that there is one real eigenvalue η_1 and $n-1$ conjugate complex eigenvalues $\eta_{2\nu+1} = \bar{\eta}_{2\nu}$, $\nu = 1, 2, \ldots, [n/2]$. (Figure 1 suggests that this is indeed the case.) Then the first eigenvector v_1 in (7.4) is real and the others occur in conjugate complex pairs, $v_{2\nu+1} = \bar{v}_{2\nu}$, $\nu = 1, 2, \ldots, [n/2]$. By (7.5) therefore,

$$\sigma_1 v_1 + \sum_{\nu=1}^{[n/2]} (\sigma_{2\nu} v_{2\nu} + \sigma_{2\nu+1} \bar{v}_{2\nu}) = \pi e_1.$$

Conjugating this, gives

$$\sigma_1 v_1 + \sum_{\nu=1}^{[n/2]} (\bar{\sigma}_{2\nu+1} v_{2\nu} + \bar{\sigma}_{2\nu} \bar{v}_{2\nu}) = \pi e_1.$$

By the nonsingularity of V_n, hence the uniqueness of σ, there follows $\sigma_{2\nu+1} = \bar{\sigma}_{2\nu}$ for $\nu = 1, 2, \ldots, [n/2]$, proving the second part of the theorem. Since the sum above, as well as v_1, are real, it follows that also σ_1 is real, which proves the first part of the theorem. A similar argument applies when n is even. ∎

In Table I we display the Gauss–Christoffel formulae (to 8 decimals only, to save space) for $n = 5, 10, 20$. They were obtained (to higher precision) on the CDC 6500 computer, using the routines HQR2, CGECO and CGESL mentioned above.

EXAMPLE 7.1. $\int_0^\pi \exp(ce^{i\theta})d\theta = \pi + i[Ei(c) + E_1(c)]$, $c > 0$.

The exact answer in terms of the exponential integrals (cf. Gautschi and Cahill [5, Eqs. 5.1.1 and 5.1.2]) follows from (8.1) below (where $f(z) = \exp(cz)$) and (8.8) (where $x = 0$).

We apply the Gauss–Christoffel rule (7.1) with $g(z) = \exp(cz)$ for $n = 2, 5, 10, 20$ and $c = .2, .6, 1.0, 2.0, 6.0, 10.0$. The results are compared with the approximations furnished by the composite trapezoidal rule based on n equal subintervals of $[0, \pi]$ and by the n-point Gauss–Legendre formula on $[0, \pi]$. Since the real part of the integrand is an even function, the trapezoidal rule must produce for the real part half of the result it would obtain if it were applied over the whole interval of periodicity, $[-\pi, \pi]$, using $2n$ subintervals. In particular, the composite trapezoidal rule, like the Gauss–Christoffel rule (7.1), integrates the first $2n-1$ powers in the real part exactly. This will not be the case for the imaginary part, which is an odd function. Here the trapezoidal rule, unlike the Gauss rule, integrates

TABLE I

Gauss–Christoffel Formula for $n = 5, 10, 20$

n	ν	ζ_ν		σ_ν	
5	1,2	±0.89052727	+0.022495461i	0.0072402551	±0.30663646i
	3,4	±0.48026508	+0.11792794i	0.50270345	±0.92618932i
	5		0.22216141i	1.99138066	
10	1,2	±0.97146604	+0.0028731070i	0.0078107581	±0.074979250i
	3,4	±0.85284258	+0.015150376i	0.023571055	±0.19000917i
	5,6	±0.65232339	+0.037578303i	0.063357456	±0.35652707i
	7,8	±0.39255204	+0.072381390i	0.23196483	±0.66539219i
	9,10	±0.11928205	+0.12236097i	1.24409223	±0.83467375i
20	1,2	±0.99279481	+0.00036088122i	0.00093961488	±0.018602063i
	3,4	±0.96223284	+0.0019015682i	0.0023283767	±0.044211071i
	5,6	±0.90804700	+0.0046758976i	0.0041099345	±0.072223615i
	7,8	±0.83157445	+0.0086981042i	0.0066940217	±0.10457986i
	9,10	±0.73472727	+0.014013039i	0.010908872	±0.14441960i
	11,12	±0.61995356	+0.020739446i	0.018712830	±0.19743837i
	13,14	±0.49022929	+0.029167472i	0.035680664	±0.27542598i
	15,16	±0.34918044	+0.040007722i	0.082367746	±0.40649151i
	17,18	±0.20200473	+0.055045977i	0.26876888	±0.65608704i
	19,20	±0.061601584	+0.075471956i	1.14028539	±0.69192546i

exactly only linear terms, and the error in the imaginary part must be expected to exhibit the familiar $\mathcal{O}(h^2)$ behavior, where $h=\pi/n$. Table II shows the results (numbers in parentheses denote decimal exponents). The three pairs of entries for each c and n represent the relative errors in the real and imaginary part corresponding to the n-point Gauss–Christoffel rule (7.1), the n-point Gauss–Legendre rule on $[0, \pi]$, and the composite $(n+1)$-point trapezoidal rule, in that order. Note that the error of the Gauss–Christoffel rule, even for the real part, is usually several orders of magnitude smaller than the corresponding error of the trapezoidal rule, unless both are near the level of machine precision (3.553×10^{-15} on the CDC 6500 computer). The large errors of the trapezoidal rule in the imaginary parts, and their $\mathcal{O}(h^2)$ decay, are particularly conspicuous. Note also the relatively poor performance (compared to (7.1)) of the Gauss–Legendre rule.

The exponential integrals Ei and E_1 in Example 7.1 were computed by the FUNPACK functions EI and $EONE$, respectively (cf. Cody [3]).

EXAMPLE 7.2. $f'(a)=(1/\pi h)\int_0^\pi e^{-i\theta}\,[f(a+(h/2)e^{i\theta})-f(a-(h/2)e^{i\theta})]d\theta.$

TABLE II

Relative Errors in Real and Imaginary Parts

c		$n=2$		$n=5$		$n=10$		$n=20$	
0.2	GC	7.4(−6)	2.4(−6)	9.0(−15)	7.1(−14)	1.4(−14)	1.2(−13)	2.7(−14)	2.1(−13)
	GL	4.8(−3)	2.5(−2)	4.7(−7)	1.2(−5)	4.5(−14)	3.0(−12)	4.6(−13)	2.4(−13)
	T	6.7(−5)	2.2(−1)	1.4(−14)	3.4(−2)	1.4(−14)	8.4(−3)	2.7(−14)	2.1(−3)
0.6	GC	6.0(−4)	1.9(−4)	3.1(−12)	5.1(−13)	1.8(−14)	1.2(−13)	2.7(−14)	2.0(−13)
	GL	3.8(−2)	3.3(−2)	6.5(−5)	2.1(−5)	7.4(−11)	6.2(−10)	4.0(−13)	2.4(−13)
	T	5.4(−3)	2.8(−1)	1.7(−9)	3.9(−2)	2.3(−14)	9.6(−3)	3.2(−14)	2.4(−3)
1.0	GC	4.7(−3)	1.5(−3)	5.2(−10)	7.1(−11)	2.3(−14)	1.3(−13)	1.4(−14)	2.2(−13)
	GL	8.3(−2)	1.4(−1)	2.8(−4)	6.4(−4)	6.8(−9)	6.0(−9)	3.7(−13)	2.2(−13)
	T	4.2(−2)	3.7(−1)	2.8(−7)	5.0(−2)	1.4(−14)	1.2(−2)	5.0(−14)	3.0(−3)
2.0	GC	7.8(−2)	2.1(−2)	5.6(−7)	6.4(−8)	2.3(−14)	1.6(−13)	4.5(−15)	2.8(−13)
	GL	1.6(−1)	4.9(−1)	1.1(−2)	5.2(−3)	2.3(−7)	1.1(−6)	4.0(−13)	1.4(−13)
	T	6.7(−1)	7.1(−1)	2.8(−4)	1.1(−1)	3.9(−13)	2.5(−2)	5.4(−14)	6.2(−3)
6.0	GC	9.0(0)	6.0(−1)	5.3(−2)	1.1(−3)	4.0(−9)	4.2(−11)	1.0(−12)	8.7(−13)
	GL	4.9(1)	2.1(0)	1.3(1)	3.2(−1)	9.3(−2)	1.2(−3)	3.4(−8)	2.5(−11)
	T	1.0(2)	1.0(0)	1.7(1)	1.4(0)	1.5(−3)	2.6(−1)	3.4(−13)	5.9(−2)
10.0	GC	1.1(2)	1.0(0)	2.2(1)	2.8(−2)	2.0(−4)	1.2(−7)	5.9(−11)	1.6(−12)
	GL	1.3(3)	1.2(0)	6.4(2)	2.1(0)	8.2(1)	1.2(−2)	1.1(−4)	1.4(−6)
	T	5.5(3)	1.0(0)	2.8(3)	1.3(0)	4.1(1)	1.0(0)	1.2(−8)	1.9(−1)

Note. Gauss–Christoffel (GC), Gauss–Legendre (GL), and trapezoidal (T) integration of $\int_0^\pi \exp(ce^{i\theta})d\theta$.

TABLE III

Numerical differentiation by (7.7) with $n=2$, for $f(z)=\exp(z)$, $a=0$

h	$f'(0)\approx$
1.	0.99994199437142
0.5	0.99999638098906
0.25	0.99999977391086
0.125	0.99999998587099
0.0625	0.99999999911702
0.03125	0.99999999994522
0.015625	0.99999999999667

It is assumed here that f is analytic on some domain containing the point a and a circular neighborhood of a with radius $h/2$. The formula given for the derivative is then an easy consequence of Cauchy's theorem. Applying (7.1) to the integral on the right yields

$$f'(a)\approx\frac{1}{\pi h}\sum_{\nu=1}^{n}\frac{\sigma_\nu}{\zeta_\nu}\left[f\left(a+\frac{h}{2}\zeta_\nu\right)-f\left(a-\frac{h}{2}\zeta_\nu\right)\right]. \tag{7.6}$$

In the case where a is real, and $f(z)$ is real for real z, this can be simplified by using Theorems 5.1 and 7.1. For example, when n is even, and $\operatorname{Re}\zeta_\nu>0$ for $\nu=1, 2,..., n/2$, one finds

$$f'(a)\approx\frac{2}{\pi h}\sum_{\nu=1}^{n/2}\operatorname{Re}\left\{\frac{\sigma_\nu}{\zeta_\nu}\left[f\left(a+\frac{h}{2}\zeta_\nu\right)-f\left(a-\frac{h}{2}\zeta_\nu\right)\right]\right\}, \qquad n \text{ even.} \tag{7.7}$$

To give a numerical illustration, let $f(z)=e^z$, $a=0$ and $n=2$. Then

$$\zeta_1=\frac{1}{12}[\sqrt{48-\pi^2}+i\pi], \qquad \sigma_1=\frac{1}{2}\left[\pi+i\frac{24-\pi^2}{\sqrt{48-\pi^2}}\right],$$

$$\frac{\sigma_1}{\zeta_1}=\frac{1}{4}\left[\pi\frac{36-\pi^2}{\sqrt{48-\pi^2}}+i(12-\pi^2)\right],$$

and (7.7) for $h=2^{-k}$, $k=0(1)6$, produces the approximations in Table III.

8. An Application to Cauchy Principal Value Integrals

Let C_ε, $0<\varepsilon<1$, be the contour in the complex plane formed by the unit upper semicircle, the line segment from -1 to $-\varepsilon$, the upper semicircle of

radius ε and center at the origin, and the line segment from ε to 1. For any function f analytic on the closed upper unit half disc we then have, by Cauchy's theorem, $\lim_{\varepsilon \downarrow 0} \int_{C_\varepsilon} f(z)\, dz/z = 0$, hence

$$\int\!\!\!\!\!\!-_{-1}^{1} \frac{f(t)}{t}\, dt = i\left\{\pi f(0) - \int_0^\pi f(e^{i\theta})\, d\theta\right\}, \tag{8.1}$$

where the integral on the left is a Cauchy principal value integral. In particular, if $f(z)$ is real for real z, as we shall henceforth assume, we have

$$\int\!\!\!\!\!\!-_{-1}^{1} \frac{f(t)}{t}\, dt = \operatorname{Im} \int_0^\pi f(e^{i\theta})\, d\theta. \tag{8.2}$$

If the singularity is not at the origin, but at some arbitrary point x on $(-1, 1)$, we map x to the origin by a linear fractional transformation and obtain

$$\int\!\!\!\!\!\!-_{-1}^{1} \frac{f(t)}{t-x}\, dt = \int\!\!\!\!\!\!-_{-1}^{1} \frac{g(x,t)}{t}\, dt = \operatorname{Im} \int_0^\pi g(x, e^{i\theta})\, d\theta, \tag{8.3}$$

where

$$g(x, z) = f\frac{z+x}{xz+1}\Big/(xz+1). \tag{8.4}$$

Applying (7.1) to (8.3) yields

$$\int\!\!\!\!\!\!-_{-1}^{1} \frac{f(t)}{t-x}\, dt = \operatorname{Im}\left\{\sum_{\nu=1}^{n} \sigma_\nu g(x, \zeta_\nu) + R_n(g(x, \cdot))\right\}. \tag{8.5}$$

Note that $g(x, z)$ has a singularity at $z = -1/x$, which is farther away from the interval $[-1, 1]$ the smaller $|x|$. We expect therefore (8.5) to provide a good approximation (when R_n is neglected), unless $|x|$ is close to 1.

One might think of proceeding more directly by following the derivation at the beginning of this section, but with a contour C_ε that excludes the point x rather than 0. This would give

$$\int\!\!\!\!\!\!-_{-1}^{1} \frac{f(t)}{t-x}\, dt = i\left\{\pi f(x) - \int_0^\pi \frac{f(e^{i\theta})}{1 - xe^{-i\theta}}\, d\theta\right\}, \qquad -1 < x < 1. \tag{8.6}$$

Applying the quadrature rule (7.1) to the integral on the right of (8.6), however, would produce poor results, owing to the pole at $z = x$ of the integrand function $f(z)/(1 - xz^{-1})$.

A better alternative is to use Gauss–Legendre quadrature on (8.3) (cf., e.g., Gautschi [7, p. 106]),

$$\int_{-1}^{1} \frac{f(t)}{t-x}\,dt \approx \sum_{\nu=1}^{n} \frac{\lambda_\nu}{\tau_\nu} g(x, \tau_\nu), \qquad n \text{ even}, \tag{8.7}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the Legendre polynomial P_n and $\lambda_\nu = \lambda_\nu^{(n)}$ the associated Christoffel numbers. This requires only real arithmetic, in contrast to (8.5), but may be less stable on account of the division by the two zeros τ_ν of opposite sign closest to the origin.

EXAMPLE 8.1. $I(x, c) = \int_{-1}^{1} \frac{e^{ct}}{t-x}\,dt, \quad -1 < x < 1, \; c \in \mathbb{R}.$

A simple calculation yields

$$\begin{aligned} I(x, c) &= e^{cx}[Ei(c(1-x)) + E_1(c(1+x))] && \text{if } c > 0, \\ &= \ln[(1-x)/(1+x)] && \text{if } c = 0, \\ &= -e^{|c|x}[Ei(|c|(1+x)) + E_1(|c|(1-x))] && \text{if } c < 0, \end{aligned} \tag{8.8}$$

where Ei, E_1 are exponential integrals.

The quadrature rules (8.5) and (8.7) were found to give comparable results in this example. Both, indeed, have similar approximation properties: (8.5) is exact when g is a polynomial of degree $\leqslant 2n-1$, and (8.7) when g is a polynomial of degree $\leqslant 2n$. When n is large, however, and the truncation error near the level of machine precision, (8.5) was observed to produce somewhat more accurate results on account of better stability. Measuring cancellation in the respective quadrature sums by the ratio of the absolutely largest quadrature term and the modulus of the quadrature sum, it was found, for example, that for $n = 40$ and $c = 0.5$ the degree of cancellation is 1–2 orders of magnitude larger in (8.7) than in (8.5).

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17.2. [104] “Polynomials Orthogonal on the Semicircle. II”

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CONSTRUCTIVE APPROXIMATION

Polynomials Orthogonal on the Semicircle, II

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Abstract. Generalizing previous work [2], we study complex polynomials $\{\pi_k\}$, $\pi_k(z)=z^k+\cdots$, orthogonal with respect to a complex-valued inner product $(f,g)=\int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})\,d\theta$. Under suitable assumptions on the "weight function" w, we show that these polynomials exist whenever $\operatorname{Re}\int_0^\pi w(e^{i\theta})\,d\theta\neq 0$, and we express them in terms of the real polynomials orthogonal with respect to the weight function $w(x)$. We also obtain the basic three-term recurrence relation. A detailed study is made of the polynomials $\{\pi_k\}$ in the case of the Jacobi weight function $w(z)=(1-z)^\alpha(1+z)^\beta$, $\alpha>-1$, $\beta>-1$, and its special case $\alpha=\beta=\lambda-\frac{1}{2}$ (Gegenbauer weight). We show, in particular, that for Gegenbauer weights the zeros of π_n are all simple and, if $n\geq 2$, contained in the interior of the upper unit half disc. We strongly suspect that the same holds true for arbitrary Jacobi weights. Finally, for the Gegenbauer weight, we obtain a linear second-order differential equation for $\pi_n(z)$. It has regular singular points at $z=1,-1,\infty$ (like Gegenbauer's equation) and an additional regular singular point on the negative imaginary axis, which depends on n.

1. Introduction

Let w be a weight function which is positive and integrable on the open interval $(-1,1)$, though possibly singular at the endpoints, and which can be extended to a function $w(z)$ holomorphic in the half disc $D_+=\{z\in\mathbf{C}:|z|<1,\ \operatorname{Im} z>0\}$. Consider the following two inner products,

$$[f,g]=\int_{-1}^{1} f(x)\overline{g(x)}w(x)\,dx, \tag{1.1}$$

$$(f,g)=\int_\Gamma f(z)g(z)w(z)(iz)^{-1}\,dz=\int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})\,d\theta, \tag{1.2}$$

where Γ is the circular part of ∂D_+ and all integrals are assumed to exist (possibly) as appropriately defined improper integrals. The first inner product is positive definite and therefore generates a unique set of real orthogonal polynomials $\{p_k\}$,

$$[p_k,p_l]\begin{cases}=0 & \text{if } k\neq l,\\ >0 & \text{if } k=l,\end{cases}\qquad k,l=0,1,2,\ldots, \tag{1.3}$$

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where p_k is assumed monic of degree k. The second inner product, on the other hand, is not Hermitian; we deliberately did not conjugate the second factor g and did not integrate with respect to the measure $|w(e^{i\theta})|\,d\theta$. The existence of corresponding orthogonal polynomials, therefore, is not guaranteed. We call a system of complex polynomials $\{\pi_k\}$ *orthogonal on the semicircle* if

$$(\pi_k, \pi_l)\begin{cases} =0 & \text{if } k \neq l, \\ \neq 0 & \text{if } k = l, \end{cases} \qquad k, l = 0, 1, 2, \ldots; \tag{1.4}$$

we assume π_k monic of degree k.

Our interest here is in the orthogonal polynomials $\{\pi_k\}$, their existence, relationship to the polynomials $\{p_k\}$, difference and differential equations, and zeros. A study of these polynomials was initiated in [2], where we considered $w(z) \equiv 1$ and used moment information to construct the polynomials $\{\pi_k\}$. This necessitated lengthy preliminary computations of moment determinants [2, Section 2]. We now obtain these polynomials more directly, and for more general weight functions, using orthogonality as the principal tool of construction.

The paper is organized as follows. In Section 2 we establish the existence of the orthogonal polynomials $\{\pi_k\}$, assuming only that

$$\operatorname{Re}(1, 1) = \operatorname{Re} \int_0^{\pi} w(e^{i\theta})\,d\theta \neq 0. \tag{1.5}$$

We furthermore represent π_n as a linear (complex) combination of p_n and p_{n-1}. This then leads quickly to the basic three-term recurrence relation, as is shown in Section 3. The case of Jacobi weights $w(z) = (1-z)^{\alpha}(1+z)^{\beta}$, $\alpha > -1$, $\beta > -1$, is considered in Section 4 and is further specialized to Gegenbauer weights ($\alpha = \beta = \lambda - \frac{1}{2}$) in Section 5. Section 6 is devoted to a study of the zeros of π_n in the case of Jacobi and Gegenbauer weights. After a brief discussion of numerical methods, it is shown that, for Gegenbauer weights with $\lambda > -\frac{1}{2}$, the zeros of π_n, $n \geq 2$, are all contained in the upper unit half disc D_+. Numerical evidence seems to suggest that the same is true for arbitrary Jacobi weights. The simplicity of the zeros is shown in the case of Gegenbauer weights. The polynomial π_n then satisfies a linear second-order differential equation, which is derived in Section 7.

2. Existence and Representation of π_n

We assume that w is a weight function, positive on $(-1, 1)$, holomorphic in $D_+ = \{z \in \mathbf{C}: |z| < 1, \operatorname{Im} z > 0\}$, and such that the integrals in (1.1) and (1.2) exist for smooth f and g (possibly) as improper integrals. We shall also assume (1.5). If C_ε, $\varepsilon > 0$, denotes the boundary of D_+ with small circular parts of radius ε and centers at ± 1 spared out, we have by Cauchy's theorem, for any polynomial g,

$$\begin{aligned} 0 &= \int_{C_\varepsilon} g(z)w(z)\,dz \\ &= \left(\int_{\Gamma_\varepsilon} + \int_{C_{\varepsilon,-1}} + \int_{C_{\varepsilon,1}}\right) g(z)w(z)\,dz + \int_{-1+\varepsilon}^{1-\varepsilon} g(x)w(x)\,dx, \qquad g \in \mathbf{P}, \end{aligned} \tag{2.1}$$

where Γ_ε and $c_{\varepsilon,\pm 1}$ are the circular parts of C_ε (with radii 1 and ε, respectively). We assume that w is such that

$$\lim_{\varepsilon \downarrow 0} \int_{c_{\varepsilon,\pm 1}} g(z)w(z)\,dz = 0, \qquad \text{all} \quad g \in \mathbf{P}. \tag{2.2}$$

Then, letting $\varepsilon \downarrow 0$ in (2.1), we obtain

$$0 = \int_C g(z)w(z)\,dz = \int_\Gamma g(z)w(z)\,dz + \int_{-1}^{1} g(x)w(x)\,dx, \qquad g \in \mathbf{P}. \tag{2.3}$$

The (monic, real) polynomials $\{p_k(z)\}$, orthogonal with respect to the inner product (1.1), as well as the associated polynomials of the second kind,

$$q_k(z) = \int_{-1}^{1} \frac{p_k(z) - p_k(x)}{z - x}\, w(x)\,dx, \qquad k = 0, 1, 2, \ldots, \tag{2.4}$$

are known to satisfy a three-term recurrence relation of the form

$$y_{k+1} = (z - a_k)y_k - b_k y_{k-1}, \qquad k = 0, 1, 2, \ldots, \tag{2.5}$$

where

$$\begin{aligned} &y_{-1} = 0, \qquad y_0 = 1 \qquad \text{for } \{p_k\}, \\ &y_{-1} = -1, \qquad y_0 = 0 \qquad \text{for } \{q_k\}. \end{aligned} \tag{2.6}$$

We denote by m_k and μ_k the moments associated with the inner products (1.1) and (1.2), respectively,

$$m_k = [x^k, 1], \qquad \mu_k = (z^k, 1), \qquad k \geq 0. \tag{2.7}$$

It is assumed, in (2.5), that

$$b_0 = m_0. \tag{2.8}$$

Theorem 2.1. *Let w be a weight function, positive on $(-1, 1)$, holomorphic in $D_+ = \{z \in \mathbf{C}: |z| < 1, \operatorname{Im} z > 0\}$, and such that (2.2) is satisfied and the integrals in (2.3) exist (possibly) as improper integrals. Assume in addition that (1.5) holds. Then there exists a unique system of (monic, complex) orthogonal polynomials $\{\pi_k\}$ relative to the inner product (1.2). Denoting by $\{p_k\}$ the (monic, real) orthogonal polynomials relative to the inner product (1.1), we have*

$$\pi_n(z) = p_n(z) - i\theta_{n-1}p_{n-1}(z), \qquad n = 0, 1, 2, \ldots, \tag{2.9}$$

where

$$\theta_{n-1} = \frac{\mu_0 p_n(0) + iq_n(0)}{i\mu_0 p_{n-1}(0) - q_{n-1}(0)}, \qquad n = 0, 1, 2, \ldots. \tag{2.10}$$

Alternatively,

$$\theta_n = ia_n + \frac{b_n}{\theta_{n-1}}, \quad n = 0, 1, 2, \ldots; \qquad \theta_{-1} = \mu_0, \tag{2.11}$$

where a_k, b_k are the recursion coefficients in (2.5) *and $\mu_0 = (1, 1)$. In particular, all θ_n are real (in fact, positive) if $a_n = 0$ for all $n \geq 0$. Finally,*

$$(2.12)\quad (\pi_n, \pi_n) = \theta_{n-1}[p_{n-1}, p_{n-1}] \neq 0, \qquad n = 1, 2, 3, \ldots, \qquad (\pi_0, \pi_0) = \mu_0.$$

Proof. Assume first that the orthogonal polynomials $\{\pi_k\}$ exist. Putting $g(z) = (1/i)\pi_n(z)z^{k-1}$, $1 \leq k < n$, in (2.3), we find

$$\begin{aligned} 0 &= \int_\Gamma \pi_n(z) z^k (iz)^{-1} w(z)\, dz - i \int_{-1}^{1} \pi_n(x) x^{k-1} w(x)\, dx \\ &= (\pi_n, z^k) - i[\pi_n, x^{k-1}] = -i[\pi_n, x^{k-1}], \qquad 1 \leq k < n, \end{aligned}$$

hence, upon expanding π_n in the polynomials $\{p_k\}$,

$$(2.13)\qquad \pi_n(z) = p_n(z) - i\theta_{n-1} p_{n-1}(z), \qquad n = 0, 1, 2, \ldots,$$

for some constants θ_{n-1}. To determine these constants, put

$$g(z) = [\pi_n(z) - \pi_n(0)](iz)^{-1} = \frac{1}{i}\left\{\frac{p_n(z) - p_n(0)}{z} - i\theta_{n-1}\frac{p_{n-1}(z) - p_{n-1}(0)}{z}\right\}$$

in (2.3) and use the first expression for g to evaluate the first integral, and the second to evaluate the second integral in (2.3). This gives

$$(2.14)\qquad 0 = (\pi_n, 1) - \pi_n(0)(1, 1) + \frac{1}{i}[q_n(0) - i\theta_{n-1} q_{n-1}(0)], \qquad n \geq 1.$$

Since $(\pi_n, 1) = 0$, $(1, 1) = \mu_0$, and using (2.13) with $z = 0$, we get (2.10) for $n \geq 1$. Note that the denominator in (2.10) (and the numerator, for that matter) does not vanish, since $\operatorname{Re} \mu_0 \neq 0$ by (1.5) and $p_k(0)$, $q_k(0)$ cannot vanish simultaneously, $\{p_k\}$ and $\{q_k\}$ being linearly independent solutions of (2.5). For $n = 0$, (2.10) yields, by virtue of (2.6), $\theta_{-1} = \mu_0$, which is the definition given in (2.11).

To show the first relation in (2.11), replace n by $n+1$ in (2.10), and use (2.5) for $z = 0$, to obtain

$$\begin{aligned} \theta_n &= \frac{\mu_0 p_{n+1}(0) + i q_{n+1}(0)}{i\mu_0 p_n(0) - q_n(0)} \\ &= \frac{\mu_0[-a_n p_n(0) - b_n p_{n-1}(0)] + i[-a_n q_n(0) - b_n q_{n-1}(0)]}{i\mu_0 p_n(0) - q_n(0)} \\ &= \frac{ia_n[i\mu_0 p_n(0) - q_n(0)] - b_n[\mu_0 p_{n-1}(0) + i q_{n-1}(0)]}{i\mu_0 p_n(0) - q_n(0)} \\ &= ia_n + \frac{b_n}{\theta_{n-1}}, \qquad n \geq 1. \end{aligned}$$

Using (2.10) with $n = 1$, (2.5) with $k = 0$, and (2.6), yields

$$\theta_0 = \frac{\mu_0(-a_0) + ib_0}{i\mu_0} = ia_0 + \frac{m_0}{\mu_0},$$

since $b_0 = m_0$ [cf. (2.8)]. Therefore, (2.11) also holds for $n = 0$.

If all $a_n = 0$, then w is symmetric and the reality of the θ_n follows from (2.11) and (5.2) below.

Conversely, defining π_n by (2.9) and (2.10), it follows readily, for $n \geq 2$, from (2.3) that

$$(\pi_n, z^k) = \frac{1}{i}\int_\Gamma \pi_n(z) z^{k-1} w(z)\, dz = i\int_{-1}^{1} \pi_n(x) x^{k-1} w(x)\, dx = 0, \qquad 1 \leq k < n,$$

and from (2.14), (2.10), and (2.9) for $z = 0$, that $(\pi_n, 1) = 0$, $n \geq 1$. Furthermore,

$$\begin{aligned}(\pi_n, \pi_n) &= \int_\Gamma \pi_n(z) z^n w(z)(iz)^{-1}\, dz \\ &= \frac{1}{i}\int_\Gamma \pi_n(z) z^{n-1} w(z)\, dz = i\int_{-1}^{1} \pi_n(x) x^{n-1} w(x)\, dx \\ &= i\int_{-1}^{1} [p_n(x) - i\theta_{n-1} p_{n-1}(x)] x^{n-1} w(x)\, dx \\ &= \theta_{n-1}\int_{-1}^{1} p_{n-1}^2(x) w(x)\, dx,\end{aligned}$$

proving (2.12). ∎

We note from (2.9) that

$$(p_n, 1) = i\theta_{n-1}(p_{n-1}, 1) = \cdots = \prod_{\nu=1}^{n} (i\theta_{\nu-1})(1, 1), \tag{2.15}$$

and, similarly,

$$(p_n, \pi_k) = i\theta_{n-1}(p_{n-1}, \pi_k), \qquad 1 \leq k < n,$$

which, applied repeatedly, gives

$$\begin{aligned}(p_n, \pi_k) &= \left(\prod_{\nu=k+1}^{n} i\theta_{\nu-1}\right)(p_k, \pi_k) \\ &= i^{-1}\left(\prod_{\nu=k}^{n} i\theta_{\nu-1}\right)[p_{k-1}, p_{k-1}], \qquad 1 \leq k \leq n.\end{aligned} \tag{2.16}$$

Here, (2.12) has been used in the last step. From (2.15) and (2.16) there follows

$$p_n(z) = \sum_{k=0}^{n} \left(\prod_{\nu=k+1}^{n} i\theta_{\nu-1}\right)\pi_k(z), \tag{2.17}$$

the inversion of (2.9). (When $k = n$, the empty product in (2.17) is to be interpreted as 1.)

Example 2.1. $w(z) = 1 + z$.

Here, $\mu_0 = (1, 1) = \pi + 2i$, Re $\mu_0 \neq 0$, so that the orthogonal polynomials $\{\pi_k\}$ exist. Furthermore, $b_0 = m_0 = 2$, $a_n = (2n+1)^{-1}(2n+3)^{-1}$ for $n \geq 0$, $b_n = n(n+1)(2n+1)^{-2}$ for $n \geq 1$, so that by (2.11),

$$\theta_0 = \frac{\pi - 4i}{3(2 - i\pi)}, \quad \theta_1 = \frac{3\pi + 8i}{5(4 + i\pi)}, \quad \ldots,$$

by (2.5) and (2.6),

$$p_0(z)=1, \quad p_1(z)=z-\tfrac{1}{3}, \quad p_2(z)=z^2-\tfrac{2}{5}z-\tfrac{1}{5}, \quad \ldots,$$

and by (2.9),

$$\pi_0(z)=1, \quad \pi_1(z)=z-\frac{2}{2-i\pi}, \quad \pi_2(z)=z^2-\frac{i\pi}{4+i\pi}z-\frac{4}{3(4+i\pi)}, \quad \ldots.$$

Example 2.2. $w(z)=z^2$.

Here, $\mu_0=\int_0^\pi e^{2i\theta}\,d\theta=0$, so that (1.5) is violated and thus the polynomials $\{\pi_k\}$ do not exist, even though $w(x)\geq 0$ on $[-1,1]$ and the polynomials $\{p_k\}$ do exist. It is easily seen, in fact, that $q_k(0)=0$ when k is even, so that θ_{n-1} in (2.10) is zero for n even, and undefined for n odd. For an explanation of Example 2.2, see Theorem 5.1.

3. Recurrence Relation

We assume (1.5), so that the orthogonal polynomials $\{\pi_k\}$ exist. Since $(zf, g)=(f, zg)$, it is known that they must satisfy a three-term recurrence relation. In analogy to Section 3 of [2] we write it in the form

$$\begin{aligned}\pi_{k+1}(z)&=(z-i\alpha_k)\pi_k(z)-\beta_k\pi_{k-1}(z), \qquad k=0,1,2,\ldots,\\ \pi_{-1}(z)&=0, \qquad \pi_0(z)=1.\end{aligned} \tag{3.1}$$

Using (2.9) in (3.1), we get, for $k\geq 1$,

$$p_{k+1}(z)-i\theta_k p_k(z)=(z-i\alpha_k)[p_k(z)-i\theta_{k-1}p_{k-1}(z)]-\beta_k[p_{k-1}(z)-i\theta_{k-2}p_{k-2}(z)],$$

and substituting here for $zp_k(z)$ and $zp_{k-1}(z)$ the expressions obtained from the basic recurrence relation (2.5) yields

$$\begin{aligned}&[a_k+i(\theta_k-\theta_{k-1}-\alpha_k)]p_k(z)+[b_k-\beta_k-\theta_{k-1}(\alpha_k+ia_{k-1})]p_{k-1}(z)\\ &\qquad +i[\beta_k\theta_{k-2}-b_{k-1}\theta_{k-1}]p_{k-2}(z)\equiv 0, \qquad k\geq 1.\end{aligned}$$

By the linear independence of the polynomials $\{p_r\}$ we conclude that

$$\begin{aligned}a_k+i(\theta_k-\theta_{k-1}-\alpha_k)&=0, \qquad k\geq 1,\\ b_k-\beta_k-\theta_{k-1}(\alpha_k+ia_{k-1})&=0, \qquad k\geq 1,\\ \beta_k\theta_{k-2}-b_{k-1}\theta_{k-1}&=0, \qquad k\geq 2.\end{aligned} \tag{3.2}$$

From the last relation in (3.2), and (2.11), we get

$$\beta_k=\frac{\theta_{k-1}}{\theta_{k-2}}b_{k-1}=\theta_{k-1}(\theta_{k-1}-ia_{k-1}) \tag{3.3}$$

for $k\geq 2$. The first relation (3.2) gives

$$\alpha_k=\theta_k-\theta_{k-1}-ia_k, \qquad k\geq 1. \tag{3.4}$$

To verify that (3.3) also holds for $k=1$, it suffices to apply the second relation (3.2) for $k=1$, in combination with (2.11) and (3.4) for $k=1$. With α_k, β_k thus determined, the second relations in (3.2) are automatically satisfied, as follows easily from (2.11). Finally, from $\pi_1(z)=z-i\alpha_0=p_1(z)-i\theta_0=z-a_0-i\theta_0$, one finds

$$\alpha_0=\theta_0-ia_0. \tag{3.4$_0$}$$

Alternatively, by (2.11), we may write (3.4) and (3.4$_0$) as

$$\begin{aligned}\alpha_k&=-\theta_{k-1}+\frac{b_k}{\theta_{k-1}}, \qquad k\geq 1,\\ \alpha_0&=\frac{b_0}{\theta_{-1}}=\frac{m_0}{\mu_0}.\end{aligned} \tag{3.5}$$

We have proved:

Theorem 3.1. *Under the assumption* (1.5), *the* (*monic, complex*) *polynomials* $\{\pi_k\}$ *orthogonal with respect to the inner product* (1.2) *satisfy the recurrence relation*

$$\begin{aligned}\pi_{k+1}(z)&=(z-i\alpha_k)\pi_k(z)-\beta_k\pi_{k-1}(z), \qquad k=0,1,2,\ldots,\\ \pi_{-1}(z)&=0, \qquad \pi_0(z)=1,\end{aligned} \tag{3.6}$$

where the coefficients α_k, β_k *are given by* (3.4) [*or* (3.5)] *and* (3.3), *respectively, with the* θ_n *defined in* (2.10) [*or* (2.11)]. (The coefficient β_0 in (3.6) is arbitrary; the definition $\beta_0=\mu_0$, however, is sometimes convenient.)

By comparing the coefficient of z^k on the left and right of (3.6), one obtains from (3.4$_0$), (3.4) that

$$\pi_n(z)=z^n-\left(i\theta_{n-1}+\sum_{m=0}^{n-1}a_m\right)z^{n-1}+\cdots, \qquad n\geq 1. \tag{3.7}$$

4. Jacobi Weight

We consider now the case of the Jacobi weight function

$$w(z)=w^{(\alpha,\beta)}(z)=(1-z)^\alpha(1+z)^\beta, \qquad \alpha>-1, \quad \beta>1, \tag{4.1}$$

where fractional powers are understood in terms of their principal branches. We first establish the existence of the corresponding orthogonal polynomials $\{\pi_k\}$.

Theorem 4.1. *We have*

$$\mu_0=\mu_0^{(\alpha,\beta)}=\int_0^\pi w^{(\alpha,\beta)}(e^{i\theta})\,d\theta=\pi+i\int_{-1}^{1}\frac{w^{(\alpha,\beta)}(x)}{x}\,dx, \tag{4.2}$$

where the integral on the right is a Cauchy principal value integral, hence $\operatorname{Re}\mu_0\neq 0$.

Proof. Let C_ε, $\varepsilon > 0$, be the contour formed by ∂D_+, with a small semicircle of radius ε about the origin spared out. Then, by Cauchy's theorem,

$$0 = \int_\Gamma \frac{w(z)}{iz}\,dz + \left(\int_{-1}^{-\varepsilon} + \int_{\varepsilon}^{1}\right)\frac{w(x)}{ix}\,dx + \int_{c_\varepsilon}\frac{w(z)}{iz}\,dz, \tag{4.3}$$

where Γ and c_ε are the circular parts of C_ε (with radii 1 and ε, respectively). Letting $\varepsilon \downarrow 0$ in (4.3) yields

$$0 = \mu_0 - i\int_{-1}^{1}\frac{w(x)}{x}\,dx - \pi w(0),$$

which proves (4.2). ∎

By Theorem 2.1 we therefore have

$$\pi_n(z) = \pi_n^{(\alpha,\beta)}(z) = \hat{P}_n^{(\alpha,\beta)}(z) - i\theta_{n-1}^{(\alpha,\beta)}\hat{P}_{n-1}^{(\alpha,\beta)}(z), \tag{4.4}$$

where $\hat{P}_k^{(\alpha,\beta)}$ are the monic Jacobi polynomials and $\theta_{n-1}^{(\alpha,\beta)}$ is given by (2.10) with the identifications

$$p_k(z) = \hat{P}_k^{(\alpha,\beta)}(z), \qquad q_k(z) \text{ as in (2.4).}$$

Theorem 4.2. *We have*

$$\pi_n^{(\beta,\alpha)}(z) = (-1)^n\bar{\pi}_n^{(\alpha,\beta)}(-z), \tag{4.5}$$

where $\bar{\pi}_n$ denotes the polynomial π_n with all coefficients conjugated, $\bar{\pi}_n(z) = \overline{\pi_n(\bar{z})}$.

Proof. As is well known, $\hat{P}_k^{(\beta,\alpha)}(z) = (-1)^k\hat{P}_k^{(\alpha,\beta)}(-z)$. Since $w^{(\beta,\alpha)}(z) = w^{(\alpha,\beta)}(-z)$, there follows from (4.2) that

$$\mu_0^{(\beta,\alpha)} = \overline{\mu_0^{(\alpha,\beta)}}$$

and from (2.4) that

$$q_k^{(\beta,\alpha)}(z) = (-1)^{k+1}q_k^{(\alpha,\beta)}(-z).$$

Consequently, by (2.10),

$$\theta_{n-1}^{(\beta,\alpha)} = \overline{\theta_{n-1}^{(\alpha,\beta)}},$$

so that, finally,

$$\pi_n^{(\beta,\alpha)}(z) = (-1)^n[\hat{P}_n^{(\alpha,\beta)}(-z) + \overline{i\theta_{n-1}^{(\alpha,\beta)}}\hat{P}_{n-1}^{(\alpha,\beta)}(-z)].$$

This, in view of (4.4), is equivalent to (4.5). ∎

The quantity $\mu_0^{(\alpha,\beta)}$ is needed to generate the $\theta_{n-1}^{(\alpha,\beta)}$ by (2.11), and the recursion coefficients α_k, β_k by (3.5) and (3.3). It is of some interest, therefore, to discuss its numerical evaluation. In principle, μ_0 can be computed from the second expression in (4.2), since the principal value integral appearing there can be expressed in terms of the Jacobi function $Q_0^{(\alpha,\beta)}(\xi)$ on the cut, evaluated at $\xi = 0$. This evaluation, however, is not easy, particularly near integer values of α, where it is plagued by cancellation phenomena (see [3]).

It appears much more convenient to use the first expression in (4.2), rewritten in the form

$$\mu_0^{(\alpha,\beta)} = 2^{\alpha+\beta} e^{-i\alpha\pi/2} \int_0^{\pi} e^{i(\alpha+\beta)\theta/2} \sin^{\alpha}\frac{\theta}{2} \cos^{\beta}\frac{\theta}{2}\, d\theta, \tag{4.6}$$

and to note that the integrand has a singularity of type θ^{α} at $\theta = 0$ and of type $(\pi-\theta)^{\beta}$ at $\theta = \pi$. This suggests the use of Gauss-Jacobi quadrature with parameters (β, α) (note the reversal of parameters!). Changing variables, $\theta = (t+1)\pi/2$, indeed yields

$$\mu_0^{(\alpha,\beta)} = 2^{\alpha+\beta-1}\pi e^{i(\beta-\alpha)\pi/4} \times \int_{-1}^{1} e^{i(\alpha+\beta)t\pi} \left[\frac{\sin((t+1)\pi/4)}{t+1}\right]^{\alpha} \left[\frac{\cos((t+1)\pi/4)}{1-t}\right]^{\beta} w^{(\beta,\alpha)}(t)\, dt, \tag{4.7}$$

where the integrand (except for the weight function $w^{(\beta,\alpha)}$) is now regular on $[-1, 1]$.

5. Symmetric Weights and Gegenbauer Weight

We begin by establishing (1.5) for arbitrary symmetric weights not vanishing at the origin.

Theorem 5.1. *If the weight function w, in addition to the assumptions stated at the beginning of Section 2, satisfies*

$$w(-z) = w(z) \quad \textit{and} \quad w(0) > 0, \tag{5.1}$$

then

$$\mu_0 = (1, 1) = \pi w(0), \tag{5.2}$$

and the system of orthogonal polynomials $\{\pi_k\}$ exists uniquely.

Proof. Proceeding as in the proof of Theorem 4.1, we find

$$0 = \mu_0 - i \int_{-1}^{1} \frac{w(x)}{x}\, dx - \pi w(0).$$

Here, the Cauchy principal value integral on the right vanishes because of symmetry of w. This proves (5.2). ∎

Under the assumption (5.1) we have $a_k = 0$, all $k \geq 0$, in (2.5), hence, by (3.4_0), (3.4), and (3.3),

$$\alpha_0 = \theta_0, \qquad \alpha_k = \theta_k - \theta_{k-1}, \qquad \beta_k = \theta_{k-1}^2, \qquad k \geq 1. \tag{5.3}$$

Furthermore, by (2.11),

$$\left.\begin{aligned} \theta_0 &= \frac{m_0}{\mu_0}, \qquad \theta_1 = \frac{b_1}{\theta_0}, \\ \theta_{2m} &= \theta_0 \frac{b_2 b_4 \cdots b_{2m}}{b_1 b_3 \cdots b_{2m-1}} \\ \theta_{2m+1} &= \frac{1}{\theta_0} \frac{b_1 b_3 \cdots b_{2m+1}}{b_2 b_4 \cdots b_{2m}} \end{aligned}\right\} \qquad m = 1, 2, 3, \ldots . \tag{5.4}$$

In particular, for the Gegenbauer weight

$$w(z) = (1-z^2)^{\lambda - 1/2}, \qquad \lambda > -\tfrac{1}{2}, \tag{5.5}$$

we have $p_k(z) = \hat{C}_k^{\lambda}(z)$—the monic Gegenbauer polynomials—for which, as is well known,

$$\begin{aligned} b_0 &= m_0 = \sqrt{\pi}\,\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda+1)}, \\ b_k &= \frac{k(k+2\lambda-1)}{4(k+\lambda)(k+\lambda-1)}, \qquad k \geq 1. \end{aligned} \tag{5.6}$$

Therefore, by (2.11),

$$\theta_n = \frac{n(n+2\lambda-1)}{4(n+\lambda)(n+\lambda-1)} \frac{1}{\theta_{n-1}}, \quad n = 1, 2, \ldots, \qquad \theta_0 = \frac{\Gamma(\lambda+\frac{1}{2})}{\sqrt{\pi}\Gamma(\lambda+1)},$$

and thus, by induction,

$$\theta_0 = \frac{\Gamma(\lambda+\frac{1}{2})}{\sqrt{\pi}\Gamma(\lambda+1)}, \qquad \theta_k = \frac{1}{\lambda+k} \frac{\Gamma((k+2)/2)\Gamma(\lambda+(k+1)/2)}{\Gamma((k+1)/2)\Gamma(\lambda+(k/2))}, \tag{5.7}$$

$$k = 1, 2, 3, \ldots .$$

For $\lambda = \frac{1}{2}$ (i.e., $w(z) \equiv 1$), this reduces to equation (3.3) of [2].

6. The Zeros of $\pi_n(z)$

6.1. *Computation of the Zeros*

It follows from (3.1) that the zeros of $\pi_n(z)$ are the eigenvalues of the (complex, tridiagonal) matrix

$$J_n = \begin{bmatrix} i\alpha_0 & 1 & & & 0 \\ \beta_1 & i\alpha_1 & 1 & & \\ & \beta_2 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & 1 \\ 0 & & & \beta_{n-1} & i\alpha_{n-1} \end{bmatrix}. \tag{6.1}$$

The elements of J_n are easily computed from (3.4$_0$), (3.4), (3.3), and (2.11), once the recursion coefficients a_k, b_k for the orthogonal polynomials $\{p_k\}$ are known.

The value of μ_0 required in this computation is best obtained from the definition (2.7) by numerical integration, as is described, e.g., in the case of the Jacobi weight at the end of Section 4. To compute the eigenvalues of (6.1) in the general case, we recommend the EISPACK routine COMQR (see, e.g., p. 277 of [4]).

If the weight w is symmetric, then $\beta_k = \theta_{k-1}^2$ is positive [cf. (5.4)], and (6.1) can be transformed into a real matrix. It follows indeed by a similarity transformation with the diagonal matrix $D_n = \operatorname{diag}(1, i\theta_0, i^2\theta_0\theta_1, i^3\theta_0\theta_1\theta_2, \ldots) \in \mathbf{C}^{n\times n}$ that the eigenvalues of (6.1) are equal to $\zeta_\nu = i\eta_\nu$, where η_ν are the eigenvalues of the real nonsymmetric tridiagonal matrix

$$(6.2)\quad -iD_n^{-1}J_nD_n = \begin{bmatrix} \alpha_0 & \theta_0 & & & 0 \\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ 0 & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix} \quad (w \text{ symmetric}).$$

These can be computed by the EISPACK routine HQR (p. 330 of [4]).

6.2. *Jacobi Weight*

For the general Jacobi weight (4.1), with parameters $\alpha > -1$, $\beta > -1$, we have only numerical results; they were obtained by the procedure described in the preceding subsection. All indications are, however, that the zeros of $\pi_n^{(\alpha,\beta)}$ for $n \geq 2$ are always contained in the upper unit half disc $D_+ = \{z \in \mathbf{C}: |z| < 1, \operatorname{Im} z > 0\}$. This was verified numerically for:

(i) $\alpha = -0.75(0.25)1.0$, $\beta = -0.75(0.25)\alpha$ [when $\beta > \alpha$, the analogous fact follows from (4.5)] and $n = 2(1)13, 16, 17, 24, 25$;
(ii) $\alpha = -0.75(0.25)1.0$, $\beta = -0.9, -0.99, -0.999, -0.9999$ and n as in (i);
(iii) miscellaneous values $\alpha > 1$, $\beta < \alpha$ and n as in (i).

A proof of this remarkable property will be given in the next subsection in the special case $\alpha = \beta > -1$, in which case we also show that all zeros are simple.

6.3. *Symmetric Weights and Gegenbauer Weight*

We first assume that w is any symmetric weight function (subject to the conditions of Theorem 2.1),

$$(6.3)\qquad w(-z) = w(z), \qquad w(0) > 0.$$

Then all $\theta_{n-1} > 0$ [cf. (5.4)].

Exactly as in Section 5 of [2] one proves:

Theorem 6.1. *If $\zeta \in \mathbf{C}$ is a zero of π_n, then so is $-\bar{\zeta}$. The zeros of π_n are thus located symmetrically with respect to the imaginary axis. Moreover, all zeros have positive imaginary parts and, in fact, are contained in the half strip $S_+ = \{z \in \mathbf{C}: \operatorname{Im} z > 0, -\xi_n \leq \operatorname{Re} z \leq \xi_n\}$, where ξ_n is the largest zero of p_n.*

More detailed information about the zeros is provided by the following theorem.

Theorem 6.2. *All zeros of π_n are contained in $D_+ = \{z \in \mathbf{C}: |z| < 1, \operatorname{Im} z > 0\}$ (in fact, in $D_+ \cap S_+$; cf. Theorem 6.1), with the possible exception of a single (simple) zero on the positive imaginary axis.*

Proof. Consider first a zero ζ of π_n not on the imaginary axis (hence $n \geq 2$). By Theorem 6.1 it suffices to prove $|\zeta| < 1$. Since, again by Theorem 6.1, there is another zero, $-\bar{\zeta}$, we have

$$\pi_n(x) = p_n(x) - i\theta_{n-1}p_{n-1}(x) = (x-\zeta)(x+\bar{\zeta})r_{n-2}(x), \tag{6.4}$$

where $r_{n-2} \not\equiv 0$ is a polynomial of degree $n-2$. Therefore,

$$0 = \int_{-1}^{1} \pi_n(x)\overline{r_{n-2}(x)}w(x)\,dx = \int_{-1}^{1} (x-\zeta)(x+\bar{\zeta})|r_{n-2}(x)|^2 w(x)\,dx, \tag{6.5}$$

where the first relation in (6.5) follows from the first relation (6.4) and the orthogonality of the p_k. Since

$$(x-\zeta)(x+\bar{\zeta}) = x^2 - 2ix\operatorname{Im}\zeta - |\zeta|^2,$$

there follows, by taking the real part of (6.5),

$$\int_{-1}^{1} (x^2 - |\zeta|^2)|r_{n-2}(x)|^2 w(x)\,dx = 0,$$

which implies $|\zeta| < 1$.

By the same argument one shows that π_n cannot have two distinct zeros, or a double zero, on the imaginary axis, all with imaginary parts ≥ 1. ∎

We specialize now to Gegenbauer weights,

$$w(z) = (1-z^2)^{\lambda - 1/2}, \qquad \lambda > -\tfrac{1}{2}, \tag{6.6}$$

and denote the corresponding polynomials π_n by

$$\pi_n^\lambda(z) = \hat{C}_n^\lambda(z) - i\theta_{n-1}^\lambda \hat{C}_{n-1}^\lambda(z), \qquad \theta_{n-1}^\lambda \text{ given by (5.7)}. \tag{6.7}$$

Here, $\hat{C}_k^\lambda$ denote the monic Gegenbauer polynomials. We shall abbreviate, when convenient, $\theta_{n-1} = \theta_{n-1}^\lambda$.

For a more detailed study of the zeros of π_n^λ, we need the following lemmas.

Lemma 6.3. *For $x > 0$, $0 < s < 1$, one has*

$$x^{1-s} < \frac{\Gamma(x+1)}{\Gamma(x+s)} < (x+1)^{1-s}. \tag{6.8}$$

Proof. See [1].

Lemma 6.4. *The quantities $\theta_{n-1} = \theta_{n-1}^\lambda$ [cf. (5.7)] satisfy*

$$\begin{aligned} &\theta_{n-1}^\lambda < \tfrac{1}{2} \quad \text{if } -\tfrac{1}{2} < \lambda < 0 \text{ or } \lambda > 1, \\ &\tfrac{1}{2} < \theta_{n-1}^\lambda \leq \max(\theta_1^\lambda, \theta_2^\lambda) \quad \text{if } 0 < \lambda < 1, \qquad n = 2, 3, \ldots. \\ &\theta_{n-1}^\lambda = \tfrac{1}{2} \quad \text{if } \lambda = 0 \text{ or } \lambda = 1. \end{aligned} \tag{6.9}$$

Proof. An elementary computation, based on (5.7), shows that

$$\theta_{k+2}^{\lambda} \gtreqless \theta_k^{\lambda} \quad \text{if and only if} \quad \lambda(\lambda-1) \gtreqless 0. \tag{6.10}$$

Furthermore, by Stirling's formula applied to (5.7),

$$\lim_{k\to\infty} \theta_k^{\lambda} = \tfrac{1}{2}. \tag{6.11}$$

Therefore, if $-\frac{1}{2}<\lambda<0$ or $\lambda>1$, we have $\theta_{k+2}^{\lambda}>\theta_k^{\lambda}$, $k=1,2,3,\ldots$, hence, by (6.11), $\theta_{n-1}^{\lambda}<\frac{1}{2}$, all $n\geq 2$. This proves the first inequality in (6.9). Suppose, next, that $0<\lambda<1$. Then, $\theta_{k+2}^{\lambda}<\theta_k^{\lambda}$, $k=1,2,3,\ldots$, hence, again by (6.11), $\frac{1}{2}<\theta_{n-1}^{\lambda}\leq \max(\theta_1^{\lambda}, \theta_2^{\lambda})$ for all $n\geq 4$ (and trivially for $n=2$ and 3), proving the second relation in (6.9). Finally, if $\lambda=0$ or $\lambda=1$, then $\theta_{n-1}^{\lambda}=\frac{1}{2}$, all $n\geq 2$. ∎

Theorem 6.5. *If $\lambda>-\frac{1}{2}$, then all zeros of $\pi_n^{\lambda}(z)$, $n\geq 2$, are contained in $D_+=\{z\in\mathbf{C}: |z|<1, \operatorname{Im} z>0\}$.*

Proof. By virtue of Theorem 6.2, it suffices to show that π_n^{λ}, $n\geq 2$, can have no purely imaginary zero with imaginary part ≥ 1.

Thus, consider a zero $\zeta=iy$ of π_n^{λ}. By (2.9) [or (6.7)],

$$p_n(iy)-i\theta_{n-1}p_{n-1}(iy)=0,$$

where $p_n=\hat{C}_n^{\lambda}$ and $\theta_{n-1}=\theta_{n-1}^{\lambda}$. Therefore,

$$\frac{p_n(iy)}{ip_{n-1}(iy)}=\theta_{n-1}. \tag{6.12}$$

Letting

$$\omega_k(y)=\frac{p_k(iy)}{ip_{k-1}(iy)}, \qquad k=1,2,3,\ldots, \tag{6.13}$$

one finds from the recurrence formula for the p_k [cf. (2.5) and (2.6)] that

$$\omega_1(y)=y, \qquad \omega_k(y)=y+\frac{b_{k-1}}{\omega_{k-1}(y)}, \quad k=2,3,\ldots,$$

hence, since $b_{k-1}>0$,

$$\omega_k(y)\geq 1 \qquad \text{for} \quad y\geq 1.$$

Therefore, the left-hand side of (6.12) is ≥ 1 for $y\geq 1$ and $n\geq 1$. We now show that

$$\theta_{n-1}<1, \qquad n\geq 2, \tag{6.14}$$

so that (6.12) cannot hold for $y\geq 1$, when $n\geq 2$, and thus π_n^{λ}, $n\geq 2$, cannot have a zero iy with $y\geq 1$.

By Lemma 6.4, the inequality (6.14) is certainly true if $-\frac{1}{2}<\lambda\le 0$ or $\lambda\ge 1$, and if $0<\lambda<1$ will follow from $\theta_1<1$, $\theta_2<1$. Now using (5.7) and the upper bound in Lemma 6.3 (with $x=\lambda$, $s=\frac{1}{2}$), one gets

$$\theta_1=\frac{\sqrt{\pi}\Gamma(\lambda+1)}{2(\lambda+1)\Gamma(\lambda+\frac{1}{2})}<\frac{\sqrt{\pi}}{2(\lambda+1)}(\lambda+1)^{1/2}=\frac{\sqrt{\pi}}{2(\lambda+1)^{1/2}}<\frac{\sqrt{\pi}}{2}<1,$$

if $\lambda>0$. Likewise,

$$\theta_2=\frac{2}{\sqrt{\pi}(\lambda+2)}\frac{\Gamma(\lambda+\frac{3}{2})}{\Gamma(\lambda+1)}<\frac{2}{\sqrt{\pi}(\lambda+2)}(\lambda+\tfrac{3}{2})^{1/2}<\sqrt{\frac{5}{2\pi}}<1,\qquad 0<\lambda<1.\ \blacksquare$$

Theorem 6.5 does not hold for $n=1$, $-\frac{1}{2}<\lambda\le 0$, since the zero $i\alpha_0=i\theta_0$ then has a modulus that increases from 1 to ∞ when λ decreases from 0 to $-\frac{1}{2}$. It does hold, however, for $n=1$, $\lambda>0$, as can be shown.

An alternative proof of Theorem 6.5, valid however only for $\lambda>0$, can be given on the basis of Rouché's theorem, as in [2].

To prove the simplicity of the zeros of π_n^λ, we need

Lemma 6.6. *The quantity $\theta_{n-1}=\theta_{n-1}^\lambda$ satisfies the inequality*

$$4(n+\lambda-1)^2\theta_{n-1}^2<n(n+2\lambda-1),\qquad n\ge 2,\quad \lambda>-\tfrac{1}{2}. \tag{6.15}$$

Proof. The right-hand side of (6.15) is positive, since $n+2\lambda-1>n-2\ge 0$. From (5.7) we have

$$\begin{aligned}4(n+\lambda-1)^2\theta_{n-1}^2&=\left(2\frac{\Gamma((n+1)/2)\Gamma(\lambda+(n/2))}{\Gamma(n/2)\Gamma(\lambda+(n-1)/2)}\right)^2\\&=\left[2\cdot\frac{n}{2}\cdot\left(\lambda+\frac{n-1}{2}\right)\right]^2\left(\frac{\Gamma((n+1)/2)\Gamma(\lambda+(n/2))}{\Gamma((n/2)+1)\Gamma(\lambda+(n+1)/2)}\right)^2,\end{aligned}$$

so that (6.15) becomes

$$\left(\frac{\Gamma((n/2)+1)\Gamma(\lambda+(n+1)/2)}{\Gamma((n+1)/2)\Gamma(\lambda+(n/2))}\right)^2>\tfrac{1}{4}n(n+2\lambda-1). \tag{6.16}$$

This follows immediately from the lower bound in Lemma 6.3, first applied with $x=\frac{1}{2}n$, $s=\frac{1}{2}$, and then with $x=\lambda+\frac{1}{2}n-\frac{1}{2}$, $s=\frac{1}{2}$. $\blacksquare$

Theorem 6.7. *If $\lambda>-\frac{1}{2}$, all zeros of $\pi_n^\lambda(z)$ are simple.*

Proof. The proof is analogous to the one given in Section 5 of [2] for the case $\lambda=\frac{1}{2}$. It suffices, of course, to assume $n\ge 2$.

Let ζ be a zero of $\pi_n=\pi_n^\lambda$. By (2.9),

$$p_n(\zeta)=i\theta_{n-1}p_{n-1}(\zeta).$$

Therefore, using again (2.9),

$$\pi_n'(\zeta) = p_n'(\zeta) - i\theta_{n-1}p_{n-1}'(\zeta) \tag{6.17}$$
$$= \frac{1}{p_{n-1}(\zeta)}[p_n'(\zeta)p_{n-1}(\zeta) - p_n(\zeta)p_{n-1}'(\zeta)].$$

Using

$$(1-\zeta^2)p_k'(\zeta) = (k+2\lambda)\zeta p_k(\zeta) - 2(k+\lambda)p_{k+1}(\zeta)$$

to remove the derivatives on the right of (6.17), and employing the recurrence relation

$$p_{k+1}(\zeta) = \zeta p_k(\zeta) - \frac{k(k+2\lambda-1)}{4(k+\lambda-1)(k+\lambda)}p_{k-1}(\zeta),$$

yields, after some computation,

$$\pi_n'(\zeta) = \frac{p_{n-1}(\zeta)}{2(1-\zeta^2)(n+\lambda-1)}[n(n+2\lambda-1) - 4(n+\lambda-1)^2\theta_{n-1}^2$$
$$-2(2n+2\lambda-1)(n+\lambda-1)\zeta i\theta_{n-1}].$$

If $\zeta = \alpha + i\beta$, the expression in brackets becomes

$$n(n+2\lambda-1) - 4(n+\lambda-1)^2\theta_{n-1}^2 + 2(2n+2\lambda-1)(n+\lambda-1)\beta\theta_{n-1}$$
$$-2(2n+2\lambda-1)(n+\lambda-1)\alpha i\theta_{n-1}$$

and is clearly nonzero by virtue of Lemma 6.6 and $\beta > 0$. ■

7. Differential Equation

The following theorem generalizes Theorem 6.1 of [2].

Theorem 7.1. *The polynomial* $\pi_n^\lambda(z)$ *in* (6.7) *satisfies the differential equation*

$$P(z)y'' + Q(z)y' + R(z)y = 0, \tag{7.1}$$

where

$$P(z) = (1-z^2)[n(n+2\lambda-1) - 4(n+\lambda-1)^2\theta_{n-1}^2$$
$$-2(2n+2\lambda-1)(n+\lambda-1)zi\theta_{n-1}],$$
$$Q(z) = -(2\lambda+1)[n(n+2\lambda-1) - 4(n+\lambda-1)^2\theta_{n-1}^2]z \tag{7.2}$$
$$+2(2n+2\lambda-1)(n+\lambda-1)(1+2\lambda z^2)i\theta_{n-1},$$
$$R(z) = n^2(n+2\lambda)(n+2\lambda-1) - 4(n-1)(n+2\lambda-1)(n+\lambda-1)^2\theta_{n-1}^2$$
$$-2n(n+2\lambda-1)(2n+2\lambda-1)(n+\lambda-1)zi\theta_{n-1}.$$

Proof. We only sketch the proof, since it is analogous to the one given in Section 6 of [2]. We put $u = \hat{C}_{n-1}^{\lambda}(z)$, $v = 2(n+\lambda-1)\pi_n^{\lambda}(z)$ and define

$$\omega(z) = (z-1)^{(1/2)(n+2\lambda-1)-i(n+\lambda-1)\theta_{n-1}}(z+1)^{(1/2)(n+2\lambda-1)+i(n+\lambda-1)\theta_{n-1}}.$$

Then,

$$(z^2-1)[\omega(z)u]' = \omega(z)v. \tag{7.3}$$

Substituting u, u', u'' from (7.3) into Gegenbauer's differential equation

$$(z^2-1)u'' + (2\lambda+1)zu' - (n-1)(n+2\lambda-1)u = 0$$

gives

$$\frac{1}{b(z)}v' + \frac{a(z)}{b(z)}v + \int \frac{\omega}{z^2-1}v\,dz = 0, \tag{7.4}$$

where

$$a(z) = (z^2-1)^{-1}[-nz + 2(n+\lambda-1)i\theta_{n-1}],$$

$$b(z) = [\omega(z)(z^2-1)]^{-1}[n(n+2\lambda-1) - 4(n+\lambda-1)^2\theta_{n-1}^2 - 2(2n+2\lambda-1)(n+\lambda-1)zi\theta_{n-1}].$$

Now differentiating (7.4) and multiplying the result by $-\omega(z)(z^2-1)^2b^2(z)$ yields (7.1) and (7.2) after some computation. ∎

We remark that (7.1) has regular singular points at 1, −1, ∞, and an additional regular singular point which depends on n and, by Lemma 6.6, is located on the negative imaginary axis.

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ON THE ZEROS OF POLYNOMIALS ORTHOGONAL ON THE SEMICIRCLE*

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Abstract. It is shown that the polynomials $\pi_n(\cdot; w)$ orthogonal in the sense of [W. Gautschi, H. J. Landau, and G. V. Milovanović, *Constr. Approx.*, 3 (1987), pp. 389-404] on the unit upper semicircle need not necessarily have all their zeros in the interior of the unit upper semidisc, not even for weight functions w that are symmetric, $w(-z)=w(z)$. A symmetric weight function w_a (depending on a parameter a) is exhibited, which has the property that $\pi_n(\cdot; w_a)$ for any fixed even n has a zero on the imaginary axis with imaginary part greater than one, provided a is large enough. Similarly, a weight function w^a is constructed for which the analogous property holds for $\pi_n(\cdot; w^a)$, n odd.

Key words. complex orthogonal polynomials, indefinite inner product, zeros

AMS(MOS) subject classifications. 30C10, 30C15, 33A65

1. In [3], [4] we introduced polynomials that are orthogonal on the semicircle with respect to the (non-Hermitian) inner product

$$(p, q)=\int_0^\pi p(e^{i\theta})q(e^{i\theta})w(e^{i\theta})\,d\theta. \tag{1.1}$$

Here, w is a "weight function" analytic on the semidisc $D_+=\{z\in\mathbb{C}: |z|<1, \operatorname{Im} z>0\}$, nonnegative on $(-1, 1)$ and integrable over ∂D_+. We have shown that under the assumption

$$\operatorname{Re}\int_0^\pi w(e^{i\theta})\,d\theta\neq 0 \tag{1.2}$$

there exists a unique system $\{\pi_n\}_{n=0}^\infty$ of monic polynomials $\pi_n(\cdot)=\pi_n(\cdot; w)$ such that

$$\deg \pi_n=n,\quad n=0, 1, 2, \cdots, \qquad (\pi_k, \pi_l)\begin{cases}=0, & k\neq l,\\ \neq 0, & k=l.\end{cases} \tag{1.3}$$

They possess many of the properties familiar from orthogonal polynomials on the real line, such as satisfying a three-term recurrence relation and a second-order linear differential equation (for special weight functions), and in fact can be expressed as (complex) linear combinations of two successive polynomials orthogonal on the interval $(-1, 1)$ with respect to the same weight function w. They give rise to Gauss-type quadrature rules for integration over the semicircle and to new, possibly more stable, quadrature formulae for evaluating Cauchy principal value integrals (see [3, §§ 7, 8]). Since the nodes of these quadrature rules involve the zeros of the polynomials π_n in (1.3), a study of the qualitative properties of these zeros is of interest.

In [4] we have shown that for weight functions analytic in $D=\{z\in\mathbb{C}: |z|<1\}$, symmetric in the sense

$$w(-z)=w(z)\quad \text{for all } z\in D, \tag{1.4}$$

and satisfying

$$w(x)\geqq 0\quad \text{on } (-1, 1),\quad w(0)>0, \tag{1.5}$$

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all zeros of π_n are contained in D_+ with the possible exception of a single (simple) zero iy, $y \geqq 1$. For the Gegenbauer weight $w(z) = (1-z^2)^{\lambda-1/2}$, the exceptional case can only arise if $n = 1$ and $-\frac{1}{2} < \lambda \leqq 0$. Likewise, no exceptional cases seem to occur for Jacobi weights $w(z) = (1-z)^\alpha (1+z)^\beta$, $\alpha > -1$, $\beta > -1$, if $n \geqq 2$, as was observed by numerical computation. We might be led to believe that this absence of exceptional cases prevails for arbitrary weight functions w. In this note we show, however, that this is not so, not even for symmetric weight functions. We exhibit symmetric functions w for which $\pi_n(\cdot; w)$, for arbitrary fixed n, has a zero iy with $y \geqq 1$.

2. Let $b_k = b_k(w)$, $k = 1, 2, 3, \cdots$, be the coefficients in the recurrence formula

$$y_{k+1} = xy_k - b_k y_{k-1}, \quad k = 0, 1, 2, \cdots, \qquad y_{-1} = 0, \quad y_0 = 1 \tag{2.1}$$

satisfied by the polynomials $p_n(x; w)$ orthogonal on the interval $(-1, 1)$ relative to the symmetric weight function w. We recall from the proof of Theorem 6.5 and equations (5.2), (5.4) of [4] that iy is a zero of $\pi_n(\cdot; w)$ if and only if

$$\omega_n(y) - \theta_{n-1} = 0, \tag{2.2}$$

where

$$\omega_1(y) = y, \quad \omega_k(y) = y + \frac{b_{k-1}}{\omega_{k-1}(y)}, \quad k = 2, 3, \cdots, \tag{2.3}$$

$$\theta_{n-1} = \begin{cases} \dfrac{b_1 b_3 \cdots b_{n-1}}{b_2 b_4 \cdots b_{n-2}} \dfrac{\pi}{m_0}, & n \text{ even}, \\ \dfrac{b_2 b_4 \cdots b_{n-1}}{b_1 b_3 \cdots b_{n-2}} \dfrac{m_0}{\pi}, & n \text{ odd}, \end{cases} \tag{2.4}$$

and

$$m_0 = \int_{-1}^{1} w(x)\, dx = 2 \int_0^1 w(x)\, dx, \tag{2.5}$$

the weight function w having been normalized to satisfy

$$w(0) = 1. \tag{2.6}$$

If $n = 1$ or $n = 2$, empty products in (2.4) are assumed to be one. Equation (2.2) holds for some $y \geqq 1$ if and only if

$$\omega_n(1) - \theta_{n-1} \leqq 0. \tag{2.7}$$

Indeed, since $\omega_n(y) \to \infty$ as $y \to \infty$, inequality (2.7) trivially implies (2.2) for some $y \geqq 1$. Conversely, if (2.2) holds for some $y \geqq 1$, but (2.7) (if $n \geqq 2$) does not, the left-hand side of (2.2), hence $\pi_n(iy)$, would have either two distinct zeros > 1, or a double zero > 1, which is impossible by Theorem 6.2 of [4]. By (2.3), we can write (2.7) in the form

$$1 + \frac{b_{n-1}}{1+} \frac{b_{n-2}}{1+} \cdots \frac{b_1}{1} \leqq \theta_{n-1}. \tag{2.8}$$

We now show that (2.8), for any fixed $n \geqq 1$, can always be achieved for some suitable weight function w.

3. It is necessary to distinguish the cases n even and n odd. In the former case, (2.8) becomes

$$1 + \frac{b_{n-1}}{1+} \frac{b_{n-2}}{1+} \cdots \frac{b_1}{1} \leqq \frac{b_1 b_3 \cdots b_{n-1}}{b_2 b_4 \cdots b_{n-2}} \frac{\pi}{m_0}. \tag{3.1}$$

It is clear that we can enforce (3.1) to hold if we can find a family of weight functions w for which m_0 tends to zero and the b_k remain bounded and bounded away from zero. Such a family of weight functions (keeping in mind that they should be analytic in D, satisfy (1.4), and be normalized by (2.6)) is given by

$$w(z)=w_a(z)=\frac{1+\sqrt{a/\pi}\,e^{-az^2}}{1+\sqrt{a/\pi}}, \qquad a>0. \tag{3.2}$$

The fact that w_a also satisfies (1.2) follows from Theorem 5.1 of [4]. We note that the second term in the numerator of (3.2), for real $z=x$, is an approximation to the Dirac delta function $\delta(x)$, to which it converges as $a\to\infty$. It follows that, for any polynomial p,

$$\begin{aligned}\left(1+\sqrt{\frac{a}{\pi}}\right)\int_{-1}^{1} w_a(x)p(x)\,dx &\to \int_{-1}^{1}[1+\delta(x)]p(x)\,dx \\ &= \int_{-1}^{1} p(x)\,dx+p(0) \quad \text{as } a\to\infty.\end{aligned} \tag{3.3}$$

In particular, putting $p(x)\equiv 1$,

$$m_0\sim 3\sqrt{\pi/a}, \qquad a\to\infty. \tag{3.4}$$

Furthermore,

$$\lim_{a\to\infty} b_k(w_a)=b_{k,\infty}>0, \quad \cdot\ k=1,2,3,\cdots, \tag{3.5}$$

where $b_{k,\infty}$ are the recursion coefficients of the monic polynomials orthogonal with respect to the weight function $1+\delta(x)$ on $[-1,1]$ (Legendre weight plus Dirac function centered at the origin). It follows from (3.4) and (3.5) that for a sufficiently large, (3.1) will be true (even with strict inequality). The proof of (3.5) is deferred to § 4.

Assume next that n is odd. Then, (2.8) becomes

$$1+\frac{b_{n-1}}{1+}\,\frac{b_{n-2}}{1+}\cdots\frac{b_1}{1}\leqq\frac{b_2b_4\cdots b_{n-1}}{b_1b_3\cdots b_{n-2}}\,\frac{m_0}{\pi}. \tag{3.6}$$

We now want m_0 to be large and may choose, for example,

$$w(z)=w^a(z)=1+az^2, \qquad a>0. \tag{3.7}$$

Then

$$m_0=\tfrac{2}{3}a+2 \tag{3.8}$$

and

$$\lim_{a\to\infty} b_k(w^a)=b_k^{\infty}>0, \qquad k=1,2,3,\cdots, \tag{3.9}$$

where b_k^{∞} are the recursion coefficients of the monic polynomials orthogonal with respect to the weight function x^2 on $[-1,1]$. Again, from (3.8) and (3.9) it follows that (3.6) will be true for a sufficiently large. It remains to prove (3.5) and (3.9).

4. We denote the moments of w by m_k,

$$m_{2r+1}=0, \qquad m_{2r}=2\int_0^1 x^{2r}w(x)\,dx>0. \tag{4.1}$$

The recursion coefficients $b_k(w)$ can be expressed in terms of Hankel determinants:

$$\Delta_n(m)=\det\,(m_{i+j})_{\substack{i=0,1,\cdots,n-1\\ j=0,1,\cdots,n-1}}, \qquad \Delta_0=1, \tag{4.2}$$

by means of [1, p. 19]

$$b_k(w)=\frac{\Delta_{k-1}(m)\Delta_{k+1}(m)}{[\Delta_k(m)]^2}, \qquad k=1,2,3,\cdots. \tag{4.3}$$

In the case of $w(x)=w_a(x)$ [cf. (3.2)], we have by (3.3)

$$m_r\sim\sqrt{\pi/a}\,m_{r,\infty}, \qquad a\to\infty, \quad r=0,1,2,\cdots, \tag{4.4}$$

where $m_{r,\infty}$ are the moments of the weight function $1+\delta(x)$ on $[-1,1]$. Therefore,

$$\Delta_n(m)\sim\left(\frac{\pi}{a}\right)^{n/2}\Delta_n(m_\infty), \qquad a\to\infty,$$

and, consequently, by (4.3),

$$b_k(w_a)\sim\frac{\Delta_{k-1}(m_\infty)\Delta_{k+1}(m_\infty)}{[\Delta_k(m_\infty)]^2}, \qquad a\to\infty,$$

that is,

$$b_k(w_a)\to b_{k,\infty} \quad \text{as } a\to\infty. \tag{4.5}$$

Likewise, for $w(x)=w^a(x)$ [cf. (3.7)],

$$m_r\sim am_r^\infty, \quad a\to\infty, \quad r=0,1,2,\cdots,$$

where m_r^∞ are the moments of the weight function x^2 on $[-1,1]$, and thus,

$$\Delta_n(m)\sim a^n\Delta_n(m^\infty), \qquad a\to\infty,$$

giving

$$b_k(w^a)\to b_k^\infty \quad \text{as } a\to\infty. \tag{4.6}$$

This proves the assertions in (3.5) and (3.9).

We remark that instead of one in (2.7) we could have selected any number larger than one, which means that the zeros of $\pi_n(\cdot;w_a)$ and $\pi_n(\cdot;w^a)$ on the imaginary axis can be made to have arbitrarily large imaginary parts by choosing a sufficiently large.

5. We now confirm the validity of the construction in § 3 numerically by computing the zeros of $\pi_n(\cdot;w_a)$, n even, and of $\pi_n(\cdot;w^a)$, n odd, for the critical value $a=a_n^*$ (which should yield a zero at i) and a few selected values $a>a_n^*$. We compute these zeros in terms of eigenvalues of a real tridiagonal (nonsymmetric) matrix, as indicated in [4, § 6.1], the coefficients $b_k(w_a)$ and $b_k(w^a)$ being generated by the "discretized Stieltjes procedure" (cf. [2, § 2.2]).

Table 5.1 shows the values of a_n^* for $n=2(1)10$ obtained to eight significant decimal digits by using the bisection method on (2.2) where $y=1$. The zeros of $\pi_n(\cdot;w_a)$

TABLE 5.1
Values of a_n^* for $n=2(1)10$.

n	a_n^*	n	a_n^*
2	55.274946	3	17.009652
4	250.25427	5	46.413430
6	798.58573	7	89.537192
8	1951.2926	9	146.34390
10	4037.4957		

TABLE 5.2
Zeros of $\pi_n(\cdot\,; w_a)$, $a=(1+\kappa)a_n^*$, $\kappa=0, \frac{1}{2}, 1, \infty$, *where* $n=2(2)10$.

n	κ	Zeros					
2	0	$.225i$	$1.000i$				
	.5	$.177i$	$1.264i$				
	1.0	$.152i$	$1.472i$				
	∞	0	∞i				
4	0	$.065i$	$1.000i$	$\pm.797+.038i$			
	.5	$.053i$	$1.237i$	$\pm.791+.035i$			
	1.0	$.046i$	$1.435i$	$\pm.788+.032i$			
	∞	0	∞i	$\pm.775$			
6	0	$.031i$	$1.000i$	$\pm.912+.011i$	$\pm.559+.051i$		
	.5	$.025i$	$1.251i$	$\pm.911+.010i$	$\pm.553+.044i$		
	1.0	$.022i$	$1.461i$	$\pm.910+.009i$	$\pm.550+.039i$		
	∞	0	∞i	$\pm.906$	$\pm.538$		
8	0	$.018i$	$1.000i$	$\pm.951+.004i$	$\pm.751+.022i$	$\pm.421+.046i$	
	.5	$.015i$	$1.262i$	$\pm.951+.004i$	$\pm.749+.019i$	$\pm.416+.039i$	
	1.0	$.013i$	$1.479i$	$\pm.950+.004i$	$\pm.747+.017i$	$\pm.413+.034i$	
	∞	0	∞i	$\pm.949$	$\pm.742$	$\pm.406$	
10	0	$.012i$	$1.000i$	$\pm.969+.002i$	$\pm.841+.011i$	$\pm.623+.026i$	$\pm.335+.040i$
	.5	$.010i$	$1.269i$	$\pm.969+.002i$	$\pm.840+.010i$	$\pm.620+.022i$	$\pm.331+.033i$
	1.0	$.008i$	$1.492i$	$\pm.969+.002i$	$\pm.839+.009i$	$\pm.618+.019i$	$\pm.330+.029i$
	∞	0	∞i	$\pm.968$	$\pm.836$	$\pm.613$	$\pm.324$

TABLE 5.3
Zeros of $\pi_n(\cdot\,; w^a)$, $a=(1+\kappa)a_n^*$, $\kappa=0, \frac{1}{2}, 1, \infty$, *where* $n=3(2)9$.

n	κ	Zeros				
3	0	$1.000i$	$\pm.781+.046i$			
	.5	$1.356i$	$\pm.776+.038i$			
	1.0	$1.710i$	$\pm.774+.032i$			
	∞	∞i	$\pm.775$			
5	0	$1.000i$	$\pm.909+.012i$	$\pm.541+.057i$		
	.5	$1.407i$	$\pm.908+.010i$	$\pm.536+.044i$		
	1.0	$1.807i$	$\pm.907+.008i$	$\pm.535+.035i$		
	∞	∞i	$\pm.906$	$\pm.538$		
7	0	$1.000i$	$\pm.951+.005i$	$\pm.747+.023i$	$\pm.405+.051i$	
	.5	$1.429i$	$\pm.950+.004i$	$\pm.744+.018i$	$\pm.402+.038i$	
	1.0	$1.847i$	$\pm.950+.003i$	$\pm.743+.015i$	$\pm.401+.030i$	
	∞	∞i	$\pm.949$	$\pm.742$	$\pm.406$	
9	0	$1.000i$	$\pm.969+.002i$	$\pm.839+.012i$	$\pm.618+.027i$	$\pm.321+.044i$
	.5	$1.440i$	$\pm.969+.002i$	$\pm.838+.009i$	$\pm.615+.020i$	$\pm.320+.032i$
	1.0	$1.868i$	$\pm.968+.002i$	$\pm.837+.008i$	$\pm.614+.016i$	$\pm.320+.025i$
	∞	∞i	$\pm.968$	$\pm.836$	$\pm.613$	$\pm.324$

and $\pi_n(\cdot; w^a)$ for $n = 2(2)10$ and $n = 3(2)9$, respectively, where $a = (1+\kappa)a_n^*$, $\kappa = 0$, $\frac{1}{2}$, 1, ∞, are listed in Tables 5.2 and 5.3. Although they were computed to eight significant digits, only three-digit values are shown because of space considerations. If $a \to \infty$ (i.e., $\kappa \to \infty$), it follows from $\pi_n = p_n - i\theta_{n-1}p_{n-1}$ (cf. [4, eq. (2.9)]) and $\theta_{n-1} \to \infty$ that the (finite) zeros of π_n tend to those of p_{n-1}, the orthogonal polynomial of degree $n-1$ relative to the limiting weight function $w_\infty(x) = 1 + \delta(x)$ and $w^\infty(x) = x^2$, for n even and odd, respectively. These limiting weights are not as unrelated as we might think at first. We have, in fact,

$$p_{n-1}(x; w_\infty) = xp_{n-2}(x; w^\infty), \qquad n(\text{even}) \geqq 2,$$

since each side is easily seen to be orthogonal on $[-1, 1]$ to all powers of degree $\leqq n-2$ with respect to the constant weight function $w \equiv 1$, and hence equal to the monic Legendre polynomial of degree $n-1$. This is why the limiting zeros for $\kappa = \infty$ in Table 5.2 and Table 5.3 are the same.

It can be seen that for n even, there are two zeros on the imaginary axis moving in opposite directions as a increases from a_n^* to ∞, one up from i to $i\infty$ (cf. the remark at the end of § 4), the other down from some iy_n^*, $0 < y_n^* < 1$, to zero. For n odd, there is one zero on the imaginary axis moving up from i to $i\infty$.

It is also easy to compute the coefficients $b_{k,\infty}$ and b_k^∞ and to observe numerically the convergence in (3.5) and (3.9).

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18

Papers on Chebyshev Quadrature

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On Chebyshev-Type Quadratures

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Abstract. According to a result of S. N. Bernstein, n-point Chebyshev quadrature formulas, with all nodes real, do not exist when $n = 8$ or $n \geqq 10$. Modifications of such quadrature formulas have recently been suggested by R. E. Barnhill, J. E. Dennis, Jr. and G. M. Nielson, and by D. Kahaner. We establish here certain empirical observations made by these authors, notably the presence of multiple nodes. We also show how some of the quadrature rules proposed can be constructed by solving single algebraic equations, and we compute the respective nodes to 25 decimal digits. The same formulas also arise in recent work of P. Rabinowitz and N. Richter as limiting cases of optimal Chebyshev-type quadrature rules in a Hilbert space setting.

1. Introduction.

The quadrature rule with equal coefficients,

$$\int_{-1}^{1} f(t)\,dt = \frac{2}{n}\sum_{k=1}^{n} f(t_k) + R_n(f), \tag{1.1}$$

is called a *Chebyshev quadrature formula* if it has polynomial degree n, i.e., if $R_n(t^i) = 0$ for $i = 0, 1, \cdots, n$. (The requirement for $i = 0$ is automatically satisfied.) By a classical result, due to S. N. Bernstein [3], Chebyshev quadrature formulas with all nodes t_k real do not exist if $n = 8$ or $n \geqq 10$. Even if Chebyshev's requirement is relaxed to $R_n(t^i) = 0$, $i = 0, 1, \cdots, p$, $p < n$, we can have t_k all real in (1.1) only if (S. N. Bernstein [3])

$$p < 4n^{1/2}. \tag{1.2}$$

In the light of these negative results it is natural to consider the following two problems.

Problem I. Let p and q be integers such that $0 \leqq p < n \leqq q \leqq \infty$. Determine real nodes $\{t_k\}_{k=1}^{n}$ (hopefully contained in the interval $[-1, 1]$) such that

$$\sum_{j=p+1}^{q} [R_n(t^j)]^2 = \min, \tag{1.3}$$

subject to

$$R_n(t^j) = 0, \qquad j = 1, 2, \cdots, p. \tag{1.4}$$

(The constraints (1.4) drop out if $p = 0$.)

Problem I′ ("*symmetric problem*"). Same as Problem I, but with the additional symmetry constraints

$$t_{n+1-k} = -t_k, \qquad k = 1, 2, \cdots, n. \tag{1.5}$$

If $q = n$, and $n \leqq 7$ or $n = 9$, Problems I and I′ are solved by the

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classical Chebyshev formulas, which drive the objective function in (1.3) to zero. We assume therefore, in the following, that $n = 8$ or $n \geqq 10$. Problems I and I′ for $p = 0$ are considered by R. E. Barnhill et al. [2], Problem I′ for $q = n$, $p \neq 0$ by D. Kahaner [4]. Their approach is largely computational. Some of the results reported in [2] seem to indicate that Problem I in fact has a symmetric solution, but this remains unproved. All we show (Theorem 2.1) is that the solution to Problem I is symmetric if it is unique. Another empirical observation made in [2], [4] is the presence of multiple nodes. We prove (Theorems 2.2 and 3.1) that Problems I and I′, in the case $q = n$, indeed give rise to multiple nodes. We subsequently concentrate on Problem I′ with $p = n - 1$ (if n is even), $p = n - 2$ (if n is odd), and show how its solution can be reduced to the solution of single algebraic equations (Theorem 3.2 and Section 4). Computational results, based on these procedures, reveal (Section 5) that the problem again cannot be solved if $n = 12$ or $14 \leqq n \leqq 19$. By (1.2) it has no solution for $n \geqq 20$ either. For the remaining values of n ($n = 8, 10, 11, 13$) the optimal nodes are computed to 25 decimals. They have previously been obtained (to 12 decimal digits) in a different context by P. Rabinowitz and N. Richter [5].

2. Problem I. In this and the subsequent sections we denote by m_j the moments

$$m_j = \int_{-1}^{1} t^j \, dt = 0 \qquad \text{if } j \text{ is odd,}$$

$$= 2/(j+1) \qquad \text{if } j \text{ is even.}$$

THEOREM 2.1. *If the solution to Problem* I *is unique (up to a permutation), then it is symmetric.*

Proof. We assume the nodes ordered, say,

$$t_1 \geqq t_2 \geqq \cdots \geqq t_n. \tag{2.1}$$

Our assumption then implies that Problem I has exactly one solution $\mathbf{t} = [t_1, t_2, \cdots, t_n]$ satisfying (2.1). Now, if $\mathbf{t}$ is a solution of Problem I, then so is $-\mathbf{t}$. Indeed, neither the objective function in (1.3), nor the constraints (1.4) are affected if $\mathbf{t}$ is replaced by $-\mathbf{t}$, the remainder $R_n(t^j)$ either remaining the same (j even), or merely changing sign (j odd). Consequently, if (2.1) represents a solution, so does

$$-t_n \geqq -t_{n-1} \geqq \cdots \geqq -t_1.$$

By the assumed uniqueness, it follows that $t_{n+1-k} = -t_k$, $k = 1, 2, \cdots, n$, that is, symmetry as asserted.

THEOREM 2.2. *Let* $q = n$, *and* $n = 8$ *or* $n \geqq 10$. *If the constraints* (1.4) *admit real solutions, then every solution of Problem* I *has at least one multiple node.*

Proof. We observe, first of all, that under the assumptions made, Problem I has a solution, and that any solution must occur at a finite point $\mathbf{t} = [t_1, t_2, \cdots, t_n] \in \mathbf{R}^n$. The latter, if $p \geqq 2$, follows immediately from (1.4) with $j = 2$, which restricts $\mathbf{t}$ to the sphere with radius $(nm_2/2)^{1/2}$ and center at the origin. If $p < 2$, we may argue that the objective function in (1.3) is never less than $[R_n(t^2)]^2 = ((2/n)\sum_{k=1}^{n} t_k^2 - m_2)^2$ and thus tends with $\|\mathbf{t}\|$ to infinity. It suffices, therefore, to consider Problem I on a sufficiently large, but finite, ball in $\mathbf{R}^n$. The existence of a solution then follows from the fact that we are minimizing a continuous function on a nonempty compact set.

From the theory of Lagrange multipliers [1, p. 153] it follows that the minimum point either satisfies the equations

$$\frac{\partial}{\partial t_i}\left\{\sum_{j=p+1}^{n}[R_n(t^j)]^2 - \sum_{j=1}^{p}\lambda_j R_n(t^j)\right\} = 0, \qquad i = 1, 2, \cdots, n, \tag{2.2}$$

$$R_n(t^j) = 0, \qquad j = 1, 2, \cdots, p, \tag{2.3}$$

or else in such that the Jacobian matrix of the system (2.3) has rank $<p$. (In the case $p = 0$, only (2.2), without multipliers, need be considered.) We first consider (2.2), (2.3). Carrying out the differentiations, we can write these equations more explicitly in the form

$$\sum_{j=p+1}^{n}\left(\frac{2}{n}\sum_{k=1}^{n}t_k^j - m_j\right)jt_i^{j-1} + \frac{1}{2}\sum_{j=1}^{p}\lambda_j jt_i^{j-1} = 0, \qquad i = 1, 2, \cdots, n, \tag{2.2'}$$

$$\frac{2}{n}\sum_{k=1}^{n}t_k^j - m_j = 0, \qquad j = 1, 2, \cdots, p. \tag{2.3'}$$

We interpret (2.2') as a system of n linear homogeneous equations in the n "unknowns"

$$u_j = \tfrac{1}{2}j\lambda_j \quad (j = 1, 2, \cdots, p), \qquad u_j = j\left(\frac{2}{n}\sum_{k=1}^{n}t_k^j - m_j\right) \quad (j = p+1, \cdots, n).$$

Not all of these can vanish, since otherwise (2.3') would hold not only for $j = 1, 2, \cdots, p$, but also for $j = p+1, \cdots, n$, which is impossible by Bernstein's result. Consequently, the determinant of the system (2.2'), a Vandermondian, must vanish, giving

$$\begin{vmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \cdots & t_2^{n-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & t_n & t_n^2 & \cdots & t_n^{n-1} \end{vmatrix} = \prod_{j>i}(t_j - t_i) = 0.$$

There exists, therefore, at least one pair of distinct indices $i \neq j$ such that $t_i = t_j$, i.e., t_i is a multiple node. The same conclusion is reached by considering the other alternative, concerning the rank of the Jacobian of (2.3'), since the latter is also a Vandermonde matrix. This completes the proof of Theorem 2.2.

It is likely that multiple nodes occur also for $q > n$, but we have no proof for this.

3. The Symmetric Problem. In view of (1.5) there are now only $[n/2]$ independent variables, which we assume ordered decreasingly,

$$t_1 \geqq t_2 \geqq \cdots \geqq t_\nu \geqq 0, \qquad \nu = [n/2]. \tag{3.1}$$

If n is odd, one node, say $t_{\nu+1}$, must vanish and therefore does not appear among the independent variables (3.1).

We consider Problem I′ for $q = n$ only. Letting $\pi = [p/2]$, the problem is then equivalent to

$$\sum_{j=\pi+1}^{\nu}[R_n(t^{2j})]^2 = \min, \quad R_n(t^{2j}) = 0, \qquad j = 1, 2, \cdots, \pi, \tag{3.2}$$

since $R_n(t^j) = 0$ for j odd. We assume $\pi < \nu$ to insure a nonvoid objective function in (3.2). (If n is even, this is always satisfied.) More explicitly, (3.2) can be written in the form

$$(3.2') \quad \sum_{i=\pi+1}^{\nu} \left(\frac{4}{n} \sum_{k=1}^{\nu} t_k^{2i} - m_{2i} \right)^2 = \min, \quad \frac{4}{n} \sum_{k=1}^{\nu} t_k^{2i} - m_{2i} = 0, \quad j = 1, 2, \cdots, \pi.$$

THEOREM 3.1. *Let $q = n$, and $n = 8$ or $n \geqq 10$. If the constraints in* (3.2') *admit real solutions, then every solution of Problem* I' *has at least one multiple node.*

Proof. Existence and boundedness of a solution of Problem I' follows as in the proof of Theorem 2.2. If $t_\nu = 0$, then the origin is a multiple node, since nodes occur in pairs, if n is even, and include the extra node $t_{\nu+1} = 0$, if n is odd. Any solution with $t_\nu > 0$, on the other hand, by the theory of Lagrange multipliers must satisfy

$$\sum_{i=\pi+1}^{\nu} \left(\frac{4}{n} \sum_{k=1}^{\nu} t_k^{2i} - m_{2i} \right) j t_i^{2i-1} + \frac{1}{2} \sum_{i=1}^{\pi} \lambda_i j t_i^{2i-1} = 0, \qquad i = 1, 2, \cdots, \nu,$$

or be such that the Jacobian matrix of the constraint equations has rank $< \pi$. As before, this implies

$$(3.3) \quad \begin{vmatrix} t_1 & t_1^3 & \cdots & t_1^{2\nu-1} \\ t_2 & t_2^3 & \cdots & t_2^{2\nu-1} \\ \cdots & \cdots & \cdots & \cdots \\ t_\nu & t_\nu^3 & \cdots & t_\nu^{2\nu-1} \end{vmatrix} = t_1 t_2 \cdots t_\nu \prod_{j>i} (t_j^2 - t_i^2) = 0.$$

Since $t_\nu > 0$, we conclude ${t_i}^2 = {t_j}^2$ for some $i \neq j$, and thus $t_i = t_j$, by virtue of (3.1). This proves Theorem 3.1.

In the case $\pi = \nu - 1$ (considered by Kahaner [4]), the method of Lagrange multipliers is actually more powerful. It permits us to reduce the problem to the much simpler problem of solving at most $\pi + 2$ single algebraic equations of degree $\leqq \pi$. The following theorem is a step in this direction.

THEOREM 3.2. *Let $q = n$, $n = 8$ or $n \geqq 10$, and $\pi = \nu - 1$, where $\pi = [p/2]$, $\nu = [n/2]$. If Problem* I' *admits solution, then one or both of the following conditions must hold:*

(A) *The system of equations*

$$\sum_{k=1}^{\pi} x_k^j = \frac{n}{4} m_{2j}, \qquad j = 1, 2, \cdots, \pi,$$

has nonnegative solutions.

(B) *The system of equations*

$$\sum_{k=1}^{\pi-1} x_k^j + 2x_\pi^j = \frac{n}{4} m_{2j}, \qquad j = 1, 2, \cdots, \pi,$$

has nonnegative solutions.

Putting

$$(3.4) \quad t_k^* = x_k^{1/2} \quad (k = 1, 2, \cdots, \pi), \qquad t_\nu^* = 0$$

for a solution in case (A), *and*

$$(3.5) \quad t_k^* = x_k^{1/2} \quad (k = 1, 2, \cdots, \pi - 1), \qquad t_\pi^* = t_\nu^* = x_\pi^{1/2}$$

for a solution in case (B), *let* $\{t_k\}_{k=1}^{\nu}$ *denote the permutation of* $\{t_k^*\}_{k=1}^{\nu}$ *which satisfies* (3.1). *The solution of problem* (3.2′) *is then given by that set of nodes* $t_1, t_2, \cdots, t_\nu$ *which gives the smallest value to the objective function in* (3.2′). *If the nodes derive from case* (A), *then the solution to Problem* I′ *has a multiple node at the origin; if they derive from case* (B), *then there is a nonzero multiple node among the solution.*

Proof. We already know from the proof of Theorem 3.1 that the solution $\mathbf{t} = [t_1, t_2, \cdots, t_\nu]$ of problem (3.2′) must satisfy (3.3) and the constraints in (3.2′). Corresponding to the $\nu(\nu + 1)/2$ factors in (3.3), there are as many possibilities to consider, which in view of (3.1) we may list as follows in terms of $x_k = t_k^2$:

$$
\begin{aligned}
x_\nu &= 0 && (1, 1)\\
x_{\nu-1} = x_\nu &= 0 && (1, 2)\\
&\cdots\cdots\cdots && \cdots\cdots\\
x_1 = x_2 = \cdots = x_\nu &= 0 && (1, \nu)\\
x_{\nu-1} &= x_\nu && (2, 1)\\
x_{\nu-2} = x_{\nu-1} &= x_\nu && (2, 2)\\
&\cdots\cdots\cdots && \cdots\cdots\\
x_1 = x_2 = \cdots = x_{\nu-1} &= x_\nu && (2, \nu - 1)\\
x_{\nu-2} &= x_{\nu-1} && (3, 1)\\
x_{\nu-3} = x_{\nu-2} &= x_{\nu-1} && (3, 2)\\
&\cdots\cdots\cdots && \cdots\cdots\\
x_1 = x_2 = \cdots = x_{\nu-2} &= x_{\nu-1} && (3, \nu - 2)\\
&\cdots\cdots\cdots && \cdots\cdots\\
x_1 &= x_2 && (\nu, 1)
\end{aligned}
$$

Condition (1, 1), together with the constraints in (3.2′), gives the system in case (A) of the theorem. The subsequent conditions (1, 2), $\cdots$, (1, ν) simply imply that this system has a solution with one or more zero components. (We see later in examples that this is not possible.) Condition (2, 1), together with the constraints, gives rise to the system of case (B). The subsequent conditions through (2, $\nu - 1$) simply mean that this system has multiple solutions. The conditions in group 3 are either a permutation of those in group 2, or in fact identical with them if $x_{\nu-1} = x_\nu$. Similar arguments apply to all subsequent groups. We thus see that if $\mathbf{t} = [t_1, t_2, \cdots, t_\nu]$ is a solution of (3.1), (3.2′), then the corresponding $\mathbf{x} = [x_1, x_2, \cdots, x_\nu]$ (with $x_k = t_k^2$) is such that either $x_\nu = 0$ and the remaining components solve the system of case (A), or there is a permuted vector $\mathbf{x}$, say, $\mathbf{x}^* = [x_1^*, x_2^*, \cdots, x_{\nu-1}^*, x_\nu^*]$ such that $x_{\nu-1}^* = x_\nu^*$ and $x_1^*, x_2^*, \cdots, x_\nu^*$ solves the system of case (B). This proves the part of Theorem 3.2 concerning (A) and (B). The rest of the theorem is a consequence of Lagrange multiplier theory.

The solution of the systems in (A) and (B) of Theorem 3.2 is discussed in the next section.

4. The Solution of Some Auxiliary Systems of Algebraic Equations. We consider first the system

$$\sum_{k=1}^{n} x_k^j = s_j, \qquad j = 1, 2, \cdots, n. \tag{4.1}$$

The lemma which follows is well known.

LEMMA 4.1. (NEWTON'S IDENTITIES). *If* $\{x_k\}_{k=1}^n$ *is a solution of* (4.1) *and*

$$\xi(x) = \prod_{k=1}^{n} (x - x_k) = x^n + a_1 x^{n-1} + \cdots + a_n, \tag{4.2}$$

then

$$\begin{aligned} &s_1 + a_1 = 0, \\ &s_2 + a_1 s_1 + 2a_2 = 0, \\ &\cdots\cdots\cdots\cdots\cdots \\ &s_n + a_1 s_{n-1} + \cdots + a_{n-1} s_1 + n a_n = 0. \end{aligned} \tag{4.3}$$

Conversely, if the constants $\{a_k\}_{k=1}^n$ *satisfy* (4.3), *then the zeros of* $\xi(x)$ *in* (4.2) *solve* (4.1).

The solution of (4.1) is thus reduced to the solution of a single algebraic equation, viz., $\xi(x) = 0$.

Together with (4.1) we now consider the system

$$\sum_{k=1}^{n} y_k^j = s_j - z^j, \qquad j = 1, 2, \cdots, n, \tag{4.4}$$

where z is an arbitrary parameter.

LEMMA 4.2. *Let* $\{x_k\}_{k=1}^n$, $\{y_k\}_{k=1}^n$ *be solutions of* (4.1) *and* (4.4), *respectively. If*

$$\xi(x) = \prod_{k=1}^{n} (x - x_k) = x^n + a_1 x^{n-1} + \cdots + a_n, \tag{4.5}$$

$$\eta(x) = \prod_{k=1}^{n} (x - y_k) = x^n + b_1 x^{n-1} + \cdots + b_n, \tag{4.6}$$

then

$$b_r = z^r + a_1 z^{r-1} + \cdots + a_r, \qquad r = 1, 2, \cdots, n. \tag{4.7}$$

Proof. By virtue of (4.1) and (4.4), we have, for large x,

$$\frac{\xi'(x)}{\xi(x)} = \sum_{k=1}^{n} \frac{1}{x - x_k} = \sum_{j=0}^{n} \frac{s_j}{x^{j+1}} + O(x^{-n-2}),$$

$$\frac{\eta'(x)}{\eta(x)} = \sum_{k=1}^{n} \frac{1}{x - y_k} = \sum_{j=0}^{n} \frac{s_j}{x^{j+1}} - \sum_{j=1}^{n} \frac{z^j}{x^{j+1}} + O(x^{-n-2}),$$

where $s_0 = n$. Consequently,

$$\frac{\eta'(x)}{\eta(x)} = \frac{\xi'(x)}{\xi(x)} - \left(\frac{1}{x - z} - \frac{1}{x}\right) + O(x^{-n-2}),$$

which, upon integration, yields

$$\eta(x) = \text{const}\,\frac{x\xi(x)}{x - z}\,[1 + O(x^{-n-1})].$$

Since $\eta(x)$ and $\xi(x)$ are both polynomials with leading coefficient 1, the constant in this identity is 1, and we get

$$(x - z)\eta(x) = x\xi(x)[1 + O(x^{-n-1})].$$

Comparing coefficients of the powers $x^n, x^{n-1}, \cdots, x$ on either side, we find

$$a_r = b_r - zb_{r-1}, \qquad r = 1, 2, \cdots, n,$$

where $b_0 = 1$, which, when solved for the b's, gives (4.7).

LEMMA 4.3. *Let* $\{x_k\}_{k=1}^n$, $\{y_k\}_{k=1}^n$ *be solutions, respectively, of*

$$\sum_{k=1}^{n} x_k^j = s_j, \qquad \sum_{k=1}^{n-1} y_k^j + 2y_n^j = s_j, \qquad j = 1, 2, \cdots, n, \tag{4.8}$$

and

$$\xi(x) = \prod_{k=1}^{n} (x - x_k) = x^n + a_1x^{n-1} + \cdots + a_n. \tag{4.9}$$

Then y_n *is a root of the algebraic equation*

$$(d/dy)[y\xi(y)] = 0. \tag{4.10}$$

Proof. Put $z = y_n$ in Lemma 4.2. The system (4.4) then becomes the second system in (4.8), and from (4.6) we see that $\eta(y_n) = 0$, i.e., in view of (4.7),

$$\sum_{r=0}^{n} \left(\sum_{s=0}^{r} a_s y_n^{r-s} \right) y_n^{n-r} = 0.$$

Inverting the order of summation, we get

$$\sum_{s=0}^{n} (n - s + 1)a_s y_n^{n-s} = 0,$$

which is the desired result.

Lemma 4.3 suggests a method for solving the second system in (4.8). We first solve (4.10), where Lemma 4.1 is used to obtain $\xi(x)$. For each root y_n of (4.10), we then solve

$$\sum_{k=1}^{n-1} y_k^j = s_j - 2y_n^j, \qquad j = 1, 2, \cdots, n - 1, \tag{4.11}$$

which is again a problem of the type considered in Lemma 4.1.

We note that if the equation $\xi(x) = 0$ has m ($\leqq n$) distinct real nonvanishing roots, then Eq. (4.10) has at least m such roots. This is a simple consequence of Rolle's theorem.

5. Numerical Results. According to Bernstein [cf. (1.2)] Problem I′ for $q = n$, $\pi = \nu - 1$ cannot have a real solution if $n - 2 \geqq 4n^{1/2}$, i.e., if $n \geqq 20$. Hence, we explore the integers $n = 8$ and $10 \leqq n \leqq 19$ for possible real solutions, following the procedures outlined in Theorem 3.2 and Lemmas 4.1, 4.3. It turns out that the problem

TABLE 1.

Search for optimal nodes

n	π	*primary* ξ	*object. fct.*	$(x\xi)'$	*secondary* ξ	*object. fct.*
			(in 10^{-7})			(in 10^{-7})
8	3	*.809*		.659	no pos. zeros	—
		.328		.266	1 pos. zero	—
		.197	40.9	.074	.801, .384	293.
10	4	.846		.730	no pos. zeros	—
		.439		.375	1 pos. zero	—
		.288		.190	2 pos. zeros	—
		.093	23.5	*.038*	*.847, .416, .326*	14.2
11	4	2 pos. zeros	—	.750	no pos. zeros	—
				.419	1 pos. zero	—
				.228	.856, .514, .008	24.1
				.070	*.860, .455, .378*	3.27
12	5	1 pos. zero	—	.777	no pos. zeros.	—
				.456	2 pos. zeros	—
				.297	2 pos. zeros	—
				.097	2 pos. zeros	—
				.040	2 pos. zeros	—
13	5	1 pos. zero	—	.791	no pos. zeros	—
				.491	*.882, .159, .118, .026*	1.48
				.327	2 pos. zeros	—
				.139	2 pos. zeros	—
				.057	.882, .525, .450, .197	1.94
14	6	2 pos. zeros	—	.811	no pos. zeros	—
				.516	2 pos. zeros	—
				.390	2 pos. zeros	—
				.011	1 pos. zero	—
15	6	2 pos. zeros	—	.822	no pos. zeros	—
				.545	2 pos. zeros	—
				.413	2 pos. zeros	—
				.183	2 pos. zeros	—
				.148	2 pos. zeros	—
				.032	1 pos. zero	—
16	7	1 pos. zero	—	.836	no pos. zeros	—
				.560	2 pos. zeros	—
				.470	2 pos. zeros	—
17	7	1 pos. zero	—	.845	no pos. zeros	—
				.586	2 pos. zeros	—
				.486	2 pos. zeros	—
18	8	1 pos. zero	—	.856	no pos. zeros	—
				.592	2 pos. zeros	—
				.541	2 pos. zeros	—
19	8	2 pos. zeros	—	.862	no pos. zeros	—
				.617	2 pos. zeros	—
				.550	2 pos. zeros	—
				.009	1 pos. zero	—

again has no solution if $n = 12$ or $n \geqq 14$. The results of our computation are summarized in Table 1. In the first two columns of this table we record the values of n

and $\pi = [n/2] - 1$, respectively. The third column provides information concerning the positive zeros* of the "primary" polynomial ξ. This is the polynomial ξ (of degree π) defined in Lemma 4.1, which corresponds to the system (A) of Theorem 3.2. We list all its positive zeros, if there are π of them, and only state their number, otherwise. A complete set of π positive zeros of ξ constitutes a candidate for an optimal solution. The fourth column contains the corresponding value of the objective function in (3.2′). In the next column are listed all positive zeros* of $(x\xi)'$ [cf. Lemma 4.3]. To each of these zeros corresponds a "secondary" polynomial ξ (of degree $\pi - 1$), which is the ξ-polynomial belonging to the system (4.11). Information concerning its positive zeros* is given in column six. Any complete set of $\pi - 1$ positive zeros, together with the corresponding zero of $(x\xi)'$, again constitutes a candidate for an optimal solution. The corresponding value of the objective function is given in the last column. Entries printed in italic type correspond to optimal solutions.

We note that all zeros listed in Table 1 correspond to x_k-values in Theorem 3.2; the desired nodes are the square roots $t_k = x_k^{1/2}$. The optimal nodes to 25 decimals, as computed in double precision arithmetic on the CDC 6500 computer, are as follows:

$n = 8$

$$
\begin{aligned}
-t_8 = t_1 &= .89917\ 93430\ 79596\ 08730\ 30645\\
-t_7 = t_2 &= .57261\ 84272\ 82722\ 13153\ 89072\\
-t_6 = t_3 &= .44375\ 44129\ 90497\ 74722\ 36463\\
-t_5 = t_4 &= 0
\end{aligned}
$$

$n = 10$

$$
\begin{aligned}
-t_{10} = t_1 &= .92019\ 94551\ 46763\ 72230\ 02697\\
-t_9 = t_2 &= .64533\ 80565\ 58410\ 15617\ 64507\\
-t_8 = t_3 &= .57137\ 69273\ 35333\ 94337\ 27524\\
-t_7 = t_4 &= .19617\ 19004\ 85916\ 40260\ 18800 = -t_6 = t_5
\end{aligned}
$$

$n = 11$

$$
\begin{aligned}
-t_{11} = t_1 &= .92750\ 15617\ 64337\ 25089\ 95943\\
-t_{10} = t_2 &= .67480\ 04201\ 44051\ 83360\ 39625\\
-t_9 = t_3 &= .61476\ 53471\ 66840\ 31224\ 97967\\
-t_8 = t_4 &= .26436\ 91993\ 73049\ 18149\ 65951 = -t_7 = t_5\\
t_6 &= 0
\end{aligned}
$$

$n = 13$

$$
\begin{aligned}
-t_{13} = t_1 &= .93913\ 47142\ 41241\ 62154\ 14039\\
-t_{12} = t_2 &= .70075\ 43220\ 36606\ 99992\ 84358 = -t_{11} = t_3\\
-t_{10} = t_4 &= .39893\ 86129\ 44348\ 55731\ 47686\\
-t_9 = t_5 &= .34310\ 66664\ 50818\ 91837\ 46133\\
-t_8 = t_6 &= .16032\ 84566\ 34386\ 73493\ 97197\\
t_7 &= 0
\end{aligned}
$$

Comparison with Table 2 in [5] reveals agreement in all twelve digits given there.

* None of the zeros vanish; we could thus equally well speak of "nonnegative" zeros.

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18.2. [50] "Nonexistence of Chebyshev-type Quadratures on Infinite Intervals"

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Nonexistence of Chebyshev-Type Quadratures on Infinite Intervals*

By Walter Gautschi

Dedicated to D. H. Lehmer on his 70th birthday

Abstract. Quadrature rules on semi-infinite and infinite intervals are considered involving weight functions of the Laguerre and Hermite type. It is shown that such quadrature rules cannot have equal coefficients and real nodes unless the algebraic degree of accuracy is severely limited.

1. Introduction. Given a nonnegative weight function $w(x)$ on the interval (a, b), with finite moments

$$m_k = \int_a^b x^k w(x)dx, \qquad k = 0, 1, 2, \cdots, \quad m_0 > 0,$$

a quadrature rule of the form

$$\int_a^b f(x)w(x)dx = \frac{m_0}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f) \tag{1.1}$$

is called a *Chebyshev quadrature formula* if the nodes $x_k^{(n)}$ are mutually distinct and located in (a, b), and if (1.1) has polynomial degree of accuracy n, i.e., $R_n(f) = 0$ whenever f is a polynomial of degree $\leqslant n$. In the following we are going to relax these requirements in two respects: Firstly, we shall drop the requirement that the nodes be distinct, or even contained in (a, b), assuming merely that all be real. Secondly, we shall allow for polynomial degree of accuracy $< n$. Since we are interested in questions of nonexistence, both modifications only strengthen our results. We shall refer to quadrature rules (1.1), under these relaxed conditions, as *Chebyshev-type quadrature formulas.*

We focus our attention on two special cases of (1.1): the Chebyshev-Laguerre formula

$$\int_0^\infty x^\alpha e^{-x} f(x)dx = \frac{\Gamma(\alpha + 1)}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f), \qquad \alpha > -1, \tag{1.2}$$

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and the Chebyshev-Hermite formula

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)dx = \frac{\sqrt{\pi}}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f). \tag{1.3}$$

In 1955, H. E. Salzer [5] first observed (by computation) that a Chebyshev formula (1.2), in the strict sense, for $\alpha = 0$, exists for $n = 1$ and $n = 2$, but does not exist for $3 \leqslant n \leqslant 10$. He found similarly that (1.3) exists for $n = 1, 2$ and 3, but not for $4 \leqslant n \leqslant 10$. Shortly thereafter, V. I. Krylov [4] proved that in fact (1.2) (with $\alpha = 0$) and (1.3) do not exist for *any* $n \geqslant 3$ and $n \geqslant 4$, respectively. This was proved again later on, independently, by H. S. Wilf [6] and L. Gatteschi [3]. We shall prove below analogous results for Chebyshev-type quadratures. In particular, we show that formulas (1.2) and (1.3) with polynomial degrees of accuracy $p_n \geqslant \tau n^{\gamma}$, $\tau > 0$, $\frac{1}{2} < \gamma < 1$, as $n \to \infty$, cannot exist.

Both Krylov's and Gatteschi's proofs are based on an inequality of Bernstein, which was used by Bernstein to settle the existence of Chebyshev quadratures in the classical case $w(x) = 1$ on $[-1, 1]$. We shall continue using Bernstein's method, but simplify its application and also establish its validity in the case of nodes not necessarily distinct.

2. Bernstein's Inequalities. The lemmas in this section are slight extensions or modifications of results due to S. Bernstein [2], which in turn, according to Bernstein [loc. cit., p. 180], are "but more or less immediate applications or modifications of a proposition due to Chebyshev". Our extension is to arbitrary weight functions (which is immediate), and our modification is prompted by our reluctance to assume mutually distinct nodes.

Let $\xi_r^{(m)}$ and $\lambda_r^{(m)}$ be the abscissas and weights of the m-point Gaussian quadrature rule

$$\int_a^b f(x)w(x)dx = \sum_{r=1}^{m} \lambda_r^{(m)} f(\xi_r^{(m)}) + R_m(f), \qquad \xi_m^{(m)} < \xi_{m-1}^{(m)} < \cdots < \xi_1^{(m)}. \tag{2.1}$$

Thus, $R_m(f) = 0$ for all polynomials of degree $\leqslant 2m - 1$. The abscissas $\xi_r^{(m)}$ are the zeros of the mth degree orthogonal polynomial associated with the weight function $w(x)$, while the weights $\lambda_r^{(m)}$ are the corresponding Christoffel numbers.

LEMMA 2.1. *If the Chebyshev-type quadrature formula* (1.1) *has polynomial degree of accuracy* $2m - 1$, $m < n$, *then either*

$$x_r^{(n)} = \xi_r^{(m)} \ (n_r\text{-times}), \qquad \lambda_r^{(m)} = (m_0/n)n_r, \qquad r = 1, 2, \cdots, m, \tag{2.2}$$

where $n_r \geqslant 1$ *are integers summing up to* n, *or*

$$x_k^{(n)} > \xi_1^{(m)} \tag{2.3}$$

for at least one value of k, $1 \leqslant k \leqslant n$. *The same statement holds true with* (2.3) *replaced by*

$$x_k^{(n)} < \xi_m^{(m)}. \tag{2.3'}$$

The proof utilizes the polynomial $p(x) = p_m^2(x)/(x - \xi_1^{(m)})$, where p_m is the mth degree orthogonal polynomial associated with the weight function $w(x)$. We have, on the one hand $\int_a^b p(x)w(x)dx = 0$, and on the other, by assumption,

$$\sum_{k=1}^{n} p(x_k^{(n)}) = 0. \tag{2.4}$$

There are the following alternatives:

(i) All $x_k^{(n)} \leqslant \xi_1^{(m)}$. Since $p(x) \leqslant 0$ for $x \leqslant \xi_1^{(m)}$, and $p(x) = 0$ only for $x = \xi_r^{(m)}$, $r = 1, 2, \cdots, m$, it follows from (2.4) that all $x_k^{(n)}$ must be placed at Gaussian nodes $\xi_r^{(m)}$, that is,

$$x_r^{(n)} = \xi_r^{(m)} \quad (n_r\text{-times}), \qquad r = 1, 2, \cdots, m,$$

where $n_r \geqslant 0$ are integers with $n_1 + n_2 + \cdots + n_m = n$. The quadrature rule (1.1) then becomes

$$\int_a^b f(x)w(x)dx = \frac{m_0}{n} \sum_{r=1}^{m} n_r f(\xi_r^{(m)}) + R_n(f).$$

Since it has polynomial degree of accuracy $2m - 1$, and since the Gaussian quadrature rule (2.1) is unique, we conclude (2.2), and in particular, $n_r \geqslant 1$ for all r, by virtue of $\lambda_r^{(m)} > 0$. This proves the first alternative (2.2).

(ii) At least one $x_k^{(n)} > \xi_1^{(m)}$. This gives the second alternative (2.3).

The statement concerning (2.2) and (2.3') follows similarly by using $p(x) = p_m^2(x)/(x - \xi_m^{(m)})$.

LEMMA 2.2. *If the Chebyshev-type quadrature formula* (1.1) *has polynomial degree of accuracy* $2m - 2$, *then*

$$\sigma(\xi_1^{(m)})m_0/n \leqslant \lambda_1^{(m)} \quad \text{and} \quad \tau(\xi_m^{(m)})m_0/n \leqslant \lambda_m^{(m)}, \tag{2.5}$$

where $\sigma(\xi_1^{(m)})$ *and* $\tau(\xi_m^{(m)})$ *are the number of nodes* $x_k^{(n)}$ *with* $x_k^{(n)} \geqslant \xi_1^{(m)}$ *and* $x_k^{(n)} \leqslant \xi_m^{(m)}$, *respectively.*

The proof of Bernstein, utilizing $p(x) = p_m^2(x)(x - \xi_r^{(m)})^{-2}[p_m'(\xi_r^{(m)})]^{-2}$, $r = 1$ or $r = m$, applies essentially unchanged.

LEMMA 2.3. *If the Chebyshev-type quadrature formula* (1.1) *has polynomial degree of accuracy* $2m - 1$, $m < n$, *then*

$$m_0/n \leqslant \min\{\lambda_1^{(m)}, \lambda_m^{(m)}\}. \tag{2.6}$$

Proof. By Lemma 2.1 we have either (2.2), or else both (2.3) and (2.3'). In the first case, (2.6) results from putting $r = 1$ and $r = m$ in (2.2) and noting that $n_r \geqslant 1$. In the second case, (2.6) is a consequence of (2.5).

3. Nonexistence of Chebyshev-Laguerre Type Formulas.

THEOREM 3.1. *A Chebyshev-type quadrature formula* (1.2) *having polynomial*

degree of accuracy $n - s$, $s \geqslant 0$, *does not exist if*

$$n \geqslant s + \tfrac{1}{2}\{\alpha + 5 + \sqrt{(\alpha+1)(\alpha+5+4s)}\} \quad \textit{and} \quad n - s \ (\textit{even}) \geqslant 4, \tag{3.1}$$

or if

$$n \geqslant s - 1 + \tfrac{1}{2}\{\alpha + 5 + \sqrt{(\alpha+1)(\alpha+1+4s)}\} \quad \textit{and} \quad n - s \ (\textit{odd}) \geqslant 3. \tag{3.2}$$

Remark. For $n - s = 2$ it is easily shown that Chebyshev-type formulas (1.2) do indeed exist. The same, of course, is true if $n - s = 1$.

Proof of Theorem 3.1. Let $\pi_0(x), \pi_1(x), \cdots$ denote the normalized Laguerre polynomials $L_0^{(\alpha)}(x), L_1^{(\alpha)}(x), \cdots$, and $\xi_r^{(m)}$ the zeros of π_m, ordered decreasingly. The associated Christoffel numbers are

$$\lambda_r^{(m)} = 1 \Big/ \sum_{k=0}^{m-1} [\pi_k(\xi_r^{(m)})]^2. \tag{3.3}$$

V. I. Krylov [4] showed that

$$\xi_1^{(m)} > 2m + \alpha - 1 \qquad (m \geqslant 2, \alpha > -1). \tag{3.4}$$

Since

$$\pi_0 = [\Gamma(\alpha+1)]^{-1/2}, \qquad \pi_1(x) = [\Gamma(\alpha+2)]^{-1/2}(\alpha + 1 - x),$$

it follows from (3.3) that

$$\lambda_1^{(m)} \leqslant \frac{1}{\pi_0^2 + [\pi_1(\xi_1^{(m)})]^2} = \frac{\Gamma(\alpha+1)}{1 + [\xi_1^{(m)} - (\alpha+1)]^2/(\alpha+1)},$$

and thus from (3.4) that

$$\lambda_1^{(m)} < \frac{\Gamma(\alpha+1)}{1 + 4(m-1)^2/(\alpha+1)}, \qquad m \geqslant 2.$$

We first consider the case where $n - s$ is even. Let $n - s = 2m$, $m \geqslant 2$. By Bernstein's inequality (2.6) we have nonexistence of (1.2) if $\Gamma(\alpha+1)/n > \lambda_1^{(m)}$, hence, a fortiori, if

$$\frac{1}{n} \geqslant \frac{1}{1 + 4(m-1)^2/(\alpha+1)}, \qquad m \geqslant 2. \tag{3.5}$$

Since $n = 2m + s$, the last inequality is equivalent to

$$4m^2 - (2\alpha + 10)m + \alpha + 5 - s(\alpha+1) \geqslant 0,$$

and is satisfied if

$$m \geqslant \tfrac{1}{4}\{\alpha + 5 + \sqrt{(\alpha+1)(\alpha+5+4s)}\}, \qquad m \geqslant 2.$$

Since $m = (n - s)/2$, this proves (3.1).

It remains to consider the case $n - s$ odd, $n - s = 2m - 1$, $m \geqslant 2$. Nonexistence of (1.2) now results if (3.5) holds with $n = 2m + s - 1$, i.e., if

$$4m^2 - (2\alpha + 10)m + 2\alpha + 6 - s(\alpha + 1) \geqslant 0, \qquad m \geqslant 2,$$

or, in particular, if

$$m \geqslant \tfrac{1}{4}\{\alpha + 5 + \sqrt{(\alpha + 1)(\alpha + 1 + 4s)}\}, \qquad m \geqslant 2.$$

Since $m = (n - s + 1)/2$, this gives (3.2), and the proof of Theorem 3.1 is completed.

COROLLARY. *There is no sequence* $\{C_n\}$ *of Chebyshev-type formulas* (1.2), *corresponding to a sequence* S *of integers* $n = n_j$, $n_j \longrightarrow \infty$, *such that* C_n *has polynomial degree of accuracy* $p_n \geqslant \tau n^\gamma$, $\tau > 0$, $\frac{1}{2} < \gamma < 1$, *for each* $n \in S$.

Proof. Letting $p_n = n - s_n$, we have $s_n \leqslant n - \tau n^\gamma$, and (3.1), (3.2) are both satisfied for $s = s_n$ and n sufficiently large.

We remark that (3.1) and (3.2) in the case $\alpha = 0$ are sharp for $s = 0$ and $s = 1$, giving the correct bounds $n \geqslant 3$ and $n \geqslant 4$, respectively, but are not quite sharp for $s \geqslant 2$. If $s = 2$, the inequalities (3.1), (3.2) yield $n = 5$ or $n \geqslant 7$. In reality, $n \geqslant 5$, as can be seen from Bernstein's inequality by verifying $n^{-1} > \lambda_1^{(2)}$ for $n = 6$. For $s = 3$ we obtain $n \geqslant 8$, while in reality $n \geqslant 6$. The latter follows from Bernstein's inequality when $n = 6$, and from computations performed in [1] when $n = 7$.

4. Nonexistence of Chebyshev-Hermite Type Formulas. We call (1.3) a *symmetric* Chebyshev-type quadrature formula if the nodes $x_k^{(n)}$ are located symmetrically with respect to the origin. Symmetric formulas are trivially exact for odd functions. We can assume therefore that the polynomial degree of accuracy of a symmetric formula is odd.

THEOREM 4.1. *A symmetric Chebyshev-type quadrature formula* (1.3) *having polynomial degree of accuracy* $2[n/2] - 2s + 1$, $s \geqslant 0$, *does not exist if*

$$s = 0 \quad \textit{and} \quad n \geqslant 4, \quad s = 1 \quad \textit{and} \quad n \geqslant 8,$$

$$s > 1 \quad \textit{and} \quad n \geqslant \begin{cases} 2(s + 1 + \sqrt{s}), & n \text{ even}, \\ 2s + 3 + \sqrt{4s + 2}, & n \text{ odd}. \end{cases} \tag{4.1}$$

Proof. The normalized Hermite polynomials $\pi_0(x), \pi_1(x), \cdots$ can be expressed in terms of Laguerre polynomials by means of

$$\pi_n(x) = \left\{\frac{\Gamma(n/2 + 1)}{\Gamma((n + 1)/2)}\right\}^{1/2} L_{n/2}^{(-1/2)}(x^2), \qquad n \text{ even},$$

$$\pi_n(x) = \left\{\frac{\Gamma((n + 1)/2)}{\Gamma(n/2 + 1)}\right\}^{1/2} xL_{(n-1)/2}^{(1/2)}(x^2), \qquad n \text{ odd}. \tag{4.2}$$

The largest zero $\xi_1^{(m)}$ of π_m, by (3.4) and (4.2), thus satisfies

$$[\xi_1^{(m)}]^2 > m - 3/2 \quad \text{for} \quad m \geq 4, \tag{4.3}$$
$$[\xi_1^{(m)}]^2 = m - 3/2 \quad \text{for} \quad m = 2 \text{ and } 3.$$

Since

$$\pi_0 = \pi^{-1/4}, \qquad \pi_1(x) = 2^{1/2}\pi^{-1/4}x, \qquad \pi_2(x) = 2^{-1/2}\pi^{-1/4}(2x^2 - 1),$$

we obtain for the corresponding Christoffel number, using again (3.3),

$$\lambda_1^{(m)} \leq \frac{1}{\pi_0^2 + [\pi_1(\xi_1^{(m)})]^2 + [\pi_2(\xi_1^{(m)})]^2} = \frac{2\sqrt{\pi}}{2 + 4[\xi_1^{(m)}]^2 + (2[\xi_1^{(m)}]^2 - 1)^2},$$

and thus, from (4.3),

$$\lambda_1^{(m)} < \frac{\sqrt{\pi}}{2[m - 1 + (m-2)^2]}, \qquad m \geq 4,$$

$$\lambda_1^{(m)} = \frac{\sqrt{\pi}}{2[m - 1 + (m-2)^2]}, \qquad m = 2 \text{ and } 3.$$

We first consider the case when n is even, $n = 2\nu$. Since we are assuming polynomial degree of accuracy $2[n/2] - 2s + 1 = 2\nu - 2s + 1$, we have $m = \nu - s + 1$ in Bernstein's inequality (2.6). Nonexistence of (1.3) thus follows in either of the following two cases:

$$\frac{1}{2\nu} \geq \frac{1}{2[\nu - s + (\nu - s - 1)^2]} \quad \text{and} \quad \nu \geq s + 3,$$

$$\frac{1}{2\nu} > \frac{1}{2[\nu - s + (\nu - s - 1)^2]} \quad \text{and} \quad \nu = s + 1 \text{ or } s + 2.$$

The first case is equivalent to

$$\nu^2 - 2(s+1)\nu + s^2 + s + 1 \geq 0 \quad \text{and} \quad \nu \geq s + 3,$$

and is realized if

$$n \geq 2(s + 1 + \sqrt{s}), \qquad n(\text{even}) \geq 2s + 6. \tag{4.4}$$

The second case occurs if

$$n > 2(s + 1 + \sqrt{s}), \qquad n = 2s + 2 \text{ or } 2s + 4. \tag{4.5}$$

Now $n = 2s + 2$ in (4.5) implies $0 > 2\sqrt{s}$, which is impossible, while $n = 2s + 4$ implies $s = 0$, hence $n = 4$. Putting in turn $s = 0$ and $s = 1$ in (4.4) gives $n(\text{even}) \geq 6$ and $n(\text{even}) \geq 8$, respectively, while for $s \geq 2$ we get $n(\text{even}) \geq 2(s + 1 + \sqrt{s})$.

Since in all these cases a symmetric formula (1.3) does not exist, Theorem 4.1 is proved for all even $n \geqslant 4$.

Consider now the case of odd n, $n = 2\nu + 1$. The degree of accuracy still being $2\nu - 2s + 1$, we can again use $m = \nu - s + 1$ in Bernstein's inequality and infer nonexistence of (1.3) in either of the following two cases:

$$\frac{1}{2\nu + 1} \geqslant \frac{1}{2[\nu - s + (\nu - s - 1)^2]} \quad \text{and} \quad \nu \geqslant s + 3,$$

$$\frac{1}{2\nu + 1} > \frac{1}{2[\nu - s + (\nu - s - 1)^2]} \quad \text{and} \quad \nu = s + 1 \text{ or } s + 2.$$

As before one sees that these cases hold if

$$n \geqslant 2s + 3 + \sqrt{4s + 2}, \qquad n(\text{odd}) \geqslant 2s + 7$$

and

$$n > 2s + 3 + \sqrt{4s + 2}, \qquad n = 2s + 3 \text{ or } 2s + 5,$$

respectively. The latter is possible only if $s = 0$, giving $n = 5$. Putting $s = 0$ in the former gives $n(\text{odd}) \geqslant 7$, while for $s \geqslant 1$ we get $n(\text{odd}) \geqslant 2s + 3 + \sqrt{4s + 2}$. This proves Theorem 4.1 for all odd $n \geqslant 5$.

COROLLARY. *There is no sequence* $\{C_n\}$ *of symmetric Chebyshev-type formulas* (1.3), *corresponding to a sequence* S *of integers* $n = n_j$, $n_j \longrightarrow \infty$, *such that* C_n *has polynomial degree of accuracy* $p_n \geqslant \tau n^\gamma$, $\tau > 0$, $\frac{1}{2} < \gamma < 1$, *for each* $n \in S$.

We remark that Theorem 4.1 is sharp for $s = 0$, as follows from Krylov's result, and also for $s = 1$, 2 and 3, as can be seen from calculations performed in [1].

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18.3. [55] “Advances in Chebyshev Quadrature”

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Advances in Chebyshev Quadrature*

Walter Gautschi

1. Introduction

Let $d\mu(x)$ be a positive measure on the interval (a,b) admitting finite moments of all orders,

$$\mu_r = \int_a^b x^r d\mu(x) < \infty, \qquad r = 0,1,2,\ldots . \tag{1}$$

We consider quadrature rules of the type

$$\int_a^b f(x)d\mu(x) = \sum_{k=1}^{n} \gamma_k^{(n)} f(x_k^{(n)}) + R_n(f) \tag{2}$$

having equal weights

$$\gamma_1^{(n)} = \gamma_2^{(n)} = \cdots = \gamma_n^{(n)} . \tag{3}$$

Equally-weighted quadrature sums have the property of minimizing the effect of random errors in the function values $f(x_k^{(n)})$, which may be a useful feature if these errors are considerably larger than the truncation error $|R_n(f)|$. Another, though minor, advantage of equal coefficients results from the fact that only one multiplication is required, as opposed to n, to evaluate the quadrature sum in (2) (not counting the work in evaluating f).

To be widely useful, quadrature rules of the type (2), (3) should have real distinct nodes $x_k^{(n)}$, preferably all located in (a,b). In addition, they should be reasonably accurate. We say that (2), (3) is a Chebyshev quadrature rule, if all nodes are real and if the formula has algebraic degree of exactness n, i.e.,

$$R_n(f) = 0, \quad \text{all } f \in \mathbb{P}_n . \tag{4}$$

($\mathbb{P}_n$ denotes the class of polynomials of degree $\leq n$.) Letting $f \equiv 1$ in (2) then gives immediately

$$\gamma_k^{(n)} = \frac{\mu_0}{n}, \qquad k = 1,2,\ldots,n . \tag{5}$$

We call (2), (5) a Chebyshev quadrature rule in the strict sense, if (4) holds and the nodes $x_k^{(n)}$ are not only real, but pairwise distinct and all contained in (a,b).

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Any quadrature rule (2), (3), on the other hand, with only real nodes, will be referred to as a Chebyshev-type quadrature formula. Such a quadrature rule, therefore, need not have algebraic degree of exactness n, in fact, need not even integrate constants exactly, and is permitted to have repeated nodes, i.e., $x_k^{(n)} = x_l^{(n)}$ for some $k \neq l$.

The monic polynomial of degree n whose zeros are $x_k^{(n)}$, $k = 1,2,\ldots,n$, will be denoted, throughout, by $p_n(x; d\mu)$,

$$p_n(x; d\mu) = \prod_{k=1}^{n} (x - x_k^{(n)}) = x^n + a_1 x^{n-1} + \cdots + a_n . \tag{6}$$

Requirements (4) and (5) uniquely determine the polynomial $p_n(x; d\mu)$ (cf. §3.2). We may say, therefore, alternatively, that (2), (3) constitutes a Chebyshev quadrature rule if and only if the polynomial $p_n(x; d\mu)$ has only real zeros. We shall have occasion to consider also the polynomials which are orthogonal with respect to the measure $d\mu(x)$; these will be denoted by $\pi_n(x; d\mu)$, $n = 0,1,2,\ldots$.

The study of Chebyshev quadratures began in 1874 with a classical memoir of Chebyshev (Chebyshev [1874]). Important progress has subsequently been made by Bernstein [1937], [1938], Ullman [1966], Geronimus [1946], [1969], and others. Apart from a brief review in Wilf [1967], and traditional treatments in textbooks, no comprehensive account seems to be available. In the following we attempt to review recent advances in this field, covering roughly the period 1945-1975.

2. The classical Chebyshev quadrature formula

2.1 Bernstein's result. The quadrature formula §1(2), (4), (5), in which $d\mu(x) = dx$ on $[-1,1]$, will be referred to as the classical Chebyshev quadrature formula. It was computed by Chebyshev for $n = 2,3,\ldots,7$ and found, in these cases, to have only real nodes, all contained in $[-1,1]$. Radau [1880b] adds to this the case $n=9$, which also yields real nodes, but notes that the formula with $n=8$ involves complex nodes. It took some fifty years after that, until Bernstein, by extremely ingenious arguments, succeeded in proving that the formulas found by Chebyshev and Radau are in fact the only ones which have all nodes real. If $n > 9$, and $n=8$, the polynomial $p_n(x; d\mu)$ necessarily has complex zeros. A simplified version of Bernstein's proof is given by Krylov [1957] (and is also reproduced in Krylov [1962, p.192ff]). Kahaner [1969] interprets the presence of complex nodes as the result of a conflict between the equal coefficients requirement and the polynomial exactness requirement, the former tending to impose a uniform distribution on the real zeros, the latter a non-uniform distribution (as the zeros of orthogonal polynomials), when $n \to \infty$.

There is a fair amount of numerical information available on classical

Chebyshev quadrature. Salzer [1947] exhibits the polynomials $p_n(x; d\mu)$ in exact rational form for $n = 1(1)12$, and also gives the zeros to 10 decimal places for $n = 2(1)7$ and $n = 9$. (The latter are reprinted in Abramowitz and Stegun [1964, p.920].) On the microfiche addendum to Kahaner [1971] the zeros of $p_n(x; d\mu)$, including the complex ones, are tabulated to 14 decimals for $2 \leq n \leq 47$.

2.2 Geometry of the zeros of $p_n(x; d\mu)$. The distribution of the zeros of $p_n(x; d\mu)$ in the complex plane, when $d\mu(x) = dx$ on $[-1,1]$, is studied in detail by Kuzmin [1938]. It turns out that for large n, all zeros (except the zero at the origin, when n is odd) accumulate near the curve

$$(1) \qquad \omega(z) = \omega(1), \qquad \omega(z) = \int_{-1}^{1} \ln|z-t|\,dt,$$

familiar from potential theory. (This is an eye-shaped curve, centred at the origin, which intersects the real axis at ± 1, and the imaginary axis at about $\pm .52$.) More precisely, Kuzmin shows that for n sufficiently large and $h = \sqrt{\ln n/n}$, all zeros of $p_n(z; d\mu)$ (with the exception noted) are either located inside the circles about ± 1, with radii $3h$, or in the narrow band bounded by the curves $\omega(z) = \omega(1)$ and $\omega(z) = \omega(1-12h)$. The zeros thus approach the logarithmic potential curve (1) from the inside. The case $n = 20$ is depicted in Kahaner [1971]. Kuzmin also proves that the number of real zeros of $p_n(z; d\mu)$ is $O(\ln n)$ as $n \to \infty$. Additional properties of the zeros can be found in Mayot [1950] and Kahaner [1971].

3. Mathematical techniques

A number of analytic tools have been developed to deal with the construction of Chebyshev quadratures, or with proofs of nonexistence. We briefly review four of them, and illustrate some by examples.

3.1 Chebyshev's method. This is the method used by Chebyshev in his original memoir (Chebyshev [1874]). The polynomial $p_n(z; d\mu)$ is represented explicitly in the form

$$(1) \qquad p_n(z; d\mu) = E\{\exp(\frac{n}{\mu_0} \int_a^b \ln(z-x)d\mu(x))\}$$

$$= E\{z^n \exp(-\frac{n}{\mu_0} \sum_{k=1}^{\infty} \frac{\mu_k}{kz^k})\},$$

where $E\{\cdot\}$ denotes the polynomial part of $\{\ \}$. Based on this formula, Chebyshev computes his original quadrature rules (with $d\mu(x) = dx$) for $n = 2,3,\ldots,7$.

In the case of $d\mu(x) = (1-x^2)^{-\frac{1}{2}}$ on $[-1,1]$, formula (1) gives

$$p_n(z;\, d\mu) = E\{(\frac{z + \sqrt{z^2-1}}{2})^n\}$$

$$= E\{(\frac{z + \sqrt{z^2-1}}{2})^n + (\frac{z - \sqrt{z^2-1}}{2})^n\} = \frac{1}{2^{n-1}} T_n(z) ,$$

where $T_n(z)$ is (what is now called) the Chebyshev polynomial of the first kind. In this way, Chebyshev recovers the classical Gauss-type quadrature rule

$$(2) \qquad \int_{-1}^{1} f(x)(1-x^2)^{-\frac{1}{2}}dx = \frac{\pi}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f), \qquad x_k^{(n)} = \cos(\frac{2k-1}{2n}\pi) ,$$

which he ascribes to Hermite.

An interesting recent extension of (2) is due to Ullman [1966a,b], who considers

$$(3) \qquad d\mu(x) = (1-x^2)^{-\frac{1}{2}}(1+ax)(1+a^2+2ax)^{-1} \quad \text{on} \quad [-1,1], \qquad -1 < a < 1 ,$$

and finds that

$$z \exp(-\frac{1}{\mu_0} \sum_{k=1}^{\infty} \frac{\mu_k}{kz^k}) = \tfrac{1}{2}(z + \sqrt{z^2-1} + a), \qquad |z| > 1 .$$

Application of (1) thus gives

$$p_n(z;\, d\mu) = E\{(\frac{z + \sqrt{z^2-1} + a}{2})^n\}$$

$$= E\{(\frac{z + \sqrt{z^2-1} + a}{2})^n + (\frac{z - \sqrt{z^2-1} + a}{2})^n - (\frac{a}{2})^n\}$$

$$= \frac{1}{2^{n-1}} T_n^{(a)}(z) ,$$

where $T_n^{(a)}(z)$ is a polynomial of degree n generalizing the Chebyshev polynomial $T_n(z) = T_n^{(0)}(z)$. Ullman shows that $T_n^{(a)}(z)$, for each n, has only real zeros, whenever $-\frac{1}{2} < a < \frac{1}{2}$, thus exhibiting his celebrated example of a weight function, other than the classical one in (2), which admits Chebyshev quadrature for each n. Work along this line is continued by Geronimus [1969] (cf. §5.1).

3.2 Method based on Newton's identity. If the quadrature formula

$$(4) \qquad \int_a^b f(x)d\mu(x) = \frac{\mu_0}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f)$$

is to have algebraic degree of exactness n, then the nodes $x_k = x_k^{(n)}$ must satisfy

$$\sum_{k=1}^{n} x_k^r = \frac{n}{\mu_0}\mu_r , \qquad r = 1,2,\ldots,n .$$

Since the moments μ_r are known, these equations determine the first n power sums $s_r = \sum_{k=1}^{n} x_k^r$ of the nodes,

$$s_r = \frac{n}{\mu_0}\mu_r , \qquad r = 1,2,\ldots,n . \tag{5}$$

These in turn determine the coefficients a_k in the polynomial $p_n(x; d\mu)$ by virtue of Newton's identities,

$$\begin{cases} s_1 + a_1 = 0 , \\ s_2 + a_1 s_1 + 2a_2 = 0 , \\ \cdots\cdots\cdots\cdots \\ s_n + a_1 s_{n-1} + \cdots + a_{n-1} s_1 + n a_n = 0 . \end{cases} \tag{6}$$

The desired nodes x_k in (4) can thus be computed by finding the roots of the algebraic equation $x^n + a_1 x^{n-1} + \cdots + a_n = 0$, where the coefficients a_k are obtained recursively from (6), the s_r being given by (5). This method, first used by Radau [1880a,b], is the one generally applied to compute Chebyshev quadratures. It is extended in Gautschi and Yanagiwara [1974] and Anderson and Gautschi [to appear] to deal with Chebyshev-type quadratures involving repeated nodes.

3.3 Bernstein's method. This is a powerful method for proving nonexistence results. Although Bernstein [1937] deals only with the case of a constant weight function, his method extends immediately to arbitrary measures $d\mu(x)$.

Bernstein's idea is to confront Chebyshev's n-point quadrature formula

$$\int_a^b f(x)d\mu(x) = \frac{\mu_0}{n}\sum_{k=1}^{n} f(x_k^{(n)}) + R_n^{Ch}(f) \tag{7}$$

with the m-point Gauss formula

$$\int_a^b f(x)d\mu(x) = \sum_{r=1}^{m} \lambda_r^{(m)} f(\xi_r^{(m)}) + R_m^{G}(f) , \tag{8}$$

where $\xi_r^{(m)}$ are the zeros of $\pi_m(x; d\mu)$, assumed in decreasing order,

$$a < \xi_m^{(m)} < \xi_{m-1}^{(m)} < \cdots < \xi_1^{(m)} < b ,$$

and $\lambda_r^{(m)}$ are the corresponding Christoffel numbers. Assuming distinct nodes $x_k^{(n)}$

in (7), all contained in (a,b), and assuming that (7) has polynomial degree of exactness $2m-1$, $m < n$, then Bernstein shows that, necessarily,

$$\frac{\mu_0}{n} \leq \min(\lambda_1^{(m)}, \lambda_m^{(m)}) \ . \tag{9}$$

This inequality remains valid under the weaker assumption of mere reality of the nodes $x_k^{(n)}$ (Gautschi [1975]).

The road from Bernstein's inequality (9) to nonexistence results is still fraught with considerable technical difficulties, particularly in the case of finite intervals. For measures on infinite intervals, the method appears to apply more easily, as we illustrate with the example of the Laguerre measure, $d\mu(x) = x^\alpha e^{-x}dx$. Here, (4) takes the form

$$\int_0^\infty f(x)x^\alpha e^{-x}dx = \frac{\Gamma(\alpha+1)}{n}\sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f), \qquad \alpha > -1 \ . \tag{10}$$

The orthonormal polynomials are the normalised Laguerre polynomials,

$$\pi_0(x) = [\Gamma(\alpha+1)]^{-\frac{1}{2}} \ , \quad \pi_1(x) = [\Gamma(\alpha+2)]^{-\frac{1}{2}}(\alpha+1-x), \ldots, \tag{11}$$

and

$$\lambda_1^{(m)} = \Big(\sum_{k=0}^{m-1} [\pi_k(\xi_1^{(m)})]^2\Big)^{-1} \leq (\pi_0^2 + [\pi_1(\xi_1^{(m)})]^2)^{-1} \ , \qquad m \geq 2 \ .$$

Using the known inequality (Krylov [1958])

$$\xi_1^{(m)} > 2m + \alpha - 1 \qquad (m \geq 2, \ \alpha > -1) \ ,$$

and the explicit expressions in (11), we can further estimate

$$\lambda_1^{(m)} < \frac{\Gamma(\alpha+1)}{1 + 4(m-1)^2/(\alpha+1)} \ , \qquad m \geq 2 \ . \tag{12}$$

Now suppose n is even, $n = 2m$ $(m \geq 2)$, and the quadrature rule (10) has degree of exactness n. Then, a fortiori, it has degree of exactness $2m-1$, and hence by Bernstein's inequality,

$$\frac{\Gamma(\alpha+1)}{n} \leq \lambda_1^{(m)} \ . \tag{13}$$

If (13) is violated, then Chebyshev quadrature in (10) is impossible. By virtue of (12), this will be the case if

$$\frac{1}{n} \geq \frac{1}{1 + 4(m-1)^2/(\alpha+1)} \ , \qquad m \geq 2 \ .$$

Since $n = 2m$, the last inequality amounts to $n^2 - (\alpha+5)n + \alpha + 5 \geq 0$, $n \geq 4$, that

is, to

$$n \geq \tfrac{1}{2}\{\alpha + 5 + \sqrt{(\alpha+1)(\alpha+5)}\} \quad \text{and} \quad n \geq 4 \,. \tag{14}$$

For all even values of n satisfying (14), therefore, the Chebyshev formula (10) does not exist. A similar argument applies for n odd, and also for Chebyshev-type quadratures (10) of given degree of exactness $< n$ (Gautschi [1975]).

3.4 Methods based on moment sequences. We already observed in (5) that for (4) to be a Chebyshev quadrature formula, it is necessary and sufficient that the nodes be real and

$$s_r = \frac{n}{\mu_0}\,\mu_r \quad , \quad r = 1,2,\ldots,n,$$

where $s_r = \sum_{k=0}^{n} x_k^r$ are the power sums in the nodes $x_k = x_k^{(n)}$. Any general property valid for power sums s_r in real variables thus immediately translates into a property for the moments μ_r, $r = 1,2,\ldots,n$, which in turn represents a necessary condition for (4) to be a Chebyshev quadrature rule. Violation of this property implies nonexistence of (4).

One such property, used by Wilf [1961], is Jensen's inequality, which states that for nonnegative numbers, $\xi_k \geq 0$, the quantities $\sigma_r = (\sum_{k=1}^{n} \xi_k^r)^{1/r}$ are nonincreasing in r for $r > 0$, i.e., $\sigma_r \geq \sigma_s$ whenever $0 < r < s$ (Hardy, Littlewood and Pólya [1952, p.28]). Consequently, if all $x_k \geq 0$, then

$$\tau_r = (\frac{n}{\mu_0}\,\mu_r)^{\frac{1}{r}} \text{ is nonincreasing for } r = 1,2,\ldots,n, \tag{15}$$

and if all x_k are arbitrary real,

$$\tau_r^* = (\frac{n}{\mu_0}\,\mu_{2r})^{\frac{1}{r}} \text{ is nonincreasing for } r = 1,2,\ldots,[\tfrac{n}{2}] \,. \tag{15*}$$

Tureckiĭ [1962] and, subsequently, Janovič [1971] and Nutfullin and Janovič [1972] use the more obvious inequalities

$$\begin{aligned} s_n &\leq s_{n-2r}s_{2r} \qquad (n \text{ even}; \quad r = 1,2,\ldots,\tfrac{n}{2}), \\ s_{n-1} &\leq s_{n-1-2r}s_{2r} \quad (n \text{ odd}\ ; \quad r = 1,2,\ldots,\tfrac{n-1}{2}) \,, \end{aligned}$$

valid for arbitrary real x_k, to obtain the necessary conditions

$$\begin{cases} \dfrac{\mu_n}{n\mu_{n-2r}} \leq \dfrac{\mu_{2r}}{\mu_0} & (n \text{ even}; \ r = 1,2,\ldots,\tfrac{n}{2}) \,, \\[2ex] \dfrac{\mu_{n-1}}{n\mu_{n-1-2r}} \leq \dfrac{\mu_{2r}}{\mu_0} & (n \text{ odd}\ ; \ r = 1,2,\ldots,\tfrac{n-1}{2}) \,. \end{cases} \tag{16}$$

To illustrate (15), consider again the Laguerre weight $x^{\alpha} e^{-x}$, $\alpha > -1$, for which $\mu_r = \Gamma(\alpha+r+1)$, $r = 0,1,2,\ldots$. Requiring nonnegative nodes x_k, we can apply (15), i.e., $\tau_{r-1} \geqslant \tau_r$ for $2 \leqslant r \leqslant n$, which, for $r = n$, gives

$$\left(\frac{n}{\mu_0}\,\mu_{n-1}\right)^{\frac{1}{n-1}} \geqslant \left(\frac{n}{\mu_0}\,\mu_n\right)^{\frac{1}{n}},$$

or, equivalently,

$$\frac{n}{\Gamma(\alpha+1)}\,\frac{\Gamma(\alpha+n+1)}{(\alpha+n)^n} \geqslant 1 . \tag{17}$$

Since the left-hand side is asymptotically equal to $\sqrt{2\pi}e^{-\alpha}\,[\Gamma(\alpha+1)]^{-1}n^{\alpha+3/2}e^{-n}$ as $n \to \infty$, it is clear that (17) will be false for all n sufficiently large, hence Chebyshev quadrature (in the strict sense) not possible.

Similarly, putting $r = 1$ in the first of (16), we find the necessary condition (Tureckiĭ [1962])

$$n^2 - (\alpha^2+\alpha+3)n + \alpha(\alpha-1) \leqslant 0 , \qquad n(\text{even}) \geqslant 4 ,$$

which leads to a nonexistence result similar to, but not as sharp as, the one obtained in (14) by Bernstein's method.

4. Chebyshev quadrature and Gaussian quadrature

We noted before in §3(2) that the Gauss quadrature formula for $d\mu(x) = (1-x^2)^{-\frac{1}{2}}dx$ on $[-1,1]$ is also a Chebyshev formula. One naturally wonders whether there are other Gauss-type quadrature formulas whose coefficients are all equal. The question was settled negatively at a surprisingly early stage (Posse [1875], Sonin [1887], Krawtchouk [1935], Bailey [1936]). An elegant proof of a rather more far-reaching result is due to Geronimus [1944], [1946] (and also reproduced in Krylov [1962, p.183ff] and Natanson [1965, p.150 ff]).

Let $d\mu(x)$ be a measure which admits a set of orthogonal polynomials, $\{\pi_n(x; d\mu)\}_{n=0}^{\infty}$. Positivity of the measure neednot be assumed. Let $\{\xi_k^{(n)}\}_{k=1}^{n}$ be the zeros of $\pi_n(x; d\mu)$, and consider

$$\int_a^b f(x)d\mu(x) = \frac{\mu_0}{n} \sum_{k=1}^{n} f(\xi_k^{(n)}) + R_n(f) . \tag{1}$$

Then Geronimus proves the following: If for each $n = 1,2,3,\ldots$ we have $R_n(f) = 0$ whenever $f(x) = x$ and $f(x) = x^2$ (if $n > 1$), then $d\mu$ is the Chebyshev measure $d\mu(x) = (1-x^2)^{-\frac{1}{2}}dx$, except for a linear transformation.

The proof can be sketched in a few lines. Introducing the power means in the nodes $\xi_k^{(n)}$,

$$m_r^{(n)} = \left(\frac{1}{n}\sum_{k=1}^{n}[\xi_k^{(n)}]^r\right)^{\frac{1}{r}},$$

the hypothesis implies

$$m_1^{(n)} = \frac{\mu_1}{\mu_0} = m_1, \quad m_2^{(n)} = \left(\frac{\mu_2}{\mu_0}\right)^{\frac{1}{2}} = m_2,$$

that is, $m_1^{(n)}$ and $m_2^{(n)}$ are <u>independent of</u> n. Assuming the polynomials $\pi_n(x) = \pi_n(x; d\mu)$ normalised to have leading coefficients 1, we have on the one hand, by Newton's identities, that

$$\pi_n(x) = x^n - nm_1x^{n-1} + \frac{n}{2}(nm_1^2 - m_2^2)x^{n-2} - \dots, \tag{2}$$

and on the other, that

$$\begin{cases} \pi_n(x) = (x-\alpha_n)\pi_{n-1}(x) - \beta_n\pi_{n-2}(x), & n = 1,2,3,\dots, \\ \pi_{-1} = 0, \quad \pi_0 = 1 \end{cases} \tag{3}$$

for some constants α_n, β_n. Inserting (2) into (3), and comparing coefficients of x^{n-1} and x^{n-2} on either side, gives

$$\alpha_n = \alpha, \qquad n = 1,2,3,\dots,$$

$$\beta_n = \beta, \qquad n = 3,4,5,\dots, \quad \beta_2 = 2\beta,$$

where

$$\alpha = m_1, \quad \beta \equiv \tfrac{1}{2}(m_2^2 - m_1^2).$$

It then follows from (3) that

$$\pi_n(x) = \left(\frac{x-\alpha+\sqrt{(x-\alpha)^2-4\beta}}{2}\right)^n + \left(\frac{x-\alpha-\sqrt{(x-\alpha)^2-4\beta}}{2}\right)^n,$$

which is essentially the Chebyshev polynomial of the first kind, $T_n(x) = \frac{1}{2}\{(x+\sqrt{x^2-1})^n + (x-\sqrt{x^2-1})^n\}$, except for a linear transformation in the independent variable and a numerical factor (cf. Rivlin [1974, p.5]).

If the measure $d\mu$ is positive, then all $\xi_k^{(n)}$ are real and $|m_1| < m_2$ by the well-known monotonicity of the power mean $m_r^{(n)}$ as a function of r. It then follows that $\beta > 0$.

5. Existence and nonexistence results

Given a positive measure $d\mu(x)$ on (a,b), we say that Chebyshev quadrature is possible for n [in the strict sense] if there exist n real numbers $x_k^{(n)}$ [pairwise distinct in (a,b)] such that

(1) $$\int_a^b f(x)d\mu(x) = \frac{\mu_0}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f)$$

has algebraic degree of exactness n. The finite or infinite sequence $\{n_j\}$ of all those integers $n_j \geq 1$ for which Chebyshev quadrature is possible will be called the T-sequence of $d\mu(x)$. It will be denoted by $T(d\mu)$, or simply by T. We say that the measure $d\mu(x)$ has property T if its T-sequence consists of all natural numbers, property T^∞, if its T-sequence is infinite, and property T^0, if it is finite. In this terminology, Bernstein's result may be rephrased by saying that the uniform measure $d\mu(x) = dx$ on $[-1,1]$ has the T-sequence $T = \{1,2,3,4,5,6,7,9\}$, hence property T^0. The Chebyshev measure $d\mu(x) = (1-x^2)^{-\frac{1}{2}}dx$, on the other hand, has property T.

Bernstein's method, as well as the methods based on moment sequences (cf. §3.3, 3.4) yield necessary conditions for $d\mu(x)$ to have property T^∞, hence, by default, also proofs for property T^0.

5.1 Measures with property T or T^∞. Measures $d\mu(x)$ with property T are rare; in fact, they occur with probability zero, if viewed as moment sequences in appropriate moment spaces (Salkauskas [1975]). Up until Ullman's discovery (cf. §3.1), Chebyshev's measure indeed was the only known measure with property T. Geronimus [1969] continues Ullman's work by first establishing an interesting sufficient condition for Chebyshev quadrature to be possible for n. To describe it, let $d\mu(x) = \omega(x)dx$ on $[-1,1]$, and assume

$$\omega(\cos\theta) = \frac{1}{\pi \sin\theta} \sum_{k=0}^{\infty} a_k \cos k\theta\,, \qquad 0 \leq \theta \leq \pi\,, \qquad a_0 = 1\,.$$

Define the constants $\{A_m^{(n)}\}_{m=0}^{\infty}$ by

$$\exp(-n \sum_{k=1}^{\infty} \frac{a_k}{k z^k}) = \sum_{m=0}^{\infty} \frac{A_m^{(n)}}{z^m}\,, \qquad A_0^{(m)} = 1\,, \qquad |z| > 1\,.$$

Then Chebyshev quadrature is possible for n if the polynomial $\sum_{m=0}^{n-1} A_m^{(n)} z^m + \frac{1}{2}A_n^{(n)} z^n$ has all its zeros in $|z| > 1$. In this case, moreover,

$$2^{n-1} p_n(x;d\mu) = \sum_{m=0}^{n-1} A_m^{(n)} \cos(n-m)\theta + \tfrac{1}{2}A_n^{(n)}\,, \qquad x = \cos\theta\,.$$

Ullman's measure with property T falls out as a simple example, by taking

$a_k = (-a)^k$. Geronimus also gives several examples of even weight functions $\omega(x)$ admitting Chebyshev quadratures for all even integers $n = 2\nu$. (These automatically have degree of exactness $2\nu + 1$.)

A measure $d\mu(x)$ on $(-\infty,\infty)$ with infinite support (i.e., with positive mass outside of every finite interval) cannot have property T^∞ unless its T-sequence contains very large gaps. For example, if $\{2\nu_j\}$ is the even subsequence of $T(d\mu)$, and m any fixed integer, then one has $\nu_j > \nu_{j-1}^m$ for infinitely many j (Wilf [1961]). Similarly for the odd subsequence. It follows, in particular, that a measure with property T necessarily has finite support. Wilf in fact conjectures that property T^∞ already implies finite support. This, however, is disproved by Ullman [1962], [1963], who in turn poses the question (still open) of formulating criteria in terms of the gaps of an infinite T-sequence, which would allow to discriminate between measures with infinite, and measures with finite, support.

Kahaner and Ullman [1971] establish conditions on the measure $d\mu(x)$ on $(-\infty,\infty)$ which either imply the absence of property T, or property T^0. The conditions involve the limit behaviour (as $n \to \infty$) of certain discrete measures concentrated at the zeros of the orthogonal polynomials $\pi_n(x;d\mu)$.

5.2 Chebyshev quadrature on finite intervals. Soon after Bernstein obtained his classical result, Akhiezer [1937], in a little-known paper, proved that the Jacobi measure $d\mu(x) = (1-x)^\alpha(1+x)^\beta dx$ on $[-1,1]$ has property T^0 whenever $-\frac{1}{2} \leq \alpha \leq \frac{1}{2}$, $-\frac{1}{2} \leq \beta \leq \frac{1}{2}$ (excepting $\alpha = \beta = -\frac{1}{2}$). More recently, using Bernstein's method, Gatteschi [1963/64] proves property T^0 for all $\alpha = \beta > -\frac{1}{2}$, while Ossicini [1966] extends it to $\alpha > -\frac{1}{2}$, $\beta > -1$, hence, by symmetry, also to $\alpha > -1$, $\beta > -\frac{1}{2}$. In the remaining square $-1 < \alpha \leq -\frac{1}{2}$, $-1 < \beta \leq -\frac{1}{2}$ (with $\alpha = \beta = -\frac{1}{2}$ deleted), the matter appears to be still unsettled.

Greenwood and Danford [1949] consider the integral $\int_0^1 xf(x)dx$ (which amounts to Jacobi's case $\alpha = 0$, $\beta = 1$) and find by computation that Chebyshev quadrature is possible (in the strict sense) if $n = 1,2,3$, but not if $4 \leq n \leq 10$. A similar result is stated in Greenwood, Carnahan and Nolly [1959] for the integral $\int_{-1}^1 x^2 f(x)dx$ (which can be reduced to the case $\alpha = 0$, $\beta = \frac{1}{2}$). The exact T-sequence has not been established in either case.

5.3 Chebyshev quadrature on infinite intervals. Computational results of Salzer [1955] suggested that the T-sequence for the Laguerre measure $d\mu(x) = e^{-x}dx$ on $(0,\infty)$, as well as the one for the Hermite measure $d\mu(x) = e^{-x^2}$ on $(-\infty,\infty)$, must be rather short, in fact $T = \{1,2\}$ in the former, and $T = \{1,2,3\}$ in the latter case. This was first proved by Krylov [1958], by an application of Bernstein's method, and again later, independently, by Gatteschi [1964/65]. Burgoyne [1963],

unaware of Krylov's result, confirms it up to $n = 50$ by computing the maximum number of nonnegative, resp. real, nodes. For more general Laguerre measures $d\mu(x) = x^{\alpha}e^{-x}$, $\alpha > -1$, property T^{o} is proved by Wilf [1961], Tureckiĭ [1962] and Gautschi [1975], using methods already illustrated in §3.3, 3.4.

Nutfullin and Janovič [1972], using the method of Tureckiĭ, prove property T^{o} for the measures

$$d\mu(x) = (x^{2p+1}/\sinh \pi x)dx , \quad p = 0,1,2,\ldots,$$

$$d\mu(x) = (x^{2p}/\cosh \pi x)dx , \quad p = 0,1,2,\ldots,$$

and

$$d\mu(x) = |x|^{\alpha}e^{-x^2}dx , \quad \alpha > -1 ,$$

all on $(-\infty,\infty)$, and for each give an upper bound for $\max_{n_j \in T(d\mu)} n_j$. They also determine the T-sequence for some of these measures. For example, the first, when $p = 0$, has $T = \{1,2,3\}$, while the last has $T = \{1,2,3\}$ for $-1 < \alpha < 1/3$, $T = \{1,2,3,5\}$ for $1/3 \leq \alpha < 1$, $T = \{1,2,3,4,5\}$ for $1 \leq \alpha \leq 7$, $T = \{1,2,3,4\}$ for $7 < \alpha < 15$. For $\alpha \geq 15$, Chebyshev quadrature is possible when $n = 1,2,3,4,6$ but the exact T-sequence is not known.

Janovič [1971] previously used Tureckiĭ's method to show that a certain measure $d\mu(x)$ on $(0,\infty)$, of interest in the theory of Wiener integrals, has $T = \{1,2\}$.

5.4 Chebyshev-type quadrature. If a measure $d\mu(x)$ has property T^{o}, and $p_n = p_n(d\mu)$ is the maximum degree of exactness of (1), subject to the reality of all nodes, it becomes of interest to determine upper bounds for p_n as $n \to \infty$. In the classical case $d\mu(x) = dx$, Bernstein [1937] already showed that $p_n < 4\sqrt{n}$. For Jacobi measures $d\mu(x) = (1-x)^{\alpha}(1+x)^{\beta}dx$, Costabile [1974] establishes $p_n < c(\alpha,\beta)n^{1/(2\alpha+2)}$, as has previously been found by Meir and Sharma [1967] in the ultraspherical case $\alpha = \beta > -\frac{1}{2}$. In this latter case, Costabile further expresses the constant c explicitly in terms of gamma and Bessel functions. For more general weight functions on $[-1,1]$, having branch point and other singularities at the endpoints, the problem is studied extensively by Geronimus [1969], [1970]. For the Laguerre measure $d\mu(x) = x^{\alpha}e^{-x}dx$, $\alpha > -1$, one finds by Bernstein's method that $p_n < 2 + \sqrt{(\alpha+1)(n-1)}$ if $p_n \geq 3$. Similar bounds hold for symmetric Hermite quadrature rules (Gautschi [1975]; see also Tureckiĭ [1962]).

Chebyshev-type quadratures having degree of exactness 1 always exist. The most familiar example is the composite midpoint rule on $[-1,1]$, with $d\mu(x) = dx$. Another example is the nontrivial extension of the midpoint rule to integrals with arbitrary positive measure, due to Stetter [1968b], which improves upon an earlier extension of Jagerman [1966].

6. Optimal Chebyshev-type quadrature formulas

Only relatively recently have attempts been made to develop Chebyshev-type quadrature formulas in cases where true Chebyshev formulas do not exist. The approach generally consists in replacing the algebraic exactness condition by some optimality condition, unconstrained or constrained. This yields new formulas even in cases where ordinary ones exist.

6.1 Optimal formulas in the sense of Sard. For the classical weight $d\mu(x) = dx$ on $[-1,1]$, consider a Chebyshev-type quadrature formula

$$\int_{-1}^{1} f(x)dx = \frac{2}{n}\sum_{k=1}^{n} f(x_k) + R_n(f) \,. \tag{1}$$

We require that (1) has polynomial degree of exactness $p < n$,

$$R_n(f) = 0 \,, \quad \text{all } f \in \mathbb{P}_p \,, \tag{2}$$

and assume $f \in AC^p[-1,1]$. The remainder $R_n(f)$, as is well known (see, e.g., Sard [1963, p.25]), can then be represented in the form

$$R_n(f) = \int_{-1}^{1} K_p(t) f^{(p+1)}(t)dt \,,$$

where $K_p(t) = K_p(t; x_1,x_2,\ldots,x_n)$ is the Peano kernel of R_n [cf. §7(3)]. By the Schwarz inequality, therefore,

$$|R_n(f)| \leq \gamma_p \|f^{(p+1)}\|_{L_2} \,, \qquad \gamma_p = \|K_p\|_{L_2} \,, \tag{3}$$

where $\|u\|_{L_2} = \left(\int_{-1}^{1} [u(t)]^2 dt\right)^{\frac{1}{2}}$. An optimal Chebyshev-type formula in the sense of Sard is a formula (1), satisfying (2), which minimizes γ_p as a function of $x_1,x_2,\ldots,x_n$. Franke [1971] studies such formulas in the cases $p = 0$ and $p = 1$, under the additional assumption of symmetry,

$$x_{n+1-k} + x_k = 0 \,, \quad k = 1,2,\ldots,n. \tag{4}$$

The condition (2) is then automatically satisfied, so that the problem reduces to an unconstrained optimization problem. The solution for $p = 0$, as has been noted previously (Krylov [1962, pp.138-140]), is the composite midpoint rule, for which $\gamma_0 = 2/3n^2$. In the case $p = 1$, numerical answers are given for $2 \leq n \leq 11$. A similar problem, without the symmetry assumption (4), is considered in Coman [1970].

6.2 Least squares criteria. Instead of minimizing γ_p in (3), we may wish to minimize the errors of (1) which result if the formula is applied to successive

monomials. More precisely, given an integer p, with $0 \leq p < n$, and an integer q, with $q \geq n$, or $q = \infty$, we determine the nodes x_k in (1) such that

$$\sum_{j=p+1}^{q} [R_n(x^j)]^2 = \min , \tag{5}$$

subject to

$$R_n(x^j) = 0 , \quad j = 1,2,\ldots,p . \tag{6}$$

Symmetry, as in (4), may or may not be imposed.

If $n \leq 7$, or $n = 9$, and $q = n$, Problem (5), (6) is trivially solved by the classical Chebyshev formulas, which drive the objective function in (5) to zero. In the case $p = 0$, and for various choices of q, including $q = \infty$, numerical answers are given by Barnhill, Dennis and Nielson [1969] for $n = 8,10,11$. Kahaner [1970] has analogous results for $q = n$ and $p = n - 1$ or $n - 2$. An interesting (although somewhat counterproductive) feature of this work is the apparent necessity of assuming repeated nodes for the minimization procedures to converge. It is shown in Gautschi and Yanagiwara [1974] that repeated nodes are indeed unavoidable, if $q = n$, whenever the constraints in (6) admit real solutions. The same is proved in Salkauskas [1973] for the case $p = 0$, all nodes being constrained to the interval $[-1,1]$. We conjecture that the same situation prevails for arbitrary $q > n$.

There is computational evidence that the optimal formulas are indeed symmetric, but the question remains open. If we knew that Problem (5), (6) had a unique solution, modulo permutations, symmetry would follow (Gautschi and Yanagiwara [1974]).

6.3 Minimum norm quadratures. A quadrature rule, such as (1), which minimizes the norm of the error functional $R_n(f)$ in some appropriate function space is called a minimum norm quadrature formula. For Chebyshev quadratures, such formulas are studied by Rabinowitz and Richter [1970]. They consider two families of Hilbert spaces. Each space consists of functions which are analytic in an ellipse $\mathcal{E}_\rho$, $\rho > 1$, having foci at ± 1 and semiaxes summing up to ρ. ($\{\mathcal{E}_\rho\}$ is a family of confocal ellipses, which as $\rho \to 1$ shrink to the interval $[-1,1]$, and as $\rho \to \infty$ inflate into progressively more circle-like regions invading the whole complex plane.) The first space, $L^2[\mathcal{E}_\rho]$, contains functions f for which $\iint_{\mathcal{E}_\rho} |f(z)|^2 dxdy < \infty$, and is equipped with the inner product $(f,g) = \iint_{\mathcal{E}_\rho} f(z)\overline{g(z)}dxdy$. The second, $H^2[\mathcal{E}_\rho]$, consists of functions f with $\int_{\partial\mathcal{E}_\rho} |f(z)|^2 |1-z^2|^{-\frac{1}{2}} |dz| < \infty$ and carries the inner product $\int_{\partial\mathcal{E}_\rho} f(z)\overline{g(z)} |1-z^2|^{-\frac{1}{2}} |dz|$.

The norm of $R_n(f)$, in each of these spaces, can be expressed explicitly in terms of the respective orthonormal bases. Thus, in $L^2[\mathcal{E}_\rho]$,

$$(7) \qquad \|R_n\| = \frac{4}{\pi} \sum_{j=0}^{\infty} \left[\frac{j+1}{\rho^{2j+2} - \rho^{-2j-2}} R_n(U_j)\right]^2 ,$$

where U_j are the Chebyshev polynomials of the second kind, and in $H^2[\mathcal{E}_\rho]$,

$$(8) \qquad \|R_n\| = \frac{2}{\pi} \sum_{j=0}^{\infty}{}' \left[\frac{1}{\rho^{2j} + \rho^{-2j}} R_n(T_j)\right]^2 ,$$

where T_j are the Chebyshev polynomials of the first kind. (The prime indicates that the term with $j = 0$ is to be halved.) It is shown by Rabinowitz and Richter that there exists a set of nodes x_k in $[-1,1]$ for which (7), and one for which (8), is a minimum, regardless of whether the weight in the quadrature rule is fixed to be $2/n$, as in (1), or whether it is treated as a free parameter. Numerical results given by Rabinowitz and Richter suggest that the optimal nodes are mutually distinct for each $\rho > 1$, but this remains a conjecture.

Rabinowitz and Richter also investigate the behaviour of the optimal Chebyshev-type rules in the limit cases $\rho \to 1$ and $\rho \to \infty$. In the former case, the limit behaviour is somewhat bizarre, and we shall not attempt to describe it here. In the latter case, it follows from (7), (8) that, both in $L^2[\mathcal{E}_\rho]$ and $H^2[\mathcal{E}_\rho]$, the optimal rule must be such that it integrates exactly as many monomials as possible, and gives minimum error for the first monomial which cannot be integrated exactly. Thus,

$$(9) \qquad \begin{cases} R_n(x^j) = 0 , \quad j = 0,1,2,..,p, \quad p = \max(= p_n) , \\ |R_n(x^{p+1})| = \min . \end{cases}$$

We call the corresponding quadrature rules briefly E-optimal. Numerical results given by Rabinowitz and Richter for $n = 8,10,11,12,13$ show again the presence of repeated nodes.

6.4 E-optimal quadratures. An algebraic study of E-optimal Chebyshev-type quadrature rules is made in Gautschi and Yanagiwara [1974] for $n = 8,10,11,13$, and in Anderson and Gautschi [to appear] for general n. One of the key results of this work reveals that an E-optimal n-point Chebyshev-type formula can have at most p_n distinct nodes, whenever $p_n < n$. It follows from this immediately that some of the nodes must be repeated. The (generally distinct) p_n optimal nodes are found among the real solutions of systems of algebraic equations of the type

$$(10) \qquad \sum_{r=1}^{p} \nu_r x_r^{\,j} = s_j , \qquad j = 1,2,\ldots,p,$$

where ν_r are integers with $\nu_1 + \nu_2 + \cdots + \nu_p = n$ and $p = p_n$ an integer generally not known a priori (cf. Eq.(9)). Finding all real solutions of such systems is a challenging computational problem. It is solved in the cited references for $n \leq 17$ by a reduction to single algebraic equations. For other techniques, see also Yanagiwara and Shibata [1974] and Yanagiwara, Fukutake and Shibata [1975]. A summary of results is given below in Table 1, where crosses indicate the availability of E-optimal Chebyshev formulas, zeros the nonexistence of Chebyshev-type quadrature formulas, and question marks unsettled cases.

p \ n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23...
2[n/2]+1	X	X	X	X	X	X	X	0	X	0	0	0	0	0	0	0	0	0	0	0	0	0	0...
2[n/2]-1								X		X	X	0	X	0	0	0	0	0	0	0	0	0	0...
2[n/2]-3												X		X	X	0	X	0	0	0	0	0	0...
2[n/2]-5																X		?	?	?	?	0	0...

Table 1. Existence and nonexistence of n-point Chebyshev-type quadrature formulas of degree of exactness p

E-optimal formulas have been obtained also for infinite and semi-infinite intervals involving weight functions of the Hermite and Laguerre type (Anderson and Gautschi [to appear]). The confluence of nodes is rather more severe in these cases. For example, in the Laguerre case, when $3 \leq n \leq 6$, there are only two distinct nodes, one being simple, the other having multiplicity $n - 1$.

7. Error and convergence

7.1 The remainder term. Remainder terms in Chebyshev-type quadratures are generally ignored, except for the classical formulas

$$(1) \qquad \int_{-1}^{1} f(x)dx = \frac{2}{n} \sum_{k=1}^{n} f(x_k^{(n)}) + R_n(f), \qquad n = 1,2,\ldots,7,9,$$

and for the Gauss-Chebyshev formula (with $d\mu(x) = (1-x^2)^{-\frac{1}{2}}\,dx$).

Each of the formulas (1) has polynomial degree of exactness $p = 2[n/2]+1$, that is, $p = n$ if n is odd, and $p = n+1$ if n is even. Assuming $f \in C^{p+1}[-1,1]$, we obtain from Peano's theorem (see, e.g., Davis [1963, p.70])

$$(2) \qquad R_n(f) = \int_{-1}^{1} K_p(t) f^{(p+1)}(t)\,dt\,,$$

where $K_p(t)$ is the Peano kernel of the functional $R_n(f)$,

$$(3)\qquad K_p(t) = \frac{1}{p!}\left\{\frac{(1-t)^{p+1}}{p+1} - \frac{2}{n}\sum_{k=1}^{n}(x_k^{(n)} - t)_+^p\right\},$$

with

$$u_+^p = \begin{cases} u^p & \text{if } u \geq 0, \\ 0 & \text{if } u < 0, \end{cases} \qquad p \geq 0.$$

Ghizzetti and Ossicini [1970], and Kozlovskiĭ [1971], give different proofs of the fact that the Peano kernel is positive,

$$(4)\qquad K_p(t) \geq 0 \quad \text{on} \quad [-1,1].$$

From (2), it then follows that

$$(5)\qquad R_n(f) = \kappa_n f^{(p+1)}(\tau), \qquad -1 \leq \tau \leq 1,$$

where

$$(6)\qquad \kappa_n = \int_{-1}^{1} K_p(t)dt = R_n\left[\frac{x^{p+1}}{(p+1)!}\right], \qquad p = 2\left[\frac{n}{2}\right]+1.$$

Numerical values of the constants κ_n for $n = 1(1)7$ and $n = 9$ can be found in Ghizzetti and Ossicini [1970, pp.129-130]. (They have previously been tabulated by Berezin and Židkov [1965, p.262], but with an incorrect value of κ_9.)

The remainder in the Gauss-Chebyshev quadrature formula has been estimated by a number of writers; see, e.g., Stetter [1968a], Chawla and Jain [1968], Chawla [1969], Riess and Johnson [1969], Chui [1972], Jayarajan [1974].

For E-optimal quadrature rules of the type (1), the remainder $R_n(f)$ is analysed by Anderson [1974].

7.2 Convergence of Chebyshev quadrature formulas. In order to study convergence of the classical Chebyshev quadrature formulas, one must, of course, allow for complex nodes. From the known distribution of the nodes in the complex plane (cf. §2.2) it follows easily from Runge's theorem that convergence is assured for functions which are analytic in a closed domain $\mathcal{D}$ containing the curve of logarithmic potential, §2.2(1), in its interior (Kahaner [1971]). Convergence, in fact, is geometric for $\mathcal{D}$ sufficiently large.

8. Miscellaneous extensions and generalizations of Chebyshev quadrature

There are many variations on the theme of Chebyshev quadrature. A natural thing to try, e.g., is to relax the rigid requirement of equal coefficients and merely seek to minimize some measure of the variance in the coefficients. The problem, first suggested by Ostrowski [1959], is discussed by Kahaner [1969] and

Salkauskas [1971].

A more substantial modification is made by Erdős and Sharma [1965], and Meir and Sharma [1967], who associate equal coefficients only with part of the nodes and leave the coefficients for the remaining nodes, as well as the nodes themselves, variable. Even with this modification, provided the number of variable coefficients is kept fixed, and the polynomial degree of exactness maximized, some of the nodes again turn complex as n, the total number of nodes, becomes large. Erdős and Sharma show this for the measure $d\mu(x) = dx$ on $[-1,1]$, and Meir and Sharma for the ultraspherical measure $d\mu(x) = (1-x^2)^{\alpha}dx$, $\alpha > -\frac{1}{2}$. The maximum polynomial degree of exactness, p_n, subject to the reality of all nodes, when $d\mu(x) = dx$, in fact obeys the law $p_n = 0(\sqrt{n})$ familiar from Bernstein's theory of the classical Chebyshev quadratures. For Jacobi measures $d\mu(x) = (1-x)^{\alpha}(1+x)^{\beta}$, $\alpha > -\frac{1}{2}$, $\beta > -1$, Gatteschi, Monegato and Vinardi [to appear] associate variable coefficients with fixed nodes at ± 1, and equal coefficients with the remaining nodes, and for this case, too, establish the impossibility of n-point Chebyshev quadrature for n sufficiently large.

For quadrature sums involving derivative values as well as function values, the natural extension of Chebyshev's problem would be to require equal coefficients for all derivative terms involving the same order derivative. The problem, as far as we know, has not been treated in any great detail, although it is briefly mentioned by Ghizzetti [1954/55] (see also Ghizzetti and Ossicini [1970, p.43ff]).

Chebyshev quadrature rules integrating exactly trigonometric, rather than algebraic, polynomials are considered by Keda [1962] and Rosati [1968]. Rosati includes derivative terms in his quadrature sums.

Equally-weighted quadrature rules for integration in the complex plane are developed by Salzer [1947] in connection with the inversion of Laplace transforms.

An extension of Chebyshev quadrature to double and triple integrals is discussed by Georgiev [1953]. Coman [1970] derives optimal Chebyshev-type formulas in two dimensions.

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Note added in proof. In addition to the references Ghizzetti and Ossicini [1970], Kozlovskiĭ [1971] in §7.1, mention should be made of the paper T. Popoviciu, "La simplicité du reste dans certaines formules de quadrature", Mathematica (Cluj) 6 (29) (1964), 157-184 {MR32 #4848}, in which the remainder is studied not only of the classical Chebyshev quadrature rule, but also of the Chebyshev-Laguerre and Chebyshev-Hermite formulas obtained by Salzer [1955].

18.4. [58] “On Optimal Chebyshev-type Quadratures”

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Numerische Mathematik

On Optimal Chebyshev-Type Quadratures*

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Summary. A well-known result of Bernstein states that a Chebyshev quadrature formula of the form

$$\int_{-1}^{1} f(x)\,dx=\frac{2}{n}\sum_{k=1}^{n} f(t_k)+R_n(f), \qquad t_k \text{ real},$$

can have algebraic degree of exactness $p=n$ only if $1\leqq n\leqq 7$ or $n=9$. The nodes t_k are necessarily symmetric with respect to the origin, so that in fact $p=2[n/2]+1$. If symmetry of the nodes is imposed, it is known from work of Gautschi and Yanagiwara and others that next-to-highest algebraic degree $p=2[n/2]-1$, beyond the classical cases above, can be attained only when $n=8$, 10, 11, and 13. For these values of n, "optimal" formulas have been obtained which minimize $|R_n(x^{p+1})|$ among all symmetric Chebyshev quadratures of degree $p=2[n/2]-1$. We show here that these same formulas in fact minimize $|R_n(x^i)|$ for each $i\geqq p+1$.

1. Introduction

We consider symmetric Chebyshev-type quadrature formulas of "next-to-highest" algebraic degree of exactness, i.e., equally weighted quadrature formulas of the form

$$\int_{-1}^{1} f(x)\,dx=\frac{2}{n}\sum_{k=1}^{n} f(t_k)+R_n(f), \tag{1.1}$$

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subject to the following constraints,

$$\begin{aligned} &\text{all } t_k \text{ are real, } t_1 \geqq t_2 \geqq \cdots \geqq t_n, \\ &t_{n+1-k} + t_k = 0, \quad k = 1, 2, \ldots, n \text{ (symmetry)}, \\ &R_n(f) = 0 \text{ for every polynomial } f \text{ of degree } p = 2[n/2] - 1. \end{aligned} \tag{1.2}$$

If $1 \leqq n \leqq 7$, or $n = 9$, the classical Chebyshev quadratures satisfy all these conditions, the last one in the strengthened form with $p = 2[n/2] + 1$. Other Chebyshev-type formulas, satisfying (1.2), exist only for $n = 8$, 10, 11, and 13. This is shown in [6] and [1], where formulas are derived that are "optimal" in the sense of minimizing

$$\rho(t_1, t_2, \ldots, t_n) = |R_n(x^{p+1})|, \quad p = 2[n/2] - 1, \tag{1.3}$$

subject to (1.2). Each of these formulas has one pair of symmetric double nodes, or one double node at the origin, which (regretfully) means loss of the equal coefficient property. We will show here that these same formulas are in fact optimal in the much wider sense of minimizing

$$\rho_i(t_1, t_2, \ldots, t_n) = |R_n(x^i)| \quad \text{for each } i \geqq p+1, \tag{1.4}$$

subject to (1.2). (For odd integers i, the statement is trivially true, since $\rho_i = 0$ by virtue of symmetry.) In particular, they are minimum norm quadratures in the Hardy space H_2 of functions $f(z)$ analytic in $|z| < r$, $r > 1$, and square-integrable on $|z| = r$, since these quadratures minimize

$$\sum_{j=p+1}^{\infty} r^{-2j} [R_n(x^j)]^2 \quad \text{(see, e.g., [2])}.$$

As a preliminary step toward these results, we first show that for each $n = 8$, 10, 11, 13, the set of all Chebyshev-type quadrature formulas (1.1), satisfying (1.2), forms a one-parameter family, with parameter α in some finite closed interval $\lambda_n \leqq \alpha \leqq \mu_n$. By using symbolic Sturm sequences, we are able to identify λ_n and μ_n as roots of certain algebraic equations. The quadrature formulas corresponding to $\lambda_n < \alpha < \mu_n$ all have n distinct (simple) nodes in the interval $(-1, 1)$, while those corresponding to $\alpha = \lambda_n$ or $\alpha = \mu_n$ have a pair of symmetric double nodes, or a double node at the origin. The main result then follows from a (possibly new) monotonicity property satisfied by the power sums of the zeros of a polynomial. In particular, it transpires that the optimal formulas [in the general sense of minimizing (1.4)] always occur at $\alpha = \lambda_n$. They are necessarily identical with the optimal formulas found in [6] and [1].

2. One-Parameter Families of Chebyshev-Type Quadratures

We associate with (1.1) the polynomial

$$\xi(x) = \prod_{k=1}^{n} (x - t_k) = x^n + a_1 x^{n-1} + \cdots + a_n.$$

From Newton's identities it follows that the (real ordered) nodes t_k will satisfy (1.2) if and only if

$$\xi(x)=\begin{cases}x^n+a_2x^{n-2}+\cdots+a_{n-2}x^2+\alpha & (n \text{ even}),\\ x^n+a_2x^{n-2}+\cdots+a_{n-3}x^3+\alpha x & (n \text{ odd}),\end{cases} \tag{2.1}$$

where α is some real parameter and the coefficients $a_2, a_4, \ldots, a_{p-1}$ $(p=2[n/2]-1)$ are given uniquely by

$$\begin{aligned}&s_2+2a_2=0,\\ &s_4+a_2s_2+4a_4=0,\\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ &s_{p-1}+a_2s_{p-3}+\cdots+a_{p-3}s_2+(p-1)a_{p-1}=0,\end{aligned}$$

where

$$s_{2j}=\frac{n}{2}\int_{-1}^{1}t^{2j}dt=\frac{n}{2j+1}, \qquad j=1,2,\ldots,(p-1)/2.$$

It remains to determine the conditions on α under which the polynomial ξ in (2.1) has only real zeros. Letting

$$\xi(x)=\begin{cases}\xi^*(x^2) & (n \text{ even}),\\ x\xi^*(x^2) & (n \text{ odd}),\end{cases}$$

we are seeking the conditions on α under which the polynomial

$$\xi^*(x)=x^\nu+a_2x^{\nu-1}+\cdots+a_{2\nu-2}x+\alpha, \qquad \nu=[n/2], \tag{2.2}$$

has only nonnegative zeros. While the problem could easily be discussed in geometric terms, we prefer to take an algebraic approach via Sturm sequences. Among other things, this allows us to identify the limits on the parameter α as roots of certain algebraic equations with integer coefficients.

We recall that the Sturm sequence of a polynomial p_0 of degree ν is the result of applying Euclid's algorithm to p_0 and $p_1=p_0'$, where p_0' is the derivative of p_0. Thus,

$$\begin{aligned}&p_0=q_1p_1-p_2,\\ &p_1=q_2p_2-p_3,\\ &\cdots\cdots\cdots\cdots\cdots\cdots\\ &p_{\tau-2}=q_{\tau-1}p_{\tau-1}-p_\tau,\\ &p_{\tau-1}=q_\tau p_\tau,\end{aligned} \tag{2.3}$$

where $\tau\leqq\nu$, and each p_κ, $2\leqq\kappa\leqq\tau$, is the negative remainder of the division of $p_{\kappa-2}$ by $p_{\kappa-1}$. Sturm's theorem (see, e.g., [3, p. 448]) then asserts that for any $a<b$, if $p_0(a)\,p_0(b)\neq 0$, the number of distinct zeros of p_0 in $[a, b]$ is equal to $v(a)-v(b)$, where $v(x)$, for fixed x, is the number of sign changes in the numerical sequence $p_0(x), p_1(x), \ldots, p_\tau(x)$. Moreover, if x_0 is a (real or complex) zero of p_0,

then its multiplicity is m if and only if x_0 is a zero of the terminal polynomial p_τ of multiplicity $m-1$. In particular, all zeros of p_0 in $[a,b]$ are simple if and only if p_τ has no zeros in $[a,b]$.

In wishing to apply this to the polynomial $p_0=\xi^*$ in (2.2), one has to be prepared to operate on polynomials whose coefficients depend rationally on the parameter α. This is best done with the help of symbolic formula manipulation systems. We indeed generated the Sturm sequences symbolically, using the MACSYMA system available to one of us at Stanford University, and repeating the computations with the SAC-1 system on the UNIVAC 1110 computer at the University of Wisconsin. The results of both computations were identical, and are summarized below.

Writing

$$p_\kappa(x)=c_{\kappa\kappa}x^{\nu-\kappa}+c_{\kappa,\kappa+1}x^{\nu-\kappa-1}+\cdots+c_{\kappa\nu},\qquad \kappa=0,1,\ldots,\nu,$$

the coefficients $c_{\kappa\lambda}$, $\kappa\leqq\lambda$, are polynomials or rational functions of α, with rational coefficients, the degrees of which are as indicated in the schedules below. Zero degree always represents a non-vanishing (rational) constant; slashes separate numerator degree from denominator degree in case of rational functions. In all rational functions on the diagonal, the denominator polynomial is the square of the numerator polynomial in the rational function preceding it

$n=8$ $(\nu=4)$

0	0	0	0	1
	0	0	0	0
		0	0	1
			1	1
				3/2

$n=10,\ 11$ $(\nu=5)$

0	0	0	0	0	1
	0	0	0	0	0
		0	0	0	1
			0	1	1
				2	2
					4/4

$n=13$ $(\nu=6)$

0	0	0	0	0	0	1
	0	0	0	0	0	0
		0	0	0	0	1
			0	0	1	1
				1	1	1
					3/2	3/2
						7/6

on the diagonal. The numerator polynomials in the terminal entries are irreducible over the field of rationals, except in the case of $n=13$, where the numerator polynomial of c_{66} factors into the square of a linear polynomial and a polynomial of degree five.

According to Sturm's theorem, the polynomial ξ^* has ν distinct positive zeros (necessarily all simple) if and only if $v(0)=\nu$ and $v(\infty)=0$, that is, if and only if

$$c_{\kappa\kappa}>0 \quad\text{and}\quad (-1)^{\nu-\kappa}c_{\kappa\nu}>0 \quad\text{for } \kappa=0,1,2,\ldots,\nu. \tag{2.4}$$

By examining the explicit form of these (polynomial) inequalities for the four values of n under study, one finds that (2.4) is equivalent to

$$\lambda_n<\alpha<\mu_n, \tag{2.5}$$

where λ_n and μ_n are either zero, or equal to one of the zeros $\alpha_1^{(n)}<\alpha_2^{(n)}<\alpha_3^{(n)}<\cdots$ of $c_{\nu\nu}(\alpha)$, as indicated in Table 2.1. Numerical values of λ_n, μ_n, and the numerator

Table 2.1. Parameter intervals for symmetric Chebyshev-type formulas of next-to-highest degree

n	λ_n	μ_n
8	0	$\alpha_2^{(8)}$
10	$\alpha_2^{(10)}$	0
11	$\alpha_2^{(11)}$	$\alpha_3^{(11)}$
13	$\alpha_2^{(13)}$	$\alpha_3^{(13)}$

polynomial $c_{\nu\nu}^N$ of $c_{\nu\nu}$ in exact integer form (of which $\alpha_2^{(n)}$, $\alpha_3^{(n)}$ are zeros) are shown below.[1]

By verifying that $v(1)=v(\infty)=0$ for α in the interval (2.5), one finds that all ν zeros of ξ^* are in fact strictly between 0 and 1.

$$n=8$$

$$c_{44}^N(\alpha)=107661642834375\alpha^3-1739295676125\alpha^2+1639058085\alpha+1698929$$

$$\lambda_8=0$$

$$\mu_8=1.69631522630102201927350 8\times 10^{-3}$$

$$n=10$$

$$c_{55}^N(\alpha)=10383610167954115312 5\alpha^4-699972937051972500\alpha^3$$
$$-118379410645986\alpha^2+59483935980\alpha+10026277$$

$$\lambda_{10}=-1.70502634454170245879544 6\times 10^{-4}$$

$$\mu_{10}=0$$

$$n=11$$

$$c_{55}^N(\alpha)=435520176618906176716800000000000000000\alpha^4$$
$$-137486584840547265026457600000000000\alpha^3$$
$$-325179089998374326256267264000000\alpha^2$$
$$-178193695673498844238099200000\alpha-227128006189569593411 8607$$

$$\lambda_{11}=-7.23172944337750944027322 7\times 10^{-4}$$

$$\mu_{11}=-1.84381436540578659211115 8\times 10^{-4}$$

$$n=13$$

$$c_{66}^N(\alpha)=-51194312382380064490010308979821320628862976000000000000000\alpha^5$$
$$+17204030294473717738937992559890853617729536000000000000\alpha^4$$
$$-90386642710548216876719871881367691915689984000000000\alpha^3$$
$$+18029285809619921776960292383189983695831040000000\alpha^2$$
$$-15569598749195624684549602965438692780605440 0\alpha$$
$$+49094135596835984770993643505846928157 57$$

$$\lambda_{13}=1.02426094095810347493167 1\times 10^{-4}$$

$$\mu_{13}=1.32597928458533371559055 3\times 10^{-4}.$$

The Sturm sequence terminates prematurely [i.e., $\tau<\nu$ in (2.3)] if and only if α is a zero of one of the diagonal entries $c_{\kappa\kappa}$. We examined the Sturm sequence

[1] For $n=13$, only the factor (of degree 5) of $c_{\nu\nu}^N$ is shown which is relevant

in each one of these cases and found, as expected, that ξ^* has the desired number of nonnegative zeros precisely when α is a nonzero endpoint of the parameter intervals in Table 2.1. In each case, ξ^* has one double zero and $\nu-2$ simple zeros in the open interval $(0,1)$.

The remaining endpoint $\alpha=0$ in the cases $n=8$ and $n=10$ can be handled by forming the Sturm sequences at $x=\varepsilon>0$ sufficiently small, and at $x=1$. One finds $\nu-1$ simple zeros of ξ^* in $(0,1)$, which together with the zero at $x=0$ again yields the desired number of zeros in $(0,1)$.

We may summarize our findings in terms of the polynomial ξ in (2.1) as follows: *If* $n=8$, 10, 11, *or* 13, *the polynomial* ξ *has n real (symmetric) zeros, counting multiplicities, exactly if* α *is in the interval* $\lambda_n \leqq \alpha \leqq \mu_n$. *If* α *is an interior point of that interval, all zeros of* ξ *are in fact simple and contained in the open interval* $(-1,1)$. *If* α *is one of the endpoints of* $[\lambda_n, \mu_n]$, *then* ξ *has a pair of (symmetric) double zeros in* $(-1,1)$, *if* $\alpha \neq 0$, *and a double zero at the origin, if* $\alpha=0$, *all other zeros being simple and located in* $(-1,1)$.

The intervals $[\lambda_n, \mu_n]$ found here are in agreement with the (less accurate) intervals given in [4, Table I] for $n=8$, 10, and 11. Our results for $n=8$ and $n=10$ contradict a theorem of Pecka [5], which indeed is false because of computational errors in the proof.

3. Optimal Chebyshev-Type Formulas

In each one-parameter family of Chebyshev-type quadratures, obtained in Section 2, we now wish to single out one that minimizes the objective function ρ_i in (1.4). We may assume $i=2j$, with $j \geqq \nu$, where $\nu=[n/2]$. Letting $t_\kappa^*(\alpha)$ denote the zeros of ξ^*, and

$$s_j^*(\alpha)=\sum_{\kappa=1}^{\nu}[t_\kappa^*(\alpha)]^j, \qquad j=0,1,2,\ldots,$$

their power sums, and assuming $\lambda_n \leqq \alpha \leqq \mu_n$, the objective function is easily found to be

$$\rho_{2j}^*(\alpha)=\frac{4}{n}\left|s_j^*(\alpha)-\frac{n}{2(2j+1)}\right|, \qquad j \geqq \nu. \tag{3.1}$$

We thus wish to minimize $\rho_{2j}^*(\alpha)$ on the interval $\lambda_n \leqq \alpha \leqq \mu_n$. The lemmas which follow will lead us to the solution of this problem.

Lemma 3.1. *Suppose the algebraic equation*

$$g(x):=x^m+c_1x^{m-1}+\cdots+c_{m-1}x+c_m=0,$$

with real coefficients c_μ, *has m distinct nonnegative roots* $x_k=x_k(c_1,c_2,\ldots,c_m)$, $k=1,2,\ldots,m$. *Let* s_j *denote their j-th power sum,*

$$s_j(c_1,c_2,\ldots,c_m)=\sum_{k=1}^{m}[x_k(c_1,c_2,\ldots,c_m)]^j, \qquad j=0,1,2,\ldots.$$

Then

$$\frac{\partial s_j}{\partial c_\mu}<0 \quad \text{if } j\geqq\mu, \qquad \text{and} \qquad \frac{\partial s_j}{\partial c_\mu}=0 \quad \text{if } j<\mu. \tag{3.2}$$

Proof. Since, by Newton's identities, s_j depends only on $c_1, c_2, \ldots, c_j$, the second half of (3.2) is self-evident. It suffices, therefore, to consider $j\geqq\mu$, $1\leqq\mu\leqq m$.

Differentiating the identity $g(x_k(c_1, c_2, \ldots, c_m))\equiv 0$ with respect to c_μ, one finds

$$\frac{\partial x_k}{\partial c_\mu}=-\frac{x_k^{m-\mu}}{g'(x_k)}=-\frac{x_k^{m-\mu}}{\prod\limits_{l\neq k}(x_k-x_l)},$$

hence

$$\frac{\partial s_j}{\partial c_\mu}=j\sum_{k=1}^{m} x_k^{j-1}\frac{\partial x_k}{\partial c_\mu}=-j\sum_{k=1}^{m}\frac{x_k^{m-\mu+j-1}}{\prod\limits_{l\neq k}(x_k-x_l)}. \tag{3.3}$$

The sum on the far right is precisely the $(m-1)$-st divided difference $[x_1, x_2, \ldots, x_m]f$ of the function $f(x)=x^{m-\mu+j-1}$. Since

$$[x_1, x_2, \ldots, x_m]f=f^{(m-1)}(\bar{x})/(m-1)!=\binom{m-\mu+j-1}{m-1}\bar{x}^{j-\mu},$$

where $\bar{x}$ is in the open interval spanned by $x_1, x_2, \ldots, x_m$, and since all $x_k\geqq 0$, it follows that $\bar{x}>0$, and the sum in question is positive. This proves the lemma.

We remark that the proof of Lemma 3.1 also yields $\dfrac{\partial s_j}{\partial c_\mu}\geqq 0$ if $j<0$, if we assume all $x_k>0$, but we will not need this fact in what follows.

Lemma 3.2. *If* $n=8$, 10, 11, *or* 13, *we have*

$$s_j^*(\lambda_n)<\frac{n}{2(2j+1)} \quad \text{for } j\geqq\nu. \tag{3.4}$$

Proof. Since the quadrature formula (1.1) has polynomial degree of exactness $p=2\nu-1$, it is certainly exact for $f(x)=x^{2\nu-2}$, which yields

$$s_{\nu-1}^*=\frac{n}{2(2\nu-1)}. \tag{3.5}$$

For any $j\geqq\nu$, we have

$$s_j^*(\alpha)=\sum_{\kappa=1}^{\nu}[t_\kappa^*(\alpha)]^{j-\nu+1}[t_\kappa^*(\alpha)]^{\nu-1}<[t_1^*(\alpha)]^{j-\nu+1}s_{\nu-1}^*, \qquad \lambda_n\leqq\alpha\leqq\mu_n,$$

where $t_1^*(\alpha)$ is the largest among the roots $t_\kappa^*(\alpha)$. The lemma will hold for any value of j for which

$$[t_1^*(\lambda_n)]^{j-\nu+1}s_{\nu-1}^*<\frac{n}{2(2j+1)}.$$

By virtue of (3.5), this is equivalent to

$$t_1^*(\lambda_n) < \left(\frac{2\nu-1}{2j+1}\right)^{\frac{1}{j-\nu+1}}. \tag{3.6}$$

An elementary computation shows that the right-hand expression in (3.6) is an increasing function of j for $j \geqq \nu$. By consulting the numerical values of $t_1(\lambda_n)$ in [1], and noting that $t_1^*(\lambda_n) = [t_1(\lambda_n)]^2$, it is possible to verify the validity of (3.6) for $j = \nu+2$ when $n=8$, for $j=\nu+3$ when $n=10$, for $j=\nu+4$ when $n=11$, and for $j=\nu+5$ when $n=13$. The inequality therefore holds for these and all larger values of j. For the few remaining values of j, one can verify (3.4) directly, from the data available in [1]. This completes the proof of Lemma 3.2.

The problem of minimizing $\rho_{2j}^*(\alpha)$ in (3.1) is now easily solved.

Theorem 3.1. *If* $n=8$, 10, 11, *or* 13, *then for each* $j \geqq \nu$,

$$\rho_{2j}^*(\lambda_n) < \rho_{2j}^*(\alpha) \quad \text{for } \lambda_n < \alpha \leqq \mu_n. \tag{3.7}$$

Proof. Applying Lemma 3.1 to the polynomial ξ^* in (2.2), the zeros of which are $t_\kappa^*(\alpha)$, we find that each $s_j^*(\alpha)$, $j \geqq \nu$, is strictly decreasing on $\lambda_n < \alpha < \mu_n$, hence

$$s_j^*(\alpha) < s_j^*(\lambda_n) \quad \text{for } \lambda_n < \alpha \leqq \mu_n. \tag{3.8}$$

Combining (3.8) with Lemma 3.2 gives

$$s_j^*(\alpha) < \frac{n}{2(2j+1)}, \quad \lambda_n < \alpha \leqq \mu_n,$$

for each $j \geqq \nu$. Since $s_j^*(\alpha)$ decreases on $\lambda_n < \alpha < \mu_n$, it follows that $\rho_{2j}^*(\alpha)$ is an increasing function of α, hence (3.7).

Corollary. *Let* $\{w_j\}$ *be any sequence of weights* $w_j \geqq 0$, *with* $w_j > 0$ *for some* $j \geqq \nu$, *satisfying*

$$\sum_{j=\nu}^{\infty} j^{-2} w_j < \infty, \tag{3.9}$$

and let

$$\rho^*(\alpha) = \sum_{j=\nu}^{\infty} w_j [\rho_{2j}^*(\alpha)]^2, \quad \lambda_n \leqq \alpha \leqq \mu_n. \tag{3.10}$$

Then

$$\rho^*(\lambda_n) < \rho^*(\alpha) \quad \text{for } \lambda_n < \alpha \leqq \mu_n. \tag{3.11}$$

Proof. Since $s_j^*(\alpha) < \nu[t_1^*(\alpha)]^j$, where $t_1^*(\alpha)$ is the largest among the roots $t_\kappa^*(\alpha)$, and since $t_1^*(\alpha) < 1$ for $\lambda_n \leqq \alpha \leqq \mu_n$, the sequence $s_j^*(\alpha)$ tends to zero at least geometrically, and consequently $\rho_{2j}^*(\alpha) \sim j^{-1}$ as $j \to \infty$. The infinite series in (3.10), therefore, converges by virtue of (3.9), and (3.11) is an immediate consequence of (3.7).

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NUMERICAL QUADRATURE IN THE PRESENCE OF A SINGULARITY*

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1. Introduction. We denote by $M[-1, 1)$ the class of functions f which are continuous on the half-open interval $[-1, 1)$, monotonic in some neighborhood of 1, and such that $\lim_{x\uparrow 1} \int_{-1}^{x} f(t)\,dt$ exists. The classes $M(-1, 1]$ and $M(-1, 1)$ are defined similarly, in an obvious manner. M designates the union of the three classes. If $f \in M$ is bounded, then $f \in C[-1, 1]$, that is, f is continuous on $[-1, 1]$. We are interested in numerical quadrature of functions $f \in M$ not necessarily bounded. By definition of M,

$$I(f) = \int_{-1}^{1} f(t)\,dt \tag{1.1}$$

exists as an improper integral.

Consider a sequence of quadrature rules

$$Q_n(f) = \sum_{k=1}^{n} w_{n,k} f(x_{n,k}), \tag{1.2}$$

$$-1 = x_{n,n+1} \leqq x_{n,n} < \cdots < x_{n,1} \leqq 1 = x_{n,0}.$$

Extending an argument due to Pólya [6], [7, p. 39], Rabinowitz [8] showed that

$$\lim_{n\to\infty} Q_n(f) = I(f) \tag{1.3}$$

for all $f \in M[-1, 1)$, provided the following two conditions are satisfied:

(i) $\lim_{n\to\infty} Q_n(g) = I(g)$ for all $g \in C[-1, 1]$;

(ii) there exist constants $c > 0$, $\delta > 0$ such that $|w_{n,k}| \leqq c(x_{n,k-1} - x_{n,k})$ for all n sufficiently large and for all $k \geqq 1$ such that $1 - \delta \leqq x_{n,k} \leqq 1$.

If (ii) is replaced by the condition

(ii′) there exist constants $c > 0$, $\delta > 0$ such that $|w_{n,k-1}| \leqq c(x_{n,k-1} - x_{n,k})$ for all n sufficiently large and for all $k \leqq n + 1$ such that $-1 \leqq x_{n,k-1} \leqq -1 + \delta$,

then clearly (i) and (ii′) imply (1.3) for all $f \in M(-1, 1]$. Conditions (ii) and (ii′) are equivalent if the quadrature formulas (1.2) are symmetric,

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i.e., if

$$x_{n,n+1-k} = -x_{n,k}, \qquad w_{n,n+1-k} = w_{n,k}, \qquad k = 1, 2, \cdots, n. \tag{1.4}$$

The three conditions (i), (ii) and (ii′) together insure convergence (1.3) for all $f \in M$.

Many quadrature schemes, such as Romberg integration, Gauss-Legendre and a class of Gauss-Jacobi quadrature formulas, as well as composite quadrature rules (rectangular, midpoint, trapezoidal, Simpson, etc.) can thus be shown [8], [1] to converge not only for continuous functions, but also for functions having monotonic singularities at one or both endpoints of the basic interval. In the present note we deal with two particular quadrature formulas of interpolatory type, already considered by Fejér [2]. These are the quadrature formulas of maximum algebraic degree with the abscissas $x_{n,k}$ being the zeros of the Chebyshev polynomial of the first kind, $T_n(x)$, or the zeros of the Chebyshev polynomial of the second kind, $U_n(x)$. The weights $w_{n,k}$ of these quadrature formulas are known explicitly [2], [5, p.458]; a short derivation is given in §2. In §3 we verify the conditions (i) and (ii) above, and thus establish convergence, in M, of both these quadrature formulas. The result is of interest in the generation of Gauss-type quadrature formulas, an application which we hope to describe in a future paper. Some numerical examples are given in §4.

2. The quadrature formulas. Let

$$x_{n,k} = \cos\theta_{n,k}, \qquad \theta_{n,k} = \frac{2k-1}{2n}\pi, \qquad k = 1, 2, \cdots, n, \tag{2.1}$$

denote the zeros of the Chebyshev polynomial $T_n(x)$, and

$$x^*_{n,k} = \cos\theta^*_{n,k}, \qquad \theta^*_{n,k} = \frac{k}{n+1}\pi, \qquad k = 1, 2, \cdots, n, \tag{2.2}$$

the zeros of the Chebyshev polynomial $U_n(x)$. Denote by

$$Q_n(f) = \sum_{k=1}^{n} w_{n,k} f(x_{n,k}), \qquad Q_n^*(f) = \sum_{k=1}^{n} w^*_{n,k} f(x^*_{n,k}) \tag{2.3}$$

the respective quadrature formulas of maximum algebraic degree. Fejér [2] observed that

$$w_{n,k} = \frac{2}{n}\left(1 - 2\sum_{m=1}^{[n/2]} \frac{\cos 2m\theta_{n,k}}{4m^2-1}\right) \tag{2.4}$$

and

$$w^*_{n,k} = \frac{2}{n+1}\left(1 - 2\sum_{m=1}^{[(n-1)/2]} \frac{\cos 2m\theta^*_{n,k}}{4m^2-1} - \frac{1}{p}\cos(p+1)\theta^*_{n,k}\right), \tag{2.5}$$

where $p = 2[(n+1)/2] - 1$ is the largest odd integer $\leqq n$. Alternatively,

$$(2.5a) \qquad w_{n,k}^* = \frac{4 \sin \theta_{n,k}^*}{n+1} \sum_{m=1}^{[(n+1)/2]} \frac{\sin (2m-1)\theta_{n,k}^*}{2m-1}.$$

As a consequence of (2.4), we have [2]

$$\frac{2}{n^2} < w_{n,k} < \frac{4}{n}.$$

In particular, all weights $w_{n,k}$ are positive. A similar inequality holds for the weights $w_{n,k}^*$. To obtain it, let

$$S_n(\theta) = \sum_{m=1}^{n} \frac{\sin (2m-1)\theta}{2m-1}.$$

Clearly,

$$S_n(\theta) = \tfrac{1}{2}[s_{2n-1}(\theta) + s_{2n-1}(\pi - \theta)],$$

where

$$s_n(\theta) = \sum_{m=1}^{n} \frac{\sin m\theta}{m}.$$

Since [3]

$$(2.6) \quad 0 < s_n(\theta) < \sigma, \quad 0 < \theta < \pi, \qquad \sigma = \int_0^{\pi} \frac{\sin t}{t}\, dt = 1.8519 \cdots,$$

one obtains $0 < S_n(\theta) < \sigma$, $0 < \theta < \pi$, and consequently, by (2.5a),

$$(2.7) \qquad 0 < w_{n,k}^* < \frac{4\sigma \sin \theta_{n,k}^*}{n+1} < \frac{4\sigma}{n+1}, \qquad \sigma = 1.8519 \cdots.$$

For the derivation of (2.4) we recall [4, p. 80] that

$$(2.8) \qquad w_{n,k} = \frac{1}{T_n'(x_{n,k})} \int_{-1}^{1} \frac{T_n(x)\, dx}{x - x_{n,k}}.$$

Letting $y = x_{n,k}$ in the Christoffel-Darboux formula

$$1 + 2\sum_{m=1}^{n} T_m(x)T_m(y) = \frac{T_{n+1}(x)T_n(y) - T_n(x)T_{n+1}(y)}{x - y},$$

we obtain

$$1 + 2\sum_{m=1}^{n-1} T_m(x)T_m(x_{n,k}) = -\frac{T_n(x)T_{n+1}(x_{n,k})}{x - x_{n,k}},$$

so that (2.8) can be brought into the form

$$(2.9) \quad w_{n,k} = -\frac{2}{T_n'(x_{n,k})T_{n+1}(x_{n,k})} \left(1 + \sum_{m=1}^{n-1} T_m(x_{n,k}) \int_{-1}^{1} T_m(x)\, dx\right).$$

Using $T_n(\cos\theta) = \cos n\theta$, $T_n'(\cos\theta) = n(\sin n\theta)/\sin\theta$, one evaluates

$$T_n'(x_{n,k}) = T_n'(\cos\theta_{n,k}) = (-1)^{k-1} n/\sin\theta_{n,k},$$

$$T_{n+1}(x_{n,k}) = \cos(n+1)\theta_{n,k} = (-1)^k \sin\theta_{n,k},$$

$$\int_{-1}^{1} T_m(x)\,dx = \int_0^{\pi} \cos m\theta \sin\theta\,d\theta = \begin{cases} -2/(m^2-1) & \text{if } m \text{ is even,} \\ 0 & \text{if } m \text{ is odd.} \end{cases}$$

Substitution in (2.9) gives (2.4). The result (2.5a), and thus (2.5), may be obtained in like manner.

3. Convergence of the quadrature formulas. Both quadrature formulas (2.3) are symmetric. To prove convergence for $f \in M$, it suffices therefore to verify conditions (i) and (ii). The first of these is an immediate consequence of a well-known theorem of Pólya [4, p. 264], the weights being positive and both quadrature formulas being trivially convergent for every polynomial. As to condition (ii), we shall prove that

$$(3.1)\qquad 0 < \frac{w_{n,k}}{x_{n,k-1} - x_{n,k}} < \pi^2 + 4, \qquad 0 < \frac{w^*_{n,k}}{x^*_{n,k-1} - x^*_{n,k}} < 2\sigma\pi,$$

for all $n \geqq 3$, and all $k \geqq 1$ for which $x_{n,k} \geqq 0$, $x^*_{n,k} \geqq 0$. The constant σ is defined in (2.6).

Assume first $k \geqq 2$. We have

$$x_{n,k-1} - x_{n,k} = \cos\theta_{n,k-1} - \cos\theta_{n,k} = 2\sin\left(\frac{k-1}{n}\pi\right)\sin\frac{\pi}{2n}.$$

Using $\sin\theta \geqq 2\theta/\pi$, $0 \leqq \theta \leqq \pi/2$, we get

$$(3.2)\qquad x_{n,k-1} - x_{n,k} > \frac{4(k-1)}{n^2}.$$

We now recall that

$$\sum_{m=1}^{\infty} \frac{\cos 2m\theta}{4m^2-1} = \frac{1}{2} - \frac{\pi}{4}\sin\theta, \qquad 0 \leqq \theta \leqq \pi.$$

From (2.4) we therefore have

$$\begin{aligned} w_{n,k} &= \frac{2}{n}\left\{1 - 2\left(\frac{1}{2} - \frac{\pi}{4}\sin\theta_{n,k}\right) + 2r_{n,k}\right\} \\ &= \frac{2}{n}\left(\frac{\pi}{2}\sin\theta_{n,k} + 2r_{n,k}\right), \end{aligned}$$

where

$$\begin{aligned} |r_{n,k}| &= \left|\sum_{m=[n/2]+1}^{\infty} \frac{\cos 2m\theta_{n,k}}{4m^2-1}\right| < \sum_{m=[n/2]+1}^{\infty} \frac{1}{4m^2-1} \\ &= \frac{1}{2\left(2\left[\frac{n}{2}\right]+1\right)} \leqq \frac{1}{2n}. \end{aligned}$$

Hence, using $\sin\theta < \theta$ and (2.1), we obtain

$$w_{n,k} < \frac{2k-1}{2n^2}\pi^2 + \frac{2}{n^2}. \tag{3.3}$$

Combining (3.3) and (3.2) now gives

$$\frac{w_{n,k}}{x_{n,k-1} - x_{n,k}} < \frac{2k-1}{8(k-1)}\pi^2 + \frac{1}{2(k-1)} \leqq \frac{3}{8}\pi^2 + \frac{1}{2}, \qquad k \geqq 2. \tag{3.4}$$

We next consider $k = 1$. Here we have

$$x_{n,0} - x_{n,1} = 1 - \cos\frac{\pi}{2n} = 2\sin^2\frac{\pi}{4n} > \frac{1}{2n^2},$$

so that by (3.3), with $k = 1$,

$$\frac{w_{n,1}}{x_{n,0} - x_{n,1}} < \pi^2 + 4.$$

This, together with (3.4), establishes the first inequality in (3.1). The second inequality follows similarly, using (2.7) in place of (3.3).

4. Numerical examples. The quadrature formula

$$\int_0^1 f(t)\,dt \doteq \frac{1}{2}\sum_{k=1}^{n} w_{n,k} f(t_{n,k}), \qquad t_{n,k} = \frac{1}{2}(1 + x_{n,k}), \tag{4.1}$$

TABLE 1

	n	Fejér	Gauss-Chebyshev	Midpoint
$a = -\frac{1}{2}$	32	161 986	67 856	1 017 759
	64	88 478	33 978	772 104
	128	47 985	17 004	583 029
	256	25 859	8 509	438 475
	512	13 866	4 263	328 588
	1024	7 501	2 160	245 467
$a = 0$	32	55	2 131	10 790
	64	14	602	5 405
	128	3	167	2 706
$a = \frac{1}{2}$	32	12	212	1 543
	64	2	51	626
	128	1	12	250
$a = 1$	32	.4	200	234
	64	.2	50	66
	128	.3	12	18

with $x_{n,k}$ and $w_{n,k}$ given by (2.1) and (2.4), was applied to compute

$$\int_0^1 t^a \ln(e/t)\, dt = \frac{a+2}{(a+1)^2}, \qquad a > -1, \tag{4.2}$$

for various values of a. The moduli of the errors, in units of 10^{-6}, are shown in Table 1 in the column headed Fejér. For comparison, the midpoint, trapezoidal, and Simpson rules, with the same number of points, were also tried. Among these, the midpoint rule invariably gave the most accurate results (a phenomenon observed previously in [1]). The respective errors are shown in the last column. The column headed Gauss-Chebyshev displays the errors of the quadrature formula

$$\int_0^1 f(t)\, dt \doteq \frac{\pi}{n} \sum_{k=1}^{n} [t_{n,k}(1 - t_{n,k})]^{1/2} f(t_{n,k}), \tag{4.3}$$

when applied to (4.2). This quadrature formula is also known [8] to converge for $f \in M$.

It is seen that (4.1) consistently gives the most accurate results, except when $a = -\frac{1}{2}$, in which case (4.3) is more accurate. This exception is probably due to the fact that the singular factor t^a in f happens to be cancelled in the quadrature sum of (4.3) when $a = -\frac{1}{2}$. The presence of two coalescent singularities in (4.2), when $a < 0$, evidently causes all quadrature formulas to converge extremely slowly. Convergence is seen to accelerate as a increases from 0 to 1. In this range, (4.1) is remarkably effective, considering that the first derivative of the integrand is still infinite at the origin.

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On Computing Gauss-Kronrod Quadrature Formulae*

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Abstract. We discuss the use of Newton's method for computing Gauss-Kronrod quadrature formulae from modified moments. The underlying nonlinear maps are analyzed from the point of view of numerical condition. A method is indicated of computing the polynomial whose zeros are the Kronrod nodes. Examples include Gauss-Kronrod formulae for integrals with a logarithmic and algebraic singularity at one endpoint. Pertinent numerical results are tabulated in the supplements section at the end of this issue.

1. Introduction. Given a positive measure $d\sigma(t)$ on the real line, whose support contains infinitely many points and all of whose moments exist, we call

$$\int_{\mathbf{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f) \tag{1.1}$$

a *Gauss-Kronrod quadrature formula* if $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes associated with $d\sigma$ and the nodes τ_μ^* and weights σ_ν, σ_μ^* are chosen so as to maximize the degree of exactness of (1.1). Since there are $3n + 2$ unknowns, we can achieve degree of exactness $d = 3n + 1$, i.e., $R_n(f) = 0$ whenever $f = \mathbf{P}_{3n+1}$. It is well known, in fact, that the nodes τ_μ^* must be the zeros of π_{n+1}^*, the (monic) polynomial of degree $n + 1$ satisfying the orthogonality property

$$\int_{\mathbf{R}} \pi_{n+1}^*(t)\pi_n(t)t^i d\sigma(t) = 0, \qquad i = 0, 1, \ldots, n, \tag{1.2}$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ is the nth degree orthogonal polynomial belonging to the measure $d\sigma$. Note that the measure $d\sigma^*(t) = \pi_n(t; d\sigma)d\sigma(t)$, with respect to which π_{n+1}^* is orthogonal, changes sign. We cannot expect, therefore, that π_{n+1}^* has all its zeros necessarily real.

We are interested here only in Gauss-Kronrod formulae (1.1) with *real* nodes τ_μ^*, all contained in $[a, b]$—the smallest interval containing the support of $d\sigma$—and with *positive* weights σ_μ^*. Then the interlacing property holds (Monegato [17, Theorem 1]),

$$a \leqslant \tau_{n+1}^* < \tau_n < \tau_n^* < \tau_{n-1} < \cdots < \tau_1 < \tau_1^* \leqslant b. \tag{1.3}$$

Our concern is with the actual computation of these nodes and the corresponding weights (provided they exist), given the integer $n \geqslant 1$ and the positive measure $d\sigma$.

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Constructive methods for this problem have been considered before. For the Legendre measure $d\sigma(t) = dt$ on $[-1, 1]$, Kronrod [16] in his original work obtains π_{n+1}^* in power form by solving (1.2). Patterson [22] expands π_{n+1}^* in Legendre polynomials, while Piessens and Branders [23] use Chebyshev polynomials, the nodes τ_μ^* each time being computed by an appropriate rootfinding procedure. The weights can be obtained by interpolation. Monegato [17], [19], Baratella [1], and Dagnino and Fiorentino [3] use similar procedures to compute π_{n+1}^* for Gegenbauer measures and other classical measures. Kahaner et al. [13], in the case of the Laguerre measure, and assuming $k \geq n + 1$ Kronrod nodes τ_μ^* in (1.1), expand $L_n\pi_k^*$ in Laguerre polynomials L_j. All these methods require three distinct phases to obtain (1.1): The computation of the appropriate polynomial, say π_{n+1}^*, finding the zeros of π_{n+1}^*, and computing the weights σ_ν, σ_μ^*. An entirely different approach is taken by Kautsky and Elhay [15] and Elhay and Kautsky [5], who compute the nodes τ_μ^* as eigenvalues of a certain matrix derived by matrix decomposition methods—an approach which extends the well-known method of Golub and Welsch [12] for ordinary Gaussian quadratures and its extension by Golub and Kautsky [11]. The weights are then obtained using general methods for constructing interpolatory quadrature rules [14], [6].

Here we propose to compute (1.1) directly by solving a set of nonlinear equations that express the exactness of (1.1) for a given set of $3n + 2$ polynomials. These polynomials are chosen so as to generate a well-conditioned problem. The respective system of nonlinear equations is solved by Newton's method, careful attention being given to the choice of initial approximations and to monitoring the progress of the iteration. We make no claims for our method to be superior in any way to other methods, but merely demonstrate its feasibility and stability. It would indeed be interesting to undertake a detailed comparative study of the various methods now in use.

While aiming directly at the unknown quantities is certainly a virtue if our method is successful, it is less than satisfactory otherwise, since no information about π_{n+1}^* is generated when the method fails. Nevertheless, if one wishes to examine the polynomial π_{n+1}^*, one can express it in terms of the orthogonal polynomials $\{\pi_k(\cdot; d\sigma)\}$ and obtain the coefficients by solving a triangular system of linear equations.

The implementation of Newton's method for computing the Gauss-Kronrod rule (1.1) is discussed in Section 2. In Section 3 we study the condition of the underlying problem. Section 4 deals with the computation of the polynomial π_{n+1}^*. Examples will be given in Section 5, and numerical results for $d\sigma(t) = t^\alpha \ln(1/t)\, dt$ on $[0, 1]$, $\alpha = 0, \pm \frac{1}{2}$, are tabulated in the supplements section at the end of this issue.

For additional questions related to Gauss-Kronrod quadrature we refer the reader to surveys by Monegato [20], [21].

2. The Computation of Gauss-Kronrod Rules by Newton's Method. The Gaussian nodes τ_ν for the measure $d\sigma$ can be computed by well-known methods; see, e.g., [8, p. 290]. We assume therefore that they are available. For a given system of monic polynomials $\{p_k(\cdot)\}$, with $\deg p_k = k$, $k = 0, 1, 2, \ldots$, we further assume that the

first $3n + 2$ modified moments of $d\sigma$,

$$m_k = \int_{\mathbb{R}} p_k(t)\, d\sigma(t), \qquad k = 0, 1, \ldots, 3n + 1, \tag{2.1}$$

are known. The system of nonlinear equations defining the Gauss-Kronrod formula (1.1) then is

$$\sum_{\nu=1}^{n} \sigma_\nu p_k(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* p_k(\tau_\mu^*) = m_k, \qquad k = 0, 1, \ldots, 3n + 1. \tag{2.2}$$

We propose to solve this system for the $3n + 2$ unknowns τ_μ^*, σ_ν, σ_μ^* by Newton's method. A number of practical issues need to be addressed.

First the choice of polynomials p_k. We assume that they satisfy a three-term recurrence relation,

$$\begin{aligned} p_{-1}(t) &= 0, \qquad p_0(t) = 1, \\ p_{k+1}(t) &= (t - a_k) p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \end{aligned} \tag{2.3}$$

with known coefficients a_k, b_k. This makes the evaluation of these polynomials, and of their derivatives, which is required in the computation of the left-hand side of the system (2.2) and its Jacobian, easy and straightforward. If, in addition, the polynomials $\{p_k\}$ are orthogonal with respect to some given measure $ds(t)$, then this computation is also numerically stable. If $d\sigma$ is one of the classical measures, the simplest choice is $p_k(\cdot) = \pi_k(\cdot; d\sigma)$, the corresponding recursion coefficients $a_k = \alpha_k(d\sigma)$, $b_k = \beta_k(d\sigma)$ then being explicitly known; the modified moments become

$$m_k = \int_{\mathbb{R}} \pi_k(t; d\sigma)\, d\sigma(t) = \beta_0 \delta_{0,k}, \qquad k = 0, 1, 2, \ldots, \tag{2.4}$$

where $\beta_0 = \int_{\mathbb{R}} d\sigma(t)$ and $\delta_{0,k}$ is the Kronecker delta, $\delta_{0,0} = 1$, $\delta_{0,k} = 0$ if $k > 0$. For nonclassical measures $d\sigma$, the choice of p_k is usually dictated by the necessity of being able to compute the modified moments (2.1).

The next important issue is the computation of the initial approximations for the Kronrod nodes τ_μ^* and for the weights σ_ν, σ_μ^*. Since we are interested only in Gauss-Kronrod formulae with nodes in $[a, b]$ and with positive weights σ_μ^*, we can assume the interlacing property (1.3). This suggests as initial approximations $\mathring{\tau}_\mu^*$, $2 \leqslant \mu \leqslant n$, the midpoints

$$\mathring{\tau}_\mu^* = \tfrac{1}{2}(\tau_{\mu-1} + \tau_\mu), \qquad \mu = 2, 3, \ldots, n, \tag{2.5}$$

between the Gaussian nodes $\tau_{\mu-1}$ and τ_μ. The choice of the initial approximations $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$ is less obvious. If the endpoint b is finite, we select a number of trial values $\mathring{\tau}_1^*$ equally spaced between τ_1 and b. If a is also finite, we do the same for $\mathring{\tau}_{n+1}^*$ in the interval (a, τ_n) and let both $\mathring{\tau}_{n+1}^*$ and $\mathring{\tau}_1^*$ move inward simultaneously, or, if necessary, let them move independently from one another. If an endpoint, say b, is infinite, we select $\mathring{\tau}_1^* = \tau_1 + (\tau_1 - \tau_2)$, or try a number of values $\mathring{\tau}_1^*$ equally spaced between τ_1 and, say, $\tau_1 + 2(\tau_1 - \tau_2)$. For each set of initial approximations $\mathring{\tau}_\mu^*$ we compute corresponding approximations $\mathring{\sigma}_\nu$, $\mathring{\sigma}_\mu^*$ to the weights by solving the first $2n + 1$ equations in (2.2), where τ_μ^* is replaced by $\mathring{\tau}_\mu^*$. Since the matrix of this system forms part of the Jacobian matrix used in the first Newton step, the only overhead of this computation is the solution of the linear system.

Each Newton step is monitored as to the location of the iterates of τ_μ^*. If at any stage one of these iterates falls outside the interval $[a, b]$ (if either a or b is finite), the iteration is terminated and restarted with a new set of initial approximations. The same action is taken if the number of Newton iterates exceeds a preset limit. If none of the initial approximations leads to a convergent process, the attempt of computing (1.1) is declared a failure. This is usually an indication (not a proof!) that the desired Gauss-Kronrod rule does not exist.

If $d\sigma(t) = d\sigma(-t)$ is an even measure and the support of $d\sigma$ is symmetric with respect to the origin, then both the Gaussian nodes τ_ν and the Kronrod nodes τ_μ^* are located symmetrically with respect to the origin, and weights corresponding to symmetric nodes are equal. As a result, (2.2) is trivially true if $p_k(t)$ is an odd polynomial. If we choose for $\{p_k\}$ a system of polynomials satisfying

$$p_k(-t) = (-1)^k p_k(t), \qquad k = 0, 1, 2, \ldots, \tag{2.6}$$

the system (2.2), therefore, is equivalent to the system

$$\sum_{\nu=1}^{n/2} \sigma_\nu p_{2k}(\tau_\nu) + \sum_{\mu=1}^{n/2} \sigma_\mu^* p_{2k}(\tau_\mu^*) + \frac{1}{2}\sigma_{(n/2)+1}^* p_{2k}(0) = \frac{1}{2} m_{2k}, \tag{2.7e}$$

$$k = 0, 1, \ldots, 3n/2,$$

if n is even, and to the system

$$\sum_{\nu=1}^{[n/2]} \sigma_\nu p_{2k}(\tau_\nu) + \frac{1}{2}\sigma_{[n/2]+1} p_{2k}(0) + \sum_{\mu=1}^{[n/2]+1} \sigma_\mu^* p_{2k}(\tau_\mu^*) = \frac{1}{2} m_{2k}, \tag{2.7o}$$

$$k = 0, 1, \ldots, (3n+1)/2,$$

if n is odd. This in effect reduces the size of the problem by a factor of 2.

3. The Condition of the Underlying Problem. Let $m^T = [m_0, m_1, \ldots, m_{3n+1}]$ be the vector of modified moments, and $\gamma^T = [\sigma_1, \ldots, \sigma_n, \sigma_1^*, \ldots, \sigma_{n+1}^*, \tau_1^*, \ldots, \tau_{n+1}^*]$ the vector of the weights and Kronrod nodes of the Gauss-Kronrod formula (1.1). The procedure of Section 2 is an attempt of carrying out the nonlinear map

$$G_n: \mathbf{R}^{3n+2} \to \mathbf{R}^{3n+2} \qquad m \to \gamma,$$

where the Gauss-Kronrod formula is assumed to have real nodes. We now wish to examine the sensitivity of the map G_n to perturbations in the modified moments. The development parallels the treatments given for Gaussian formulae in Gautschi [8], [9]; see also Gautschi [10, Section 5].

We assume that the polynomials $\{p_k\}$ defining the modified moments are orthogonal on the real line with respect to some measure ds. The support of this measure normally coincides with the support of $d\sigma$, but does not have to. We define normalized modified moments by

$$\tilde{m}_k = d_k^{-1} m_k, \qquad d_k^2 = \int_{\mathbf{R}} p_k^2(t)\, ds(t), \tag{3.1}$$

and consider, in place of G_n, the map

$$\tilde{G}_n: \mathbf{R}^{3n+2} \to \mathbf{R}^{3n+2} \qquad \tilde{m} \to \gamma, \tag{3.2}$$

where $\tilde{m}^T = [\tilde{m}_0, \tilde{m}_1, \ldots, \tilde{m}_{3n+1}]$. We analyze the sensitivity of $\tilde{G}_n$ by computing the Frobenius norm of the Jacobian matrix, $J_{\tilde{G}_n}$, of the map $\tilde{G}_n$.

The basic equations can be written in the form

$$\Phi(\gamma) = \tilde{m}, \tag{3.3}$$

where

$$\Phi_k(\gamma) = d_k^{-1}\left\{ \sum_{\nu=1}^{n} \sigma_\nu p_k(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* p_k(\tau_\mu^*) \right\}, \tag{3.4}$$

$$k = 0, 1, 2, \ldots, 3n+1.$$

Since the map $\tilde{G}_n$ amounts to solving (3.3) for γ, the Jacobian of $\tilde{G}_n$ is the inverse of the Jacobian $\partial\Phi/\partial\gamma$ of Φ,

$$J_{\tilde{G}_n} = (\partial\Phi/\partial\gamma)^{-1}. \tag{3.5}$$

An elementary computation shows that

$$\partial\Phi/\partial\gamma = D^{-1}P\Sigma^*, \tag{3.6}$$

where $D = \operatorname{diag}(d_0, d_1, \ldots, d_{3n+1})$, $\Sigma^* = \operatorname{diag}(1, \ldots, 1, 1, \ldots, 1, \sigma_1^*, \ldots, \sigma_{n+1}^*)$, and

(3.7)

$$P = \begin{bmatrix} p_0(\tau_1) & \cdots & p_0(\tau_n) & p_0(\tau_1^*) & \cdots & p_0(\tau_{n+1}^*) & p_0'(\tau_1^*) & \cdots & p_0'(\tau_{n+1}^*) \\ p_1(\tau_1) & \cdots & p_1(\tau_n) & p_1(\tau_1^*) & \cdots & p_1(\tau_{n+1}^*) & p_1'(\tau_1^*) & \cdots & p_1'(\tau_{n+1}^*) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ p_{3n+1}(\tau_1) & \cdots & p_{3n+1}(\tau_n) & p_{3n+1}(\tau_1^*) & \cdots & p_{3n+1}(\tau_{n+1}^*) & p_{3n+1}'(\tau_1^*) & \cdots & p_{3n+1}'(\tau_{n+1}^*) \end{bmatrix}.$$

Therefore,

$$J_{\tilde{G}_n} = (\Sigma^*)^{-1}P^{-1}D. \tag{3.8}$$

For the inversion of P, define g_ν, h_μ, k_μ to be the elementary Hermite interpolation polynomials of degree $3n+1$, belonging to the nodes τ_ν and τ_μ^*, defined by

$$\left.\begin{aligned} &g_\nu(\tau_\lambda) = \delta_{\nu\lambda}, \quad \lambda = 1, 2, \ldots, n \\ &g_\nu(\tau_\mu^*) = 0, \quad g_\nu'(\tau_\mu^*) = 0, \qquad \mu = 1, 2, \ldots, n+1 \end{aligned}\right\},$$

$$\nu = 1, 2, \ldots, n,$$

$$\left.\begin{aligned} &h_\mu(\tau_\lambda) = 0, \quad \lambda = 1, 2, \ldots, n \\ &h_\mu(\tau_\nu^*) = \delta_{\mu\nu}, \quad h_\mu'(\tau_\nu^*) = 0, \qquad \nu = 1, 2, \ldots, n+1 \\ &k_\mu(\tau_\lambda) = 0, \quad \lambda = 1, 2, \ldots, n \\ &k_\mu(\tau_\nu^*) = 0, \quad k_\mu'(\tau_\nu^*) = \delta_{\mu\nu}, \qquad \nu = 1, 2, \ldots, n+1 \end{aligned}\right\}, \tag{3.9}$$

$$\mu = 1, 2, \ldots, n+1.$$

Writing

$$g_\nu(t) = \sum_{\rho=1}^{3n+2} a_{\nu\rho}p_{\rho-1}(t), \quad h_\mu(t) = \sum_{\rho=1}^{3n+2} b_{\mu\rho}p_{\rho-1}(t), \quad k_\mu(t) = \sum_{\rho=1}^{3n+2} c_{\mu\rho}p_{\rho-1}(t),$$

it is easily seen that

$$P^{-1} = \begin{bmatrix} A \\ B \\ C \end{bmatrix}, \quad A = [a_{\nu\rho}], \quad B = [b_{\mu\rho}], \quad C = [c_{\mu\rho}]. \tag{3.10}$$

By a computation similar to the one in [8, pp. 303–304] one finds from (3.8) and (3.10) that the Frobenius norm of $J_{\tilde{G}_n}$ is given by

$$\|J_{\tilde{G}_n}\|_F = \left\{ \int_{\mathbf{R}} \left[\sum_{\nu=1}^{n} g_\nu^2(t) + \sum_{\mu=1}^{n+1} \left(h_\mu^2(t) + \frac{1}{\sigma_\mu^{*2}} k_\mu^2(t) \right) \right] ds(t) \right\}^{1/2}. \tag{3.11}$$

Its magnitude, therefore, is critically influenced by the magnitude of the polynomial

$$f_n(t) = \sum_{\nu=1}^{n} g_\nu^2(t) + \sum_{\mu=1}^{n+1} \left(h_\mu^2(t) + \frac{1}{\sigma_\mu^{*2}} k_\mu^2(t) \right) \tag{3.12}$$

on the support of ds. The degree of f_n is $6n + 2$. The integral in (3.11) can therefore be computed exactly (up to rounding errors) by a $(3n + 2)$-point Gaussian quadrature rule belonging to the measure ds.

Explicit forms of the polynomials g_ν, h_μ, k_μ can easily be given in terms of the fundamental Lagrange polynomials

$$l_\nu(t) = \prod_{\substack{\lambda=1 \\ \lambda \neq \nu}}^{n} \frac{t - \tau_\lambda}{\tau_\nu - \tau_\lambda}, \qquad l_\mu^*(t) = \prod_{\substack{\lambda=1 \\ \lambda \neq \mu}}^{n+1} \frac{t - \tau_\lambda^*}{\tau_\mu^* - \tau_\lambda^*}$$

belonging to the nodes τ_ν and τ_μ^*, respectively. One obtains

$$g_\nu(t) = l_\nu(t) \left[\frac{\pi_{n+1}^*(t)}{\pi_{n+1}^*(\tau_\nu)} \right]^2, \qquad \nu = 1, 2, \ldots, n,$$

$$h_\mu(t) = \frac{\pi_n(t)}{\pi_n(\tau_\mu^*)} \left[l_\mu^*(t) \right]^2 \left\{ 1 - (t - \tau_\mu^*) \left[\frac{\pi_n'(\tau_\mu^*)}{\pi_n(\tau_\mu^*)} + 2 l_\mu^{*\prime}(\tau_\mu^*) \right] \right\}, \tag{3.13}$$

$$\mu = 1, 2, \ldots, n+1,$$

$$k_\mu(t) = \frac{\pi_n(t)}{\pi_n(\tau_\mu^*)} \left[l_\mu^*(t) \right]^2 (t - \tau_\mu^*), \qquad \mu = 1, 2, \ldots, n+1,$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ and $\pi_{n+1}^*(t) = \prod_{\lambda=1}^{n+1}(t - \tau_\lambda^*)$. We also note the following properties of f_n, which follow directly from (3.9) and (3.12),

$$\begin{aligned} &f_n(t) > 0 \quad \text{for all } t \in \mathbf{R}, \\ &f_n(\tau_\nu) = 1, \quad f_n'(\tau_\nu) = 2g_\nu'(\tau_\nu), \qquad \nu = 1, 2, \ldots, n, \\ &f_n(\tau_\mu^*) = 1, \quad f_n'(\tau_\mu^*) = 0, \qquad \mu = 1, 2, \ldots, n+1. \end{aligned} \tag{3.14}$$

These conditions, of course, are not sufficient to determine the polynomial f_n. There are $2n + 1$ degrees of freedom left, which allow f_n considerable room for movement.

4. Computation of the Polynomial π_{n+1}^*. Expressing the polynomial π_{n+1}^* in terms of the orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\sigma)$,

$$\pi_{n+1}^*(t) = \pi_{n+1}(t) + c_0 \pi_n(t) + c_1 \pi_{n-1}(t) + \cdots + c_n \pi_0(t), \tag{4.1}$$

and replacing the powers t^i in (1.2) by the polynomials $\pi_i(t)$, one obtains the conditions

$$\int_{\mathbf{R}} \left[\pi_{n+1}(t) + \sum_{k=0}^{n} c_k \pi_{n-k}(t) \right] \pi_n(t) \pi_i(t)\, d\sigma(t) = 0, \qquad i = 0, 1, \ldots, n,$$

hence the linear system

$$\sum_{k=0}^{n} a_{ik}c_k = b_i, \qquad i = 0,1,\ldots,n, \tag{4.2}$$

for the coefficients c_k, where

$$\begin{aligned} a_{ik} &= \int_{\mathbb{R}} \pi_i(t)\pi_{n-k}(t)\pi_n(t)\,d\sigma(t), \qquad i,k = 0,1,\ldots,n, \\ b_i &= -\int_{\mathbb{R}} \pi_i(t)\pi_{n+1}(t)\pi_n(t)\,d\sigma(t), \qquad i = 0,1,\ldots,n. \end{aligned} \tag{4.3}$$

By orthogonality, $a_{ik} = 0$ if $i < k$, so that the matrix $A = [a_{ik}]$ is lower triangular, and $a_{ii} = \int_{\mathbb{R}} \pi_n^2(t)\,d\sigma(t) > 0$, so that A is nonsingular. The solution of (4.2), therefore, can be effected by forward substitution.

The coefficients a_{ik} and $b_i = -a_{i,-1}$ satisfy a two-dimensional recursion relation, which could be used for their computation (see [2]). Noting, however, that the integrands in (4.3) are polynomials of degree at most equal to $3n + 1$, we can also use m-point Gauss-Christoffel quadrature relative to the measure $d\sigma$, with $m = [(3n + 3)/2]$, to compute a_{ik} and b_i. This might be preferable, since it requires nothing beyond standard software.

While this procedure of generating π_{n+1}^* is similar to Kronrod's original method, it is significantly more stable, since the use of powers as a polynomial basis is completely avoided.

5. Examples. It is known that for $d\sigma(t) = (1 - t^2)^{\lambda - 1/2}\,dt$ on $[-1,1]$ all Gauss-Kronrod formulae exist if $0 \leqslant \lambda \leqslant 2$. Furthermore, the interlacing property (1.3) holds and $\sigma_\mu^* > 0$ for $\mu = 1,2,\ldots,n+1$ (Monegato [17]). If $0 \leqslant \lambda \leqslant 1$, one has in addition $\sigma_\nu > 0$ for $\nu = 1,2,\ldots,n$ (Monegato [18]). Our first example deals with the case $\lambda = \frac{1}{2}$, i.e., with the Legendre measure. All computations reported were done on the CDC 6500 computer in single precision (machine precision $\approx 3.55 \times 10^{-15}$), unless noted otherwise.

Example 5.1. $d\sigma(t) = dt$ on $[-1,1]$.

Taking advantage of symmetry, we apply Newton's method to the system (2.7), using for p_{2k} the (monic) Legendre polynomials of degree $2k$. The required modified moments are then given by (2.4). We had no difficulty with convergence. By symmetry, only *one* "trial" initial approximation, $\hat{\tau}_1^*$, is needed, which was programmed to move in nine equal steps of length $h = (1 - \tau_1)/10$ from $1 - h$ to $\tau_1 + h$. Convergence was invariably achieved for the first choice of $\hat{\tau}_1^*$. Moreover, the problem, suitably scaled, turns out to be extremely stable. In the first four columns of Table 5.1 we report on the number of iterations required for 12 decimal place accuracy, the maximum of $f_n(t)$ (cf. Eq. (3.12)) on $[-1,1]$ and the value of $\|J_{\hat{G}_n}\|_F$ (cf. Eq. (3.11)) for $n = 5, 10, 20, 40, 80$. The maximum of $f_n(t)$—an even function of t—is typically assumed between τ_2 and τ_2^*, if n is even, there being a couple of smaller maxima on either side of it. If n is odd, the maximum seems to occur at $t = 1$. Through most of the interval $(-1,1)$, however, f_n remains $\leqslant 1$.

TABLE 5.1

Performance and stability characteristics of Newton's method for generating the $(2n+1)$*-point Gauss-Kronrod formula with* $d\sigma(t) = dt$ *on* $[-1,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\hat{G}_n}\|_F$	cond_1	cond_2	cond_1 (scaled)	cond_2 (scaled)
5	6	1.126	1.293	1.4(3)	3.3(4)	1.2(1)	1.4(1)
10	6	2.456	1.397	1.5(6)	5.2(8)	1.8(1)	2.3(1)
20	6	2.520	1.333	1.5(12)	5.3(17)	4.1(1)	4.8(1)
40	6	2.535	1.310	1.6(24)	5.8(35)	6.6(1)	7.7(1)
80	6	2.540	1.302	—	—	1.3(2)	1.7(2)

The linear systems of equations for determining the initial approximations $\mathring{\sigma}_\nu$, $\mathring{\sigma}_\mu^*$ for the weights, as well as the Jacobian matrices in Newton's method, appear to become rapidly ill-conditioned as n increases. Typical condition number estimates (furnished by the LINPACK routine SGECO; cf. [4, Chapter 1]) for the former are shown in the fifth column of Table 5.1, while those for the latter are shown in the sixth column. (Numbers in parentheses indicate decimal exponents.) In spite of the large condition numbers, numerical difficulties were not observed, except in the case $n = 80$, when the computation was aborted due to an arithmetic error. We believe that the apparent ill-conditioning is caused by the use of monic polynomials p_{2k} in (2.7); their L_2-norm goes to zero rather quickly,

$$\|p_{2k}\|_2 = \frac{2^{2k}(2k)!^2}{(4k)!}\sqrt{\frac{2}{4k+1}} \sim \sqrt{\pi}\,2^{-2k} \quad \text{as } k \to \infty,$$

thereby introducing a systematic diminution of the rows down the matrices. If the row involving p_{2k} is scaled by dividing it by $2^{2k}(2k)!^2/(4k)!$, the condition numbers indeed become much more reasonable (the solutions remaining the same); they are shown in the last two columns of Table 5.1.

Example 5.2. $d\sigma(t) = \ln(1/t)\,dt$ on $[0,1]$.

It appears that this measure also admits Gauss-Kronrod formulae for all n, satisfying the interlacing property (1.3) and having all weights positive. A summary of our numerical experience with Newton's method is given in Table 5.2; it contains information analogous to the one given in Table 5.1 for Example 5.1.

TABLE 5.2

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = \ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\hat{G}_n}\|_F$	cond_1	cond_2	cond_1 (scaled)	cond_2 (scaled)
5	6	2.90(4)	12.14	2.0(6)	6.9(9)	5.8(1)	2.7(3)
10	6	4.09(5)	24.35	2.2(12)	7.5(18)	2.8(1)	1.6(4)
20	6	5.77(6)	47.43	2.4(24)	8.2(36)	9.8(2)	1.0(5)
40	6	8.86(7)	94.59	—	—	3.8(3)	6.4(5)

We have used modified moments with respect to the (monic) shifted Legendre polynomials, $p_k(t) = [k!^2/(2k)!]P_k^*(t)$; they are known to be (cf., e.g., Gautschi [7])

$$m_0 = 1, \qquad m_k = \int_0^1 p_k(t)\ln(1/t)\,dt = \frac{k!^2}{(2k)!}\frac{(-1)^k}{k(k+1)}, \qquad k = 1,2,\ldots.$$

Row scaling of the matrices was performed through division by $k!^2/(2k)!$ (of the row numbered $k + 1$).

The initial approximations $\dot\tau_1^*$ and $\dot\tau_{n+1}^*$ were programmed to first move inward symmetrically in nine steps of length $h = (1 - \tau_1)/10$ and $h' = \tau_n/10$, respectively, and if this did not work, $\dot\tau_1^*$ was varied independently over the same set of points for each fixed $\dot\tau_{n+1}^*$. Convergence, in general, was achieved for the very first choice of $\dot\tau_1^*$ and $\dot\tau_{n+1}^*$, i.e., for $\dot\tau_1^* = 1 - h$ and $\dot\tau_{n+1}^* = h'$, except when n is small, for example, $n = 1$ and $n = 3$, in which cases convergence was realized when $\dot\tau_{n+1}^* = h'$ and $\dot\tau_1^* = 1 - 4h$ (for $n = 1$), $\dot\tau_1^* = 1 - 2h$ (for $n = 3$).

The polynomial $f_n(t)$ invariably assumes its global maximum at $t = 1$, has a few much smaller relative maxima between the first few neighboring nodes τ_μ^* and τ_ν, and then settles down to magnitudes around 1 for the remaining portion of the interval [0, 1]. The condition of the problem, though slightly worse than in Example 5.1, is still remarkably good.

Numerical results for the nodes and weights of the $(2n + 1)$-point Gauss-Kronrod formula for $n = 5(5)25$ can be found in Table S.1 of the supplements section at the end of this issue. They have been computed in double precision to an accuracy of 25 decimal places after the decimal point. As the results are displayed in D-format, some of the end figures may not be reliable in those numbers that are much smaller than 1.

We used Example 5.2 to further experiment with alternative choices of initial approximations. In particular, we examined how inaccuracies in individual initial approximations affect the speed of convergence. To obtain a basis for meaningful comparison, we first obtained "reference" values for the number of iterations required when all initial approximations are at the same level of accuracy. This was achieved by imposing on the "exact" results for σ_ν, σ_μ^*, τ_μ^* (computed to 12 decimal digits) a random perturbation at level ε, i.e., by taking $\dot\sigma_\nu = \sigma_\nu(1 + r_\nu\varepsilon)$, $\dot\sigma_\mu^* = \sigma_\mu^*(1 + r_\mu^*\varepsilon)$, $\dot\tau_\mu^* = \tau_\mu^*(1 + s_\mu^*\varepsilon)$, where r_ν, r_μ^*, s_μ^* are random numbers from $[-1, 1]$. The results for $\varepsilon = 10^{-2}$, 10^{-5}, 10^{-8}, and 10^{-11} are shown in Table 5.3. (For $\varepsilon = 10^{-2}$ and $n = 40$, Newton's method did not converge within 20 iterations.)

TABLE 5.3

The number of iterations required for initial approximations at accuracy level ε.

ε	$n = 5$	$n = 10$	$n = 20$	$n = 40$
10^{-2}	6	6	5	—
10^{-5}	3	3	3	4
10^{-8}	2	2	2	2
10^{-11}	2	2	2	2

TABLE 5.4

The number of iterations required when two pairs of initial approximations (with indices μ and $n + 2 - \mu$) are inaccurate.

ε	$\mu = 1$				$\mu \approx n/4$				$\mu = n/2$			
	$n = 5$	$n = 10$	$n = 20$	$n = 40$	$n = 5$	$n = 10$	$n = 20$	$n = 40$	$n = 5$	$n = 10$	$n = 20$	$n = 40$
10^{-2}	5	4	6	6	5	4	6	5	4	4	5	6
10^{-5}	3	3	3	4	3	3	3	3	3	3	3	3
10^{-8}	2	2	2	2	2	2	2	2	2	2	2	2
10^{-11}	2	2	2	2	2	2	2	2	2	2	2	2

We now contrast this with the case in which all initial approximations are at the accuracy level $\frac{1}{2}10^{-12}$ of the initially computed results, except for two pairs of Kronrod nodes and weights (situated symmetrically with respect to the midpoint of the interval [0, 1]), which are randomly perturbed at level ε. Choosing the inaccurate pairs $\hat{\tau}_\mu^*$, $\hat{\sigma}_\mu^*$ to be those corresponding to $\mu = 1$, $\mu \approx n/4$, and $\mu \approx n/2$ (and to the symmetric indices $n + 2 - \mu$), we observed the results shown in Table 5.4.

Comparing Tables 5.3 and 5.4, we note some improvement, particularly for $\mu \approx n/2$, in the case $\varepsilon = 10^{-2}$, when only two pairs of initial approximations are inaccurate (though for $n = 20$ there are two instances of deterioration), but in all other cases the performance of Newton's iteration is practically the same. This seems to suggest that it is the maximum relative error in the initial approximations (usually associated with a Kronrod or Gauss node near the end of the interval) which determines the speed of convergence.

The choice of initial approximations proposed in Section 2 leads to initial (relative) errors that are reasonably small for "interior" nodes, but comparatively larger near the "boundary". Specifically, if we regard the three Kronrod nodes nearest to each of the endpoints of [0, 1], and the two Gauss nodes between them, as belonging to the "boundary", and all others to the "interior", then the relative errors of the initial approximations in our scheme range for $n = 10$, 20, 40 respectively from 2.0(−3) to 9.5(−2), 2.4(−5) to 5.5(−2), and 4.3(−6) to 2.9(−2) in the interior, and from 4.3(−3) to 5.4(−1), 1.3(−3) to 5.6(−1), and 3.3(−4) to 5.7(−1), respectively, at the boundary. The relatively large number of 6 iterations reported in Table 5.2 appears to be due to the large maximum error of the initial approximations in the boundary zones.

Attempts to improve the initial approximations for σ_ν by using, for example, $\sigma_\nu = \frac{1}{2}\sigma_\nu^{(n)}$,** where $\sigma_\nu^{(n)}$ are the Christoffel numbers for $d\sigma$, and by obtaining the remaining initial approximations σ_μ^* from a reduced system (2.2) of $n + 1$ linear equations, do not speed up Newton's iteration (in fact, require 7 iterations, instead of 6, when $n = 5$ and $n = 10$), precisely because of the initial approximations in the boundary zones remaining at the same low accuracy level.

Example 5.3. $d\sigma(t) = t^\alpha \ln(1/t)\,dt$ on [0, 1], $\alpha = \pm \frac{1}{2}$.

Modified moments with respect to the shifted Legendre polynomials are again available (Gautschi [7]) and suggest the same scaling as in Example 5.2. Results for

** This approximation was proposed to us by the referee.

TABLE 5.5

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = t^{1/2}\ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1 (scaled)	cond_2 (scaled)
5	6	1.03(4)	7.542	3.8(3)	7.8(4)
10	6	1.35(5)	14.64	7.3(4)	1.0(6)
20	6	2.06(6)	29.60	5.2(5)	1.4(7)
40	6	3.40(7)	61.04	1.4(7)	3.0(8)

TABLE 5.6

Newton's method for Gauss-Kronrod formulae with $d\sigma(t) = t^{-1/2}\ln(1/t)\,dt$ *on* $[0,1]$.

n	#iter.	$\|f_n\|_\infty$	$\|J_{\tilde{G}_n}\|_F$	cond_1 (scaled)	cond_2 (scaled)
4	7	9.78(6)	272.21	1.3(2)	9.0(5)
8	9	3.66(8)	889.01	2.0(3)	1.3(7)
16	9	1.52(10)	2961.5	6.3(3)	2.0(8)
32	—	6.56(11)	9907.2	8.8(3)	3.1(9)

$\alpha = \frac{1}{2}$ are summarized in Table 5.5. (The computation was done in double precision, the number of iterations referring again to 12 decimal place accuracy.) The performance of Newton's method is similar as in Example 5.2, except for the (scaled) matrices now being more ill-conditioned. The ill-conditioning of the Jacobian matrices is still worse in the case $\alpha = -\frac{1}{2}$, as can be seen from Table 5.6. For this value of α the independent variation of the starting approximations $\mathring{\tau}_1^*$, $\mathring{\tau}_{n+1}^*$ proved to be rather essential, since convergence was *never* achieved for the first choices of these starting values. This is in contrast to the case $\alpha = \frac{1}{2}$, where the first choice of $\mathring{\tau}_1^*$ and $\mathring{\tau}_{n+1}^*$ *always* worked.

When $\alpha = -\frac{1}{2}$, Newton's method could not be made to converge for $n = 32$, using the implementation described in Section 2. The difficulty, we believe, is caused by the smallest Kronrod node being almost equal to zero. Computing (in double precision) π_{33}^* by the procedure of Section 4, and applying Newton's method to π_{33}^*, we find $\tau_{33}^* = 3.05867\ldots \times 10^{-9}$. Using all zeros of π_{33}^* computed in this way as initial approximations to Newton's method, and lowering the accuracy requirement to 20 decimal places, indeed restores convergence and yields the data for $n = 32$ in Table 5.6 after 1 iteration.

Nonconvergence (in the case $\alpha = -\frac{1}{2}$) was also observed for odd values of n, this time because of the presence of negative Kronrod nodes. When $n = 1$, for example, one computes directly $\pi_2^*(t) = t^2 - (198/343)t - (3671/117649)$, which has the zeros $\tau_1^* = .627023\ldots$ and $\tau_2^* = -.0497636\ldots$. We verified that for all odd $n < 32$ the polynomial π_{n+1}^* has exactly one negative zero, while all other zeros are between 0 and 1.

Numerical results for $\alpha = \frac{1}{2}$, $n = 5(5)25$, computed in double precision, are given in Table S.2 and for $\alpha = -\frac{1}{2}$, $n = 4(4)24$, in Table S.3 of the supplements section at the end of this issue.

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Supplement to On Computing Gauss-Kronrod Quadrature Formulae

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Table S.1. Nodes and weights for (2n+1)-point Gauss-Kronrod quadrature with respect to the weight function ln(1/t) on [0,1], n=5(5)25.

n=5

nodes	weights
9.67031701131318416289952 6e-01	1.81767499850900484492328 0e-03
8.94771361031008283638886 2e-01	9.82051471045946484940182 0e-03
7.94645767443236515060041 3e-01	2.52814327985086117375012 0e-02
6.77314174582820380701802 7e-01	4.83594866241926530841399 4e-02
5.47424157227210764616793 8e-01	8.11198787994263227055992 9e-02
4.11702520284902043174931 9e-01	1.19288706310164035849216 8e-01
2.83390971298221704204244 1e-01	1.51525428452066710744088 0e-01
1.73977213320897628701139 7e-01	1.71520396734757562805552 2e-01
8.79312024647970401929077 8e-02	1.78553297070489267028154 7e-01
2.91344721519720533037267 6e-02	1.51862437516305822122338 8e-01
3.05545345037404760852227 6e-03	6.08507459871205442290839 6e-02

n=10

nodes	weights
9.90401456634661039922810 4e-01	1.53356918420764362300368 3e-04
9.68847988718633539391504 5e-01	8.48706824070665931073607 0e-04
9.37565090924901304376684 4e-01	2.28455683274578234646262 2e-03
8.98161091219003538166953 2e-01	4.67121172489448435671321 9e-03
8.50306269983725144609514 2e-01	8.46727336990677915455342 6e-03
7.94190416011966217358509 3e-01	1.37350742247182155487421 5e-02
7.31987286608171582474970 2e-01	2.00987429726411370129816 0e-02
6.65775205516424597222381 3e-01	2.76432528248589850930559 0e-02
5.96117116996000209231776 0e-01	3.68659535228178105859621 8e-02
5.23792317971843201161163 8e-01	4.71838278413364158790965 8e-02
4.51094020978795526121672 1e-01	5.73461316917431556072574 9e-02
3.80212539609332339723413 0e-01	6.73349195447911548765094 4e-02
3.11932719341955603323743 3e-01	7.78475891669607958237950 3e-02
2.47052416287159824222545 4e-01	8.74825885266359436050286 8e-02
1.87572713081066381251392 7e-01	9.38182691070552392235618 9e-02
1.35311824639250774870232 1e-01	9.68554451577195298865681 2e-02
9.06891671909172237641670 0e-02	9.79444646162853683897934 8e-02
5.39712662225006295042012 3e-02	9.45663602996504140017826 9e-02
2.64056462496855773849341 6e-02	8.19090031692669954909549 3e-02
9.04263096219965063694662 8e-03	5.77412517471011018682132 3e-02
1.28356233580538611425934 2e-03	2.52020199163792475393434 7e-02

n=15

nodes	weights
9.955062032210203065436479d-01	3.357815654243661548948029d-05
9.853644681221319389269624d-01	1.867299006875115946524248 8d-04
9.705026873648731297474113d-01	5.072275002553377098340643d-04
9.515061887434099027258391d-01	1.050963965210986765850134d-03
9.280162364465907698779526d-01	1.933104011942378729208846d-03
8.998820501208980843296834d-01	3.190889865704233456490884d-03
8.678381091713744037653244d-01	4.779034704112885950987212d-03
8.325480338661895892571129d-01	6.761018715645906314403643d-03
7.939725057930610180934046d-01	9.288478735472569416427278d-03
7.521788833787857987876117d-01	1.229726258478325504072739d-02
7.079314919075917433738803d-01	1.560484457034490029545047d-02
6.619629190124564213899423d-01	1.928734485028152522456972d-02
6.144114316079393925056921d-01	2.354129846195501191136131d-02
5.654734737918173064251632d-01	2.816306202293781318011909d-02
5.159281197251698686643213d-01	3.279359102818710839191692d-02
4.665243289647065826763175d-01	3.753740401570121850593575d-02
4.174740401607727232892736d-01	4.266259975028707391875499d-02
3.690151271397429438163725d-01	4.779519235886964106927171d-02
3.218836311092453561370282d-01	5.236357887389227516672947d-02
2.767728387061020243943043d-01	5.653057204376319250072220d-02
2.338769341974417732800076d-01	6.067668308282592292092547d-02
1.933952623740071159826138d-01	6.422040606380861029765769d-02
1.559511206003269465750938d-01	6.733689456591986450848039d-02
1.221019340733316033298185d-01	6.727951219688497202086968d-02
9.194826698918039456243045d-02	6.754806739613383019504674d-02
6.559609541231624525414253d-02	6.624118747605014469353877d-02
4.348667054615062384492759d-02	6.221849986611900460665585d-02
2.593589810533061610233579d-02	5.580103629888099937933513d-02
1.288587659395193488317299d-02	4.706544967830100544061973d-02
4.383110175475403834849363d-03	3.334061514932781411657855d-02
5.544989787418253709377232d-04	1.296387300298296570951722d-02

n=20

nodes	weights
9.974051747754021726815112d-01	1.119120386135197331240513d-05
9.915380814387119726524614d-01	6.234751867566481278122572d-05
9.829097100719784115576 80d-01	1.699213822344778312809097d-04
9.718227410752631937384774d-01	3.537458228177945904745 82d-04
9.580235839107271112957833d-01	6.541024959595038379628446d-04
9.413697491290916763026514d-01	1.086469275609816363649001d-03
9.222189523583085372003105d-01	1.640460188864980451721585d-03
9.008796808544175942234388d-01	2.343174789793118945570437d-03
8.772492102901398438038662d-01	3.251666542556207314358937d-03
8.512808927891257272221675d-01	4.353743132969725370633632d-03
8.233246692255883677771127d-01	5.600865664991813383103788d-03
7.937096719870858177436895d-01	7.030712225954972070510475d-03
7.624225990213010114195479d-01	8.719937994416142525644214d-03
7.294840839296874988710464d-01	1.061765292401797709138894d-02
6.952523574328258135406468d-01	1.262611533487395717731370d-02
6.600734133149094139120981d-01	1.479752460822837432037302d-02
6.239895863343987426462166d-01	1.723383714774471792170947d-02
5.870640449144099151324930d-01	1.983576301748516647055005d-02
5.496581314321561031264430d-01	2.244533076595314561155444d-02
5.121225946789673361956659d-01	2.513555268116814567548939d-02
4.745282547483664360892560d-01	2.804325139797733619155811d-02
4.369571400907683184866372d-01	3.101132662721120125912722d-02
3.997604567933887465725919d-01	3.380933829342717825506397d-02
3.632774298578589045379837d-01	3.654039370029929610073875d-02
3.275828306689844846935035d-01	3.939061773496089695800781d-02
2.927549609415458329919803d-01	4.213420134431541634237262d-02
2.591185891213443228759480d-01	4.445188330801194279595702d-02
2.269837872602025033612951d-01	4.648868081272922970010393d-02
1.964072043115371981322821d-01	4.850033897703557142277773d-02
1.674428562753296857182839d-01	5.017586276076158588044332d-02
1.403725658417845314584782d-01	5.107866276681074308046991d-02
1.154605264876331505588940d-01	5.140557152353493568631314d-02
9.272636361692522683481713d-02	5.150934294025731019836121d-02
7.218161381587390643496765d-02	5.095958907930292428817528d-02
5.404991045642136079431372d-02	4.912845927977704823331800d-02
3.853655037216532795984797d-02	4.623790878250996363663192d-02
2.560818311490157653026807d-02	4.277242840871254454932234d-02
1.520966234956023172065596d-02	3.807927322821316086752015d-02
7.485340063583503492186069d-03	3.094007479903797052858831d-02
2.588327955921955428332736d-03	2.079484873867849035127780d-02
3.694444650593027343659999d-04	8.577830778258255066645536d-03

n=45

nodes	weights
9.983128986278789961661727d-01	4.729985754717521273346377d-06
9.944848697646927524797932d-01	2.647340507732136315151368d-05
9.888707018544905070619272d-01	7.199064300278025408454537d-05
9.816252725992549675149930d-01	1.502106716669550701254493d-04
9.725798827984935169482453d-01	2.784375046786605260889035d-04
9.616242619673757147608422d-01	4.638338091686261124915172d-04
9.489694797742318211236809d-01	7.030013585363309559084309d-04
9.347912842966051819430816d-01	1.008639472797857140463509d-03
9.189964680454576632653927d-01	1.406182206148140074339552d-03
9.015261575671396041060695d-01	1.892437937744082111843870d-03
8.825755888546463808008079d-01	2.449660792497222859835327d-03
8.623241609572156561755193d-01	3.096482034768542390293309d-03
8.407290426227791410059593d-01	3.867639355338351711869998d-03
8.177687343472579e41766653d-01	4.745545010317325519987375d-03
7.936380012585329233399983d-01	5.694307421074741186615433d-03
7.685227343520897819970126d-01	6.740099545722766423514155d-03
7.424142881943629420746711d-01	7.928732158632907210959958d-03
7.153184705742639531113880d-01	9.224633590253314317443249d-03
6.874323255864890444271265d-01	1.057006525250185916087603d-02
6.585966883596468602996559d-01	1.200069918709648864070296d-02
6.298760168905099694178551d-01	1.357587857152964266004495d-02
6.002446666992273705187849d-01	1.523866396876478781028388d-02
5.702499338656883525432245d-01	1.690573309480445567093723d-02
5.400836112987538809360160d-01	1.862482598418693593120474d-02
5.097739109651696368322621d-01	2.047214000003285767200002d-02
4.793555262000715691454639d-01	2.236597150091422686086380d-02
4.490216872094010799525427d-01	2.419345798727057842045739d-02
4.185959764874968971593518940-01	2.601771135037998987e50332d-02
3.882032480187998615929326d-01	2.793602749240390594804615d-02
3.597894506450982806557797d-01	2.983822658434194257e655511d-02
3.309020855010095615519533d-01	3.157747162604635192411693d-02
3.027179664597163042391690-01	3.323623992979833823865307d-02
2.752681778745490731973764d-01	3.493787282825680011970966d-02
2.485857025771854935199340d-01	3.653916308723857770543239d-02
2.228388124017029203218251d-01	3.785406450471582696354310d-02
1.981872403062508468259920d-01	3.898867780858078184566833d-02
1.746530164035288454722222d-01	4.009693370952813168888747d-02
1.522591278588089225362797d-01	4.099605123816250223196770d-02
1.311523567594944725896411d-01	4.165449988655061776091333d-02
1.114683666474060405652694e-01	4.160496193672403588504229d-02
9.321492439096544167459447d-02	4.163137141338749000859714d-02
7.640165348265870132682356e-02	4.129905777685603175617267d-02
6.114754710816483918926005d-02	4.032437745861597724169167d-02
4.755526608752405384819518e-02	3.886247780176191811488868d-02
3.561500389827781933660593e-02	3.709691452349115977272900d-02
2.532505988961362761827773d-02	3.469902641990007619953950d-02
1.676872331051512741335331d-02	3.133194281532546447971416d-02
9.994559916853792794865875d-03	2.714251848602312161568686d-02
4.969956845265078995266501d-03	2.203114174961010079467786d-02
1.710007201966834333767190d-03	1.500267297611801902145656d-02
2.274019670687735033139105d-04	5.800224682854019005446604d-03

Table 5.2. Nodes and weights for (2n+1)-point Gauss-Kronrod quadrature with respect to the weight function $t^{\frac{1}{2}}\ln(1/t)$ on [0,1], n=5(5)25.

n=5

nodes	weights
9.696166053194431386034569d-01	1.518621703245064911238920d-03
9.029354976302693697440326d-01	7.918209630488931068085090d-03
8.101107288035271090849330d-01	1.940997445389493706984277d-02
7.001427291341351349085560-01	3.492536726049289162501093d-02
5.769087058030322490077738d-01	5.363653907515083214871332d-02
4.467123731948644671815189d-01	6.997805838224885451283229d-02
3.210905075966306604889925d-01	7.702597204357045876511760d-02
2.096522296417729123298881d-01	7.333914141939224778997501d-02
1.173877740538859158364745d-01	5.955012620582518424233754d-02
4.947701955575340163420805d-02	3.592188934246314021399989d-02
1.084416999952998905225187d-02	1.122054492767190248450108d-02

n=10

nodes	weights
9.908249255501930516574412 7d-01	1.394496855568403266934975 3d-04
9.702208699408183350814147d-01	7.635011344553433632030752d-04
9.402965553572893169161932d-01	2.024857904781604108051194d-03
9.025384582552350528421821d-01	4.063789872820607031523504d-03
8.566056607706870801969932d-01	7.183481599155638368766751d-03
8.026806142819284908704270d-01	1.128838106348526528619264d-02
7.427730638296861355174625d-01	1.592794681832925691177951d-02
6.787559328976017347207577 8d-01	2.101497313410452297902945d-02
6.111733227010825676487500d-01	2.665053956302234899354840d-02
5.408058388275156878481092d-01	3.214786468419731667118785d-02
4.697468016339130402377083d-01	3.658881203763763977491126d-02
3.999403178414447653361729d-01	3.990410808867376829491568d-02
3.322045316253965362431151d-01	4.223059844283214427758878d-02
2.674429071474993800705367d-01	4.276994109906270652661152d-02
2.074532308974391232607778d-01	4.082837576698908224519390d-02
1.538036758794403479214318d-01	3.688016299546247515745820-02
1.070797600006763569921467d-01	3.153900421376590286697619d-02
6.781818479343935804646819d-02	2.465406934320781026244711d-02
3.710840258661342680972846d-02	1.655591948554056584312295d-02
1.575165506971142895456201d-02	8.675097358006968358765139d-03
3.621722872729035900182115d-03	2.614018969261302497394738d-03

n=15

nodes	weights
9.95643773504402150269212 8d-01	3.14818808132415231982902 5d-05
9.85813045002747422228591 7d-01	1.74167937136333039660010 7d-04
9.71404533648623326617067 0d-01	4.69756633145998800004835 1d-04
9.52975452459569156189718 1d-01	9.64753385128543184524991 8d-04
9.30174686380313878023626 5d-01	1.75360863625944783678503 6d-03
9.02859719144113302853755 8d-01	2.85202344462342076240477 8d-03
8.71728710301631437341549 0d-01	4.20050174580017262404945 0d-03
8.37400182093495259748101 9d-01	5.83123952391102693376728 1d-03
7.99837056555364819815934 5d-01	7.83318517901293743461158 2d-03
7.59116871228825146022575 4d-01	1.01066362043361459428482 8d-02
7.15954258819360112972048 0d-01	1.24719464015280999522421 9d-02
6.71019668475771175520320 3d-01	1.49504227920329233082634 9d-02
6.24459214590402974184142 4d-01	1.76177831442071147466843 6d-02
5.76490752780406373079820 3d-01	2.02646872144811464010682 7d-02
5.27831062128445321115028 5d-01	2.26273967207295867078382 7d-02
4.79152057388494954674830 2d-01	2.47455218614955925251277 7d-02
4.30689335818532526257864 4d-01	2.66999359713331511904743 8d-02
3.82723076002376492348376 2d-01	2.82313154944806723761480 1d-02
3.35916718894954142246438 0d-01	2.90787380097467142062726 6d-02
2.90874452045300225063502 9d-01	2.93451934272609582974009 2d-02
2.47839518360907807481377 8d-01	2.91455373570220953004134 3d-02
2.07082744689410151841533 4d-01	2.82655423544220253732716 0d-02
1.69146520271921761905695 4d-01	2.65620717914509597528614 0d-02
1.34491320965156630672279 4d-01	2.42376257089911497672462 3d-02
1.03300200316981886145954 6d-01	2.14565766522664076656160 6d-02
7.57810623767204512737852 8d-02	1.81562838592545394030843 4d-02
5.22872658176984456788307 3d-02	1.44292115520404413432944 1d-02
3.30509104396267654458240 0d-02	1.05897201260988749850160 8d-02
1.81435740826475099625096 9d-02	6.86279382377153240933974 9d-03
7.69254299620694700608764 5d-03	3.49095842238695857616794 4d-03
1.75621755117794337533381 1d-03	9.97827189269862074502781 6d-04

n=20

nodes	weights
9.97466022372376299437749 5d-01	1.06584490553030992055462 7d-05
9.91736739732511708786748 9d-01	5.92014104890475414579590 7d-05
9.83310716080334187396099 8d-01	1.60678257552511762389867 6d-04
9.72479871445854812929755 5d-01	3.32771998396384782921741 5d-04
9.58996547497761359309517 5d-01	6.11097581106972947208056 3d-04
9.42722710065275214094708 0d-01	1.00639477984416420101220 5d-03
9.24003756107721584891853 7d-01	1.50491848427865341734177 3d-03
9.03133696854357605235889 7d-01	2.12628590326550202974534 9d-03
8.80012734782268122722629 8d-01	2.91320306836358780291751 4d-03
8.54599094304298524726738 4d-01	3.84426523352744852702245 0d-03
8.27226574822221080206685 2d-01	4.86841477561343576683866 0d-03
7.98204561960728583473498 0d-01	6.00765508761516857796831 4d-03
7.67523380570257552143191 5d-01	7.30864132189547514823056 5d-03
7.35210774414612521089336 7d-01	8.71189760439523163314043 7d-03
7.01604322215684147159254 1d-01	1.01288668936937520814403 1d-02
6.67024890961004688789463 1d-01	1.15866727280043360620213 0d-02
6.31521464352945896793477 3d-01	1.31361353397019766753838 5d-02
5.95168658509472565913101 4d-01	1.46833471183971201215840 3d-02
5.58302654760847952874149 9d-01	1.61114765890671555601347 3d-02
5.21243889165180447657242 4d-01	1.74586697317151112102806 4d-02
4.84075057321444614064871 55d-01	1.87832199291413452372070 9d-02
4.46896089573740410077705 1d-01	1.99692846558914680665965 8d-02
4.10028746522739753844117 6d-01	2.08893019030078795018431 5d-02
3.73777049353812307651423 9d-01	2.16001162330703032887477 4d-02
3.38234980216904485515077 7d-01	2.21721860984273186376655 9d-02
3.03507206093409080161319 3d-01	2.24868414621199634588616 5d-02
2.69884989144889183476237 2d-01	2.24288248340376869595301 0d-02
2.37638587301869290867022 5d-01	2.20804412794793108022673 9d-02
2.06853097717301087250328 5d-01	2.15279576676504101872172 2d-02
1.77619075174026913509047 6d-01	2.06723761082958011334714 4d-02
1.50180911704963792021103 1d-01	1.94353671917850482637646 1d-02
1.24758625047309300084531 5d-01	1.79279358548122326516915 4d-02
1.01411058557466667970698 1d-01	1.62535231761763615702102 5d-02
8.01978306432190934371848 8d-02	1.43560765852390394376271 3d-02
6.13015118801036415273969 4d-02	1.22169385315832828557214 3d-02
4.48786685751817689110744 6d-02	9.97636211505646882198368 9d-03
3.09468750244732678229702 7d-02	7.75974931937185584228273 6d-03
1.95155612358625214096384 7d-02	5.58204083518154685688934 d-03
1.06900982252147862857719 6d-02	3.51154664385278629091286 2d-03
4.55710823085100849820210 3d-03	1.74436587109262487753657 6d-03
1.05724317430265423667851 2d-03	4.98735794856762925371436 9d-04

n=25

nodes	weights
9.98344941085195078874402 1d-01	4.54810652661602385447256 9d-06
9.94599575389403546478010 9d-01	2.53091814193558414379201 5d-05
9.89082292025395282167094 0d-01	6.88979407164686546549374 3d-05
9.81973249178507450854444 2d-01	1.43271351566927513184116 5d-04
9.73096951932482148139114 3d-01	2.64380792207994813896508 4d-04
9.62346064735606517265490 8d-01	4.37963892228574925153016 6d-04
9.49926066867810058992925 0d-01	6.59625017110547381120773 7d-04
9.36006280343012622004119 5d-01	9.39739832836576620933004 9d-04
9.20495787224812234455288 7d-01	1.29931657729586401431800 8d-03
9.03338865524546560358325 4d-01	1.73227425119208922699909 4d-03
8.84723663517615236185270 9d-01	2.21982439675567788620928 3d-03
8.64820904271289343962113 3d-01	2.77540271940868629434072 0d-03
8.43590369114769034300048 8d-01	3.42417844140385227296932 2d-03
8.21014703390483505539451 9d-01	4.14510530034216538087922 8d-03
7.97279525604112463948846 7d-01	4.90361576951212706762285 3d-03
7.72559528535307428095447 5d-01	5.71671013389834946235638 8d-03
7.46849856397256259525608 1d-01	6.61315990100241062480474 1d-03
7.20162180274694218365676 9d-01	7.55626200440913699327439 6d-03
6.92682094972462289762739 1d-01	8.49669780170625645066258 2d-03
6.64586565188070662175996 9d-01	9.45591113279043036371214 2d-03
6.35895786126892598153024 1d-01	1.04661502362708299408066 5d-02
6.06642420398621586160115 36d-01	1.14768476020953312245106 9d-02
5.77009886396847520839104 1d-01	1.24274313452305233599935 8d-02
5.47173353448994964291402 3d-01	1.33450403929231899204879 5d-02
5.17169457888487783168630 8d-01	1.42655825780008526502789 7d-02
4.87044379140900347053730 4d-01	1.51287401895915668241057 6d-02
4.56974961969209566787342 0d-01	1.59884391678380504019323 5d-02
4.27129127116891546602465 0d-01	1.65188333121035579078940 0d-02
3.97552211837879238215883 8d-01	1.71196225642254402258893 4d-02
3.68296908275107603697547 0d-01	1.76067893593213332109863 0d-02
3.39527953722527429879549 3d-01	1.79162990997700911188329 5d-02
3.11399822052623671826413 0d-01	1.80902080223208903818625 7d-02
2.83959567542329100933859 1d-01	1.81715875507831479929432 1d-02
2.57260083491817334870659 2d-01	1.81001562068210664172390 2d-02
2.31447979240492959651258 3d-01	1.78226433134698386770825 2d-02
2.06657736585740219554441 0d-01	1.73888943638469066509046 8d-02
1.82932097367493227891886 9d-01	1.68439104560607169461305 8d-02
1.60318918195364400160088 0d-01	1.61394136829415507091998 9d-02
1.38940558268083079881309 88d-01	1.52421607972753377099470 2d-02
1.18904749119466541838769 4d-01	1.42083363566594004622198 9d-02
1.00245130631171715920649 9d-01	1.30822982852452077448009 1d-02
8.30009822040467726865569 9d-02	1.18366160744680404141419 0d-02
6.72642256840261551392252 5d-02	1.04676198880435559397278 9d-02
5.31082748473585877582409 6d-02	9.03551764182410601566365 0d-03
4.05544395113324594352962 8d-02	7.58159110249551988060199 5d-03
2.96327609544314286608260 6d-02	6.10997893132680565041176 3d-03
2.03975590488842400457926 4d-02	4.65815822380410437417471 5d-03
1.28755776788508931260996 9d-02	3.29152272063615135103980 3d-03
7.07280865915908581513269 9d-03	2.05517915204459160510854 1d-03
3.01545136223804377572067 2d-03	1.01303981304542816972524 0d-03
6.97454156103497918301235 5d-04	2.83642469631202005037019 9d-04

Table S.3. Nodes and weights for (2n+1)-point Gauss-Kronrod quadrature with respect to the weight function $t^{-\frac{1}{2}}\ln(1/t)$ on [0,1], n=4(4)24.

n=4

nodes	weights
9.46782386026081035032978 6d-01	4.89144005517918967237944 3d-03
8.32363768005759233298136 9d-01	2.77089860745405504796025 3d-02
6.80240349974324967179175 7d-01	7.57059508271950545423702 9d-02
5.14881089681188841074348 8d-01	1.54317530868933016163795 1d-01
3.49181092451776995876838 9d-01	2.89761009739017933257416 0d-01
1.95904505085884889417651 7d-01	5.13996393777814613178289 6d-01
7.84601808074503320660082 4d-02	8.34339417797833973686756 4d-01
1.60535125642731376395901 8d-02	1.09994310944647588665382 0d-00
8.02823938819877645287090 4d-04	9.99336161414009883626568 9d-01

n=8

nodes	weights
9.84710059921132691392047 2d-01	3.92691534644518531068525 1d-04
9.50551750261925188629962 47d-01	2.20211715324734315868157 4d-03
9.01497665509406246421451 6d-01	6.02399417222038803937204 0d-03
8.40790896415611993124758 5d-01	1.25439144556417729473186 7d-02
7.68613576466316286100272 6d-01	2.33879478999152417191066 4d-02
6.85966844443030567474398 8d-01	3.93944449197497028905148 2d-02
5.97284655108182627107116 9d-01	6.00143241865705856186630 0d-02
5.06989043048905204048091 4d-01	8.62407279962108205852229 4d-02
4.16648192244743176979481 0d-01	1.22184635936007787361305 0d-01
3.27851320433035244645676 0d-01	1.68888256384243453102285 1d-01
2.44975670316874579664341 6d-01	2.22396775268892149514232 8d-01
1.72265349694669771462838 9d-01	2.84223297053195736289458 6d-01
1.10611662416523745756170 7d-01	3.72561924014321746301673 5d-01
6.02663731942119449424290 5d-02	5.01616513356098043873999 7d-01
2.42043054826994488027387 6d-02	6.64037774861738878572255 9d-01
5.07944542153419435651866 8d-03	8.06064607386342503543205 0d-01
1.42845551968855828505632 9d-04	6.27826030068707581141016 4d-01

n=12

nodes	weights
9.928826120909483027505245d-01	8.458735678948550037906433d-05
9.768566552363760599297629d-01	4.733122955476183293624621d-04
9.534839312427130712288346d-01	1.295334109572110901102865d-03
9.238428533052712944323204d-01	2.706731683127645324403101d-03
8.875285378330856871129993d-01	5.043077178842719760579588d-03
8.444757119500635772136230d-01	8.464378140053237244756604d-03
7.961003718805113291006520d-01	1.290184488023427186184698d-02
7.437592675800603295615879d-01	1.860574263854033135894625d-02
6.876293672741867836731351d-01	2.620807444877358112292989d-02
6.280255610314505048355104d-01	3.574276734938528850187790d-02
5.664847326900428451563138d-01	4.674578998978516431564844d-02
5.045314832870891371017139d-01	5.967444746985659301284190d-02
4.425648565847031835767200d-01	7.589043686446729665694696d-02
3.809913524608552951366326d-01	9.526118334566874264250961d-02
3.213287813866706015400765d-01	1.163886052639084540070262d-01
2.650780200227866862700090d-01	1.401920773080115885220792d-01
2.125435271249162729620080d-01	1.703148279001835272137846d-01
1.639230168101155957295188d-01	2.067657388086946130994607d-01
1.205253501937517224566087d-01	2.453472778680508216014776d-01
8.364282470170227024739391d-02	2.878107462572700670782938d-01
5.319956262510167405639963d-02	3.488252075194488774741921d-01
2.890555423183584924268035d-02	4.371382853483828410959049d-01
1.170669272088357088680876d-02	5.443017169369761164032346d-01
2.493727677631593676683112d-03	6.448506073230140879888332d-01
4.489625718700550057552605d-05	4.689672017154149189815816d-01

n=16

nodes	weights
9.959030014166557799095396d-01	2.796696253016289349963365d-05
9.866515060015691419583797d-01	1.563618047866580836374612d-04
9.730831485036508224494794d-01	4.279841410648129644923035d-04
9.557246853516667872249829d-01	8.953718434721696512597104d-04
9.342322202953951064273636d-01	1.667823441448298692849240d-03
9.084410487719504138811946d-01	2.796503270116237469008471d-03
8.790043208903614626232110d-01	4.264562009906493149375904d-03
8.465172197510391627033991d-01	6.157778404042156270426219d-03
8.109094289793264441170613d-01	8.664296784171990168965690d-03
7.721954238899551020288427d-01	1.178914548971068376229409d-02
7.310578764357724062707320d-01	1.541622902607393697490992d-02
6.881636342918276232235943d-01	1.969368431901409029855592d-02
6.435911779555280266552427d-01	2.495318554310177071923101d-02
5.974569405535026844411241d-01	3.112637634051024021346720d-02
5.504729697239363220234514d-01	3.791883042163783807914079d-02
5.033457796482281675897882d-01	4.559175304495993122835237d-02
4.562129900337846201935433d-01	5.476881407984725842184861d-02
4.092153034701697007042927d-01	6.526768640264185711280638d-02
3.630574939867149728373585d-01	7.643814766072266748027824d-02
3.184402442336167895674019d-01	8.876066795067189137014152d-02
2.754787120787447394771186d-01	1.035400689846584558875641d-01
2.342596648033869713090313d-01	1.204351082860888829429207d-01
1.954353091919325313914467d-01	1.379688245775762562052125d-01
1.596557467773047315218671d-01	1.570768111358994027147340d-01
1.269382086713585331460270d-01	1.810410049158762565639792d-01
9.724006597479101015701976d-02	2.095536713187366192274676d-01
7.112145494114210204176551d-02	2.387506330915078037381027d-01
4.914898627259817786969019d-02	2.704017225795069274341500d-01
3.117122758336660397793752d-02	3.166546359013415213957580d-01
1.694404804397794929883851d-02	3.835631688506201888693871d-01
6.907658421540979336488189d-03	4.632613073104877219193036d-01
1.485765788500239757310222d-03	5.424729284517174404220322d-01
1.760376132934953188281986d-05	3.784969915426641107134499d-01

n=20

nodes	weights
9.97341430082074078852888 4e-01	1.17640608565415398120097 2e-05
9.91329941959464751556910 7e-01	6.57461056586267644533772 3e-05
9.82490101481697629383864 4e-01	1.79967333722845322595411 1e-04
9.71134424471491162351737 9e-01	3.76705869209853411920068 7e-04
9.57004729705305042798896 1e-01	7.01614283069972076815099 5e-04
9.39953155289654632510867 0e-01	1.17591376917305673447301 7e-03
9.20350516658714471667350 1e-01	1.79367240709410291859549 1e-03
8.98520984578427643017549 5e-01	2.59150079756150982093051 4e-03
8.74358636051275474067571 6e-01	3.64496819231087692669837 8e-03
8.47811128061996338736375 2e-01	4.95568884558447040696738 9e-03
8.19245829828610557013765 6e-01	6.48151608030112537873336 7e-03
7.89013759548540766973492 7e-01	8.28390334708987954090178 6e-03
7.57097244279626538242382 7e-01	1.04855394759299321692113 5e-02
7.23507931353071860441417 9e-01	1.30579147527205746890423 9e-02
6.88626846069046075235077 2e-01	1.59021903784699575108845 9e-02
6.52828809210597149952611 5e-01	1.91194608359753963285565 7e-02
6.16147650958679064650121 8e-01	2.29109977435094364092869 1e-02
5.78631141692631459533564 9e-01	2.72030576684044437901569 6e-02
5.40669398036845432656479 6e-01	3.18033181654805407888127 9e-02
5.02649850689443529403702 1e-01	3.68780871218750884017995 8e-02
4.64627457919388903772268 6e-01	4.27692526599442855664659 7e-02
4.26658671690005019620646 2e-01	4.93336879151533405113484 9e-02
3.89130324223788061425887 6e-01	5.62130116515416195044034 9e-02
3.52427804436560129008362 6e-01	6.36869561182945153377989 4e-02
3.16598922956079496473647 0e-01	7.23732795203808385910371 2e-02
2.81681539664853008524198 7e-01	8.20203981323731311643363 2e-02
2.48044588532030900105436 1e-01	9.19435996444339483630275 0e-02
2.16056796456662742451539 0e-01	1.02633881662607361682599 4e-02
1.85732193592513180220031 1e-01	1.15326548762012899016178 8e-01
1.57063421421493444574415 3e-01	1.29612084941104222172048 5e-01
1.30388161474044082031687 8e-01	1.44066375021882285934132 0e-01
1.06046927337080359871558 9e-01	1.59603169631693438689388 9e-01
8.39950717633919876043620 1e-02	1.79172853260915034676721 0e-01
6.41539753704582268768739 5e-02	2.02336655548793707991891 3e-01
4.68203446480249255077863 5e-02	2.25608725617278235988602 7e-01
3.22999564841955059336477 8e-02	2.50688578643727590841903 3e-01
2.04637662418347808227701 5e-02	2.87879556202207695986766 6e-01
1.11348676693581177129819 5e-02	3.41682752063558146262517 0e-01
4.56252255350894770464062 8e-03	4.05051115725954175780833 5e-01
9.88134882927999300817248 4e-04	4.71014651763223442071178 6e-01
7.51226336803836780380221 3e-06	3.19359331775268676314573 8e-01

n=24

nodes	weights
9.98136704819505113011533 3e-01	5.77529485527800338734624 0e-06
9.93920329641478198031410 5e-01	3.22693667842712704668873 6e-05
9.87711703968300246654166 0e-01	8.83338941033902492415932 9e-05
9.79716862280274971388472 5e-01	1.84952919649825622418078 7e-04
9.69742741663090421154098 1e-01	3.44451511466157062793470 0e-04
9.57668976918675062360409 2e-01	5.77171534309324161828718 2e-04
9.43734345533474275111045 8e-01	8.80510082827612197256185 8e-04
9.28141105187719671366123 9e-01	1.27257357711809843577814 9e-03
9.10790262806352100190820 2e-01	1.78956237847220413576305 1e-03
8.91619184437926990976442 5e-01	2.43221101499219511881905 4e-03
8.70853380099087872914275 7e-01	3.18154412230026294016417 4e-03
8.48703799160618554707443 4e-01	4.06749693307800248986435 9e-03
8.25126927877141567283679 2e-01	5.14641601648388313241329 7e-03
8.00100361872156801857701 0e-01	6.40478550962413622106512 7e-03
7.73853031949525585113693 7e-01	7.79997142503385755458364 0e-03
7.46607421174948847291967 8e-01	9.37944177479981061589093 0e-03
7.18355922033279402018274 0e-01	1.12296458441806406382583 6e-02
6.89103392914812429345730 8e-01	1.33167473618253695038113 6e-02
6.59084755504282628454875 0e-01	1.55630306930960362941308 3e-02
6.28531952671852297242518 2e-01	1.80420563920837279979177 5e-02
5.97459063978850568078960 9e-01	2.08871013897245273134288 4e-02
5.65886335138175422384456 4e-01	2.40350345840009446218349 5e-02
5.34051985907768523693078 0e-01	2.73539100099360257772247 4e-02
5.02192799807411568002435 4e-01	3.09573814682890244738074 2e-02
4.70331977712789179048848 7e-01	3.50554227662131331130159 9e-02
4.38493533819719851664726 4e-01	3.95414726960727674094044 3e-02
4.06914002983499053433366 2e-01	4.41950090059789144546565 7e-02
3.75829269529238708210244 0e-01	4.91940853514200492286739 9e-02
3.45259801195051197313408 1e-01	5.48828128729913117885750 7e-02
3.15221895275189606052616 8e-01	6.10880964295090405951216 0e-02
2.85944671248271349804147 2e-01	6.74340256899904043026845 1e-02
2.57657331737882173811854 9e-01	7.42079378403497463123888 1e-02
2.30366315303612219468329 0e-01	8.20102491997376197566461 0e-02
2.04068931105995019238901 2e-01	9.05636653230684928231809 3e-02
1.78981482333654905299301 6e-01	9.91922113563599643653142 8e-02
1.55321627883886718174138 6e-01	1.08381611960941600396604 4e-01
1.33071058199322669224966 0e-01	1.19289949049157782783004 0e-01
1.12197018914746517689495 8e-01	1.31485824659589240256743 7e-01
9.28987854055705842516807 8e-02	1.43628730619849588357352 8e-01
7.53794516228743044613801 4e-02	1.56592434554334812307439 5e-01
5.95855810901877312326743 2e-02	1.73038518760151516130016 6e-01
4.54429830805652072736084 0e-02	1.92472994039652978841087 2e-01
3.31314060294046311071861 8e-02	2.11753272361807390216779 5e-01
2.28384979097706249202119 7e-02	2.32482438201428254325534 1e-01
1.44636100798008414727384 6e-02	2.63572821168136773528652 2e-01
7.87829478980672462929712 5e-03	3.08539737066678505334205 1e-01
3.24116001346421600480497 0e-03	3.61107372927955520172454 7e-01
7.05635988016975760480240 9e-04	4.17938386824895391013820 5e-01
3.13993234848191405054430 6e-06	2.77378544174691013188757 8e-01

19.3. [103] "COMPUTING THE HILBERT TRANSFORM OF A JACOBI WEIGHT FUNCTION"

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[103] (with J. Wimp) "Computing the Hilbert Transform of a Jacobi Weight Function," *BIT* **27**, 203–215 (1987).

BIT 27 (1987), 203–215

COMPUTING THE HILBERT TRANSFORM OF A JACOBI WEIGHT FUNCTION (*)

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Abstract.

We discuss the evaluation of the Hilbert transform $\int_{-1}^{1}(t-\xi)^{-1}w^{(\alpha,\beta)}(t)dt$, $-1<\xi<1$, of the Jacobi weight function $w^{(\alpha,\beta)}(t)=(1-t)^{\alpha}(1+t)^{\beta}$ by analytic and numerical means and also comment on the recursive computation of the quantities $\int_{-1}^{1}(t-\xi)^{-1}\pi_n(t;w^{(\alpha,\beta)})w^{(\alpha,\beta)}(t)dt$, $n=0,1,2,\ldots$, where $\pi_n(\cdot;w^{(\alpha,\beta)})$ is the Jacobi polynomial of degree n.

AMS Categories: 65D30, 65D32, 65R10.

1. Introduction.

When computing singular integrals with a Jacobi-type weight function

$$(1.1)\quad w^{(\alpha,\beta)}(t)=(1-t)^{\alpha}(1+t)^{\beta},\qquad -1<t<1,\qquad \alpha>-1,\qquad \beta>-1,$$

as well as in the numerical solution of singular integral equations, it is often necessary to compute

$$(1.2)\quad \varrho_n(\xi;w^{(\alpha,\beta)})=\int_{-1}^{1}\frac{\pi_n(t;w^{(\alpha,\beta)})}{t-\xi}w^{(\alpha,\beta)}(t)dt,\quad -1<\xi<1,\quad n=0,1,2,\ldots,$$

where $\pi_n(\cdot;w^{(\alpha,\beta)})$ is the (monic) Jacobi polynomial of degree n and the integral on the right is a Cauchy principal value integral (see, e.g., [3, §§3.2.1–3.2.4]; the notation ϱ_n adopted here differs from the one in [3] by a sign factor). A simple way to generate the quantities $y_k=\varrho_k$ is by recursion,

$$(1.3)\quad y_{k+1}=(\xi-\alpha_k)y_k-\beta_k y_{k-1},\qquad k=0,1,2,\ldots,$$

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where

$$y_{-1} = -1, \qquad y_0 = \int_{-1}^{1} \frac{w^{(\alpha,\beta)}(t)}{t-\xi}\,dt, \tag{1.4}$$

and $\alpha_k = \alpha_k(\alpha,\beta)$, $\beta_k = \beta_k(\alpha,\beta)$ are the recursion coefficients for the monic Jacobi polynomials with parameters α, β. (It is assumed in (1.3) that $\beta_0 = \int_{-1}^{1} w^{(\alpha,\beta)}(t)dt$.) The problem, then, is reduced to the accurate computation of

$$\varrho_0^{(\alpha,\beta)}(\xi) = \varrho_0(\xi; w^{(\alpha,\beta)}) = \int_{-1}^{1} \frac{w^{(\alpha,\beta)}(t)}{t-\xi}\,dt, \quad -1 < \xi < 1,\ \alpha > -1,\ \beta > -1. \tag{1.5}$$

This is the main subject of the present note. The challenge of this problem is seen in arriving at a solution that is viable for a wide range of values of the parameters α, β. Since

$$\varrho_n(-\xi; w^{(\alpha,\beta)}) = (-1)^{n+1}\varrho_n(\xi; w^{(\beta,\alpha)}), \tag{1.6}$$

we will assume $0 \le \xi < 1$, without restriction of generality. Another concern is with the numerical stability of the recursion (1.3), (1.4).

In Section 2 we examine a number of possible alternatives for computing $\varrho_0^{(\alpha,\beta)}(\xi)$, discuss their relative merits, and end up recommending a procedure that combines numerical quadrature with analytic evaluation. Numerical illustrations and tests will be described in Section 3. In Section 4 we analyze the numerical stability of (1.3), (1.4) and exhibit a phenomenon of "pseudostability".

2. Analytic and numerical approaches.

We begin by recalling and analyzing an expression for (1.5) in terms of hypergeometric functions. We then discuss two methods based on numerical quadrature. Our method of choice is a combination of one of the latter with analytic evaluation.

2.1. *An analytic expression for* $\varrho_0^{(\alpha,\beta)}(\xi)$.

It is well known that (see, e.g. [2, §15.2, Eq. (33)])

$$\varrho_0^{(\alpha,\beta)}(\xi) = w^{(\alpha,\beta)}(\xi)\pi\cot\alpha\pi - \frac{2^{\alpha+\beta}\Gamma(\alpha)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}F(\tfrac{1}{2}-\tfrac{1}{2}\xi), \tag{2.1}$$

where

$$F(z) = {}_2F_1(1, -\alpha-\beta; 1-\alpha; z).$$

Using (see, e.g., [1, Eq. 15.3.3])

$$
\begin{aligned}
{}_2F_1(1, -\alpha-\beta; 1-\alpha; z) &= (1-z)^{\beta}\,{}_2F_1(-\alpha, 1+\beta; 1-\alpha; z) \\
&= (1-z)^{\beta}(-\alpha)\sum_{k=0}^{\infty}\frac{(1+\beta)_k}{k-\alpha}\frac{z^k}{k!},
\end{aligned}
$$

we can write (2.1) in the form

$$
\begin{aligned}
\varrho_0^{(\alpha,\beta)}(\xi) = w^{(\alpha,\beta)}(\xi)\Bigg\{\pi\cot\alpha\pi + \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}\sum_{k=0}^{\infty}\frac{(1+\beta)_k}{k!}\times \\
\times\frac{1}{k-\alpha}\left(\frac{1-\xi}{2}\right)^{k-\alpha}\Bigg\}.
\end{aligned}
\tag{2.2}
$$

This shows that for α near an integer $K \geq 0$, severe cancellation ensues (unless $\beta+1$ is small, comparable in magnitude to $|\alpha-K|$), the dominant term in the sum occurring for $k = K$ and the expression in curled parentheses assuming, approximately, the form $(\alpha-K)^{-1}+(K-\alpha)^{-1}$. Additional cancellation occurs in computing the term with $k = K$ in the summation, unless $K-\alpha$ is computed in double precision. The problem is not easily overcome and both formulae (2.2) and (2.1) are therefore unsuitable in the immediate vicinity of integer values of α. If $\beta+1$ is small, however, then either the term with $k = K$, $K > 0$, in the sum of (2.2) is no longer dominant, or, if $K = 0$, it is multiplied (outside the summation) by a quantity no longer close to unity, and the cancellation problem disappears. This observation will assume some significance later on.

Another, lesser difficulty, is associated with the fact that $\Gamma(\alpha+\beta+1)$ becomes infinite when $\alpha+\beta+1$ vanishes. It is safe, however, to neglect the second term in curled parentheses when $\alpha+\beta+1$ is close, or equal, to zero and α not close to zero.

An additional word of caution is in order concerning the use of (2.1), especially near integer values of α. To avoid loss of accuracy in the computation of the cotangent term, it is recommended that $\cot\alpha\pi$, when $|\alpha-K| \leq \frac{1}{2}$ for some integer $K \geq -1$, be computed by

$$
\cot\alpha\pi = \begin{cases} \cot(\alpha-K)\pi & \text{if } |\alpha-K| < \frac{1}{4}, \\ -\operatorname{sgn}(\alpha-K)\tan(|\alpha-K|-\frac{1}{2})\pi & \text{if } |\alpha-K| \geq \frac{1}{4}, \end{cases}
\tag{2.3}
$$

where $\alpha-K$ on the right is evaluated in double precision. It is also good practice to compute the arguments $\alpha+1$, $\beta+1$, $\alpha+\beta+1$ to the gamma function, and the argument $\frac{1}{2}-\frac{1}{2}\xi$ of F, in double precision and round the double precision arguments to single precision prior to evaluating the functions in question. This has always been done in the computations reported in Section 3.

2.2. *Contour integration.*

By Cauchy's theorem,

$$\int_{C_\varepsilon} \frac{w^{(\alpha,\beta)}(z)}{z-\xi}\,dz = 0, \tag{2.4}$$

where C_ε is the contour formed by the upper unit semicircle Γ and the interval $[-1,1]$, with ξ spared out by a small upper semicircle of radius ε. Letting $\varepsilon \downarrow 0$ yields

$$\begin{aligned}\varrho_0^{(\alpha,\beta)}(\xi) &= -i\pi w^{(\alpha,\beta)}(\xi) - \int_\Gamma \frac{w^{(\alpha,\beta)}(z)}{z-\xi}\,dz \\ &= -i\pi\left[w^{(\alpha,\beta)}(\xi) + I^{(\alpha,\beta)}(\xi)\right],\end{aligned}$$

where

$$I^{(\alpha,\beta)}(\xi) = \frac{1}{\pi}\int_0^\pi \frac{w^{(\alpha,\beta)}(e^{i\theta})}{1-\xi e^{-i\theta}}\,d\theta. \tag{2.5}$$

Therefore,

$$\varrho_0^{(\alpha,\beta)}(\xi) = \pi \operatorname{Im} I^{(\alpha,\beta)}(\xi). \tag{2.6}$$

Observing that

$$w^{(\alpha,\beta)}(e^{i\theta}) = 2^{\alpha+\beta} e^{-i\alpha\pi/2} e^{i(\alpha+\beta)\theta/2} \sin^\alpha\frac{\theta}{2}\cos^\beta\frac{\theta}{2},$$

and noting that near $\theta = 0$ this behaves like θ^α, and near π like $(\pi-\theta)^\beta$ (up to multiplicative constants), the use of Gauss-Jacobi quadrature is indicated with parameters β, α (note the reversal of parameters!); see also [6] for a similar application. Thus, transforming to the standard interval $[-1,1]$, we first write

$$I^{(\alpha,\beta)}(\xi) = 2^{\alpha+\beta-1} e^{i(\beta-\alpha)\pi/4} \int_{-1}^1 f(t;\xi) w^{(\beta,\alpha)}(t)\,dt, \tag{2.7}$$

where

$$f(t;\xi) = \frac{e^{i(\alpha+\beta)t\pi/4}}{1-\xi e^{-i(t+1)\pi/2}}\left[\frac{\sin((t+1)\pi/4)}{1+t}\right]^\alpha\left[\frac{\cos((t+1)\pi/4)}{1-t}\right]^\beta \tag{2.8}$$

is regular for $t \in [-1,1]$, and then approximate

$$I^{(\alpha,\beta)}(\xi) \approx 2^{\alpha+\beta-1} e^{i(\beta-\alpha)\pi/4} \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu;\xi), \tag{2.9}$$

where $\tau_\nu = \tau_\nu^{(n)}(\beta,\alpha)$ are the zeros of $\pi_n(\cdot\,; w^{(\beta,\alpha)})$ and $\lambda_\nu = \lambda_\nu^{(n)}(\beta,\alpha)$ the corre-

sponding Christoffel numbers. Even for moderate values of n, Eq. (2.9) in general provides a good approximation to $I^{(\alpha,\beta)}(\xi)$, and hence to $\varrho_0^{(\alpha,\beta)}(\xi)$ in (2.6), unless ξ is close to 1. If ξ is near 1, the pole

$$p_0 = -1 + \frac{2}{\pi} i \ln(1/\xi) \tag{2.10}$$

of f closest to $[-1, 1]$ inhibits convergence of the Gauss-Jacobi integration. (The other poles $p_k = p_0 + 4k$, $k = \pm 1, \pm 2, \ldots$, are sufficiently far away from $[-1, 1]$ to have much effect on convergence.) It is well known, however, how to take the pole p_0 into account in order to restore satisfactory convergence (see, e.g., [5, Eq. (3.5)]): Use

$$\int_{-1}^{1} f(t;\xi) w^{(\beta,\alpha)}(t)dt \approx \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu;\xi) + K_n(p_0)(\operatorname{res} f)_{p_0}, \tag{2.11}$$

where

$$K_n(p_0) = \frac{\varrho_n(p_0; w^{(\beta,\alpha)})}{\pi_n(p_0; w^{(\beta,\alpha)})}, \tag{2.12}$$

and $(\operatorname{res} f)_{p_0}$ denotes the residue of f at p_0,

$$\begin{aligned}(\operatorname{res} f)_{p_0} &= e^{i(\beta\varphi - (\alpha+1)\pi/2)} \left[\frac{\pi}{2} \frac{1-\xi}{\ln(1/\xi)}\right]^{\alpha} \left[\frac{\pi}{2} \frac{1+\xi}{\sqrt{(\pi^2 + \ln^2(1/\xi))}}\right]^{\beta}, \\ \varphi &= \tan^{-1}\left(\frac{1}{\pi} \ln(1/\xi)\right).\end{aligned} \tag{2.13}$$

The kernel $K_n(p_0)$ can be computed recursively: ϱ_n (as minimal solution of (1.3), where $\alpha_k = \alpha_k(\beta, \alpha)$, $\beta_k = \beta_k(\beta, \alpha)$ and ξ is to be replaced by p_0) by backward recursion and π_n by forward recursion; cf. [5, §4]. The approximation (2.11) is quite accurate, uniformly in α, β and ξ; see Section 3 for numerical examples. The main difficulty with (2.11) is the computation of ϱ_n when ξ is very close to 1; in this case, minimality of ϱ_n is weak, rendering the backward recursion process slowly convergent, and thus prohibitively expensive.

2.3. *A combined analytic-numerical approach.*

We write (2.2) in the form

$$\varrho_0^{(\alpha,\beta)}(\xi) = w^{(\alpha,\beta)}(\xi)\pi \cot \alpha\pi + \frac{2^\alpha \Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)} (1+\xi)^\beta \phi^{(\alpha,\beta)}(\tfrac{1}{2} - \tfrac{1}{2}\xi), \tag{2.14}$$

where

$$\phi^{(\alpha,\beta)}(z) = \sum_{k=0}^{\infty} \frac{(1+\beta)_k}{k-\alpha} \frac{z^k}{k!}, \tag{2.15}$$

and use the relation

$$\varrho_0^{(\alpha,\beta)}(0) = \pi\cot\alpha\pi + \frac{2^\alpha\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}\phi^{(\alpha,\beta)}(\tfrac{1}{2}) \tag{2.16}$$

to eliminate the term $\pi\cot\alpha\pi$ in (2.14); the result is

$$\begin{aligned}\varrho_0^{(\alpha,\beta)}(\xi) &= w^{(\alpha,\beta)}(\xi)\varrho_0^{(\alpha,\beta)}(0)\\ &- \frac{2^\alpha\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}(1+\xi)^\beta\left[(1-\xi)^\alpha\phi^{(\alpha,\beta)}(\tfrac{1}{2}) - \phi^{(\alpha,\beta)}(\tfrac{1}{2}-\tfrac{1}{2}\xi)\right].\end{aligned} \tag{2.17}$$

Here, $\varrho_0^{(\alpha,\beta)}(0)$ can be well approximated by numerical quadrature (cf. (2.6)–(2.9)),

$$\varrho_0^{(\alpha,\beta)}(0) \approx 2^{\alpha+\beta-1}\pi\,\mathrm{Im}\left\{e^{i(\beta-\alpha)\pi/4}\sum_{\nu=1}^{n}\lambda_\nu f(\tau_\nu;0)\right\}, \tag{2.18}$$

unless $\beta+1$ is small, in which case the quadrature sum in (2.18) may be severely inaccurate, for reasons discussed later in Section 3. Lesser inaccuracies occur also when α is large or α and β both are large, in part due to cancellation errors in the quadrature sum. Yet another problem with (2.17) arises when β is large but α is not. Then, if $\xi > 0$, the first term in brackets of (2.17) is quite large and dominates the second, so that

$$\begin{aligned}\varrho_0^{(\alpha,\beta)}(\xi) &\approx w^{(\alpha,\beta)}(\xi)\left[\varrho_0^{(\alpha,\beta)}(0) - \frac{2^\alpha\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}\phi^{(\alpha,\beta)}(\tfrac{1}{2})\right]\\ &= w^{(\alpha,\beta)}(\xi)\pi\cot\alpha\pi\end{aligned}$$

by (2.16). Here, both terms in brackets are large, but produce the result $\pi\cot\alpha\pi$, not necessarily large (unless α is near an integer). Some cancellation, therefore, is unavoidable.

Eq. (2.17), like (2.14), still suffers from severe cancellation errors when α is near an integer $K \geq 0$. The problem, however, is more easily controlled in (2.17) than in (2.14). Let, indeed,

$$K-\tfrac{1}{2} \leq \alpha < K+\tfrac{1}{2} \text{ for some integer } K \geq 0. \tag{2.19}$$

Then (2.17) is rewritten in the form

$$\begin{aligned}\varrho_0^{(\alpha,\beta)}(\xi) &= w^{(\alpha,\beta)}(\xi)\varrho_0^{(\alpha,\beta)}(0) - \frac{2^\alpha\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}(1+\xi)^\beta\times\\ &\times\left[\frac{(1+\beta)_K}{K!}\left(\frac{1-\xi}{2}\right)^K\cdot\frac{1-(1-\xi)^{\alpha-K}}{\alpha-K} + (1-\xi)^\alpha\phi_K^{(\alpha,\beta)}(\tfrac{1}{2}) - \phi_K^{(\alpha,\beta)}(\tfrac{1}{2}-\tfrac{1}{2}\xi)\right],\end{aligned} \tag{2.20}$$

where

$$\phi_K^{(\alpha,\beta)}(z) = \sum_{\substack{k=0 \\ k\neq K}}^{\infty} \frac{(1+\beta)_k}{k-\alpha} \frac{z^k}{k!}. \tag{2.21}$$

The original cancellation problem is now focused in the term $(1-(1-\xi)^{\alpha-K})/(\alpha-K)$, which, however, with some care, can be computed to full accuracy.

In summary, we have at our disposal two formulas – Eq. (2.14) and Eq. (2.20) – for computing $\varrho_0^{(\alpha,\beta)}(\xi)$. To a certain extent, they complement each other: When α is close (or equal) to an integer, (2.14) is useless, while (2.20) is quite effective. If β is large, or both α and β are large, (2.20) becomes inaccurate, while (2.14) is usually quite accurate (unless α is near an integer, of course). For β very close to -1, cancellation errors in the computation of $\varrho_0^{(\alpha,\beta)}(0)$ by quadrature may produce an inaccurate result in (2.20), whereas (2.14) is accurate, even when α is close to an integer. On the other hand, (2.20) is more expensive to compute than (2.14), since it requires the generation of Jacobi quadrature rules and the determination of an appropriate n in (2.18). Note, however, that in the case $\alpha = \beta$, since $\varrho_0^{(\alpha,\beta)}(0) = 0$ by symmetry, no quadrature is required in (2.20).

Our recommended procedure, therefore, is to first apply (2.14) (unless α is exactly an integer) and to monitor the amount of cancellation between the two terms in (2.14). If this amount is not excessive, we accept the result of (2.14) as our final answer. Otherwise, we proceed to (2.20) and once again monitor the combined amount of cancellation between the two principal terms in (2.20) and in the quadrature sum of (2.18). If that amount is less than the one observed previously in (2.14), we accept the result of (2.20) as the final answer; otherwise, we hold on to the value computed initially by (2.14). This procedure not only produces the desired answer, but also provides us with an indication of its accuracy.

In principle, it would suffice to consider the parameter range $-1 < \alpha \leq 0$, $-1 < \beta \leq 0$, since [1])

$$\begin{aligned} \varrho_0^{(\alpha+1,\beta)}(\xi) &= \left[\frac{2(\alpha+1)}{\alpha+\beta+2} - (\xi-\alpha_0)\right]\varrho_0^{(\alpha,\beta)}(\xi) - \beta_0, \\ \varrho_0^{(\alpha,\beta+1)}(\xi) &= \left[\frac{2(\beta+1)}{\alpha+\beta+2} + (\xi-\alpha_0)\right]\varrho_0^{(\alpha,\beta)}(\xi) + \beta_0, \end{aligned} \tag{2.22}$$

as follows from [7, Eq. (4.5.4), with $n = 0$] (rewritten in terms of monic polynomials) and (1.3), with $k = 0$ and (1.4). However, we have not implemented this idea.

[1]) The authors are indebted to the referee for this remark.

3. Numerical results and tests.

All computations reported in this section were carried out on the CDC 6500 computer in single or double precision, as indicated. The machine accuracy in single precision is approx. 3.55×10^{-15}.

Table 3.1. *Relative errors incurred in Eq.* (2.14) *near integer values of* α. (Integers in parentheses denote decimal exponents.)

β	ε	$\alpha = \varepsilon$			$\alpha = 5+\varepsilon$			$\alpha = 10+\varepsilon$		
		$\xi = 0$	$\xi = .5$	$\xi = .99$	$\xi = 0$	$\xi = .5$	$\xi = .99$	$\xi = 0$	$\xi = .5$	$\xi = .99$
$-1+10^{-8}$	1.(−1)	1.(−14)	2.(−14)	2.(−14)	8.(−15)	4.(−15)	1.(−14)	4.(−14)	3.(−14)	5.(−14)
	1.(−5)	2.(−14)	2.(−14)	2.(−14)	3.(−15)	1.(−14)	3.(−15)	5.(−14)	4.(−14)	5.(−14)
	1.(−9)	4.(−13)	2.(−13)	4.(−13)	5.(−15)	5.(−15)	5.(−15)	1.(−13)	1.(−13)	1.(−13)
−.9	1.(−1)	3.(−14)	3.(−14)	3.(−14)	5.(−14)	4.(−14)	4.(−14)	2.(−14)	1.(−14)	4.(−14)
	1.(−5)	2.(−10)	2.(−10)	1.(−10)	9.(−12)	3.(−13)	2.(−14)	4.(−13)	5.(−15)	1.(−14)
	1.(−9)	3.(−6)	3.(−6)	2.(−6)	1.(−7)	4.(−9)	2.(−14)	1.(−10)	1.(−14)	3.(−14)
−.5	1.(−1)	1.(−13)	8.(−14)	5.(−14)	1.(−13)	5.(−14)	4.(−14)	1.(−13)	7.(−14)	6.(−14)
	1.(−5)	4.(−10)	6.(−10)	1.(−10)	4.(−11)	2.(−12)	3.(−14)	7.(−12)	5.(−14)	3.(−14)
	1.(−9)	2.(−5)	1.(−5)	3.(−6)	8.(−7)	4.(−8)	5.(−14)	4.(−8)	6.(−11)	1.(−14)
0.	1.(−1)	4.(−13)	1.(−13)	5.(−14)	7.(−14)	1.(−13)	3.(−14)	8.(−14)	7.(−14)	4.(−14)
	1.(−5)	5.(−5)	9.(−10)	2.(−10)	9.(−11)	6.(−12)	3.(−14)	6.(−12)	9.(−14)	3.(−14)
	1.(−9)	6.(+3)	1.(−5)	3.(−6)	7.(−7)	3.(−8)	3.(−14)	4.(−8)	9.(−11)	3.(−14)
2.5	1.(−1)	2.(−13)	3.(−15)	4.(−14)	7.(−14)	1.(−14)	9.(−15)	1.(−13)	8.(−14)	5.(−14)
	1.(−5)	2.(−10)	4.(−10)	3.(−11)	2.(−10)	4.(−11)	2.(−14)	5.(−10)	3.(−12)	7.(−14)
	1.(−9)	1.(−6)	4.(−6)	3.(−6)	1.(−5)	1.(−6)	4.(−14)	5.(−6)	3.(−8)	7.(−14)
5.	1.(−1)	2.(−13)	1.(−13)	8.(−15)	1.(−11)	1.(−13)	5.(−14)	1.(−13)	1.(−14)	4.(−14)
	1.(−5)	2.(−10)	1.(−9)	1.(−9)	2.(−4)	2.(−10)	1.(−14)	7.(−12)	2.(−12)	2.(−15)
	1.(−9)	6.(−8)	1.(−6)	3.(−7)	1.(0)	2.(−7)	4.(−14)	1.(−5)	1.(−7)	5.(−14)
10.	1.(−1)	6.(−14)	1.(−13)	6.(−13)	5.(−13)	1.(−12)	2.(−13)	2.(−11)	1.(−13)	1.(−13)
	1.(−5)	5.(−11)	1.(−9)	6.(−9)	2.(−9)	5.(−9)	7.(−14)	6.(−6)	2.(−11)	1.(−14)
	1.(−9)	3.(−7)	7.(−6)	3.(−5)	3.(−5)	5.(−5)	5.(−12)	3.(+6)	8.(−7)	3.(−14)

We begin by illustrating the numerical performance of Eq. (2.14) near integer values of α. We computed $\varrho_0^{(\alpha,\beta)}(\xi)$ for $\alpha = \varepsilon$, $\alpha = 5+\varepsilon$, $\alpha = 10+\varepsilon$; $\beta = -.99999999$, $-.9$, $-.5$, 0., 2.5, 5., 10.; $\xi = 0.$, .5, .99, where $\varepsilon = 10^{-1}$, 10^{-5}, 10^{-9}. The relative errors (rounded to one decimal digit) are shown in Table 3.1. (Double precision results were used as "exact" reference values.) The degradation of accuracy as $\varepsilon \downarrow 0$ is clearly visible, although it is less pronounced for ξ near 1, particularly when α is relatively large, and virtually nonexistent when β is very close to -1. Large relative errors must be expected, of course, when $\alpha \approx \beta$ and $\xi \approx 0$, since $\varrho_0^{(\alpha,\beta)}(\xi)$ then almost vanishes.

We next illustrate the use of the quadrature formulae (2.9) and (2.11), in particular, the effect of the correction term in (2.11). The results for $\alpha = 0.$, $\beta = -.5$ (computed in double precision) are displayed in Table 3.2 and are fairly representative. Shown are the relative errors for the n-point quadrature formulae,

$n = 4(4)16$, in Eq. (2.9) and Eq. (2.11), respectively. Also shown in the last two columns are the starting indices ν and ν_d required to compute ϱ_n, $1 \leq n \leq 20$, in (2.12) to 14 and 20 correct decimal digits, respectively, by backward recursion. It is seen that the correction term in (2.11) is rather effective, but costly in terms of the number of backward recurrence steps, when ξ is close to 1. Also to be noted is the fast convergence of the quadrature rule (2.9) when $\xi = 0$.

Table 3.2. *Accuracy of the quadrature formulae* (2.9) *and* (2.11) *for* $\alpha = 0.$, $\beta = -.5$, $\xi = 0., .5, .99$ *and* $n = 4(4)16$.

ξ	n	err. (2.9)	err. (2.11)	ν	ν_d
0.	4	3.(−7)	–		
	8	2.(−13)	–		
	12	1.(−19)	–		
	16	7.(−26)	–		
.5	4	4.(−3)	5.(−7)	45	55
	8	1.(−5)	2.(−13)		
	12	1.(−7)	2.(−19)		
	16	1.(−10)	2.(−25)		
.99	4	3.(−1)	5.(−8)	226	313
	8	6.(−2)	2.(−14)		
	12	2.(−2)	1.(−20)		
	16	5.(−2)	4.(−27)		

For larger values of α it was found that when $\xi > 0$ the quadrature formula (2.9) generally converges faster, and the formula (2.11) more slowly, while for $\xi = 0$ the formula (2.9) becomes more slowly convergent.

Table 3.3. *Largest Gauss-Jacobi nodes* $\tau_1 = \tau_1^{(n)}(\beta, \alpha)$ *and corresponding weights* $\lambda_1 = \lambda_1^{(n)}(\beta, \alpha)$, $n = 4(4)16$, *for* $\alpha = 0$ *and* β *near* -1.

β	n	τ_1	λ_1
−.99	4	.998...	9.8270...(1)
	8	.9996...	9.6934...(1)
	12	.9998...	9.6155...(1)
	16	.99992...	9.5604...(1)
−.9999	4	.99998...	9.998245...(3)
	8	.999996...	9.996875...(3)
	12	.999998...	9.996067...(3)
	16	.9999992...	9.995493...(3)
−.99999999	4	.999999998...	9.999998997...(7)
	8	.9999999996...	9.999998860...(7)
	12	.9999999998...	9.999998779...(7)
	16	.99999999992...	9.999998721...(7)

There is a phenomenon, however, that adversely affects both quadrature

formulae (2.9) and (2.11), even when $\xi = 0$: As β approaches -1, the largest Gauss-Jacobi node τ_1 in (2.9) [or (2.11)] approaches 1 very rapidly and causes considerable cancellation error in the evaluation of $f(\tau_1; \xi)$ in (2.8). What is worse, the corresponding weight λ_1 is unusually large, making the inaccurate term $\lambda_1 f(\tau_1; \xi)$ dominant in the quadrature sum of (2.9) [or (2.11)]. As an illustration, we show numerical values of $\tau_1 = \tau_1^{(n)}(\beta, \alpha)$ and $\lambda_1 = \lambda_1^{(n)}(\beta, \alpha)$ in Table 3.3 for $\alpha = 0.$, $\beta = -.99$, $-.9999$, $-.99999999$. One can see, for example, that for these three values of β one must expect a loss of about 4, 6 and 10 decimal digits, respectively, in the evaluation of the quadrature sums in (2.9) and (2.11), when $n = 16$.

Eq. (2.14), on the other hand, is a viable alternative, unless α is exactly an integer, or very close to an integer; see, e.g., the top rows in Table 3.1.

Other instances of cancellation error in the quadrature sum of (2.18) occur when α and β are both large and n is relatively large. For example, in the 32-point quadrature sum, a loss of 3 decimal digits was observed when $\alpha = 10$, $\beta = 20$ or $\alpha = 20$, $\beta = 10$. Also, the accuracy of the Gauss-Jacobi nodes, and hence of the terms in the quadrature sum, seems to deteriorate somewhat as α gets larger.

We now report on two tests conducted with our proposed procedure. In the first test we evaluated $\varrho_0^{(\alpha,\beta)}(\xi)$ for $\alpha, \beta = -.9, -.6, -.3, 0., .3, .6, .9, 1.5, 2., 3.5, 5., 7.5, 10., 15., 20.$ and $\xi = 0., .5, .99$ in both single and double precision and used the latter results to determine the accuracy of the former.

Table 3.4. *Accuracy test for* $\varrho_0^{(\alpha,\beta)}(\xi)$.

α	β	ξ	err	α	β	ξ	err	α	β	ξ	err
0.	−.9	0.	2.(−11)	5.	10.	0.	6.(−12)	−.3	20.	.99	1.(−11)
		.5	2.(−11)			.5	1.(−11)	0.	20.	.5	1.(−10)
		.99	1.(−11)	15.	10.	0.	4.(−11)			.99	4.(−9)
5.	−.9	0.	6.(−11)	20.	10.	0.	2.(−10)	2.	20.	0.	6.(−12)
15.	−.9	0.	9.(−11)	0.	15.	.5	2.(−11)			.5	2.(−9)
20.	−.9	0.	4.(−11)			.99	3.(−10)			.99	1.(−10)
.9	3.5	.5	6.(−12)	2.	15.	.5	5.(−11)	5.	20.	0.	6.(−12)
10.	5.	0.	7.(−12)	5.	15.	.5	4.(−10)			.5	4.(−10)
2.	7.5	.5	8.(−12)	10.	15.	0.	5.(−11)	10.	20.	0.	4.(−11)
15.	7.5	0.	4.(−11)			.5	2.(−11)			.5	1.(−10)
20.	7.5	0.	8.(−11)	20.	15.	0.	2.(−9)	15.	20.	0.	4.(−10)
0.	10.	.99	7.(−12)			.5	6.(−12)			.5	5.(−11)

We asked for convergence to 12 correct decimal digits of the Gauss-Jacobi quadrature (when applicable) in single precision, and for 20 correct decimal digits in double precision. Table 3.4 shows all instances in which the relative error exceeded $5. \times 10^{-12}$ (about 10 times the accuracy level in the Gauss-Jacobi quadrature rule). The majority of these instances (disregarding $\alpha = \beta$, $\xi = 0$) involve integer values of α, hence Eq. (2.20), and reflect inaccuracies in the Gauss

formula, either because β is near -1 (in the first four instances of Table 3.4), or because β, or both α and β, are large. Only two cases are connected with Eq. (2.14), namely $\alpha = .9$, $\beta = 3.5$, in which case α is relatively close to 1 and there is a cancellation of two digits (the maximum tolerated) in Eq. (2.14), and $\alpha = -.3$, $\beta = 20.$, when again 2 digits cancelled, but more digits would have cancelled in Eq. (2.20), owing to a large β.

The fact that among all 675 cases computed, only 36 exhibit mild inaccuracies, and then mostly for relatively large (and probably unlikely) values of the parameters α, β, attests to the viability of the procedure proposed. Also, as far as the speed of convergence of the Gauss-Jacobi quadrature rule is concerned, no unreasonably large values of n were required, typically $n = 16$ to 24 for single precision, and $n = 20$ to 28 for double precision.

In our second test we evaluated $\varrho_0^{(\alpha,\beta)}(\xi)$ for a total of 1200 values of α, β and ξ, chosen randomly in the intervals $-1 < \alpha < 1$, $-1 < \beta < 1$, $0 < \xi < 1$, in order to observe the relative frequency of usage of Eqs. (2.20) and (2.14). Interestingly (and encouragingly), the "expensive" equation (2.20) was invoked only 12 times, i.e., in 1 percent of all cases, and with one exception because of α having fallen close to an integer (-1, 0, or 1). In the exceptional case, the result $\varrho_0^{(\alpha,\beta)}(\xi)$ was unusually small. The number n of quadrature points required, almost invariably, was 12 for single precision and 16 for double precision. In only 6 cases (.5 percent) did the relative error exceed $5. \times 10^{-12}$ (but remained less than $9. \times 10^{-11}$), each time cancellation (and an exceptionally small $\varrho_0^{(\alpha,\beta)}$) having been the reason. Our error monitoring scheme diagnosed the problems correctly in every instance.

4. Stability of the recursion for $\{\varrho_n\}$.

We now discuss the stability of the recursion (1.3) for computing $y_n = \varrho_n(\xi; w^{(\alpha,\beta)})$, $n = 1, 2, 3, \ldots$, from starting values $y_{-1} = -1$, $y_0 = \varrho_0^{(\alpha,\beta)}(\xi)$. For values of α and β in the interval $(-1, 1]$, and values of ξ in $[0, 1)$, the recursion (1.3) was found to be quite stable. Curiously, and somewhat surprisingly, when α becomes large and ξ approaches 1, a phenomenon of "pseudostability" develops. To describe it, we first introduce a quantity that characterizes the stability of the initial value problem (1.3), (1.4).

Let $\{y_n\}$ be the exact solution and $\{y_n^*\}$ a perturbed solution corresponding to initial values $y_0^* = y_0(1+\varepsilon_0)$, $y_1^* = y_1(1+\varepsilon_1)$, where $|\varepsilon_i| \leq \varepsilon$, $i = 0, 1$, and ε is small. Elementary theory of difference equations then shows that

$$\frac{y_n^* - y_n}{y_n} = \frac{(z_1/y_1 - z_n/y_n)\varepsilon_0 - (z_0/y_0 - z_n/y_n)\varepsilon_1}{z_1/y_1 - z_0/y_0}, \tag{3.1}$$

where $\{z_n\}$ is any solution of (1.3), linearly independent of $\{y_n\}$. (We assume

$y_0 y_1 y_n \neq 0$.) The quantity

$$\omega_n = \frac{|z_1/y_1 - z_n/y_n| + |z_0/y_0 - z_n/y_n|}{|z_1/y_1 - z_0/y_0|} \tag{3.2}$$

therefore measures the amplification of relative error in y_n due to relative errors in y_0 and y_1. Since the left-hand side in (3.1) does not depend on the choice of the second solution $\{z_n\}$, the same must be true for the quantity ω_n. By "pseudostability" we mean that, while ω_n does not tend to infinity as $n \to \infty$, it grows rapidly and eventually "settles" at a level that may be extremely large, though bounded as $n \to \infty$.

This is precisely what seems to be happening as α increases and ξ approaches 1. We illustrate the phenomenon in Figure 3.1, where $\log_{10} \omega_n$ is depicted for $1 \leq n \leq 50$ in the case $\alpha = 10.$, $\beta = 0.$, and $\xi = .7, .9, .99$.

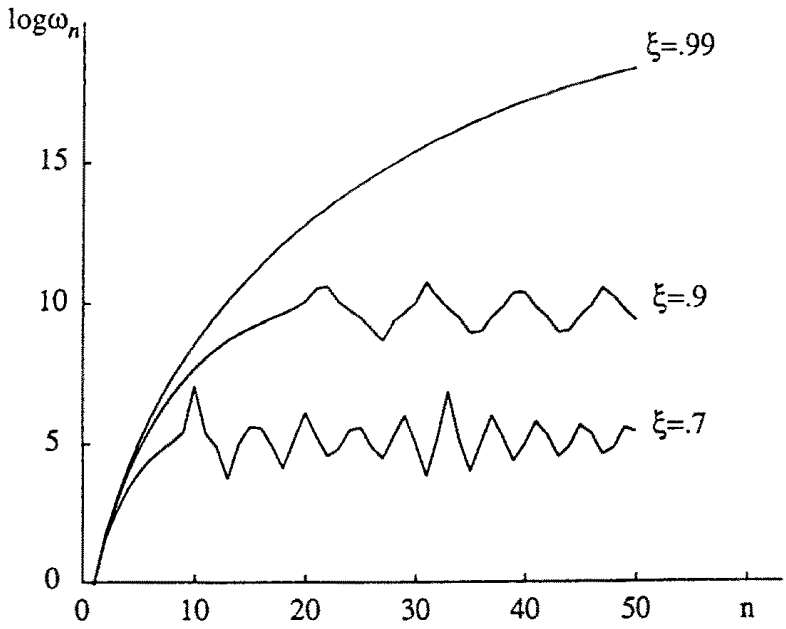

Fig. 3.1. Pseudostability of (1.3), (1.4) for $\alpha = 10$, $\beta = 0$ and $\xi = .7, .9, .99$.

As second solution $\{z_n\}$ we took the one with initial values $z_{-1} = \varrho_0$, $z_0 = 1$, so that $y_0 z_{-1} - y_{-1} z_0 = \varrho_0^2 + 1 \neq 0$, and $\{z_n\}$ is indeed linearly independent of $\{y_n\}$.

It is seen that, when $\xi = .7$, one must expect to lose about 5 decimal digits by the time n reaches 10; when $\xi = .9$, about 10 decimal digits as n becomes 20; and when $\xi = .99$, about 18 digits for $n = 50$ and even more for larger n. This was indeed observed numerically. The phenomenon becomes more pronounced with increasing α, and somewhat less pronounced with increasing β. It is also present for smaller values of ξ, even for $\xi = 0$, but in a much weaker form.

A similar case of pseudostability was observed in [4] in a different context, which was simple enough to yield to mathematical analysis. In the present case, a rigorous analysis of the phenomenon appears to be a more challenging task.

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GAUSS-KRONROD QUADRATURE - A SURVEY*

WALTER GAUTSCHI

Abstract. Kronrod in 1964 proposed to extend the n-point Gauss-Legendre quadrature rule to a $(2n + 1)$-point formula by inserting $n+1$ additional points and making the extended quadrature rule to have maximum degree of exactness, hence suitable for estimating the error in the original Gauss formula. The nodes to be inserted can be characterized as zeros of a polynomial orthogonal with respect to a certain sign-variable weight function depending on n. The same type of orthogonality has previously been considered by Stieltjes and Szegö without reference to quadrature. We survey the considerable literature on this subject that has evolved after the work of Kronrod.

1. Introduction. Historically, the subject to be discussed here comes from two different mathematical developments: One originates with Stieltjes in 1894, the other, much more recently, with the Russian mathematician Kronrod in 1964. Although their motivations were different, the ideas involved lead to the same theory.

1894 was the year that saw the publication of Stieltjes' momentous work on continued fractions and the moment problem, his last effort of will before succumbing to a long illness at the end of the same year. Underlying Stieltjes' theory is the integral

$$S(z) = \int_{\mathbb{R}} \frac{ds(t)}{z-t}, \quad z \in \mathbb{C}, \tag{1.1}$$

and its development in continued fractions, where ds is a positive measure supported on the positive real line. Having just completed this major theory, it must have seemed natural to Stieltjes to explore how it could be extended, in particular, what could be said if the measure ds were no

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longer assumed to be supported on $\mathbb{R}_+$ and to have constant sign. What, for example, would happen if one took a typical oscillatory measure, like $ds(t) = P_n(t)dt$ on $[-1,1]$, where P_n is the Legendre polynomial of degree n?

In a letter to Hermite, dated November 8, 1894 (in fact, his last letter in the life-long correspondence with Hermite; see Baillaud and Bourget [1905, v.2, pp. 439–441]), Stieltjes indeed looks at (what is now called) Legendre's function of the second kind

$$Q_n(z) = \int_{-1}^{1} \frac{P_n(t)}{z-t}\, dt, \tag{1.2}$$

expands it into descending powers of z (beginning with $z^{-(n+1)}$ by orthogonality of P_n) and then has the fortunate idea of expanding the reciprocal of Q_n,

$$\frac{1}{Q_n(z)} = z^{n+1}(\mu_0^{(n)} + \mu_1^{(n)} z^{-1} + \cdots), \quad \mu_0^{(n)} \neq 0. \tag{1.3}$$

This led him naturally to consider the polynomial part in (1.3),

$$E_{n+1}(z) = z^{n+1}(\mu_0^{(n)} + \mu_1^{(n)} z^{-1} + \cdots + \mu_{n+1}^{(n)} z^{-(n+1)}), \tag{1.4}$$

a polynomial of exact degree $n + 1$, now appropriately called *Stieltjes' polynomial*, and to investigate its properties. By a residue calculation, he first observes that

$$E_{n+1}(t) = \frac{1}{2\pi i} \oint_C \frac{dz}{(z-t)Q_n(z)}, \tag{1.5}$$

where C is a sufficiently large contour, and then goes on to multiply (1.5) by $t^k P_n(t)dt$, $k = 0, 1, \ldots, n$, and to integrate, obtaining

$$\int_{-1}^{1} E_{n+1}(t) t^k P_n(t)dt = \frac{1}{2\pi i} \oint_C \frac{dz}{Q_n(z)} \int_{-1}^{1} \frac{t^k P_n(t)}{z-t}\, dt$$

$$= \frac{1}{2\pi i} \oint_C \frac{dz}{Q_n(z)} \int_{-1}^{1} \frac{z^k - (z^k - t^k)}{z-t} P_n(t)dt$$

$$= \frac{1}{2\pi i} \oint_C \frac{z^k dz}{Q_n(z)} \int_{-1}^{1} \frac{P_n(t)}{z-t}\, dt$$

$$= \frac{1}{2\pi i} \oint_C z^k\, dz = 0,$$

where orthogonality of P_n is used in the third equality. Thus,

$$\int_{-1}^{1} E_{n+1}(t)p(t)P_n(t)dt = 0, \text{ all } p \in \mathbf{P}_n, \tag{1.6}$$

that is, Stieltjes' polynomial E_{n+1} *is orthogonal to all lower-degree polynomials relative to the* (sign-variable) *measure* $ds(t) = P_n(t)dt$.

At this point, Stieltjes conjectures (1) that E_{n+1} has $n + 1$ real simple zeros, all contained in $(-1,1)$ and (2) that they separate those of P_n. He presents a numerical example with $n = 4$. He furthermore believes (strongly so in the case of reality and simplicity of the roots, less so for the separation property) that this is a special case of "a much more general theorem".

In his reply (of November 10, 1894), Hermite expressed his delight in the polynomials E_{n+1} and "the beautiful properties" conjectured for it and encouraged Stieltjes to look for a differential equation as a possible key to these properties. Stieltjes may have already been too ill to respond. Neither he, nor anybody else after him was able to give an affirmative answer to Hermite's suggestion. (It has been found, nevertheless, that the Stieltjes polynomials, at least in the realm of Jacobi measures $d\sigma^{(\alpha,\beta)}(t) = (1-t)^{\alpha}(1+t)^{\beta}\, dt$, do *not* satisfy a three-term recurrence relation unless $|\alpha| = |\beta| = \frac{1}{2}$, in which case they do, and in fact also satisfy a differential equation; cf. Monegato [1982].)

Stieltjes' ideas seem to have gone unnoticed for many years. Geronimus in 1930, however, developed similar ideas, considering in place of (1.3) the expansion of $[Q_n(z)\sqrt{z^2-1}]^{-1}$, where $Q_n(z) = \int_{-1}^{1} \pi_n(t\,; wdt)w(t)dt/(z-t)$ and $\pi_n(\cdot\,; wdt)$ is the nth degree orthogonal polynomial associated with the weight function $w(t) = (1-t)^{\alpha}(1+t)^{\beta}\, h(t)$, h being continuous and positive on $[-1,1]$ (Geronimus [1930]). Although this approach does not lead to a perfect orthogonality result, like the one in (1.6), it nevertheless has relevance to the subject at hand; see the beginning of Subsection 3.5 below.

The first who has taken up Stieltjes' challenge in earnest was Szegö in 1935. He expresses (Szegö [1935]) Stieltjes' polynomial on the circle as a cosine polynomial,

$$E_{n+1}(\cos\theta) = \lambda_0^{(n)} \cos(n+1)\theta + \lambda_1^{(n)} \cos(n-1)\theta + \cdots, \tag{1.7}$$

and relates an extended (infinite) sequence $\lambda_\nu = \lambda_\nu^{(n)}$ to an explicitly known sequence $f_\nu = f_\nu^{(n)}$ via a reciprocity identity for the respective power series. From this he proves $\lambda_0 > 0$ and the negativity of all λ_ν, $\nu \geq 1$, as well as $\sum_{\nu=0}^{\infty} \lambda_\nu = 0$. It follows from this that the polynomial $\lambda_0 z^{n+1} + \lambda_1 z^{n-1} + \cdots$ has all its zeros in $|z| < 1$, which implies, via the argument principle, that (1.7) vanishes at least $2n + 2$ times. This proves Stieltjes' first conjecture. Szegö also proves the second conjecture, but this requires a deeper analysis involving, in particular, Legendre functions on the cut.

Szegö's analysis is not peculiar to Legendre polynomials. Indeed, he himself extends it to Gegenbauer polynomials $P_n^{(\lambda)}$, orthogonal on $[-1,1]$ with respect to the measure $d\sigma(t) = (1-t^2)^{\lambda-\frac{1}{2}}dt$, $\lambda > -\frac{1}{2}$. If $E_{n+1}^{(\lambda)}$ denotes the corresponding Stieltjes polynomial,

$$\int_{-1}^{1} E_{n+1}^{(\lambda)}(t)p(t)P_n^{(\lambda)}(t)(1-t^2)^{\lambda-\frac{1}{2}}dt = 0, \quad \text{all } p \in \mathbf{P}_n, \tag{1.8}$$

which (up to a multiplicative constant) is uniquely defined, then Szegö shows that both conjectures of Stieltjes continue to hold for $0 < \lambda \leq 2$. When $\lambda=0$, two zeros of $E_{n+1}^{(\lambda)}$ move into the endpoints ± 1; they move outside of $[-1,1]$ for $\lambda<0$, as is shown by the example $n=2$. The question of whether the same can happen for $\lambda>2$ is left unanswered by Szegö. (The answer is still unknown today, but, according to Table 3.1 below, is probably "no", at least as long as the interlacing property holds.)

Szegö concludes by considering the Gaussian quadrature formula for the (sign-variable) measure $ds(t) = P_n(t)dt$ and shows that its weights alternate in sign.

This brings us naturally to the work of Kronrod in 1964, which is also concerned with quadrature. Motivated by a desire to economically estimate the error in the classical Gaussian quadrature formula

$$\int_{-1}^{1} f(t)dt \approx \sum_{\nu=1}^{n} \gamma_\nu f(\tau_\nu), \tag{1.9}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the Legendre polynomial P_n and $\gamma_\nu = \gamma_\nu^{(n)}$ the corresponding Christoffel numbers, Kronrod [1964a,b] proposes to extend the n-point formula (1.9) to a $(2n + 1)$-point formula

$$\int_{-1}^{1} f(t)dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f), \tag{1.10}$$

in which the τ_ν are the same as in (1.9), but new nodes τ_μ^* and new weights σ_ν, σ_μ^* have been introduced and chosen to increase the degree of exactness from $2n - 1$ (for (1.9)) to $3n + 1$ (for (1.10)), i.e.,

$$R_n(f) = 0, \text{ all } f \in \mathbb{P}_{3n+1}. \tag{1.11}$$

It turns out that the nodes τ_μ^* must be precisely the zeros of Stieltjes' polynomial E_{n+1}. With all nodes τ_ν, τ_μ^* at hand, it is then easy to determine the weights σ_ν, σ_μ^* by interpolation.

In the same manner, one can try to extend the Gauss-Gegenbauer quadrature formula to a formula of the type

$$\int_{-1}^{1} f(t)(1-t^2)^{\lambda-\frac{1}{2}}\, dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f), \quad \lambda > -\tfrac{1}{2}, \tag{1.12}$$

and, more generally, to do the same for an integral with arbitrary (positive) measure $d\sigma$,

$$\int_{-1}^{1} f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f), \quad R_n(\mathbb{P}_{3n+1}) = 0. \tag{1.13}$$

(The dependence of the nodes and weights on n and $d\sigma$ will from now on be suppressed in our notation.) The new nodes τ_μ^*, similarly as before, are then the zeros of the (unique, monic) polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot\,; d\sigma)$ satisfying the orthogonality property

$$\int_{\mathbb{R}} \pi_{n+1}^*(t)p(t)\pi_n(t)d\sigma(t) = 0, \text{ all } p \in \mathbb{P}_n, \tag{1.14}$$

where $\pi_n(\cdot) = \pi_n(\cdot\,; d\sigma)$ is the orthogonal polynomial of degree n associated with the measure $d\sigma$. To be useful in practice, the formulae (1.12), (1.13) should have nodes τ_μ^* which are all contained in the support interval of $d\sigma$ and are different from the τ_ν, and they should have weights σ_ν, σ_μ^* which, if at all possible, are all positive. By Szegö's theory, we know that the former is

true for (1.12), if $0 < \lambda \leq 2$, while the latter has been proven true by Monegato [1978a] if $0 \leq \lambda \leq 1$, hence, in particular, for the original Gauss-Kronrod formula (1.10) (which corresponds to $\lambda = 1/2$).

Soon after Kronrod's work, it has occurred to a number of people (probably first to Patterson [1968a]) that other quadrature rules can be similarly extended, for example, the Gauss-Lobatto rule. In addition, it is not unreasonable to also consider the interpolatory quadrature rule based solely on the nodes τ_μ^* in (1.13). In the case of (1.10), numerical results suggest that these quadrature rules also have all weights positive and enjoy an interlacing property of their own: the zeros of E_{n+1} alternate with those of E_n; cf. Monegato [1982]. Indeed, having three quadrature rules at disposal – the one just mentioned, the Gauss rule (1.9), and (1.10) – with degrees of exactness roughly equal to n, $2n$ and $3n$, respectively, might well be an attractive feature that could be useful in automatic integration schemes (Kahaner [1987]).

Orthogonality with respect to sign-variable measures and related quadrature rules have independently been studied by Struble [1963], who develops a general theory. It might be interesting to explore this theory in the framework of more general indefinite inner product spaces (cf., e.g., Bognár [1974]).

The merit of discovering the connection between Kronrod's work and the earlier work of Stieltjes and Szegö is due to Mysovskih [1964], although it has been noted, independently, in the Western literature, by Barrucand [1970]. The relevance of Geronimus' work to Gauss-Kronrod quadrature is pointed out by Monegato [1982] and Monegato and Palamara Orsi [1985].

Brief accounts of the Kronrod and Patterson methods can be found in Davis and Rabinowitz [1984, pp. 106–109, 426] and Atkinson [1978, pp. 243–248].

2. Extended quadrature formulae. We now give a more systematic treatment of the problem of extending quadrature rules. We begin with a general theorem, which has become part of "folklore" in numerical quadrature and is difficult to attribute to any one in particular. In its key ingredients, it goes back to Jacobi [1826].

Let $d\sigma$ be a nonnegative measure on the real line $\mathbf{R}$, with bounded or unbounded support and with infinitely many points of increase. Assume that all its moments $\mu_k = \int_{\mathbf{R}} t^k d\sigma(t)$ exist and are finite. We consider quadrature rules of the form

$$\int_{\mathbf{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{N} \sigma_\nu f(\tau_\nu) + R_N(f), \tag{2.1}$$

where τ_ν, σ_ν are real and $N \geq 1$ an integer. We say that (2.1) has *degree of exactness* d if $R_N(f) = 0$ for every $f \in \mathbf{P}_d$, the class of polynomials of degree $\leq d$. We associate with (2.1) the polynomial

$$\omega(t) = \prod_{\nu=1}^{N} (t - \tau_\nu) \tag{2.2}$$

and call it the *node polynomial*. The theorem in question then reads as follows.

Theorem. *The quadrature rule* (2.1) *has degree of exactness* $d = N - 1 + k$, $k \geq 0$, *if and only if both of the following conditions are satisfied:*

(i) (2.1) *is interpolatory* (i.e., $d = N-1$);

(ii) $\int_{\mathbf{R}} \omega(t)p(t)d\sigma(t) = 0$ *for all* $p \in \mathbf{P}_{k-1}$.

We remark that polynomial degree of exactness $N-1$ (the case $k=0$ of the theorem) can always be achieved, simply by interpolating at the nodes τ_ν; this is condition (i) of the theorem. To get higher degree of exactness ($k>0$), the node polynomial, according to (ii), has to be orthogonal (relative to the measure $d\sigma$) to sufficiently many polynomials. If we have complete freedom in the choice of τ_ν and σ_ν, we can take k as large as $k=N$, in which case (ii) identifies $\omega(\cdot)$ with the (monic) orthogonal polynomial $\pi_N(\cdot\,; d\sigma)$ of degree N associated with the measure $d\sigma$, and the nodes τ_ν in (2.1) with its zeros. This, of course, is the well-known Gauss-Christoffel quadrature rule (cf., e.g., Gautschi [1981]).

The situation we are going to consider here is somewhat different: We shall assume that some of the nodes are prescribed and the rest variable. Let

$$N = N^\circ + N^*, \tag{2.3}$$

and suppose the prescribed (distinct) nodes are $\tau_1, \tau_2, \ldots, \tau_{N^\circ}$; we denote the remaining ones by

$$\tau_\mu^* = \tau_{N^\circ+\mu}, \quad \mu = 1, 2, \ldots, N^*. \tag{2.4}$$

Correspondingly, we let $\sigma_\mu^* = \sigma_{N^\circ+\mu}$ and write (2.1) in the form

$$\int_{\mathbf{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{N^\circ} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{N^*} \sigma_\mu^* f(\tau_\mu^*) + R_N(f). \tag{2.5}$$

We may interpret (2.5) as an "extension" of some quadrature rule

$$\int_{\mathbf{R}} f(t)d\sigma(t) \doteq \sum_{\nu=1}^{N^\circ} \gamma_\nu f(\tau_\nu). \tag{2.6}$$

The degree of exactness of (2.6) is quite irrelevant for what follows, as the weights γ_ν are being discarded.

Putting

$$\pi_{N^\circ}^\circ(t) = \prod_{\nu=1}^{N^\circ} (t - \tau_\nu), \quad \pi_{N^*}^*(t) = \prod_{\mu=1}^{N^*} (t - t_\mu^*), \tag{2.7}$$

the theorem above, since $\omega(t) = \pi_{N^\circ}^\circ(t)\pi_{N^*}^*(t)$, becomes:

Corollary. *The quadrature formula* (2.5) *has degree of exactness* $d = N - 1 + k$, $k \geq 0$, *with N given by* (2.3), *if and only if it is interpolatory and the polynomial* $\pi_{N^*}^*$ *satisfies*

$$\int_{\mathbf{R}} \pi_{N^*}^*(t)p(t)\pi_{N^\circ}^\circ(t)d\sigma(t) = 0, \quad \textit{all} \quad p \in \mathbf{P}_{k-1}. \tag{2.8_k}$$

One expects the maximum degree of exactness to be realized for $k = N^*$ (there are $N + N^*$ degrees of freedom!), in which case (2.8_k) becomes

$$\int_{\mathbf{R}} \pi_{N^*}^*(t)p(t)\pi_{N^\circ}^\circ(t)d\sigma(t) = 0, \quad \text{all} \quad p \in \mathbf{P}_{N^*-1}. \tag{2.8_{N^*}}$$

We call (2.5) an *optimal extension* of (2.6) if $k = N^*$, i.e., if (2.8_{N^*}) holds, and a *nonoptimal* [*interpolatory*] *extension* if (2.8_k) holds with $0 \leq k < N^*$ [k=0]. (We assume $p \equiv 0$ in (2.8_k) if k=0.) Thus, (2.5) is an optimal extension of (2.6) if and only if $\pi_{N^*}^*$ *is orthogonal to all lower-degree polynomials with respect to the* (sign-variable) *measure* $d\sigma^*(t) = \pi_{N^\circ}^\circ(t)d\sigma(t)$. Here is how sign-variable measures enter into the process of extending quadrature rules.

We now discuss a number of specific examples.

Example 2.1: Gauss-Kronrod formulae.

This is the case $N^\circ = n$, $\pi_{N^\circ}(\cdot) = \pi_n(\cdot\,; d\sigma)$, $N^* = n+1$, so that $N = 2n + 1$, $d = 3n + 1$, and (2.8_{N^*}) takes the form

$$\int_{\mathbf{R}} \pi^*_{n+1}(t)p(t)\pi_n(t\,; d\sigma)d\sigma(t) = 0, \quad \text{all} \quad p \in \mathbf{P}_n. \tag{2.9}$$

(We must necessarily have $N^* \geq n + 1$ in this case; cf. Monegato [1980].) In other words, the classical n-point Gauss-Christoffel formula is optimally extended to a $(2n + 1)$-point formula of the form

$$\int_{\mathbf{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma^*_\mu f(\tau^*_\mu) + R_n(f). \tag{2.10}$$

The measure involved in the orthogonality relation (2.9) is $d\sigma^*(t) = \pi_n(t\,; d\sigma)d\sigma(t)$, which for $d\sigma(t) = dt$ is precisely the one considered by Stieltjes. We call π^*_{n+1} in (2.9) the *Stieltjes polynomial* associated with $d\sigma$ and denote it by $\pi^*_{n+1}(\cdot) = \pi^*_{n+1}(\cdot\,; d\sigma)$. It is easily seen that π^*_{n+1} (assumed monic of degree $n+1$) is uniquely determined by (2.9).

For the weights in (2.10) one finds (see, e.g., Monegato [1976])

$$\begin{aligned} \sigma_\nu &= \gamma_\nu + \frac{\|\pi_n\|^2_{d\sigma}}{\pi^*_{n+1}(\tau_\nu)\,\pi'_n(\tau_\nu)}, \qquad \nu = 1, 2, \ldots, n; \\ \sigma^*_\mu &= \frac{\|\pi_n\|^2_{d\sigma}}{\pi_n(\tau^*_\mu)\,\pi^{*\prime}_{n+1}(\tau^*_\mu)}, \qquad \mu = 1, 2, \ldots, n+1, \end{aligned} \tag{2.11}$$

where $\gamma_\nu = \gamma_\nu^{(n)}(d\sigma)$ are the Christoffel numbers, and $\|\cdot\|_{d\sigma}$ the L_2-norm for the measure $d\sigma$.

For symmetric measures, i.e., $d\sigma(-t) = d\sigma(t)$ and the support of $d\sigma$ symmetric with respect to the origin, it follows easily from uniqueness that

$$\pi_n(-t\,; d\sigma) = (-1)^n\, \pi_n(t\,; d\sigma), \quad \pi^*_{n+1}(-t\,; d\sigma) = (-1)^{n+1}\, \pi^*_{n+1}(t\,; d\sigma) \quad (d\sigma \text{ symmetric}), \tag{2.12}$$

so that (2.9) holds trivially for even polynomials p and is therefore valid for all $p \in \mathbf{P}_{n+1}$ if n is odd. Thus, $d = 3n + 1$ if n is even, and $d = 3n + 2$ if n is odd. (In special cases, the degree of exactness can be even higher; see Subsections 3.3 and 3.5 for examples.)

Example 2.2: Kronrod extension of Gauss-Radau formulae.

For definiteness we consider only the Radau formula with fixed node τ_0 at -1. The case $\tau_0 = 1$ is treated similarly.

We assume that $d\sigma$ is supported on $[-1,1]$ and that the measure $(1+t)d\sigma(t)$ allows $(2n+1)$-point Kronrod extension, i.e., the Stieltjes polynomial $\pi^*_{n+1}(\cdot\,;(1+t)d\sigma)$ has distinct real zeros, all in $(-1,1)$ and all different from the zeros of $\pi_n(\cdot\,;(1+t)d\sigma)$. Then there exists a unique optimal extension of the Gauss-Radau formula for the measure $d\sigma$. It has the form

$$\int_{-1}^{1} f(t)d\sigma(t) = \sigma_0 f(-1) + \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma^*_\mu f(\tau^*_\mu) + R_n(f) \tag{2.13}$$

and corresponds to the case $N^\circ = n+1$, $\pi^\circ_{N^\circ}(t) = (1+t)\pi_n(t\,;(1+t)d\sigma)$, $N^* = n+1$, hence has degree of exactness (at least) $d = 3n+2$. The orthogonality condition (2.8_{N^*}) assumes the form

$$\int_{-1}^{1} \pi^*_{n+1}(t)p(t)\pi_n(t\,;(1+t)d\sigma)(1+t)d\sigma(t) = 0, \quad \text{all } p \in \mathbf{P}_n. \tag{2.14}$$

Thus, as far as the nodes τ^*_μ are concerned, we can obtain them exactly as if we were to extend the Gauss formula for the measure $(1+t)d\sigma(t)$. Also, the quantities $(1+\tau_\nu)\sigma_\nu$ and $(1+\tau^*_\mu)\sigma^*_\mu$ can be obtained by expressions which are identical to the ones on the right-hand sides of (2.11), where the Christoffel numbers and norm refer to the measure $(1+t)d\sigma(t)$. The weight σ_0 then follows from $\sigma_0 + \sum_{\nu=1}^{n} \sigma_\nu + \sum_{\mu=1}^{n+1} \sigma^*_\mu = \mu_0$, $\mu_0 = \int_{\mathbf{R}} d\sigma(t)$.

Example 2.3: Kronrod extension of Gauss-Lobatto formulae.

We assume, similarly as in Example 2.2, that the measure $(1-t^2)d\sigma(t)$, supported on $[-1,1]$, allows Kronrod extension. Then the unique optimal extension of the $(n+2)$-point Gauss-Lobatto formula for the measure $d\sigma$ is given by

$$\int_{-1}^{1} f(t)d\sigma(t) = \sigma_0 f(-1) + \sigma_{n+1} f(1) + \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma^*_\mu f(\tau^*_\mu) + R_n(f), \tag{2.15}$$

and is the case $N^\circ = n+2$, $\pi^\circ_{N^\circ}(t) = (1-t^2)\,\pi_n(t\,;(1-t^2)d\sigma)$, $N^* = n+1$ of (2.5), with the degree of exactness now being (at least) $d = 3n+3$. The orthogonality condition (2.8_{N^*}) becomes

$$\int_{-1}^{1} \pi^*_{n+1}(t)p(t)\pi_n(t\,;(1-t^2)d\sigma)(1-t^2)d\sigma(t) = 0, \quad \text{all } p \in \mathbf{P}_n, \tag{2.16}$$

and is the same as for Kronrod extension of the n-point Gauss formula for the measure $(1-t^2)d\sigma(t)$. Again, the quantities $(1-\tau_\nu^2)\sigma_\nu$ and $(1-\tau_\mu^{*2})\sigma_\mu^*$ have representations identical to those on the right of (2.11), the measure being $(1-t^2)d\sigma(t)$ throughout. The remaining weights σ_0, σ_{n+1} are most easily obtained by solving the system of two linear equations expressing exactness of (2.15) for $f(t)=1$ and $f(t)=t$.

We remark that in the special case of Jacobi measures $d\sigma^{(\alpha,\beta)}(t)=(1-t)^\alpha(1+t)^\beta dt$, $\alpha>-1$, $\beta>-1$, we have

$$\pi_n(\cdot;(1-t^2)d\sigma^{(\alpha,\beta)})=\frac{1}{n+1}\,\pi'_{n+1}(\cdot;d\sigma^{(\alpha,\beta)}), \tag{2.17}$$

as follows readily from the identity $(d/dt)P_{n+1}^{(\alpha,\beta)}(t)=\tfrac{1}{2}(n+\alpha+\beta+2)\,P_n^{(\alpha+1,\beta+1)}(t)$ for Jacobi polynomials.

Example 2.4: "Kronrod-heavy" extension of Gauss formulae.

The "Kronrod nodes" τ_μ^* and "Gauss nodes" τ_ν in the Gauss-Kronrod formula (2.10) are nicely balanced, in that exactly one Kronrod node fits into the space between two consecutive Gauss nodes and between the extreme Gauss nodes and the respective endpoints (possibly $\pm\infty$) of the support interval of $d\sigma$. There are, however, occasions (for example, in cases of nonexistence; cf. Subsection 3.4) where it might be necessary to forgo this balance in favor of more Kronrod nodes; we call such extensions *Kronrod-heavy*. These also fit into the general scheme (2.5), where $N^\circ=n$, $\pi_N^\circ(\cdot)=\pi_n(\cdot;d\sigma)$, $N^*=n+q$ with $q>1$, and give rise to the orthogonality condition

$$\int_{\mathbf{R}}\pi_{n+q}^*(t)p(t)\pi_n(t;d\sigma)d\sigma(t)=0,\quad\text{all } p\in\mathbf{P}_{n+q-1}. \tag{2.18}$$

In contrast to Gauss-Kronrod formulae, the unique existence of π_{n+q}^*, let alone the reality of its zeros, is no longer assured. Starting with the unique $\pi_{n+1}^*(\cdot;d\sigma)=\pi_{n+1,n}^*(\cdot)$, however, there is an infinite sequence $\{\pi_{n+q_m,n}^*\}_{m=1}^\infty$ of uniquely determined polynomials $\pi_{n+q_m}^*=\pi_{n+q_m,n}^*$ of exact degree $n+q_m$, $1=q_1<q_2<q_3<\cdots$, such that (2.18) holds with $q=q_m$, and such that no polynomial $\pi_{n+q_m}^*$ of degree $<n+q_m$ exists for which (2.18) holds with $q=q_m$ (Monegato [1980]).

One can try, of course, to extend in this manner other quadrature formulae, e.g., the Gauss-Radau or Gauss-Lobatto formulae.

Example 2.5: Repeated Kronrod extension of Gauss formulae.

Given an n-point Gauss formula, one can try to extend it optimally to a $(2n + 1)$-point formula as in Example 2.1, then extend this formula once again to a $(4n + 3)$-point formula (by optimally adding $2n + 2$ new nodes), and so on. The likelihood of such repeated extensions to all exist (i.e., have real distinct nodes) is probably quite small. Remarkably, however, for $n=3$ and $d\sigma(t) = dt$ on $[-1,1]$, such extensions, even with all weights positive, have been successfully computed by Patterson [1968a], [1973] up to the 255-point formula.

For the second extension, for example, the node polynomial π^*_{2n+2} must be orthogonal to all lower-degree polynomials with respect to the measure $d\sigma^*(t) = \pi_n(t\,;d\sigma)\,\pi^*_{n+1}(t\,;d\sigma)d\sigma(t)$.

Example 2.6: Extension by contraction.

As contradictory as this may sound, the point here is that one starts with a "base formula" containing a sufficiently large number of nodes, then successively removes subsets of nodes to generate a sequence of quadrature rules having fewer and fewer nodes. Looking at this sequence in the opposite direction then turns it into a sequence of (finitely often) extended quadrature rules.

More specifically, following Patterson [1968b], one takes as base formula any $(2^r + 1)$-point formula and then defines r subsets of points by successively deleting alternate points from the preceding subset (keeping the first and the last). For example, if $r=3$, the successive three subsets of the original points with index set {1,2,3,4,5,6,7,8,9} contain the points with indices {1,3,5,7,9}, {1,5,9} and {1,9}, respectively. A sequence of $r+1$ quadrature formulae can now be defined by taking the interpolatory formulae for the original node set and all r subsets of nodes. (A slightly different procedure is proposed by Rabinowitz, Kautsky and Elhay; see Rabinowitz, Kautsky, Elhay and Butcher [1987, Appendix A, p.125].)

The reality of the nodes is thereby trivially guaranteed, but not necessarily the positivity of the weights. Patterson [1968b], nevertheless, finds by computation that all weights remain posi-

tive if one starts with the 33-point, or 65-point Gauss-Legendre formula (r=5 and r=6, respectively), or with the 65-point Lobatto formula (r=6) as base formulae.

Another example of a suitable base formula, which in fact (Imhof [1963], Brass [1977, Satz 77]) has positivity of all weights built in, is the Clenshaw-Curtis formula (Clenshaw and Curtis [1960]) based on the initial point set $\tau_\nu = \cos(\nu\pi/2^r)$, $\nu = 0, 1, 2, \ldots, 2^r$.

If one is willing to delete successively one point at a time, then the following result of Rabinowitz, Kautsky, Elhay and Butcher [1987] is of interest: Given any interpolatory quadrature rule with all weights positive, it is possible to delete one of its points such that the interpolatory rule based on the reduced point set has all weights nonnegative.

All sequences of extended quadrature rules in Example 2.6 are examples of nonoptimal, in fact interpolatory, extensions. Other examples of nonoptimal, even subinterpolatory, extensions are those of product rules given by Dagnino [1983] (see also Dagnino [1986]). The severe sacrifice in polynomial degree of exactness is justified in this reference in terms of a simplified convergence and stability theory.

We restricted our discussion here to quadrature rules of the simplest type (2.1). There is little work in the literature on the extension of quadrature rules involving derivatives. Bellen and Guerra [1982], however, extend Turán-type formulae, but work them out only in very simple special cases.

3. Existence, nonexistence and remainder term. We consider here mainly the Gauss-Kronrod formula as defined in Example 2.1, that is,

$$\int_{\mathbb{R}} f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f), \quad R_n(\mathbb{P}_{3n+1}) = 0. \tag{3.1}$$

We say that the nodes τ_ν, τ_μ^* in (3.1) *interlace* if they are all real and, when arranged decreasingly, satisfy

$$-\infty < \tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^* < \infty. \tag{3.2}$$

For any given $n \geq 1$, the following properties are of interest:

(a) The nodes τ_ν, τ_μ^* interlace.

(b) All nodes τ_ν, τ_μ^*, in addition to interlacing, are contained in the interior of the smallest interval containing the support of $d\sigma$.

(c) The nodes interlace and each weight σ_ν is positive. (It is known, cf. Monegato [1976], that the interlacing property is equivalent to $\sigma_\mu^- > 0$, all μ.)

(d) All nodes, without necessarily satisfying (a) and/or (b), are real.

Little has been *proved* with regard to these properties; any new piece of information, from whatever source – computational or otherwise – should therefore be greeted with appreciation. In this section, we give an account of what is known, or what can be conjectured, for some classical and nonclassical measures.

3.1 *Gegenbauer measures* $d\sigma^{(\lambda)}(t) = (1-t^2)^{\lambda-\frac{1}{2}}dt$ *on* $[-1,1]$, $\lambda > -\frac{1}{2}$. Properties (a) and (b), as already mentioned in Section 1, have been proved for all $n \geq 1$ by Szegö [1935], when $0 < \lambda \leq 2$, and property (c) by Monegato [1978a], when $0 \leq \lambda \leq 1$. Properties (a) and (b) also hold for the extension of Lobatto formulae, if $-\frac{1}{2} < \lambda \leq 1$ (cf. Example 2.3), but nothing as yet has been proved concerning property (c). This, then, is the extent of what is known rigorously, for arbitrary n, at this time.

A good deal more, however, can be uncovered for specific values of n, if we let the parameter λ move continuously away from the above intervals and observe the resulting motion of the nodes τ_ν, τ_μ^* and the movement of the weights σ_ν, σ_μ^*. Given n, property (a) will cease to hold at the very moment a node τ_ν collides (for the first time) with a node τ_μ^*. This event is coincident with the vanishing of the resultant of $\pi_n(\cdot\,; d\sigma^{(\lambda)})$ and $\pi_{n+1}^*(\cdot\,; d\sigma^{(\lambda)})$. When λ has moved beyond this critical value, the nodes τ_ν and τ_μ^* involved in the collision have likely crossed each other, so that two Kronrod nodes now lie between consecutive Gauss nodes. Only now is it possible that two Kronrod nodes may collide and split into a pair of complex nodes, an event that is signaled by the vanishing of the discriminant of $\pi_{n+1}^*(\cdot\,; d\sigma^{(\lambda)})$. By using purely algebraic methods, it is thus possible to delineate parameter intervals in which properties (a) and (d) are valid. The

subintervals of the first of these, in which properties (b) and (c) hold, can be determined rather more easily, in an obvious manner.

This has been carried out computationally in Gautschi and Notaris [submitted] for values of n up to 40. Based on these results it is conjectured (and proved for $n \leq 4$) that property (p) holds for $\lambda_n^p < \lambda < \Lambda_n^p$, where the bounds λ_n^p and Λ_n^p for $p = a, b, c, d$ are as shown in Table 3.1.

n	λ_n^a	Λ_n^a	λ_n^b	Λ_n^b	λ_n^c	Λ_n^c	λ_n^d	Λ_n^d
1	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞
2	$-\frac{1}{2}$	∞	0	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞
3	$-\frac{1}{2}$	16	0	16	$-\frac{1}{2}$	6.552...	$-\frac{1}{2}$	16
4	$-\frac{1}{2}$	∞	0	∞	$-\frac{1}{2}$	51.78...	$-\frac{1}{2}$	∞
≥ 5	$-\frac{1}{2}$	Λ_n^a	0	Λ_n^a	$-\frac{1}{2}$	Λ_n^c	$-\frac{1}{2}$	Λ_n^d

Table 3.1. *Property (p) for Gegenbauer measures*

Here, Λ_n^a, Λ_n^c, Λ_n^d are certain constants satisfying $1 < \Lambda_n^a < \infty$, $1 < \Lambda_n^c < \Lambda_n^a$ and $\Lambda_n^d \geq \Lambda_n^a$ with equality precisely when $n = 4r - 1$, $r = 1, 2, 3, \ldots$. Numerical values of these constants, to 10 decimal places, are provided in the cited reference for $n = 5(1)20(4)40$.

The fact that Kronrod extension (satisfying properties (c) and (d)) cannot exist for all $n \geq 1$ when λ is sufficiently large, not even if the degree of exactness is lowered to $[2rn + l]$, $r > 1$, l an integer, is claimed by Monegato [1979]. (The proof given is erroneous, but can be repaired; Monegato [1987].)

3.2 *Jacobi measures* $d\sigma^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta dt$ *on* $[-1,1]$. Since interchanging the parameters α and β has the effect of changing the signs of the nodes τ_ν and τ_μ^*, hence, if the order (3.2) is maintained, of renumbering them in reverse order, and the same renumbering applies to the weights σ_ν and σ_μ^*, the validity of property (p), $p = a, b, c, d$, is unaffected by such an interchange. We will assume, therefore, that $-1 < \alpha \leq \beta$.

Except for the cases $|\alpha| = |\beta| = \frac{1}{2}$ (considered in Subsection 3.3) and the transformations to Gegenbauer measures noted below, the only known proven result is that property (b) is false for $\alpha = -\frac{1}{2}, -\frac{1}{2} < \beta < \frac{1}{2}$ when n is even, and for $\alpha = -\frac{1}{2}, \frac{1}{2} < \beta \leq 3/2$ when n is odd (Rabinowitz [1983, p.75] †).

(†) There is a misprint on p.75 of this reference: The superscript $\mu + \frac{1}{2}$ should be replaced by $\mu - \frac{1}{2}$ twice in Eq. (68), and twice in the discussion immediately following Eq. (69).

Monegato [1982] notes that $\pi_{n+1}^{*(\alpha,-\frac{1}{2})}(2t^2-1) = 2^{n+1}\, t\, \pi_{2n+1}^{*(\alpha,\alpha)}(t) - d_n$, where d_n is an explicitly given constant, and similarly, $\pi_{n+1}^{*(\alpha,\frac{1}{2})}(2t^2-1) = 2^{n+1}\, \pi_{2n+2}^{*(\alpha,\alpha)}(t)$. In the latter case, there are also simple relationships between the weights σ_ν, σ_μ^* of the respective Gauss-Kronrod formulae (3.1); cf. Gautschi and Notaris [submitted, Thm. 5.1]. The cases $\alpha > -1$, $\beta = \pm \frac{1}{2}$ can thus be reduced to the Gegenbauer case, and appeal can be made to the empirical results of Subsection 3.1, at least when $\beta = \frac{1}{2}$. A similar reduction is possible in the case $\alpha > -1$, $\beta = \alpha + 1$ (Monegato [1982, Eq. (36)]), which is of interest in connection with Kronrod extension of Gauss-Radau formulae for Gegenbauer measures (cf. Example 2.2).

The algebraic methods described in Subsection 3.1 have also been applied to general Jacobi measures (Gautschi and Notaris [submitted]) and the results for $2 \le n \le 10$ displayed by means of graphs. There are marked qualitative differences for n even and n odd, as is shown in Figure 3.1 for the cases $n=6$ and $n=7$. The region of validity for property (p) is consistently below the curve labeled "p", except for $p=b$ and n even, when it is above and to the right of the curve.

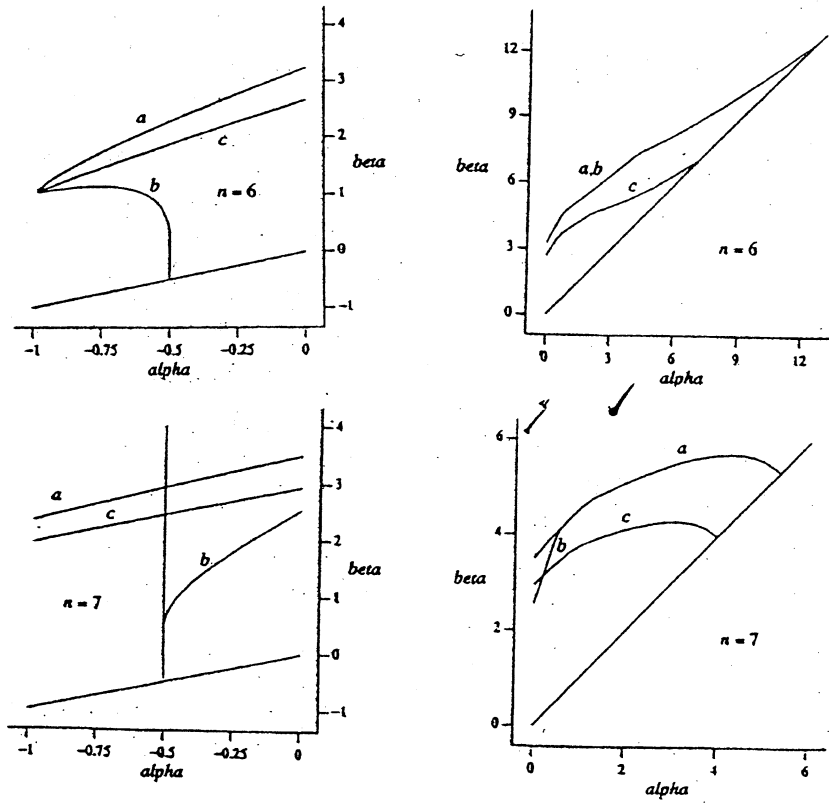

Figure 3.1. *Property (p), p = a, b, c for the Jacobi measure* $d\sigma^{(\alpha,\beta)}$ *when n=6 and n=7*

3.3 *Chebyshev measures of* 1st, 2nd *and* 3rd *kind.* These are the cases $|\alpha| = |\beta| = \frac{1}{2}$ of the Jacobi measure $d\sigma^{(\alpha,\beta)}$. They are the only known cases in which both the Gauss formulae and their Kronrod extensions can be written down explicitly (in terms of trigonometric functions). If $\alpha = \beta = -\frac{1}{2}$, the (optimal) extension of the n-point Gauss-Chebyshev formula of the first kind, when $n \geq 2$, is simply the $(2n + 1)$-point Lobatto formula for the same weight function. (For $n=1$, it is the 3-point Gauss-Chebyshev rule.) To get the Kronrod extension of the n-point Gauss-Chebyshev formula of the second kind ($\alpha = \beta = \frac{1}{2}$), it suffices to replace n by $2n + 1$ in the same formula. Finally, for $\alpha = -\frac{1}{2}$, $\beta = \frac{1}{2}$, the Kronrod extension is the Radau formula (with fixed node at 1) for the same weight function. All these extended formulae have elevated degrees of exactness, namely $4n - 1$, $4n + 1$ and $4n$, respectively, and enjoy property (p) for all $p = a, b, c$ (hence also d). These elegant relationships have been noted as early as 1964 by Mysovskih [1964]; see also Monegato [1982, p.147]. For the first two cases, Monegato [1976] points out that the formulae can be extended infinitely often in an explicit manner.

3.4 *Laguerre and Hermite measures.* Here is another instance in which a nonexistence result is known (Kahaner and Monegato [1978]): For the generalized Laguerre measure $d\sigma^{(\alpha)}(t) = t^{\alpha}e^{-t}dt$ on $[0,\infty]$, $-1 < \alpha \leq 1$, the Kronrod extension of the n-point Gauss-Laguerre formula, with real nodes and positive weights, does not exist when $n \geq 23$, and if $\alpha=0$ not even for $n>1$. As a corollary, n-point Gauss-Hermite formulae cannot be so extended, unless $n = 1, 2$ or 4, confirming earlier empirical results of Ramskii [1974]. These negative results led Kahaner, Waldvogel and Fullerton [1982], [1984] to explore the feasibility of Kronrod-heavy extensions for the Laguerre measure. Computational experience is reported for $n = 1(1)10$ and $q=8$ (11 for $n=1$ and 9 for $n=2$), where q is defined as in Example 2.4.

3.5 *Other measures.* At the heart of Geronimus' theory (Geronimus [1930]) is the measure $d\sigma_{\mu}(t) = (1-t^2)^{\frac{1}{2}}dt/(1 - \mu t^2)$ on $[-1,1]$, $-\infty < \mu \leq 1$. The corresponding polynomials $\pi_n(\cdot\,; d\sigma_{\mu})$ and $\pi^*_{n+1}(\cdot\,; d\sigma_{\mu})$ turn out to be linear combinations of Chebyshev polynomials U_n, U_{n-2} and T_{n+1}, T_{n-1}, respectively. This allows explicit construction of the associated Gauss-Kronrod extension and verification of all properties (a) – (c); cf. Gautschi and Rivlin [submitted]. In addition,

the degree of exactness is exceptionally high (Monegato [1982, p.146]). Similar expressions for π_n and π^*_{n+1} result if the denominator of $d\sigma_\mu$ is replaced by a positive, not necessarily even, polynomial of degree 2 (Monegato and Palamara Orsi [1985]).

Gautschi and Notaris [submitted, Thm. 5.2] observe that the problem of Kronrod extension for the measure $^\gamma d\sigma^{(\alpha)}(t) = |t|^\gamma(1-t^2)^\alpha dt$ on $[-1,1]$, $\alpha > -1$, $\gamma > -1$, can be reduced, when n is odd, to the analogous problem for the Jacobi measure $d\sigma^{(\alpha,(\gamma+1)/2)}$.

Very little is known for measures unrelated to classical measures. One that is likely to admit satisfactory Kronrod extension for every $n \geq 1$ (judging from numerical results of Calió, Gautschi and Marchetti [1986]) is the logarithmic measure $d\sigma(t) = \ln(1/t)dt$ on $[0,1]$ for which properties (a), (b) and (c) appear to be all true. The same is conjectured for measures $d\sigma(t) = t^\alpha \ln(1/t)dt$, $\alpha = \pm\,½$, except for $\alpha = -½$ and n odd, in which case property (b), though not (d), fails, the polynomial $\pi^*_{n+1}(\cdot\,; d\sigma)$ having exactly one negative zero.

3.6 *Remainder term.* The Gauss-Kronrod formula (3.1) can be characterized in the manner of Markov [1885] as the unique quadrature formula (if it exists) obtained by integrating the interpolation polynomial $p_{3n+1}(f\,; \tau_\nu, \tau^*_\mu, \tau^*_\mu; \cdot)$ (with simple knots τ_ν and double knots τ^*_μ) of degree $\leq 3n + 1$ and by requiring (if possible) that the coefficients of all derivative terms in the resulting quadrature sum be zero. The elementary Hermite interpolation polynomials g_ν, h_μ, k_μ associated with this interpolation process can be easily expressed in terms of the fundamental Lagrange polynomials l_ν and l^*_μ for the nodes $\tau_1, \tau_2, \ldots, \tau_n$ and $\tau^*_1, \tau^*_2, \ldots, \tau^*_{n+1}$, respectively (see, e.g., Calió, Gautschi and Marchetti [1986, Eq. (3.13)]). The coefficients $\sigma^{*\prime}_\mu$ required to be zero are then

$$\sigma^{*\prime}_\mu = \int_{\mathbb{R}} k_\mu(t)d\sigma(t), \quad \mu = 1, 2, \ldots, n+1, \tag{3.3}$$

where

$$k_\mu(t) = \frac{\pi_n(t)}{\pi_n(\tau^*_\mu)}\,[l^*_\mu(t)]^2(t - \tau^*_\mu), \quad \pi_n(\cdot) = \pi_n(\cdot\,; d\sigma). \tag{3.4}$$

Thus we must have

$$\pi^{*\prime}_{n+1}(\tau^*_\mu)\int_{\mathbb{R}} \pi_n(t)[l^*_\mu(t)]^2(t - \tau^*_\mu)d\sigma(t) = \int_{\mathbb{R}} \pi^*_{n+1}(t)l^*_\mu(t)\pi_n(t)d\sigma(t) = 0, \quad \mu = 1, 2, \ldots, n+1, \tag{3.5}$$

which, by the linear independence of the l_μ^*, is equivalent to the orthogonality condition (2.9).

From interpolation theory there follows that

$$R_n(f) = \frac{1}{(3n+2)!} \int_{\mathbf{R}} [\pi_{n+1}^*(t)]^2 f^{(3n+2)}(\tau(t))\pi_n(t)d\sigma(t). \tag{3.6}$$

provided $f \in C^{3n+2}$ on an interval containing $\operatorname{supp}(d\sigma)$. For Gegenbauer measures $d\sigma(t) = (1-t^2)^{\lambda-\frac{1}{2}}dt$ on $[-1,1]$, with $0 < \lambda < 1$, Monegato [1978b], relying heavily on Szegö's theory, shows that $|\pi_{n+1}^*(t\,; d\sigma)| < 2^{-n}$ on $[-1,1]$, which in combination with known bounds for $|\pi_n(\cdot\,; d\sigma)|$ yields an explicit upper bound for $|R_n(f)|$ in terms of $\|f^{(3n+2)}\|_\infty$. Rabinowitz [1980] improves this bound slightly and extends it to the case $1 < \lambda < 2$, as well as to Kronrod extensions of Gauss-Lobatto rules for $-\frac{1}{2} < \lambda \leq 1$, $\lambda \neq 0$. He also proves that for $0 < \lambda \leq 2$, $\lambda \neq 1$ the degrees $d = 3n+1$ and $d = 3n+2$ for n even and odd, respectively, are indeed the exact degrees of precision. (When $\lambda = 1$, one has exact degree $4n + 1$, and when $\lambda = 0$ exact degree $4n - 1$.) Analogous statements are proved for the Kronrod extension of the Gauss-Lobatto rule. Szegö's work, again, proves invaluable for this analysis, as it does, in combination with a result of Akrivis and Förster [1984, Proposition 1], to show that the remainder term $R_n(f)$ is indefinite if $0 < \lambda < 1$ and $n \geq 2$ (Rabinowitz [1986b]). For $\lambda > 1$, the question of definiteness is still open; it is also open for Kronrod extensions of Gauss-Lobatto rules for any λ (with the obvious exceptions).

Error constants in Davis-Rabinowitz type estimates of the remainder (Davis and Rabinowitz [1954]) for functions analytic on elliptic domains are given by Patterson [1968a] for his repeated extensions of the 3-point Gauss formula. They are compared with the corresponding constants for the Gauss and Clenshaw-Curtis formulae having the same number of points.

4. Computational methods, numerical tables, computer programs and applications.

4.1 *Computational methods.* Kronrod originally computed the Stieltjes polynomial $\pi_{n+1}^*(\cdot\,; dt)$ in power form, requiring it to be orthogonal (in the sense of (1.14)) to all monomials of degree $\leq n$. The zeros of π_{n+1}^* are then obtained by a rootfinding procedure, and the weights

σ_ν, σ_μ^* from a system of linear equations expressing exactness of (1.10) for the first $2n+1$ monomials. (Symmetry, of course, was used throughout.) As he himself observes, the procedure is subject to considerable loss of accuracy and therefore requires elevated precision. Patterson [1968a] achieves better stability by expanding π_{n+1}^* in Legendre polynomials and computing the coefficients recursively. He does so not only for the Kronrod extension of the Gauss formula, but likewise for the extension of the Lobatto formula. Further improvements and simplifications result from expansion in Chebyshev polynomials; cf. Piessens and Branders [1974]. Their procedure, even somewhat simplified and generalized to Gegenbauer measures, actually can be extracted from the work of Szegö [1935], as is pointed out by Monegato [1978b]; see also Monegato [1979], [1982]. For Gegenbauer measures, then, this seems to be the method of choice. Once the nodes have been computed, the weights can be obtained, e.g., by the formulae in (2.11).

Expansion of $\pi_{n+1}^*(\cdot\,; d\sigma)$ in orthogonal polynomials $\pi_k(\cdot\,; d\sigma)$, $k = 0, 1, \ldots, n+1$, however, is possible for arbitrary measures $d\sigma$. Replacing $p(\cdot)$ in (2.9) successively by $\pi_i(\cdot\,; d\sigma)$, $i = 0, 1, \ldots, n$, indeed yields a triangular system of equations which can be readily solved. Its coefficients can be computed, e.g., by Gauss-Christoffel quadrature relative to the measure $d\sigma$, using $[(3n + 3)/2]$ points; cf. Caliò, Gautschi and Marchetti [1986, Sec. 4]. (For another method, see Caliò, Marchetti and Pizzi [1984] and Caliò and Marchetti [1987].)

A rather different approach, resembling (in fact, generalizing) the well-known Golub-Welsch procedure (Golub and Welsch [1969]) for computing Gauss-Christoffel quadrature formulae is developed by Kautsky and Elhay [1984] and Elhay and Kautsky [1984] and relies on eigenvalues of suitably constructed matrices. For the weights, these authors use their own methods and software for generating interpolatory quadrature rules (Kautsky and Elhay [1982], Elhay and Kautsky [1985]).

Instead of computing, as above, the Gauss-Kronrod formula piecemeal – first the Stieltjes polynomial, then its zeros, and finally the weights – it might be preferable to compute these components all at once, for example by applying Newton's method to the system of $3n + 2$ (non-

linear) equations expressing exactness of the quadrature rule (2.10) for some set of basis functions in $\mathbb{P}_{3n+1}$. The feasibility of this idea is demonstrated in Caliò, Gautschi and Marchetti [1986], where the numerical condition of the underlying problem, hence the stability of the procedure, is also analyzed. It appears, though, that this method runs into severe ill-conditioning when one attempts to use it for repeated Kronrod extension (Gautschi and Notaris [in preparation]).

4.2. *Numerical tables.* There are a number of places where Kronrod extensions of n-point Gauss formulae can be found tabulated: Kronrod himself (Kronrod [1964b]) has them (transformed to the interval [0,1]) for $n = 1(1)40$ to 16 decimals (also in binary form!). In addition, he tabulates errors incurred when the formulae are applied to monomials. Patterson [1968a] (on microfiche) gives 20 S values for $n = 65$, and Piessens [1973] 16 S values for $n = 10$. The most accurate are the 33-decimal tables for $n = 7, 10(5)30$ in Piessens et al. [1983, pp. 19–23]. Extensions of $(n+2)$-point Lobatto formulae, $n = 1(1)7$ and $n = 63$, can be found to 20 decimals in Patterson [1968a] (on microfiche), and extensions of the $(n+1)$-point Radau formula, $n = 2(2)16$ (but incomplete), to 15 decimals in Baratella [1979].

Repeated Gauss-Kronrod extensions of the 3-point Gauss formula, as far up as the 127-point formula, are given to 20 significant digits in Patterson [1968a] (on microfiche), and the 255-point formula to the same accuracy in Patterson [1973] (in a Fortran data statement). The repeatedly extended 10-point formula, through the one with 87 points, is given to 33 decimals in Piessens et al. [1983, pp. 19, 26–27]. Extensions in the sense of Example 2.6 are tabulated to 20 decimals in Patterson [1968b] (on microfiche), using the 33-point and 65-point Gauss formula, as well as the 65-point Lobatto formula as "base formulae".

For measures other than the constant weight measure, there are 25 S tables of $(2n+1)$-point Gauss-Kronrod formulae for $d\sigma(t) = t^{\alpha} \ln(1/t)dt$ on [0,1], $\alpha = 0, \pm\frac{1}{2}$, where $n = 5(5)25$ for $\alpha = 0, \frac{1}{2}$, and $n = 4(4)24$ for $\alpha = -\frac{1}{2}$ (Caliò, Gautschi and Marchetti [1986, Suppl. S57–S63]). 15 S tables for the same weight functions, but with $n = 4$ and 12 for $\alpha = 0, \frac{1}{2}$, and $n = 6$ and 12 for $\alpha = -\frac{1}{2}$, are given in Caliò and Marchetti [1987]. Kahaner, Waldvogel and Fullerton [1984]

provide 15–18 S tables of Kronrod-heavy extensions of the Gauss-Laguerre formula ($d\sigma(t) = e^{-t}\,dt$ on $[0, \infty]$) with $n = 1$, $q = 3(1)6$ and $n = 10$, $q = 18$ (in the notation of Example 2.4).

We finally mention the 16 S tables of Piessens [1969] of the complex Gauss-Kronrod formulae, with $n = 2(1)12$, for the Bromwich integral, and the 15 S table of the interpolatory $(n+1)$-point formula based solely on the Kronrod nodes, given by Monegato [1982] for $d\sigma(t) = dt$ and $n = 2(1)9$.

4.3. *Computer programs.* Fortran programs for Kronrod extension of the n-point Gauss formula are provided in Squire [1970, p. 279] for $n = 20$, and in Piessens and Branders [1974] for arbitrary n. Dagnino and Fiorentino [1984] describe a Fortran program (listed in Dagnino and Fiorentino [1983]) generating Gauss-Kronrod formulae for Gegenbauer measures $d\sigma(t) = (1-t^2)^{\lambda - \frac{1}{2}}dt$ on $[-1,1]$, $0 \le \lambda \le 2$, $\lambda \ne 1$, using the recursive algorithm of Szegö as resurrected by Monegato (cf. Subsection 4.1). Programs for more general measures are described and listed in Calió and Marchetti [1987], [1985], respectively.

A number of routines employing Gauss-Kronrod quadrature in the context of automatic integration are discussed and listed in Piessens et al. [1983].

4.4. *Applications.* The original motivation came from a desire to estimate the error of Gaussian, or other quadrature formulae (taking the more accurate Kronrod extension as a substitute for the exact answer). The need for such error estimates has recently been highlighted in connection with the development of automatic integration schemes; see, e.g., Cranley and Patterson [1971], Patterson [1973], Piessens [1973] and Piessens et al. [1983]. For an interesting interpretation of the Kronrod scheme of error estimation, see Laurie [1985]. A rather different estimation procedure is proposed in Berntsen and Espelid [1984].

Patterson's repeated extensions of the 3-point Gauss-Legendre rule (cf. Example 2.5) has been used with some success in certain methods to compute improper integrals arising in weakly singular integral equations. One method employs the ε – algorithm to accelerate a sequence of approximants (Evans, Hyslop and Morgan [1983]), another suitable transformations of variables to attenuate the singularity (Evans, Forbes and Hyslop [1983]).

Kronrod's idea has been applied to other types of integrals, for example, as already mentioned, to the Bromwich integral for the inversion of Laplace transforms (Piessens [1969]), and to Cauchy type singular integrals involving Gegenbauer measures (Rabinowitz [1983]). These applications, especially the latter, are not entirely straightforward, as the occurrence of numerical cancellation, or derivative values, may present difficulties. They can be surmounted, to some extent, by more stable implementations (Rabinowitz [1986a]), using, in part, Kronrod-heavy extensions (with $q = 2$; see Example 2.4). For an application of Kronrod's idea to cubature formulae, see Malik [1980], Genz and Malik [1980], [1983], Laurie [1982], Neumann [1982], Cools and Haegemans [1986], [1987] and Berntsen and Espelid [1987].

An interesting application, first noted by Barrucand [1970], is the use of Gauss-Kronrod formulae for computing Fourier coefficients in orthogonal expansions,

$$c_n(f) = \|\pi_n\|_{d\sigma}^{-1} \int_{\mathbb{R}} \pi_n(t) f(t)\, d\sigma(t), \quad n = 0, 1, 2, \ldots, \tag{4.1}$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ is the nth degree orthogonal polynomial associated with the measure $d\sigma$. The $(2n+1)$-point Gauss-Kronrod formula (for the coefficient c_n), in this case, reduces to an $(n+1)$-point formula,

$$c_n(f) = \|\pi_n\|_{d\sigma}^{-1} \left[\sum_{\mu=1}^{n+1} \sigma_\mu^* \pi_n(\tau_\mu^*) f(\tau_\mu^*) + R_n(\pi_n f) \right], \tag{4.2}$$

but still has degree of exactness (at least) $2n + 1$. The new weights, $\sigma_\mu^*\, \pi_n(\tau_\mu^*)$, however, even if all σ_μ^* are positive, alternate in sign, which somewhat detracts from the usefulness of these formulae. For Gegenbauer measures $d\sigma^{(\lambda)} = (1-t^2)^{\lambda - \frac{1}{2}}$, $\lambda \neq 0,1$, Rabinowitz [1980] shows that the degree of exactness $2n + 1$ ($2n + 2$ if n is odd) is best possible. (4.2) is exact for polynomials of degree $3n - 1$, when $\lambda = 0$, and of degree $3n + 1$, when $\lambda = 1$, both of which is again best possible. The highest precision is thus obtained for Fourier-Chebyshev coefficients of the second kind.

Finite element and projection methods frequently rely on numerical integration but so far, Gauss-Kronrod formulae, unlike the Gauss formulae, have been shunned. An exception is Bellen [1980], who uses them in his "extended collocation-least squares" method.

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NEWTON'S METHOD AND GAUSS-KRONROD QUADRATURE*

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1. Introduction

One of us, jointly with CALIÒ and MARCHETTI (1986), considered the application of Newton's method (for large nonlinear systems of equations) in the context of computing Gauss-Kronrod quadrature rules. With the equations set up in an appropriate manner, it was found that, by careful choice of initial approximations and continued monitoring of the iteration process, the method could be made to work for rules with up to 81 nodes (40 Gauss and 41 Kronrod nodes). This was documented for the Legendre weight on [−1,1] (where in fact formulae with up to 161 nodes were computed) and for weight functions on [0,1] involving logarithmic and algebraic singularities. Further evidence of the feasibility of Newton's method, also for Kronrod extension of Gauss-Radau and Gauss-Lobatto formulae, is contained in NOTARIS's thesis (1988). If one attempts, however, to repeat Kronrod extension in the manner of PATTERSON (1968), one discovers that Newton's method quickly deteriorates and

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eventually fails to converge. The purpose of this note is to shed some light on the reasons for this failure of Newton's method. One of these is the excessive magnitude of the inverse Jacobian of the nonlinear system (evaluated at the solution) which comes about because of a peculiar behavior of a certain polynomial responsible for the magnitude of this inverse. Graphical evidence is provided to underscore the phenomenon.

For simplicity we consider only integrals over a finite interval (standardized by [−1,1]) with constant weight function.

2. Extension of quadrature rules

Given an N-point quadrature rule $Q_N(f)$ of the form

$$Q_N(f) = \sum_{\nu=1}^{N} \omega_\nu f(\tau_\nu), \quad -1 < \tau_N < \tau_{N-1} < \cdots < \tau_1 < 1, \tag{2.1}$$

approximating the integral $I(f)$,

$$Q_N(f) \approx I(f) = \int_{-1}^{1} f(t)dt, \tag{2.2}$$

we call *Kronrod extension* of Q_N, in notation

$$Q_N(f) \subset Q_{N'}(f), \tag{2.3}$$

the quadrature rule $Q_{N'}(f)$ with $N' = N + (N+1) = 2N + 1$ nodes, N of which being the given

nodes τ_ν in (2.1) and the additional $N+1$ (the "Kronrod nodes") and all $2N+1$ weights being determined to achieve maximum algebraic degree of exactness for $Q_{N'}(f)$. Hopefully, the $N+1$ Kronrod nodes are all real and fit nicely into the $N+1$ spaces between the nodes τ_ν and between the extreme nodes τ_1, τ_N and the corresponding endpoints 1, −1 of the interval of integration. Unfortunately, however, this is not guaranteed in general. Letting

$$\pi_N(t) = \prod_{\nu=1}^{N} (t - \tau_\nu) \tag{2.4}$$

denote the (given) node polynomial, it is known that the Kronrod nodes must be the zeros of the (monic) polynomial π^*_{N+1} of degree $N+1$ (if it exists) satisfying the orthogonality property

$$\int_{-1}^{1} \pi^*_{N+1}(t)p(t)\pi_N(t)dt = 0\,, \quad \text{all} \quad p \in \mathbf{P}_N\,. \tag{2.5}$$

Since this is orthogonality with respect to a sign-changing "weight function", π_N, the usual properties of classical orthogonal polynomials can no longer be expected to hold. Even the existence of π^*_{N+1} is in doubt, unless the Hankel matrix $H_{N+1}(\pi_N dt) = \left[\int_{-1}^{1} t^{i+k}\pi_N(t)dt\right]_{i,k=0}^{N}$ is known to be nonsingular.

By *repeated Kronrod extension* we mean a sequence of Kronrod extensions (all assumed to exist),

$$Q_{N_0}(f) \subset Q_{N_1}(f) \subset Q_{N_2}(f) \subset \cdots\,, \tag{2.6}$$

where

$$N_0 = n\,,\ N_k = 2N_{k-1} + 1\,, \quad k = 1, 2, 3, \ldots\,. \tag{2.7}$$

Example 2.1: Gauss-Kronrod formula [KRONROD (1964)].

This is the Kronrod extension

$$Q_n(f) \subset Q_{2n+1}(f) \tag{2.8}$$

of the n-point Gauss formula $Q_n(f)$. It has all the desirable properties – interlacing of nodes [SZEGÖ (1935)] and positivity of weights [MONEGATO (1978)] – for each $n = 1, 2, 3, \ldots$.

Example 2.2: Gauss-Kronrod-Patterson formulae.

These are the repeated Kronrod extensions (2.6), (2.7) for $n = 3$ and $Q_3(f)$ the 3-point Gauss formula,

$$Q_3(f) \subset Q_7(f) \subset Q_{15}(f) \subset Q_{31}(f) \subset \cdots \quad . \tag{2.9}$$

The chain of quadrature rules has been computed numerically by PATTERSON (1968), (1973) through $Q_{255}(f)$. Remarkably, both the interlacing and positivity properties appear to hold for each extension, although no proof of this has ever been given.

3. Extension by Newton's method

Traditionally, the Kronrod extension (2.3) is computed by first obtaining π^*_{N+1} in (2.5), for example by expansion in Legendre or Chebyshev polynomials, then applying a rootfinding procedure to compute the zeros of π^*_{N+1} and finally (if the zeros are all real) computing the weights of the Kronrod extension as those of an interpolatory quadrature rule. The first two

steps can be combined into one by using eigenvalue techniques [see, e.g., ELHAY and KAUTSKY (1984), FREY, and WALDVOGEL and FREY].

Here we try to obtain all quantities of interest at once, by applying Newton's method to an appropriate system of nonlinear equations. If we write (2.3) as

$$Q_N(f) \subset Q_{2N+1}(f) = \sum_{\nu=1}^{N} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{N+1} \sigma_\mu^* f(\tau_\mu^*) , \tag{3.1}$$

where the τ_ν are prescribed and σ_ν, σ_μ^*, τ_μ^* are unknowns, the system of equations is taken to be

$$Q_{2N+1}(p_k) = m_k, \quad k = 0, 1, 2, \ldots, 3N+1 , \tag{3.2}$$

where p_k is the normalized Legendre polynomial of degree k and $m_k = \int_{-1}^{1} p_k(t)dt = \sqrt{2}\,\delta_{k,0}$ with $\delta_{0,0} = 1$, $\delta_{k,0} = 0$ for $k > 0$. Letting $x^T = [\sigma_1, \ldots, \sigma_N; \ \sigma_1^*, \ldots, \sigma_{N+1}^*; \ \tau_1^*, \ldots, \tau_{N+1}^*] \in \mathbb{R}^{3N+2}$ denote the vector of unknowns, we write (3.2) in the form

$$g(x) = 0 , \quad g: \mathbb{R}^{3N+2} \to \mathbb{R}^{3N+2} , \tag{3.3}$$

where g has as kth component $Q_{2N+1}(p_k) - m_k$, $k = 0, 1, \ldots, 3N+1$. We assume here that the extension (3.1) exists and has real nodes τ_μ^*.

Newton's method for (3.3) can then be written in the form

$$x_{i+1} = x_i - \Delta_i , \ \Delta_i = [g'(x_i)]^{-1} g(x_i) , \ i = 0, 1, 2, \ldots , \tag{3.4}$$

where $x_0 \in \mathbb{R}^{3N+2}$ is a suitable initial approximation and g' denotes the Jacobian matrix of g.

If symmetry is present, as in Examples 2.1 and 2.2, the system (3.3) can be reduced to essentially half its size, and in practice Newton's method need only be applied to this reduced system. For our qualitative study we shall ignore this simplification since Newton's method applied to the full system produces the same approximations as Newton's method applied to the reduced system, if the initial approximation of the former is the symmetric extension of that of the latter. Neither shall we concern ourselves here with other practical matters, such as the choice of initial approximations, for which we refer to CALIÒ et al. (1986).

As to convergence of Newton's method (3.4), suppose that

$$\| g''(x_0) \|_F \le M_0 \text{ on } U_0 = \{x \in \mathbf{R}^{3N+2}: \| x - x_0 \| \le 2 \| \Delta_0 \| \}, \tag{3.5}$$

where $\| g'' \|_F^2$ is the sum of the squares of all second partial derivatives of all components of g, and vector norms are Euclidean norms. A sufficient condition for convergence then is [OSTROWSKI (1966, p. 187)]

$$\theta_0 < 1, \quad \theta_0 := 2M_0 \| \Delta_0 \| \cdot \| [g'(x_0)]^{-1} \|_F, \tag{3.6}$$

where now $\| \cdot \|_F$ denotes the Frobenius matrix norm.

If we denote by $\hat{x} \in \mathbf{R}^{3N+2}$ the exact solution of (3.3) and assume that $\hat{\sigma}_\mu^* \neq 0$, $\mu = 1, 2, \ldots, N+1$, then a straightforward adaptation of an argument in GAUTSCHI (1982, Thm. 3.1) yields

$$\| [g'(\hat{x})]^{-1} \|_F = \left\{ \int_{-1}^{1} \phi_N(t) dt \right\}^{1/2}, \tag{3.7}$$

where

$$\phi_N = \sum_{\nu=1}^{N} \alpha_\nu^2 + \sum_{\mu=1}^{N+1} \left(\beta_\mu^2 + \frac{1}{\hat{\sigma}_\mu^{*2}} \gamma_\mu^2 \right) \tag{3.8}$$

is a polynomial of degree $6N + 2$ expressed in terms of elementary Hermite interpolation polynomials α_ν, β_μ, γ_μ defined by

$$\begin{aligned}
&\alpha_\nu(\hat{\tau}_\lambda) = \delta_{\nu\lambda}\,, \quad \alpha_\nu(\hat{\tau}_\mu^*) = 0\,, \quad \alpha_\nu'(\hat{\tau}_\mu^*) = 0\,; \\
&\beta_\mu(\hat{\tau}_\lambda) = 0\,, \quad \beta_\mu(\hat{\tau}_\kappa^*) = \delta_{\mu\kappa}\,, \quad \beta_\mu'(\hat{\tau}_\kappa^*) = 0\,; \\
&\gamma_\mu(\hat{\tau}_\lambda) = 0\,, \quad \gamma_\mu(\hat{\tau}_\kappa^*) = 0\,, \quad \gamma_\mu'(\hat{\tau}_\kappa^*) = \delta_{\mu\kappa}\,.
\end{aligned} \tag{3.9}$$

From the definition (3.8) of ϕ_N, and (3.9), it readily follows that

$$\begin{aligned}
&\phi_N(t) > 0\,, \quad \text{all } t \in \mathbf{R}\,, \\
&\phi_N(\hat{\tau}_\nu) = 1\,, \quad \nu = 1, 2, \ldots, N\,, \\
&\phi_N(\hat{\tau}_\mu^*) = 1\,, \quad \phi_N'(\hat{\tau}_\mu^*) = 0\,, \quad \mu = 1, 2, \ldots, N+1\,.
\end{aligned} \tag{3.10}$$

We emphasize that (3.7) is an *equality,* not an inequality, and that it holds for *any* Kronrod extension with real distinct nodes and $\hat{\sigma}_\mu^* \neq 0$, including those that may arise as links in a chain of repeated Kronrod extensions.

4. Numerical behavior of Newton's method

Since notable differences were observed in the performance of Newton's method for one-time and repeated application of the Kronrod extension process, we carried out controlled experiments for the Gauss-Kronrod extension (2.8) and the Gauss-Kronrod-Patterson extensions (2.9) in order to (i) observe to what extent the sufficient condition of convergence (3.6) was satisfied (approximately) for various initial approximations at preassigned accuracy levels;

(ii) see how satisfaction or violation of (3.6) correlates with actual convergence or divergence of Newton's method; (iii) understand the principal factors responsible for convergence or divergence. All computations were carried out in double precision on the DEC VAX 11/780 computer (machine precision $\approx 2.78\times10^{-17}$).

Since accurate answers for the solutions $\hat{x}$ are available in the literature, it was easy to select initial approximations x_0 having preassigned accuracy, say $\|x_0 - \hat{x}\| \approx \varepsilon$. In reporting our results, we approximate M_0 in (3.5) by $\hat{M} = \|g''(\hat{x})\|_F$ and $\Gamma_0 = \|[g'(x_0)]^{-1}\|_F$ by $\hat{\Gamma} = \|[g'(\hat{x})]^{-1}\|_F$ as given in (3.7). The resulting approximation for θ_0 in (3.6) is denoted by $\hat{\theta}$; thus, $\hat{\theta} = 2\hat{M}\hat{\Gamma}\|\Delta_0\|$.

In our first experiment we applied Newton's method to compute the Gauss-Kronrod extension (2.8) for $n = 3, 7, 15, 31$, starting with initial approximations x_0 at accuracy levels $\varepsilon = 10^{-14}$, $\varepsilon = 10^{-10}$, and $\varepsilon = 10^{-6}$. In each case we computed the quantities $\|\Delta_0\|$, $\hat{M}$, $\hat{\Gamma}$, $\hat{\theta}$.

Table I. *Convergence study of Newton's method applied to* (2.8) *with* $n = 3, 7, 15, 31$

n	ε	$\|\Delta_0\|$	$\hat{M}$	$\hat{\Gamma}$	$\hat{\theta}$
3	10^{-14}	9.7(–15)	2.8(2)	1.6(0)	8.7(–12)
	10^{-10}	1.3(–10)			1.2(–7)
	10^{-6}	1.1(–6)			9.9(–4)
7	10^{-14}	2.1(–14)	2.4(3)	1.4(0)	1.4(–10)
	10^{-10}	1.7(–10)			1.1(–6)
	10^{-6}	1.8(–6)			1.2(–2)
15	10^{-14}	2.2(–14)	2.0(4)	1.4(0)	1.2(–9)
	10^{-10}	1.8(–10)			1.0(–5)
	10^{-6}	1.6(–6)			9.0(–2)
31	10^{-14}	2.1(–14)	1.6(5)	1.3(0)	8.7(–9)
	10^{-10}	1.9(–10)			7.9(–5)
	10^{-6}	2.4(–6)			1.0(0)

The results are displayed in Table I. (Integers in parentheses denote decimal exponents.) It can be seen that the sufficient condition (3.6) is amply satisfied at all accuracy levels shown, except for 6-digit initial approximation when $n = 31$, in which case it is just barely satisfied. Actually, Newton's method did in fact converge in all cases.

Our second experiment is an analogous study of the first four Gauss-Kronrod-Patterson extensions in (2.9), i.e., (3.1) with $N = 3$, 7, 15 and 31, and the nodes τ_ν on the right of (3.1) being those of the N-point Gauss-Kronrod-Patterson formula (the Gauss formula, when $N = 3$). The results obtained are shown in Table II. (The case $N = 3$ in Table II is identical with the case $n = 3$ in Table I.)

Tabel II. *Convergence study of Newton's method applied to* (2.9)

N	ε	$\|\|\Delta_0\|\|$	$\hat{M}$	$\hat{\Gamma}$	$\hat{\theta}$
3	10^{-14}	9.7(–15)	2.8(2)	1.6(0)	8.7(–12)
	10^{-10}	1.3(–10)			1.2(–7)
	10^{-6}	1.1(–6)			9.9(–4)
7	10^{-14}	1.9(–14)	2.3(3)	1.5(0)	1.3(–10)
	10^{-10}	1.6(–10)			1.1(–6)
	10^{-6}	2.1(–6)			1.4(–2)
15	10^{-14}	2.2(–14)	1.7(4)	7.9(0)	5.9(–9)
	10^{-10}	2.0(–10)			5.4(–5)
	10^{-6}	2.3(–6)			6.2(–1)
31	10^{-14}	1.4(–10)	1.3(5)	9.6(5)	3.5(+1)
	10^{-10}	2.6(–10)			6.5(+1)
	10^{-6}	9.5(–5)			2.4(+7)

What is most notable in Table II is the large jump of $\hat{\Gamma}$ going from $N = 15$ to $N = 31$. The value of $\hat{\Gamma}$ for $N = 31$ is about 10^6 times as large as the corresponding value in Table I. This leads to values of the convergence index $\hat{\theta}$ considerably larger than 1. (For $\varepsilon = 10^{-14}$, the relatively large value of $\|\|\Delta_0\|\|$, and hence the large value of $\hat{\theta}$, is in part due to double-

precision rounding effects.) It was observed that Newton's method with initial approximations at the accuracy levels ε shown converges only when $N = 3$, 7 and 15, but not for $N = 31$.

In order to appreciate and to understand the well-behaved and ill-behaved nature of $\hat{\Gamma}$ in the contexts of (2.8) and (2.9), respectively, we display in Figures 1 and 2 the polynomial ϕ_N of (3.8) [which determines $\hat{\Gamma}$ according to (3.7)] in the case (2.8) for $n = 3$, 7, 15, 31 and in the respective cases of (2.9). [For $n = 3$, the graphs are identical.] Only half of the graphs are shown, since they are symmetric with respect to the origin.

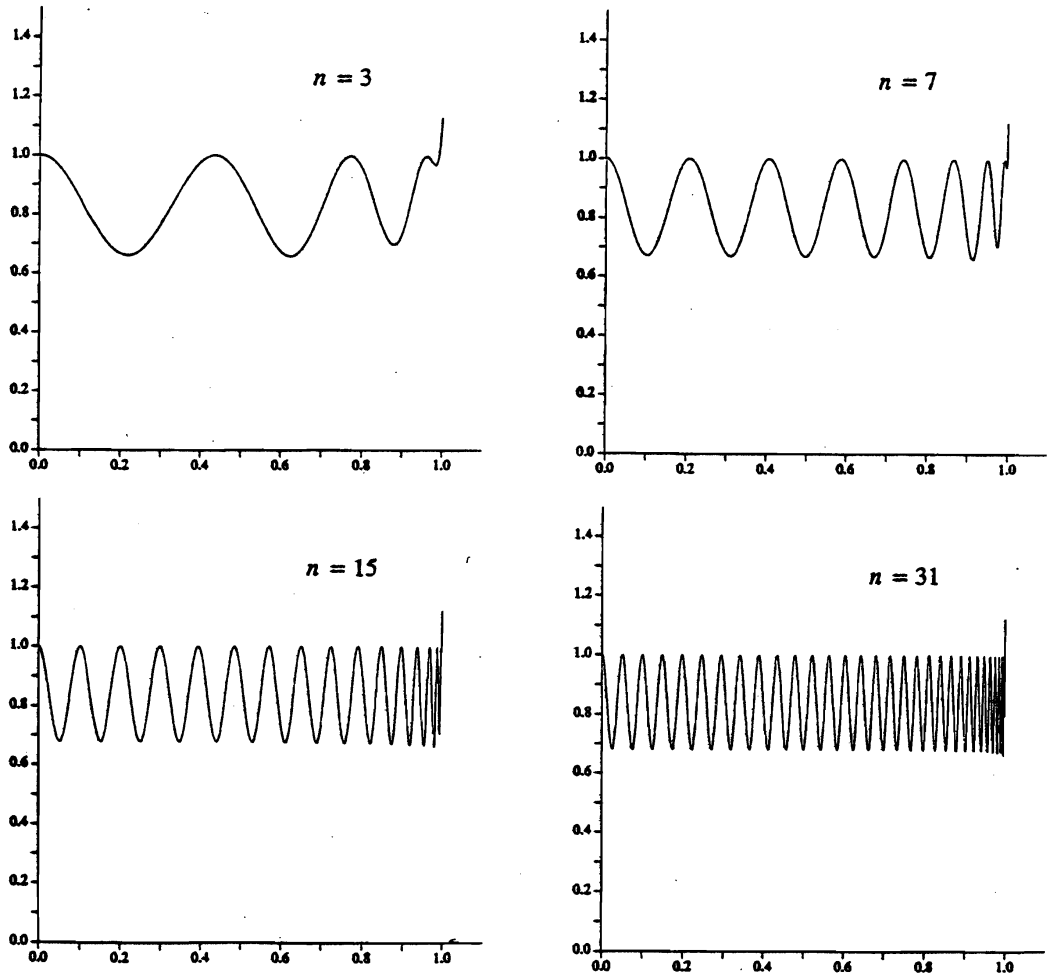

Fig. 1. *The behavior of* ϕ_N *in the case of* (2.8), $n = 3$, 7, 15, 31

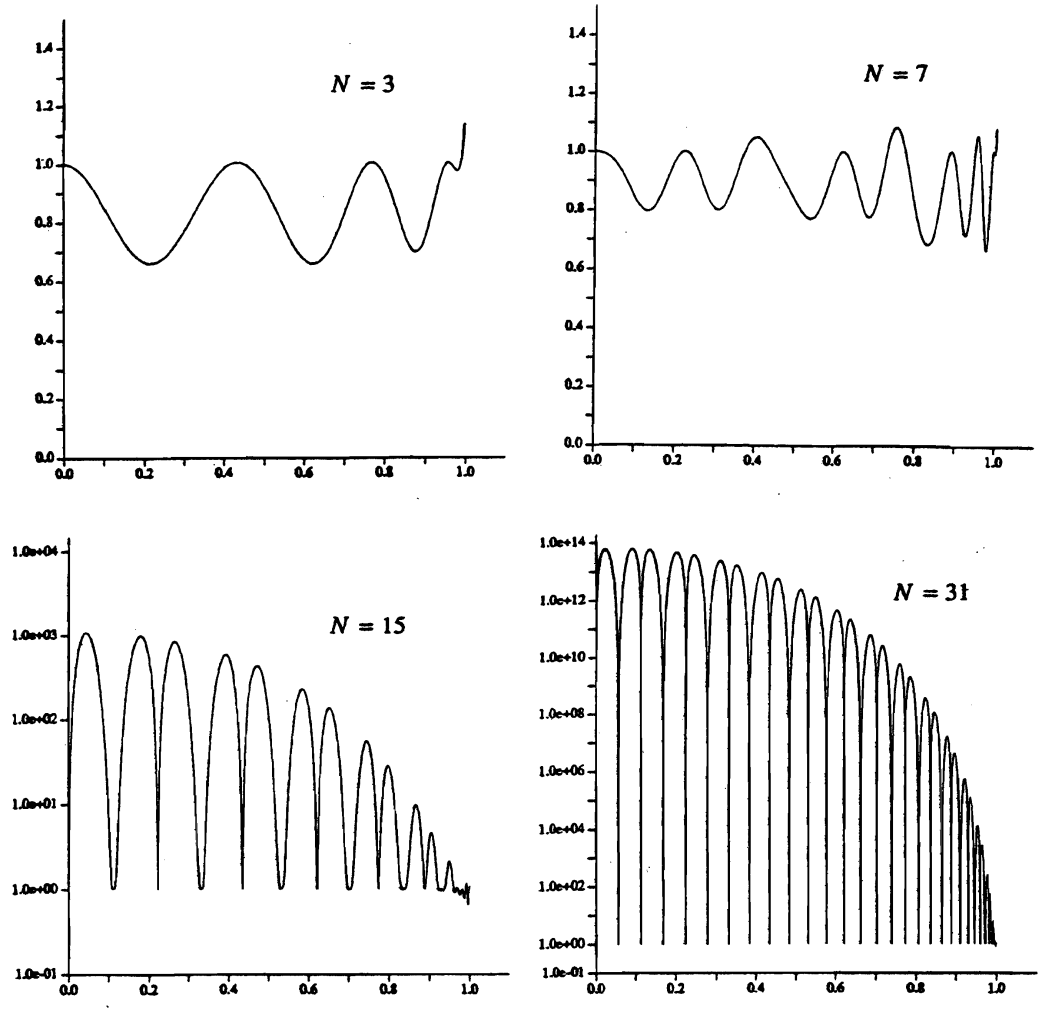

Fig. 2. *The behavior of* ϕ_N *in the first four extensions of* (2.9)

It can be seen that for one-time Kronrod extension, ϕ_N is less than 1 over most of the interval [−1,1], the exceptions occurring very close to the endpoints ± 1. For repeated Kronrod extension, the story is quite different!

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An Algebraic Study of Gauss-Kronrod Quadrature Formulae for Jacobi Weight Functions*

By Walter Gautschi and Sotirios E. Notaris

Abstract. We study Gauss-Kronrod quadrature formulae for the Jacobi weight function $w^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta$ and its special case $\alpha = \beta = \lambda - \frac{1}{2}$ of the Gegenbauer weight function. We are interested in delineating regions in the (α,β)-plane, resp. intervals in λ, for which the quadrature rule has (a) the interlacing property, i.e., the Gauss nodes and the Kronrod nodes interlace; (b) all nodes contained in $(-1,1)$; (c) all weights positive; (d) only real nodes (not necessarily satisfying (a) and/or (b)). We determine the respective regions numerically for $n = 1(1)20(4)40$ in the Gegenbauer case, and for $n = 1(1)10$ in the Jacobi case, where n is the number of Gauss nodes. Algebraic criteria, in particular the vanishing of appropriate resultants and discriminants, are used to determine the boundaries of the regions identifying properties (a) and (d). The regions for properties (b) and (c) are found more directly. A number of conjectures are suggested by the numerical results. Finally, the Gauss-Kronrod formula for the weight $w^{(\alpha,1/2)}$ is obtained from the one for the weight $w^{(\alpha,\alpha)}$, and similarly, the Gauss-Kronrod formula with an odd number of Gauss nodes for the weight function $w(t) = |t|^\gamma(1-t^2)^\alpha$ is derived from the Gauss-Kronrod formula for the weight $w^{(\alpha,(1+\gamma)/2)}$.

1. Introduction. A Gauss-Kronrod quadrature formula for the (nonnegative) weight function w on $[a,b]$ is a quadrature formula of the form

$$\int_a^b f(t)w(t)\,dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f), \tag{1.1}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes (i.e., the zeros of $\pi_n(\cdot; w\,dt)$, the nth degree (monic) orthogonal polynomial relative to the measure $d\sigma(t) = w(t)\,dt$ on $[a,b]$) and the nodes $\tau_\mu^* = \tau_\mu^{(n)*}$ (the "Kronrod nodes") and weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{(n)*}$ are determined such that (1.1) has maximum degree of exactness $3n+1$, i.e.,

$$R_n(f) = 0, \quad \text{all } f \in \mathbf{P}_{3n+1}. \tag{1.2}$$

It is well known that τ_μ^* must be the zeros of the (monic) polynomial π_{n+1}^* of degree $n+1$ orthogonal to all polynomials of degree n with respect to the "weight function"

$$w^*(t) = \pi_n(t; w\,dt)w(t) \quad \text{on } [a,b]. \tag{1.3}$$

Even though π_n, and hence w^*, changes sign on $[a,b]$, it is known that π_{n+1}^* exists uniquely (see, e.g., Gautschi [3, Section 3.1.2]). There is no guarantee, however, that the zeros τ_μ^* of π_{n+1}^* are inside the interval $[a,b]$, or real, for that matter.

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Our interest here is indeed in obtaining precise information about the reality and location of these zeros, as well as the positivity of all weights. We are studying these questions in the case where w is the Jacobi weight function,

$$w^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta, \qquad -1 < t < 1, \alpha > -1, \beta > -1, \tag{1.4}$$

or its special case, the Gegenbauer weight

$$w_\lambda(t) = w^{(\lambda-1/2,\lambda-1/2)}(t), \qquad -1 < t < 1, \lambda > -\tfrac{1}{2}. \tag{1.5}$$

We say that the nodes of (1.1) *interlace* if they are all real and, when ordered decreasingly, satisfy

$$-\infty < \tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^* < \infty. \tag{1.6}$$

Our objective is, for each fixed $n = 1, 2, 3, \ldots$, to determine domains of the parameters α, β and λ, respectively, in which either of the following properties holds:

(a) The nodes τ_ν, τ_μ^* interlace.
(b) All nodes τ_ν, τ_μ^*, in addition to satisfying (1.6), are contained in $(-1,1)$, i.e., $-1 < \tau_{n+1}^*$ and $\tau_1^* < 1$.
(c) The nodes interlace and each weight σ_ν is positive. (The positivity of σ_μ^* is equivalent to the interlacing property; see Monegato [5, Theorem 1].)
(d) All nodes, without necessarily satisfying (a) and/or (b), are real.

To answer these questions, we start from the known fact (see, e.g., Gautschi [3, Section 2.1.2]) that all properties (a)–(d) hold for the Gegenbauer weight (1.5), or the Jacobi weight (1.4) with $\alpha = \beta = \lambda - \frac{1}{2}$, when $0 < \lambda < 1$. Moving the parameters α, β, or λ, continuously away from this segment induces a continuous motion of the nodes τ_ν, τ_μ^*, which, initially, are constrained to move on the real line. The interlacing property breaks down the first time a node τ_μ^* collides with a node τ_ν. The polynomials π_n and π_{n+1}^* then have a common zero, a fact that can be detected by determining when the resultant $R(\pi_n, \pi_{n+1}^*)$ of π_n and π_{n+1}^* vanishes (for the first time). When a collision occurs, the nodes τ_ν, τ_μ^* involved most likely cross each other, so that there are now two Kronrod nodes captured between two Gauss nodes. Only now is it possible that two Kronrod nodes may collide, giving rise to a pair of complex Kronrod nodes. The occurrence of this event can be detected by determining the appropriate zero of the resultant $R(\pi_{n+1}^*, \pi_{n+1}^{*\prime})$. This allows us to settle property (d). Properties (b) and (c) are easily dealt with by examining when (for the first time) $(\tau_{n+1}^* + 1)(\tau_1^* - 1) = 0$, and $\sigma_\nu = 0$ for some ν, respectively.

In Section 2 we carry out this program for the Gegenbauer weight (1.5). The success of the calculations, particularly when n is large, depends crucially on the resultants involved being computed in a stable manner. This is discussed in Section 3. In Section 4 we report on limited explorations for the case of the Jacobi weight (1.4). Section 5 presents analytic treatments of Gauss-Kronrod formulae for Jacobi weights with parameter $\beta = \frac{1}{2}$ and for the weight function $w(t) = |t|^\gamma(1-t^2)^\alpha$, $\alpha > -1$, $\gamma > -1$, on $(-1,1)$.

2. Gegenbauer Weights. We consider here the weight function (1.5), that is,

$$w_\lambda(t) = (1-t^2)^{\lambda-1/2}, \qquad -1 < t < 1, \lambda > -\tfrac{1}{2}. \tag{2.1}$$

Using

$$\int_{-1}^{1} t^{2m}(1-t^2)^{\lambda-1/2}\,dt = \int_0^1 x^{m-1/2}(1-x)^{\lambda-1/2}\,dx$$
$$= B\left(m+\frac{1}{2},\lambda+\frac{1}{2}\right) = \frac{\Gamma(m+\frac{1}{2})\Gamma(\lambda+\frac{1}{2})}{\Gamma(m+\lambda+1)}, \qquad m=0,1,2,\ldots,$$

it is straightforward (though tedious, at times) to compute π_n, π_{n+1}^* explicitly for the first few values of n. One obtains, for $n=1,2,3$ and 4,

$$(2.2_1) \qquad \pi_1(t)=t, \qquad \pi_2^*(t)=t^2-\frac{3}{2(\lambda+2)},$$

$$(2.2_2) \qquad \pi_2(t)=t^2-\frac{1}{2(\lambda+1)}, \qquad \pi_3^*(t)=t^3-\frac{3}{\lambda+3}t,$$

$$(2.2_3) \qquad \pi_3(t)=t^3-\frac{3}{2(\lambda+2)}t, \qquad \pi_4^*(t)=t^4-\frac{5}{\lambda+4}t^2+\frac{5}{4}\frac{16-\lambda}{(\lambda+4)^2(\lambda+5)},$$

$$(2.2_4) \qquad \begin{aligned} \pi_4(t) &= t^4-\frac{3}{\lambda+3}t^2+\frac{3}{4(\lambda+2)(\lambda+3)}, \\ \pi_5^*(t) &= t^5-\frac{15}{2(\lambda+5)}t^3+\frac{15}{4}\frac{\lambda+20}{(\lambda+5)^2(\lambda+6)}t. \end{aligned}$$

Likewise, using the formula (Monegato [5, Eq. (2.5)])

$$(2.3) \qquad \sigma_\nu^{(n)} = \lambda_\nu^{(n)} + \frac{\|\pi_n\|_w^2}{\pi_{n+1}^*(\tau_\nu^{(n)})\pi_n'(\tau_\nu^{(n)})},$$

where $\lambda_\nu^{(n)}$ are the Christoffel numbers (i.e., the weights in the Gaussian quadrature rule) and $\|\cdot\|_w$ the L_2-norm for the weight function (2.1), one obtains

$$(2.4_1) \qquad \sigma_1^{(1)} = \frac{2\sqrt{\pi}}{3}\frac{\Gamma(\lambda+3/2)}{\Gamma(\lambda+2)},$$

$$(2.4_2) \qquad \sigma_1^{(2)} = \sigma_2^{(2)} = \frac{3\sqrt{\pi}}{2}\frac{\Gamma(\lambda+\frac{1}{2})(\lambda+1)^2}{\Gamma(\lambda+1)(\lambda+2)(5\lambda+3)},$$

$$(2.4_3) \qquad \sigma_1^{(3)} = \sigma_3^{(3)} = \frac{5\sqrt{\pi}}{3}\frac{\Gamma(\lambda+\frac{1}{2})(\lambda+2)^4(2\lambda+3)}{\Gamma(\lambda+2)(\lambda+3)(26\lambda^3+153\lambda^2+336\lambda+160)},$$

$$\sigma_2^{(3)} = \frac{8\sqrt{\pi}}{15}\frac{\Gamma(\lambda+5/2)(40+7\lambda-2\lambda^2)}{\Gamma(\lambda+4)(16-\lambda)},$$

$$(2.4_4) \qquad \sigma_1^{(4)} = \sigma_4^{(4)} = \frac{5\sqrt{\pi}}{2}\times$$
$$\frac{\Gamma(\lambda+3/2)(\lambda+2)(\lambda+3)^4[(\lambda+5)(\lambda+6)(2\lambda+3)+\omega(\lambda+2)(\lambda^2-15)]}{\Gamma(\lambda+5)\omega(\omega+3)(2\lambda-\omega+3)[5\lambda^4+11\lambda^3-109\lambda^2-465\lambda-450+\omega(\lambda+2)(\lambda+5)(\lambda+6)(3\lambda+5)]},$$
$$\sigma_2^{(4)} = \sigma_3^{(4)} = \text{same expression with } \omega \text{ replaced by } -\omega,$$

where $\omega=[3(2\lambda+3)/(\lambda+2)]^{1/2}$ in (2.4_4).

For $n=1$, the Gauss-Kronrod rule is the 3-point Gauss rule and therefore satisfies properties (a)–(d) for all $\lambda > -\frac{1}{2}$. If $n=2$, Eq. (2.2_2) shows that (a) [hence also (d)] holds for all $\lambda > -\frac{1}{2}$ and (b) for all $\lambda > 0$, while Eq. (2.4_2) shows that (c) holds for all $\lambda > -\frac{1}{2}$. We now discuss in detail the two cases $n=3$ and

$n = 4$ for which we have analytic expressions for all the quantities of interest. They are representative for the cases n odd and n even, respectively, to be discussed subsequently.

If $n = 3$, the polynomials π_3 and π_4^* have common zeros if and only if either $\pi_4^*(0) = 0$ (in which case 0 is a common zero) or the polynomials

$$\frac{1}{\sqrt{x}}\pi_3(\sqrt{x}) = x - \frac{3}{2(\lambda+2)} =: p_3(x),$$
$$\pi_4^*(\sqrt{x}) = x^2 - \frac{5}{\lambda+4}x + \frac{5}{4}\frac{16-\lambda}{(\lambda+4)^2(\lambda+5)} =: p_4^*(x)$$

have a common zero. The former, by (2.2_3), is true exactly for $\lambda = 16$, whereas the latter is true precisely if the resultant of p_3 and p_4^* vanishes,

$$R(p_3, p_4^*) = \begin{vmatrix} 1 & -\frac{3}{2(\lambda+2)} & 0 \\ 0 & 1 & -\frac{3}{2(\lambda+2)} \\ 1 & -\frac{5}{\lambda+4} & \frac{5}{4}\frac{16-\lambda}{(\lambda+4)^2(\lambda+5)} \end{vmatrix} = 0. \tag{2.5}$$

An easy calculation shows that

$$R(p_3, p_4^*) = -\tfrac{1}{4}(\lambda+2)^{-2}(\lambda+4)^{-2}(\lambda+5)^{-1}(26\lambda^3 + 153\lambda^2 + 336\lambda + 160). \tag{2.6$_3$}$$

The cubic polynomial on the right has one real zero at $-.6447375\ldots$ and a pair of conjugate complex zeros, hence is positive for all $\lambda > -\frac{1}{2}$. Therefore, $R(p_3, p_4^*) < 0$ for all $\lambda > -\frac{1}{2}$. It follows that (a) is true precisely for $-\frac{1}{2} < \lambda < 16$, there occurring a collision of nodes at the origin when $\lambda = 16$, but no other collisions. Since the zeros of π_4^* are symmetric with respect to the origin, π_4^* has a double zero at the origin when $\lambda = 16$, which splits into a pair of conjugate complex zeros as λ increases beyond 16. Indeed, the constant term of p_4^*, hence at least one of the zeros of p_4^*, becomes (and remains) negative, giving rise to a pair of complex zeros of π_4^*. Therefore, (d) is true exactly for $-\frac{1}{2} < \lambda \leq 16$. Property (b) is discussed most easily by noting that it is equivalent to $\pi_4^*(1) > 0$. Indeed, $\tau_1^* < 1$ clearly implies $\pi_4^*(1) > 0$, while, conversely, $\pi_4^*(1) > 0$ implies $\tau_1^* < 1$ since otherwise, by the interlacing property, $\tau_1 < 1 \leq \tau_1^*$, meaning that $\pi_4^*(1) \leq 0$. Since, by (2.2_3),

$$\pi_4^*(1) = \tfrac{1}{4}\lambda(\lambda+4)^{-2}(\lambda+5)^{-1}(2\lambda+3)(2\lambda+13), \tag{2.7$_3$}$$

we have property (b) precisely if $\lambda > 0$. The cubic polynomial in the denominator of $\sigma_1^{(3)}$ [cf. (2.4_3)] being the same as the one in (2.6_3), hence positive for all $\lambda > -\frac{1}{2}$, it follows that $\sigma_1^{(3)} > 0$ for all $\lambda > -\frac{1}{2}$. Assuming $-\frac{1}{2} < \lambda < 16$, we have, on the other hand, $\sigma_2^{(3)} > 0$ if and only if $40 + 7\lambda - 2\lambda^2 > 0$, i.e., $-\frac{1}{2} < \lambda < \frac{1}{4}(7 + 3\sqrt{41}) = 6.552343\ldots$. This settles property (c).

Now consider $n = 4$. Since $\pi_4(0) \neq 0$, the origin is never a common zero of π_4 and π_5^*, and π_4, π_5^* have a common zero if and only if the same is true for the polynomials $\pi_4(\sqrt{x}) =: p_4(x)$ and $(\sqrt{x})^{-1}\pi_5^*(\sqrt{x}) =: p_5^*(x)$. Using (2.2_4), a

somewhat lengthy computation gives

$$R(p_4, p_5^*) = -\tfrac{9}{16}(\lambda+2)^{-2}(\lambda+3)^{-2}(\lambda+5)^{-4}(\lambda+6)^{-2} \times [29\lambda^6 + 1273\lambda^5 + 11904\lambda^4 + 48385\lambda^3 + 91925\lambda^2 + 78000\lambda + 22500]. \tag{2.6$_4$}$$

The polynomial in brackets has two real zeros at $-.580667\ldots$ and $-32.863977\ldots$ and two pairs of conjugate complex zeros. Consequently, $R(p_4, p_5^*) < 0$ for all $\lambda > -\frac{1}{2}$, and property (a) [hence also (d)] holds for all $\lambda > -\frac{1}{2}$. From (2.2$_4$) we find

$$\pi_5^*(1) = \tfrac{1}{4}(\lambda+5)^{-2}(\lambda+6)^{-1}\lambda(4\lambda^2+34\lambda+25), \tag{2.7$_4$}$$

where the quadratic has the two negative zeros $-.813068\ldots$ and $-7.686931\ldots$, hence remains positive for $\lambda > -\frac{1}{2}$. Property (b), i.e., $\pi_5^*(1) > 0$, therefore holds precisely for $\lambda > 0$. Another lengthy (but elementary) computation, based on (2.4$_4$), shows that $\sigma_1^{(4)}$ is positive for all $\lambda > -\frac{1}{2}$, but $\sigma_2^{(4)} > 0$ only if $\lambda < 51.7868606883\ldots$, the unique positive root of $\lambda^3 - 47\lambda^2 - 245\lambda - 150 = 0$. Thus, property (c) holds precisely if this last condition is satisfied.

The results for $1 \le n \le 4$ are summarized in Table 2.1, which shows the interval $\lambda_n^p < \lambda < \Lambda_n^p$ in which property (p) holds, $p = a, b, c, d$. An extended table for $n = 5(1)20(4)40$ is given as Table A.1 in the appendix.** The reasonings used to compute Table A.1 were similar to the ones explained in the cases $n = 3$ and $n = 4$, and are now briefly described.

TABLE 2.1

Property (p) $(p = a, b, c, d)$ *for* $1 \le n \le 4$.

n	λ_n^a	Λ_n^a	λ_n^b	Λ_n^b	λ_n^c	Λ_n^c	λ_n^d	Λ_n^d
1	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞
2	$-\frac{1}{2}$	∞	0	∞	$-\frac{1}{2}$	∞	$-\frac{1}{2}$	∞
3	$-\frac{1}{2}$	16	0	16	$-\frac{1}{2}$	$(7+3\sqrt{41})/4$	$-\frac{1}{2}$	16
4	$-\frac{1}{2}$	∞	0	∞	$-\frac{1}{2}$	$51.786\ldots$	$-\frac{1}{2}$	∞

It is convenient to distinguish between $n = 2m$ even, in which case we write

$$\pi_{2m}(\sqrt{x}) = x^m + a_{2m,1}x^{m-1} + \cdots + a_{2m,m} =: p_{2m}(x),$$
$$\frac{1}{\sqrt{x}}\pi_{2m+1}^*(\sqrt{x}) = x^m + b_{2m+1,1}x^{m-1} + \cdots + b_{2m+1,m} =: p_{2m+1}^*(x), \tag{2.8$_{\text{even}}$}$$

and $n = 2m-1$ odd, in which case we write

$$\frac{1}{\sqrt{x}}\pi_{2m-1}(\sqrt{x}) = x^{m-1} + a_{2m-1,1}x^{m-2} + \cdots + a_{2m-1,m-1} =: p_{2m-1}(x),$$
$$\pi_{2m}^*(\sqrt{x}) = x^m + b_{2m,1}x^{m-1} + \cdots + b_{2m,m} =: p_{2m}^*(x). \tag{2.8$_{\text{odd}}$}$$

**Professor I. P. Mysovskih informed the first-named author by letter of October 28, 1987, that L. N. Puolokaĭnen [7], in a 1964 diploma paper prepared under his guidance, obtained $\lambda_n^a = -\frac{1}{2}$ for $n = 1(1)7$ and the same values of Λ_n^a, $n = 1(1)4$, as shown in Table 2.1. She furthermore calculated 6D values of Λ_n^a, $n = 5(1)7$, which agree with ours in Table A.1 to 4–5 significant digits.

(Computational details for generating the coefficients in (2.8) and for the procedures to be described will be discussed in Section 3.)

To examine property (a), note that in the case $n = 2m$, since $a_{2m,m} \neq 0$, the polynomials π_{2m} and π^*_{2m+1} have a common zero if and only if p_{2m} and p^*_{2m+1} do, i.e., precisely if the resultant $R(p_{2m}, p^*_{2m+1})$ vanishes. This resultant, of course, has a constant sign on the interval $0 < \lambda < 1$; in all cases computed, it was found that the sign on $-\frac{1}{2} < \lambda \leq 0$ remained the same. Consequently, $\lambda^a_n = -\frac{1}{2}$. The quantity Λ^a_n is the first value of λ for which the resultant vanishes. This value was determined by a preliminary search, followed by the bisection method. The case $n = 2m - 1$ is handled similarly, except for the additional possibility that the origin is a common zero of π_{2m-1} and π^*_{2m}. This was detected (if the case indeed occurs) by the coefficient $b_{2m,m}$ changing its sign. Our numerical work suggests the following

CONJECTURE 2.1. *The Kronrod nodes $\tau^{(n)*}_\mu$ and Gauss nodes $\tau^{(n)}_\nu$ for the weight function w_λ in* (2.1) *interlace if $-\frac{1}{2} < \lambda < \Lambda^a_n$, where Λ^a_n are certain constants > 1.* (For numerical values of Λ^a_n, $n = 1(1)20(4)40$, see Tables 2.1 and A.1.)

Property (b), as in the cases $n = 3, 4$, is settled by determining the subinterval of $(-\frac{1}{2}, \Lambda^a_n)$ in which $\pi^*_{n+1}(1) > 0$, and property (c) by determining the subinterval of $(-\frac{1}{2}, \Lambda^a_n)$ in which $\sigma^{(n)}_\nu > 0$ for all $\nu = 1, 2, \ldots, n$. The results can be summarized as

CONJECTURE 2.2. *The Kronrod nodes $\tau^{(n)*}_\mu$ and Gauss nodes $\tau^{(n)}_\nu$ for the weight function w_λ in* (2.1), *in addition to interlacing, are all contained in* $(-1, 1)$ *if $0 < \lambda < \Lambda^a_n$, where Λ^a_n are the constants in Conjecture* 2.1*; some Kronrod nodes are outside of* $[-1, 1]$ *if $\lambda < 0$.*

CONJECTURE 2.3. *The Kronrod nodes and Gauss nodes for the weight function w_λ in* (2.1) *interlace, and all weights $\sigma^{(n)}_\nu$ are positive, if $-\frac{1}{2} < \lambda < \Lambda^c_n$, where Λ^c_n are certain constants $1 < \Lambda^c_n < \Lambda^a_n$.* (For numerical values of Λ^c_n, $n = 1(1)20(4)40$, see Tables 2.1 and A.1.)

Property (d), finally, needs to be considered only for $\lambda \geq \Lambda^a_n$ and requires the examination of discriminants. Complex zeros (of π^*_{n+1}) indeed can only arise from multiple zeros, i.e., after $R(\pi^*_{n+1}, \pi^{*\prime}_{n+1})$ has vanished. The discussion of this again depends, in part, on the parity of n. If $n = 2m$, we write

$$\begin{aligned} \frac{1}{\sqrt{x}}\pi^*_{2m+1}(\sqrt{x}) &= x^m + b_{2m+1,1}x^{m-1} + \cdots + b_{2m+1,m} =: p^*_{2m+1}(x), \\ \pi^{*\prime}_{2m+1}(\sqrt{x}) &= (2m+1)x^m + (2m-1)b_{2m+1,1}x^{m-1} + \cdots + b_{2m+1,m} \\ &=: q^*_{2m+1}(x), \end{aligned} \tag{2.9$_{\text{even}}$}$$

and if $n = 2m - 1$,

$$\begin{aligned} \pi^*_{2m}(\sqrt{x}) &= x^m + b_{2m,1}x^{m-1} + \cdots + b_{2m,m} =: p^*_{2m}(x), \\ \frac{1}{\sqrt{x}}\pi^{*\prime}_{2m}(\sqrt{x}) &= 2mx^{m-1} + (2m-2)b_{2m,1}x^{m-2} + \cdots + 2b_{2m,m-1} \\ &=: q^*_{2m}(x). \end{aligned} \tag{2.9$_{\text{odd}}$}$$

There are two possibilities: Either the common zero of π^*_{n+1} and $\pi^{*\prime}_{n+1}$ is also a zero of π_n, or it is not. The first case can only occur if two Kronrod nodes collide with one another and simultaneously with a Gauss node. If n is even, this

is unlikely to occur and, in fact, was never observed. It is also unlikely, and was not observed, when n is odd, unless the collision takes place at the origin,

$$\pi_n(0) = \pi^*_{n+1}(0) = \pi^{*\prime}_{n+1}(0) \qquad (n = 2m-1 \text{ odd}), \tag{2.10}$$

in which case, since $\lambda \geq \Lambda^a_n$, we must have $\lambda = \Lambda^a_n$. The event (2.10) indeed seems to occur whenever m in (2.10) is even; then, moreover, $b_{2m,m}$ in (2.9_{odd}) was observed to change sign from positive to negative (cf. the discussion of property (a) above). This means that for λ immediately beyond Λ^a_n, the polynomial p^*_{2m} has at least one negative zero (since m is even!), hence π^*_{2m} a pair of conjugate complex zeros. Consequently, $\Lambda^d_n = \Lambda^a_n$ in this case.

If the common zero of π^*_{n+1} and $\pi^{*\prime}_{n+1}$ is *not* a zero of π_n, then necessarily $\Lambda^d_n > \Lambda^a_n$. It was found, then, that $b_{2m+1,m}$ and $b_{2m,m}$ in (2.9) do not vanish, so that the zero in question cannot be the origin. It then follows that π^*_{n+1} and $\pi^{*\prime}_{n+1}$ have a common zero if and only if p^*_{n+1} and q^*_{n+1} do, i.e., if $R(p^*_{n+1}, q^*_{n+1}) = 0$. This event again can be determined by a search and bisection procedure. It transpired that the resultant $R(p^*_{n+1}, q^*_{n+1})$ not only vanishes for some $\lambda = \lambda^* > \Lambda^a_n$, but also changes sign there. Since

$$R(p^*_{n+1}, q^*_{n+1}) = \prod_{\mu} p^*_{n+1}(\xi_\mu),$$

where ξ_μ are the zeros of q^*_{n+1} (cf. [10, Section 5.9]), a pair of positive zeros of p^*_{n+1} (and hence a pair of real zeros of π^*_{n+1}) coalesce and then disappear as λ passes through λ^*, i.e., p^*_{n+1} (and hence π^*_{n+1}) has a pair of conjugate complex zeros for λ immediately beyond λ^*. There follows $\lambda^* = \Lambda^d_n$. Thus we form the

CONJECTURE 2.4. *All Kronrod nodes $\tau^{(n)*}_\mu$ for the weight function w_λ in* (2.1) *are real if $-\frac{1}{2} < \lambda \leq \Lambda^d_n$, where Λ^d_n ($n \neq 1, 2, 4$) are certain constants either slightly larger than Λ^a_n, or equal to Λ^a_n, the latter precisely if $n = 4r-1$, $r = 1, 2, 3, \ldots$.* (For numerical values of Λ^d_n, $n = 1(1)20(4)40$, see Tables 2.1 and A.1.)

3. Computational Considerations. All computations were performed on the CDC 6500 computer in single or double precision (machine precision 3.55×10^{-15} and 1.26×10^{-29}, respectively).

Two different methods were used to compute the various resultants involved. One is an obvious extension of the method exemplified in Section 2. The coefficients $a_{n,k}$ of the polynomial p_n (cf. (2.8)) are first computed by a recurrence relation that results from the linear relation connecting three consecutive π_k of the same parity. The coefficients $b_{n,k}$ of p^*_{n+1} (cf. (2.8)) then satisfy a system of linear algebraic equations expressing orthogonality of π^*_{n+1} (with respect to the weight function $w^* = w_\lambda \pi_n$) to the first $[(n+1)/2]$ odd powers. This system has been solved using the LINPACK [2] routines SGECO, SGESL (and their double-precision companions), whereupon the resultants of p_n and p^*_{n+1} and of p^*_{n+1} and q^*_{n+1} can be computed in determinant form (cf. [10, Section 5.8, Eq. (5.20)]), using again the factoring routine SGECO and its double-precision version. The major weakness of this approach is the severe ill-conditioning of the determinants involved. Their condition numbers (as estimated by SGECO) range from about 10^5 for $n = 6$ to about 10^{16} for $n = 20$, precluding the safe use of our procedure in single precision, and also its use in double precision much beyond $n = 20$.

To avoid (or at least alleviate) this problem of ill-conditioning, we express the polynomial π_{n+1}^* in terms of Gegenbauer polynomials and compute the expansion coefficients from a triangular system of equations as described in [1, Section 4], using Gauss-Jacobi quadrature to generate the matrix elements. If $n = 2m$ is even, we then have [10, Section 5.9]

$$R(p_{2m}, p_{2m+1}^*) = \prod_{\mu=1}^{m} p_{2m+1}^*(\tau_\mu^2) = \prod_{\mu=1}^{m} \left[\frac{1}{\tau_\mu}\pi_{2m+1}^*(\tau_\mu)\right] \tag{3.1$_{\text{even}}$}$$

and, if $n = 2m - 1$,

$$R(p_{2m-1}, p_{2m}^*) = \prod_{\mu=1}^{m-1} p_{2m}^*(\tau_\mu^2) = \prod_{\mu=1}^{m-1} \pi_{2m}^*(\tau_\mu), \tag{3.1$_{\text{odd}}$}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of π_n in decreasing order, $\tau_1 > \tau_2 > \cdots > \tau_n$. Each factor in (3.1) is evaluated by Clenshaw's algorithm.

Similarly, the resultant of p_{n+1}^* and q_{n+1}^*, required to analyze property (d), is computed for even $n = 2m$ by

$$R(p_{2m+1}^*, q_{2m+1}^*) = \prod_{\mu=1}^{m} p_{2m+1}^*(\tau_\mu'^2) = \prod_{\mu=1}^{m} \left[\frac{1}{\tau_\mu'}\pi_{2m+1}^*(\tau_\mu')\right] \tag{3.2$_{\text{even}}$}$$

and for odd $n = 2m - 1$ by

$$R(p_{2m}^*, q_{2m}^*) = \prod_{\mu=1}^{m-1} p_{2m}^*(\tau_\mu'^2) = \prod_{\mu=1}^{m-1} \pi_{2m}^*(\tau_\mu'), \tag{3.2$_{\text{odd}}$}$$

where $\tau_1' > \tau_2' > \cdots > \tau_n'$ are the zeros of $\pi_{n+1}^{*\prime}$. To compute these zeros, we used, for the initial value $\lambda \approx \Lambda_n^a$ of λ, a simple search procedure followed by Newton's method. Then, as λ was incremented by small amounts, and during the bisection procedure for determining Λ_n^d, the zeros found for one λ were used as initial approximations for computing the zeros for the next λ by Newton's method. The factors in (3.2) again were evaluated by Clenshaw's algorithm.

The computations based on (3.1), (3.2) appear to produce rather accurate results, even for relatively large values of n. For example, when $n = 40$, we still obtained 10 correct decimal digits in single precision, as was confirmed by recomputation in double precision.

4. Jacobi Weights. We now consider property (p), $p = a, b, c$, for the general Jacobi weight $w^{(\alpha,\beta)}$ in (1.4). (Property (d) was not investigated, except for $n = 1$, since the effort involved seemed to us excessive, given the chance that the curve d could be indistinguishable from the curve a; cf. Table A.1 and Figure 4.1.) Noting that $w^{(\alpha,\beta)}(-t) = w^{(\beta,\alpha)}(t)$ and recalling the well-known fact that $\pi_n^{(\beta,\alpha)}(t) = (-1)^n \pi_n^{(\alpha,\beta)}(-t)$, it is easy to show that

$$\pi_{n+1}^{*(\beta,\alpha)}(t) = (-1)^{n+1} \pi_{n+1}^{*(\alpha,\beta)}(-t) \tag{4.1}$$

and

$$\begin{aligned} \sigma_\nu^{(\beta,\alpha)} &= \sigma_{n+1-\nu}^{(\alpha,\beta)}, \qquad \nu = 1, 2, \ldots, n, \\ \sigma_\mu^{*(\beta,\alpha)} &= \sigma_{n+2-\mu}^{*(\alpha,\beta)}, \qquad \mu = 1, 2, \ldots, n+1. \end{aligned} \tag{4.2}$$

Interchanging α and β, therefore, has no effect on the validity of property (p), $p = a, b, c$. It thus suffices to consider $\beta \geq \alpha$.

The case $n = 1$ can be handled analytically. One finds

$$R(\pi_1, \pi_2^*) = -\frac{4}{\alpha+\beta+3}\left\{\frac{(\alpha+1)(\beta+1)}{(\alpha+\beta+2)^2} + \frac{2(\alpha+2)(\beta+2)(\alpha+\beta+2)}{(\alpha+\beta+4)^2(\alpha+\beta+5)}\right\} < 0, \tag{4.3}$$

so that property (a), hence also property (d), holds for all $\alpha > -1$, $\beta > -1$. The same is true for property (c), since

$$\sigma_1 = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+2)\Gamma(\beta+2)}{\Gamma(\alpha+\beta+2)} \cdot \left\{\frac{1}{(\alpha+1)(\beta+1)} - \frac{1}{(\alpha+1)(\beta+1) + \frac{2(\alpha+2)(\beta+2)(\alpha+\beta+2)^3}{(\alpha+\beta+4)^2(\alpha+\beta+5)}}\right\} > 0. \tag{4.4}$$

For property (b) we must show $\pi_2^*(1) > 0$ and $\pi_2^*(-1) > 0$. A simple calculation gives

$$\pi_2^*(1) = \frac{4(\alpha+2)(\alpha^2+\alpha\beta+7\alpha-\beta+4)}{(\alpha+\beta+4)^2(\alpha+\beta+5)}, \tag{4.5}$$

which is positive (for $\alpha > -1$, $\beta > -1$) precisely if

$$\beta(\alpha-1) > -(\alpha^2+7\alpha+4).$$

For $\alpha > 1$, this inequality is true (since $\beta > -1$), while for $-1 < \alpha < 1$ it is true when

$$\beta < \frac{\alpha^2+7\alpha+4}{1-\alpha}, \qquad -1 < \alpha < 1. \tag{4.6}$$

This defines a curve in the (α, β)-plane that starts at the point $(-1, -1)$ and increases monotonically until it reaches a vertical asymptote at $\alpha = 1$. By (4.1), one has the same expression as in (4.5) for $\pi_2^*(-1)$, except that α and β are interchanged.

We summarize as follows: *For $n = 1$, the Gauss-Kronrod formula* (1.1) *for the Jacobi weight $w^{(\alpha,\beta)}$ satisfies properties* (a), (c) *and* (d) *for all $\alpha > -1$, $\beta > -1$, and property* (b) *precisely in the region*

$$\alpha \leq \beta < \frac{\alpha^2+7\alpha+4}{1-\alpha}, \qquad -1 < \alpha < 1, \tag{4.7}$$

and in its symmetric image with respect to the diagonal $\alpha = \beta$. (In particular, property (b) holds for all $\alpha > 1$, $\beta > 1$.)

In order to delineate the regions of validity of property (p) for values of n larger than 1, we used procedures similar to those described in Section 2. Letting α move through the interval $(-1, \Lambda_n^p - \frac{1}{2})$, for each α we started with $\beta = \alpha$ and increased β in fixed (sufficiently small!) steps to determine the first change in the truth value of property (p). Thereupon, the bisection method was used to narrow down the changeover point more accurately. The procedure had to be slightly modified for property (b), when n is even, since there are two critical values of β to be determined for α near and $\geq -\frac{1}{2}$. The smaller of the two was determined as before, the other by starting with $\beta = 0$ (instead of $\beta = \alpha$).

The validity of property (a) depends on the sign of the resultant $R(\pi_n, \pi_{n+1}^*)$, which was computed as in (3.1), except that symmetry could no longer be assumed; thus,

$$R(\pi_n, \pi_{n+1}^*) = \prod_{\nu=1}^{n} \pi_{n+1}^*(\tau_\nu). \tag{4.8}$$

Property (b) holds exactly if both of the inequalities

$$\pi_{n+1}^*(1) > 0, \qquad (-1)^{n+1}\pi_{n+1}^*(-1) > 0 \tag{4.9}$$

hold, while property (c) amounts to the positivity of all $\sigma_\nu^{(n)}$ in (2.3).

The results of our calculations are depicted graphically in Figure 4.1 for $n = 2(1)10$. The region of validity for property (p) is always located *below* the curve labeled p, except for the case $p = b$, n even, $-1 < \alpha < 0$, where property (b) holds above (or to the right) of curve b.

Figure 4.1 suggests the validity of the following conjectures.

CONJECTURE 4.1. *If n is even, property* (a) *implies property* (b) *whenever $\alpha > \alpha_n$, where $-\frac{1}{2} < \alpha_n < -.470$, $\alpha_n \to -\frac{1}{2}$ as $n \to \infty$.*

CONJECTURE 4.2. *If n is odd, property* (b) *is false for $-1 < \alpha < -\frac{1}{2}$.*

The fact that property (b) is false for n even, $\alpha = -\frac{1}{2}$, $-\frac{1}{2} < \beta < \frac{1}{2}$, and for n odd, $\alpha = -\frac{1}{2}$, $\frac{1}{2} < \beta < \frac{3}{2}$, is proved by Rabinowitz in [8, p. 75].***

Verification of properties (a) and (c), when $\alpha > 0$, was found to be delicate at times, because of the resultant (for fixed α and varying β) exhibiting near double zeros, i.e., changing sign for two β-values very close together. For example, when $n = 5$ and $\alpha = 3.75$, a first change of sign of the resultant (4.8) from negative to positive was observed between $\beta = 7.520$ and $\beta = 7.521$, which was followed by a change from positive to negative between $\beta = 7.540$ and $\beta = 7.541$. The increment in β, therefore, had to be chosen sufficiently small to detect this change of sign. Such difficulties were observed typically near points where the slope of the curve a or c undergoes a rapid change (the "kinks" in the graphs for a and c of Figure 4.1).

5. Special Weights. Simple transformations allow us to reduce special Jacobi weights with $\beta = \frac{1}{2}$ to Gegenbauer weights and Gegenbauer weights multiplied by a power of $|t|$ to Jacobi weights. Some consequences of this for Gauss-Kronrod formulae will now be explored.

5.1. *The Jacobi weight $w^{(\alpha,1/2)}$.* It is well known (see, e.g., [9, Eq. (4.1.5)]), and easily verified, that

$$t\pi_n^{(\alpha,1/2)}(2t^2 - 1) = 2^n \pi_{2n+1}^{(\alpha,\alpha)}(t), \qquad \alpha > -1. \tag{5.1}$$

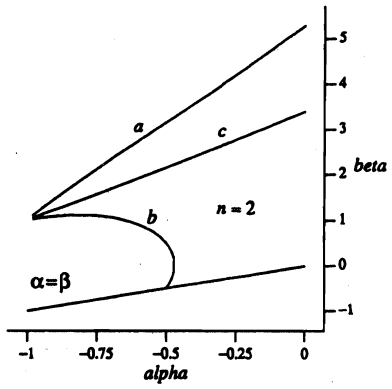
We depart from the Gauss-Kronrod formula (assumed to exist)

$$\int_{-1}^{1} f(t)w^{(\alpha,\alpha)}(t)\,dt = \sum_{\nu=1}^{2n+1} \overline{\sigma}_\nu f(\overline{\tau}_\nu) + \sum_{\mu=1}^{2n+2} \overline{\sigma}_\mu^* f(\overline{\tau}_\mu^*), \quad \text{all } f \in \mathbf{P}_{6n+4} \tag{5.2}$$

with $2n + 1$ Gauss nodes $\overline{\tau}_\nu = \tau_\nu^{(\alpha,\alpha)}$ and $2n + 2$ Kronrod nodes $\overline{\tau}_\mu^*$, ordered decreasingly as in (1.6); in particular,

$$0 < \overline{\tau}_{n+1}^* < \overline{\tau}_n < \cdots < \overline{\tau}_1 < \overline{\tau}_1^* < 1. \tag{5.3}$$

***The superscript $\mu + \frac{1}{2}$ in Eq. (68) of [8] should read $\mu - \frac{1}{2}$ (twice). The same change is required in the discussion immediately following Eq. (69).


a
c
b
n = 2
α=β
beta
alpha
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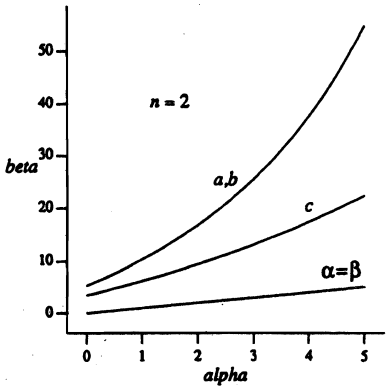
4
3
2
1
0
−1
−1
−0.75
−0.5
−0.25
0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a,b
c
α=β
beta
alpha
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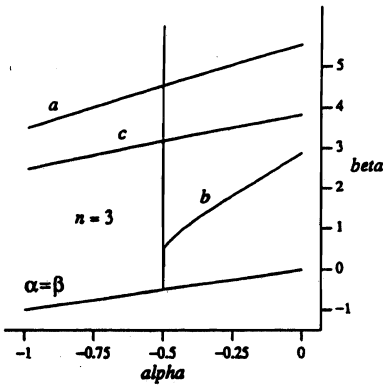
40
30
20
10
0
0
1
2
3
4
5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c
b
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α=β
beta
alpha
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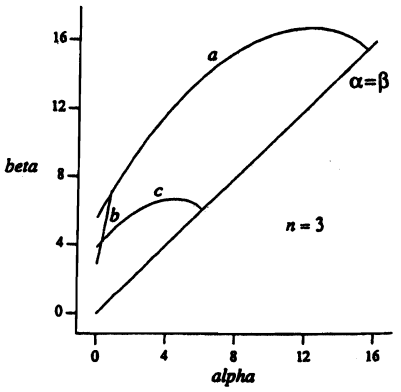
4
3
2
1
0
−1
−1
−0.75
−0.5
−0.25
0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α=β
c
b
n = 3
beta
alpha
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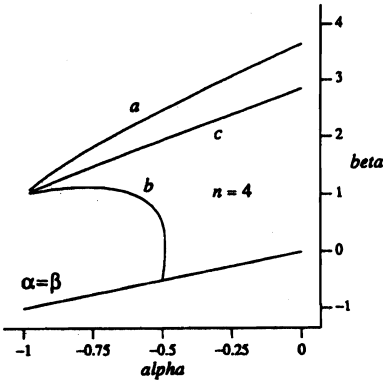
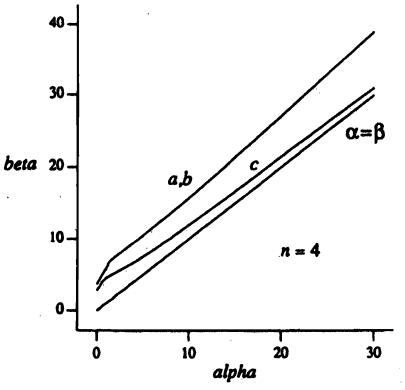
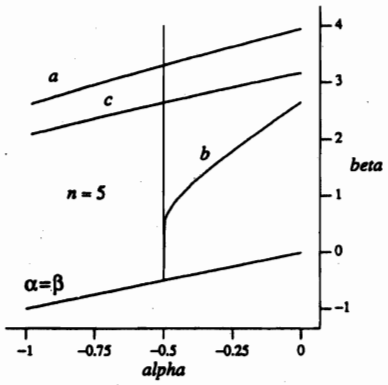
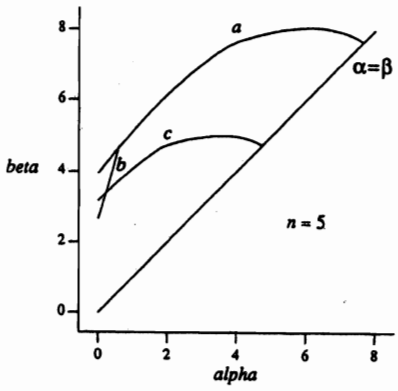
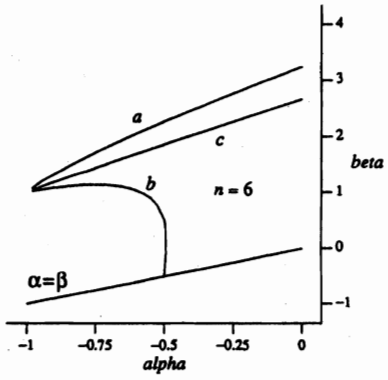
8
4
0
0
4
8
12
16

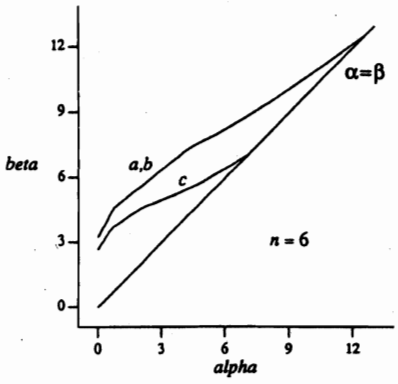

a
c
b
n = 4
α=β
beta
alpha
4
3
2
1
0
−1
−1
−0.75
−0.5
−0.25
0

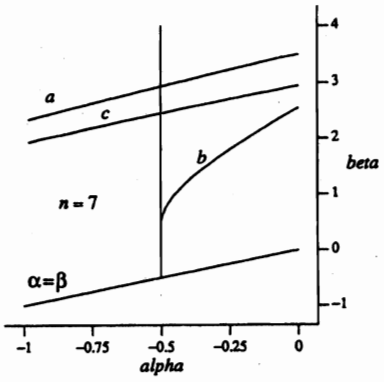

a,b
c
α=β
n = 4
beta
alpha
40
30
20
10
0
0
10
20
30

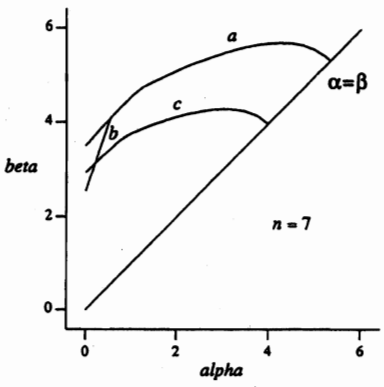

a
c
b
n = 5
α=β
beta
alpha
−1
−0.75
−0.5
−0.25
0
4
3
2
1
0
−1


a
α=β
c
b
beta
n = 5
alpha
8
6
4
2
0


a
c
b
n = 6
α=β
beta
alpha
−1
−0.75
−0.5
−0.25
0
4
3
2
1
0
−1


α=β
a,b
c
beta
n = 6
alpha
12
9
6
3
0


a
c
b
n = 7
α=β
beta
alpha
−1
−0.75
−0.5
−0.25
0
4
3
2
1
0
−1


a
α=β
c
b
beta
n = 7
alpha
6
4
2
0

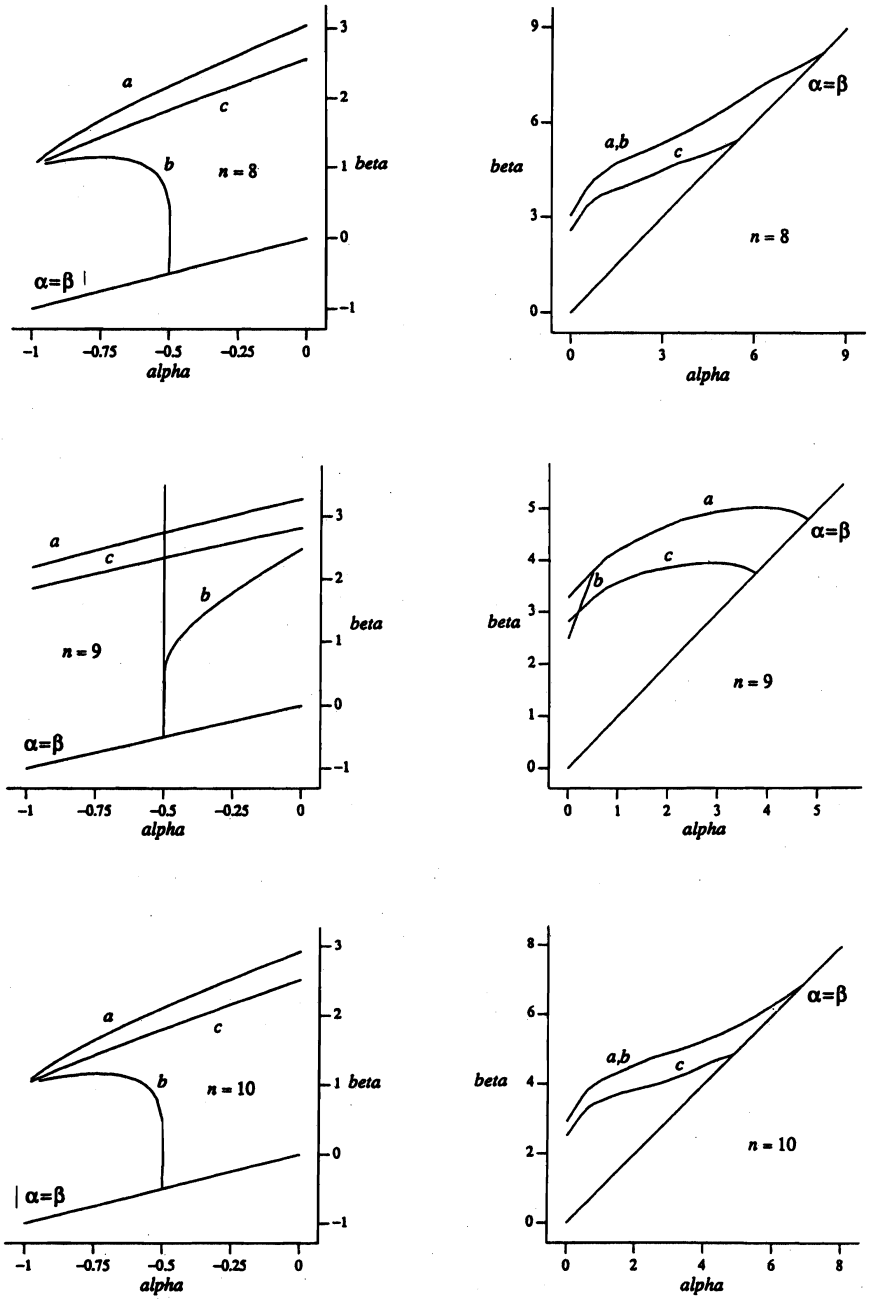


FIGURE 4.1
Property (p), $p = a, b, c$, *for the Jacobi weight* $w^{(\alpha,\beta)}$.

By (5.1), the Gauss nodes $\tau_\nu = \tau_\nu^{(\alpha,1/2)}$ for $\pi_n^{(\alpha,1/2)}$ are given by

$$\tau_\nu = 2\bar{\tau}_\nu^2 - 1, \qquad \nu = 1,2,\dots,n. \tag{5.4}$$

Now (5.2) implies (but is not necessarily implied by)

$$\int_{-1}^{1} t^2 g(t^2) w^{(\alpha,\alpha)}(t)\,dt = \sum_{\nu=1}^{2n+1} \bar{\sigma}_\nu \bar{\tau}_\nu^2 g(\bar{\tau}_\nu^2) + \sum_{\mu=1}^{2n+2} \bar{\sigma}_\mu^* \bar{\tau}_\mu^{*2} g(\bar{\tau}_\mu^{*2}), \quad \text{all } g \in \mathbf{P}_{3n+1},$$

from which, by symmetry,

$$\int_0^1 t^2 g(t^2) w^{(\alpha,\alpha)}(t)\,dt = \sum_{\nu=1}^{n} \bar{\sigma}_\nu \bar{\tau}_\nu^2 g(\bar{\tau}_\nu^2) + \sum_{\mu=1}^{n+1} \bar{\sigma}_\mu^* \bar{\tau}_\mu^{*2} g(\bar{\tau}_\mu^{*2}), \quad \text{all } g \in \mathbf{P}_{3n+1}. \tag{5.5}$$

Changing variables, $t = [(\tau+1)/2]^{1/2}$, so that $dt = \frac{1}{4}[(\tau+1)/2]^{-1/2}\,d\tau$ and $w^{(\alpha,\alpha)}(t) = 2^{-\alpha}(1-\tau)^\alpha$, yields

$$\begin{aligned}\int_{-1}^{1} g(\tau) w^{(\alpha,1/2)}(\tau)\,d\tau \\ = 2^{\alpha+5/2}\left\{\sum_{\nu=1}^{n} \bar{\sigma}_\nu \bar{\tau}_\nu^2 g(2\bar{\tau}_\nu^2 - 1) + \sum_{\mu=1}^{n+1} \bar{\sigma}_\mu^* \bar{\tau}_\mu^{*2} g(2\bar{\tau}_\mu^{*2} - 1)\right\},\end{aligned} \tag{5.6}$$

$$\text{all } g \in \mathbf{P}_{3n+1}.$$

Since, by (5.4), $2\bar{\tau}_\nu^2 - 1 = \tau_\nu$ are the Gauss nodes of $w^{(\alpha,1/2)}$, Eq. (5.6) is precisely the (unique) Gauss-Kronrod formula for $w^{(\alpha,1/2)}$ with n Gauss and $n+1$ Kronrod nodes. We have shown:

THEOREM 5.1. *The Gauss-Kronrod formula* (1.1) *for the weight function* $w^{(\alpha,1/2)}$ *is given by*

$$\tau_\nu = 2\bar{\tau}_\nu^2 - 1, \quad \sigma_\nu = 2^{\alpha+5/2}\bar{\tau}_\nu^2 \bar{\sigma}_\nu, \qquad \nu = 1,2,\dots,n; \tag{5.7}$$

$$\tau_\mu^* = 2\bar{\tau}_\mu^{*2} - 1, \quad \sigma_\mu^* = 2^{\alpha+5/2}\bar{\tau}_\mu^{*2}\bar{\sigma}_\mu^*, \qquad \mu = 1,2,\dots,n+1, \tag{5.8}$$

where $\bar{\tau}_\nu$, $\bar{\tau}_\mu^*$ *are the positive nodes in the Gauss-Kronrod formula* (5.2) *for the weight function* $w^{(\alpha,\alpha)}$ *and* $\bar{\sigma}_\nu$, $\bar{\sigma}_\mu^*$ *the corresponding weights.*

Clearly, if the formula (5.2) has property (p), $p = a,b,c,d$, so does formula (5.6). (For property (a), this has previously been observed by Monegato [6, p. 147].) From the discussion in Section 2, we expect this to be true for

$$\lambda_{2n+1}^p - \tfrac{1}{2} < \alpha < \Lambda_{2n+1}^p - \tfrac{1}{2}, \tag{5.9}$$

so that the Gauss-Kronrod formula (5.6) for the weight $w^{(\alpha,1/2)}$, and hence, by the remark at the beginning of Section 4, also the one for the weight $w^{(1/2,\alpha)}$, has property (p) if (5.9) holds. This means, in particular, that the point

$$Q_n^p = (\tfrac{1}{2}, \Lambda_{2n+1}^p - \tfrac{1}{2}) \tag{5.10}$$

must lie on or below the curve labeled p in Figure 4.1(n). More precisely, it was observed that for $p = a$ the point Q_n^a lies strictly below the curve if n is odd, and on the curve if n is even. The reason for this is the phenomenon (2.10) (where m is to be replaced by $m+1$) which was observed to hold precisely if $m+1$ (our current

n) is odd. Property (a) for (5.2) then ceases to hold because of the collision of a Kronrod node with the Gauss node $\overline{\tau}_{n+1} = 0$ at the origin. Since the latter node has no equivalent in the formula (5.6), property (a) continues to hold for (5.6) beyond the critical value $\alpha = \Lambda^a_{2n+1} - \frac{1}{2}$. If n is even, on the other hand, the collision in (5.2) is between a Kronrod node and a *nonzero* Gauss node, which gives rise to a collision also in (5.6). For the same reason, the point Q^b_n in (5.10) for property (b) is on the curve labeled b in Figure 4.1(n), when n is odd, because of the Kronrod node τ^*_{n+1} becoming equal to -1, and on the curve labeled a, b, when n is even, by virtue of property (a) ceasing to hold. For property (c), Q^c_n was observed to lie on the curve labeled c in Figure 4.1(n) when n is even, and below the curve otherwise.

5.2. *The weight* $|t|^\gamma(1-t^2)^\alpha$. We now construct the Gauss-Kronrod formula with $2n+1$ Gauss nodes and $2n+2$ Kronrod nodes for the weight function

$$(5.11) \qquad {}^\gamma w^{(\alpha)}(t) = |t|^\gamma(1-t^2)^\alpha \quad \text{on } -1 < t < 1, \alpha > -1,\ \gamma > -1.$$

It is known that the associated (monic) orthogonal polynomials are expressible in terms of Jacobi polynomials [4, p. 173]. In particular,

$$2^n \cdot {}^\gamma\pi^{(\alpha)}_{2n+1}(t) = t\pi^{(\alpha,(\gamma+1)/2)}_n(2t^2-1).$$

Therefore, if $\overline{\tau}_\nu$, $\nu = 1, 2, \dots, n$, are the zeros of the Jacobi polynomial $\pi^{(\alpha,(\gamma+1)/2)}_n$, the nodes in the $(2n+1)$-point Gauss formula for the weight (5.11) are

$$(5.12) \qquad \tau_\nu = \sqrt{\frac{\overline{\tau}_\nu + 1}{2}}, \qquad \nu = 1, 2, \dots, n; \quad \tau_{n+1} = 0;$$
$$\tau_\nu = -\tau_{2n+2-\nu}, \qquad \nu = n+2, \dots, 2n+1.$$

We now start from the Gauss-Kronrod formula (assumed to exist) for the Jacobi weight $w^{(\alpha,(\gamma+1)/2)}$,

$$(5.13) \qquad \int_{-1}^{1} f(t)w^{(\alpha,(\gamma+1)/2)}(t)\,dt = \sum_{\nu=1}^{n} \overline{\sigma}_\nu f(\overline{\tau}_\nu) + \sum_{\mu=1}^{n+1} \overline{\sigma}^*_\mu f(\overline{\tau}^*_\mu), \quad \text{all } f \in \mathbf{P}_{3n+1}.$$

Substituting $t = 2\tau^2 - 1$ in the integral on the left yields

$$\int_0^1 f(2\tau^2-1)\tau^2 \cdot \tau^\gamma(1-\tau^2)^\alpha\,d\tau$$
$$= 2^{-\alpha-(\gamma+5)/2}\left[\sum_{\nu=1}^{n} \overline{\sigma}_\nu f(\overline{\tau}_\nu) + \sum_{\mu=1}^{n+1} \overline{\sigma}^*_\mu f(\overline{\tau}^*_\mu)\right], \quad \text{all } f \in \mathbf{P}_{3n+1}.$$

Letting $f(u) = [(u+1)/2]^k$, $k = 0, 1, \dots, 3n+1$, gives

$$\int_0^1 \tau^{2k+2} \cdot \tau^\gamma(1-\tau^2)^\alpha\,d\tau$$
$$(5.14) \qquad = 2^{-\alpha-(\gamma+5)/2}\left[\sum_{\nu=1}^{n} \frac{\overline{\sigma}_\nu}{(\overline{\tau}_\nu+1)/2}\left(\sqrt{\frac{\overline{\tau}_\nu+1}{2}}\right)^{2k+2} + \sum_{\mu=1}^{n+1} \frac{\overline{\sigma}^*_\mu}{(\overline{\tau}^*_\mu+1)/2}\left(\sqrt{\frac{\overline{\tau}^*_\mu+1}{2}}\right)^{2k+2}\right],$$
$$k = 0, 1, \dots, 3n+1.$$

Defining, in analogy to (5.12),

$$\tau_\mu^* = \sqrt{\frac{\overline{\tau}_\mu^* + 1}{2}}, \qquad \mu = 1, 2, \ldots, n+1; \quad \tau_\mu^* = -\tau_{2n+3-\mu}^*, \quad \mu = n+2, \ldots, 2n+2; \tag{5.12*}$$

and letting

$$\sigma_\nu = 2^{-\alpha-(\gamma+5)/2} \frac{\overline{\sigma}_\nu}{(\overline{\tau}_\nu + 1)/2}, \qquad \nu = 1, 2, \ldots, n; \quad \sigma_{n+1} = \lambda; \tag{5.15}$$
$$\sigma_\nu = \sigma_{2n+2-\nu}, \qquad \nu = n+2, \ldots, 2n+1;$$

$$\sigma_\mu^* = 2^{-\alpha-(\gamma+5)/2} \frac{\overline{\sigma}_\mu^*}{(\overline{\tau}_\mu^* + 1)/2}, \qquad \mu = 1, 2, \ldots, n+1; \tag{5.15*}$$
$$\sigma_\mu^* = \sigma_{2n+3-\mu}^*, \qquad \mu = n+2, \ldots, 2n+2,$$

where λ will be determined shortly, we can write (5.14) equivalently in the form

$$\int_{-1}^{1} t^l \cdot {}^\gamma w^{(\alpha)}(t)\, dt = \sum_{\nu=1}^{2n+1} \sigma_\nu \tau_\nu^l + \sum_{\mu=1}^{2n+2} \sigma_\mu^* \tau_\mu^{*l}, \qquad l = 1, 2, \ldots, 6n+4, \tag{5.16}$$

where both sides are zero if l is odd. If we require (5.16) to hold also for $l = 0$ (with $\tau_{n+1}^0 = 0^0 = 1$), i.e., if λ is chosen so that

$$2\sum_{\nu=1}^{n} \sigma_\nu + \lambda + 2\sum_{\mu=1}^{n+1} \sigma_\mu^* = \int_{-1}^{1} {}^\gamma w^{(\alpha)}(t)\, dt, \tag{5.17}$$

then

$$\int_{-1}^{1} f(t)\, {}^\gamma w^{(\alpha)}(t)\, dt = \sum_{\nu=1}^{2n+1} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{2n+2} \sigma_\mu^* f(\tau_\mu^*), \quad \text{all } f \in \mathbf{P}_{6n+4} \tag{5.18}$$

is the desired Gauss-Kronrod formula for the weight ${}^\gamma w^{(\alpha)}$. We have shown:

THEOREM 5.2. *The Gauss-Kronrod formula for the weight* ${}^\gamma w^{(\alpha)}(t) = |t|^\gamma (1-t^2)^\alpha$ *on* $(-1, 1)$, *with* $2n+1$ *Gauss nodes and* $2n+2$ *Kronrod nodes, is given by* (5.18), *where the nodes* τ_ν, τ_μ^* *are expressible in terms of the nodes* $\overline{\tau}_\nu$, $\overline{\tau}_\mu^*$ *in the Gauss-Kronrod formula* (5.13) *for the Jacobi weight* $w^{(\alpha,(\gamma+1)/2)}$ *by means of* (5.12), (5.12*), *and similarly, the weights* σ_ν, σ_μ^* *are expressible in terms of the weights* $\overline{\sigma}_\nu$, $\overline{\sigma}_\mu^*$ *in* (5.13) *by means of* (5.15), (5.15*), $\sigma_{n+1} = \lambda$ *being determined by* (5.17).

Clearly, if property (p), $p = a, b, d$, holds for the Gauss-Jacobi-Kronrod formula (5.13), it also holds for formula (5.18). Property (c) for (5.13), on the other hand, does not necessarily imply property (c) for (5.18), since the positivity of $\overline{\sigma}_\nu$, $\overline{\sigma}_\mu^*$, while implying the positivity of all σ_ν, σ_μ^* other than σ_{n+1}, may or may not imply $\sigma_{n+1} > 0$, depending on whether λ, as obtained from (5.17), is positive or not.

Appendix. Property (p) $(p = a, b, c, d)$ for $n = 5(1)20(4)40$.

TABLE A.1

Property (p) for the Gegenbauer weight $w^{(\lambda-1/2,\lambda-1/2)}$ $(\lambda > -\frac{1}{2})$ holds if $\lambda_n^p < \lambda < \Lambda_n^p$. This table shows Λ_n^a, Λ_n^c and Λ_n^d, as computed by the methods of Section 2. By Conjectures 2.1–2.4, $\lambda_n^a = \lambda_n^c = \lambda_n^d = -\frac{1}{2}$, $\lambda_n^b = 0$, $\Lambda_n^b = \Lambda_n^a$ for all $n \geq 5$, and $\Lambda_n^d = \Lambda_n^a$ whenever $n = 4r - 1$, $r = 1, 2, 3, \ldots$.

n	Λ_n^a	Λ_n^c	Λ_n^d
5	8.1494082801	5.2388459015	8.1830000561
6	13.1085950564	7.6571453588	13.1107896727
7	5.8401376887	4.4759114573	Λ_7^a
8	8.7386889750	5.9524378395	8.7555343902
9	5.2935342610	4.2497937619	5.2945466651
10	7.3992715320	5.3753659922	7.4237962746
11	4.8531386151	4.0481558230	Λ_{11}^a
12	6.1920646523	5.0379559112	6.1934889120
13	4.6542480033	3.9519324055	4.6543912620
14	5.6700664070	4.6801034243	5.6700700822
15	4.4686100363	3.8582584626	Λ_{15}^a
16	5.3822674428	4.4807122988	5.3826940246
17	4.3630476637	3.8036436813	4.3630833901
18	5.1865732169	4.3552498234	5.1873227488
19	4.2595630405	3.7488473165	Λ_{19}^a
20	4.9631599397	4.2700177278	4.9632639191
24	4.7114083943	4.1057723823	4.7114508725
28	4.5422887809	4.0009291994	4.5423182352
32	4.4137444535	3.9286038916	4.4137495863
36	4.3224901583	3.8624938923	4.3225046157
40	4.2417789470	3.8175327957	4.2417792595

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A Family of Gauss-Kronrod Quadrature Formulae*

By Walter Gautschi and Theodore J. Rivlin

Dedicated with affection to Dick Varga on his 60th birthday

Abstract. We show, for each $n \geq 1$, that the $(2n+1)$-point Kronrod extension of the n-point Gaussian quadrature formula for the measure

$$d\sigma_\gamma(t) = (1+\gamma)^2(1-t^2)^{1/2}dt/((1+\gamma)^2 - 4\gamma t^2), \qquad -1 < \gamma \leq 1,$$

has the properties that its $n+1$ Kronrod nodes interlace with the n Gauss nodes and all its $2n+1$ weights are positive. We also produce explicit formulae for the weights.

1. Introduction. Given a positive measure $d\sigma$ on the real line, whose moments all exist, a quadrature rule

$$\int_{\mathbf{R}} f(t)\,d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f) \tag{1.1}$$

is called a *Gauss-Kronrod formula* if $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes for the measure $d\sigma$, i.e., the zeros of the nth degree orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$, and the nodes $\tau_\mu^* = \tau_\mu^{*(n)}$ and weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{*(n)}$ are chosen so as to maximize the degree of exactness of (1.1); thus, $R_n(f) = 0$ for all $f \in \mathbf{P}_{3n+1}$ at least. It is well known (see, e.g., the survey in [1]) that the "Kronrod nodes" τ_μ^* must be the zeros of the polynomial $\pi_{n+1}^*(\cdot; d\sigma)$ of degree $n+1$ orthogonal to all lower-degree polynomials relative to the (sign-variable) measure $d\sigma^*(t) = \pi_n(t)d\sigma(t)$:

$$\int_{\mathbf{R}} \pi_{n+1}^*(t; d\sigma)p(t)\pi_n(t; d\sigma)d\sigma(t) = 0, \quad \text{all } p \in \mathbf{P}_n. \tag{1.2}$$

While π_{n+1}^* (assumed monic) is known to exist uniquely, there is no assurance, in general, that its zeros τ_μ^* are all real and simple, and distinct from the Gaussian nodes τ_ν.

In practice, it is particularly desirable to have the following two properties satisfied:

(i) the *interlacing* property,

$$-\infty < \tau_{n+1}^{*(n)} < \tau_n^{(n)} < \tau_n^{*(n)} < \cdots < \tau_2^{*(n)} < \tau_1^{(n)} < \tau_1^{*(n)} < \infty, \tag{1.3}$$

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with all nodes contained in the support interval of $d\sigma$, and

(ii) the *positivity* of all weights,

$$\sigma_\nu^{(n)} > 0, \qquad \nu = 1, 2, \ldots, n; \qquad \sigma_\mu^{*(n)} > 0, \qquad \mu = 1, 2, \ldots, n+1. \tag{1.4}$$

(The inequalities $\sigma_\mu^* > 0$ are actually equivalent to (1.3); see Monegato [4].) Only one family of measures $d\sigma$ is presently known for which both properties (i) and (ii) hold for all $n \geq 1$, namely the Gegenbauer measure $d\sigma^\lambda(t) = (1-t^2)^{\lambda-1/2}\,dt$ on $(-1,1)$. For this measure, (1.3) (with $-1 \leq \tau_{n+1}^*$ and $\tau_1^* \leq 1$) has been established by Szegö [7] for $0 \leq \lambda \leq 2$, and (1.4) by Monegato [5] for $0 \leq \lambda \leq 1$. In this note we show that the family of measures

$$d\sigma_\gamma(t) = (1+\gamma)^2 \frac{(1-t^2)^{1/2}}{(1+\gamma)^2 - 4\gamma t^2}\,dt \quad \text{on } (-1,1), \quad -1 < \gamma \leq 1, \tag{1.5}$$

already considered by Geronimus [3] and Monegato [6], also has these same properties, i.e., (1.3) (with $-1 \leq \tau_{n+1}^*$ and $\tau_1^* \leq 1$) and (1.4) both hold for all $n \geq 1$. In addition, as is known (Monegato [6, p. 146]), the degree of precision of (1.1) for $d\sigma = d\sigma_\gamma$ is exceptionally high, namely, if $n > 1$, exactly $4n-1$ and $4n+1$ when $\gamma \neq 0$ and $\gamma = 0$, respectively, and 5 if $n = 1$.

Note that the restriction $-1 < \gamma \leq 1$ in (1.5) is a natural one, since the measure is $(1-t^2)^{1/2}\,dt/(1-\mu t^2)$, $\mu = 4\gamma/(1+\gamma)^2$, and μ runs through all admissible values $-\infty < \mu \leq 1$ as γ varies from -1 to 1.

In a sense, the results obtained here for the Geronimus measure (1.5) are more pleasing than those presently known for the Gegenbauer measure. Not only do we have higher degree of accuracy and explicit formulae, but our results cover an entire class of measures, in contrast to those for the Gegenbauer measure, which are partial at best. See, in this connection, the numerical work in [2].

The proofs of (i) and (ii) for the measure (1.5) are facilitated by the fact that both (monic) polynomials $\pi_n(\cdot; d\sigma_\gamma)$ and $\pi_{n+1}^*(\cdot; d\sigma_\gamma)$ are known explicitly,

$$\pi_n(t; d\sigma_\gamma) = 2^{-n}[U_n(t) - \gamma U_{n-2}(t)], \tag{1.6}$$

$$\begin{aligned} \pi_2^*(t; d\sigma_\gamma) &= \tfrac{1}{2}\left[T_2(t) - \tfrac{1}{2}\gamma\right], \\ \pi_{n+1}^*(t; d\sigma_\gamma) &= 2^{-n}[T_{n+1}(t) - \gamma T_{n-1}(t)], \qquad n \geq 2. \end{aligned} \tag{1.6*}$$

(Cf. Monegato [6, p. 146]; the first relation in (1.6*) is not given in this reference but follows from an elementary computation.) Here, T_m and U_m denote the mth degree Chebyshev polynomials of the first and second kind.

2. Interlacing. If $\gamma = 1$, then $d\sigma_\gamma(t) = (1-t^2)^{-1/2}\,dt$ is the Chebyshev measure of the first kind, that is, a Gegenbauer measure with $\lambda = 0$, so that (1.3) and (1.4) hold. If $\gamma < 1$, it follows from (1.6*) that the zeros of π_{n+1}^* are all in the interior of $[-1,1]$ and are separated by the extreme points of T_{n+1}. As γ is continuously decreased from $\gamma = 1$ to $\gamma = -1$, the only way (1.3) can cease to hold is that for some $\gamma = \gamma_0$, $-1 < \gamma_0 < 1$, the two polynomials π_n, π_{n+1}^* have a common zero τ_0. We now show that this is impossible.

The case $n = 1$ being trivial, we may assume $n \geq 2$. Suppose, then, that τ_0 is a common zero of π_n and π_{n+1}^*,

$$(U_n - \gamma U_{n-2})(\tau_0) = (T_{n+1} - \gamma T_{n-1})(\tau_0) = 0 \quad \text{for } \gamma = \gamma_0. \tag{2.1}$$

It is clear, first of all, that $\tau_0 \neq 0$, since otherwise, one of the two expressions on the left of (2.1) is zero and the other $\pm(1+\gamma) \neq 0$. Furthermore, $U_{n-2}(\tau_0) \neq 0$, $T_{n-1}(\tau_0) \neq 0$. We show only the first inequality; the other is proved similarly. If we had $U_{n-2}(\tau_0) = 0$, then, by (2.1), $U_n(\tau_0) = 0$, and the recurrence formula $U_n(\tau_0) = 2\tau_0 U_{n-1}(\tau_0) - U_{n-2}(\tau_0)$ would imply, since $\tau_0 \neq 0$, that $U_{n-1}(\tau_0) = 0$. This contradicts the well-known fact that two consecutive orthogonal polynomials cannot vanish at the same point.

It now follows from (2.1) that

$$\gamma_0 = \frac{U_n(\tau_0)}{U_{n-2}(\tau_0)} = \frac{T_{n+1}(\tau_0)}{T_{n-1}(\tau_0)},$$

hence

$$\Delta_n := U_n T_{n-1} - U_{n-2} T_{n+1} = 0 \quad \text{at } \tau_0. \tag{2.2}$$

Since $U_m(t)$ and $T_m(t)$ both satisfy

$$y_{m+1} = (4t^2 - 2)y_{m-1} - y_{m-3},$$

where $m \geq 3$ for T, and $m \geq 2$ for U, there follows, for $n = 3, 4, 5, \ldots$, that

$$\begin{aligned}\Delta_n &= [(4t^2-2)U_{n-2} - U_{n-4}]T_{n-1} - U_{n-2}[(4t^2-2)T_{n-1} - T_{n-3}] \\ &= U_{n-2}T_{n-3} - U_{n-4}T_{n-1} \\ &= \Delta_{n-2},\end{aligned}$$

hence $\Delta_n = \Delta_2$ for n even, and $\Delta_n = \Delta_1$ for n odd. But, for $t = \tau_0 \neq 0$, $\Delta_2 = \Delta_1 = 2\tau_0 \neq 0$, so that $\Delta_n \neq 0$, contrary to (2.2). This proves the interlacing property for $-1 < \gamma \leq 1$ and all $n \geq 1$.

3. Positivity. We actually derive explicit formulae for σ_ν and σ_μ^*, from which positivity can be read off: see Eqs. (3.9), (3.11).

Let $\tau_\nu = \cos\theta_\nu$, $0 < \theta_\nu < \pi$, and assume first $n \geq 2$ and $\tau_\nu \neq 0$, that is, $\theta_\nu \neq \pi/2$. Since $U_{n-2}(\tau_\nu) \neq 0$ (cf. Section 2), we have by (1.6), using $U_{m-1}(\cos\theta) = \sin m\theta / \sin\theta$, that

$$\gamma = \frac{\sin(n+1)\theta_\nu}{\sin(n-1)\theta_\nu} \tag{3.1}$$

for each ν.

It is well known (cf. Monegato [4]) that

$$\sigma_\nu = \lambda_\nu + \frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}, \qquad \nu = 1, 2, \ldots, n, \tag{3.2}$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma_\gamma)$ and $\lambda_\nu = \lambda_\nu^{(n)}$ are the Christoffel numbers for $d\sigma_\gamma$; for the latter, we have (see, e.g., [8, Eq. (3.4.7)])

$$\lambda_\nu = -\frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}, \qquad \nu = 1, 2, \ldots, n. \tag{3.3}$$

Putting $t = \cos\theta_\nu$ in (1.6*), and using $T_m(\cos\theta) = \cos m\theta$ and (3.1), one finds

$$\pi^*_{n+1}(\tau_\nu) = -2^{-n}\frac{\sin 2\theta_\nu}{\sin(n-1)\theta_\nu}. \tag{3.4}$$

Similarly, from (1.6), replacing n by $n+1$, one gets after a little computation

$$\pi_{n+1}(\tau_\nu) = -2^{-n-1}\frac{\sin 2\theta_\nu}{\sin(n-1)\theta_\nu}. \tag{3.5}$$

Interestingly, $\pi_{n+1}(\tau_\nu)$ has precisely half the value of $\pi^*_{n+1}(\tau_\nu)$, which, by (3.2) and (3.3), implies that the second term on the right of (3.2) is half as big (in modulus) as the first and of opposite sign. Since $\lambda_\nu > 0$, this already proves $\sigma_\nu > 0$. But we want an explicit formula for σ_ν and therefore proceed with our computation.

We first incorporate the preceding remark in (3.2) and write

$$\sigma_\nu = -\frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu)}. \tag{3.6}$$

Differentiating (1.6) gives

$$\begin{aligned}&\cos\theta\cdot\pi_n(\cos\theta) - \sin^2\theta\cdot\pi'_n(\cos\theta)\\ &\quad = n\pi^*_{n+1}(\cos\theta) + 2^{-n}[\cos(n+1)\theta + \gamma\cos(n-1)\theta].\end{aligned}$$

Now substitute from (3.1) for γ, put $\theta = \theta_\nu$ and use (3.4) to get

$$-\pi^*_{n+1}(\tau_\nu)\pi'_n(\tau_\nu) = 2^{-2n+1}\frac{\cos\theta_\nu}{\sin\theta_\nu\sin^2(n-1)\theta_\nu}[n\sin 2\theta_\nu - \sin 2n\theta_\nu]. \tag{3.7}$$

It remains to calculate the norm of π_n. For this, we use the fact that

$$\|\pi_n\|^2_{d\sigma_\gamma} = \beta_0\beta_1\beta_2\cdots\beta_n,$$

where $\beta_0 = \int_{-1}^{1} d\sigma_\gamma(t)$ and β_k are the recursion coefficients in

$$\begin{aligned}\pi_{k+1}(t) &= t\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0,1,2,\ldots,\\ \pi_0(t) &= 1, \qquad \pi_{-1}(t) = 0.\end{aligned}$$

An elementary calculation shows that

$$\beta_0 = \frac{\pi}{2}(1+\gamma), \quad \beta_1 = \frac{1}{4}(1+\gamma), \quad \beta_2 = \beta_3 = \cdots = \frac{1}{4}.$$

Therefore,

$$\|\pi_n\|^2_{d\sigma_\gamma} = \frac{\pi}{2}\left(\frac{1+\gamma}{2^n}\right)^2, \qquad n \geq 1, \tag{3.8}$$

or, alternatively, using (3.1) once again,

$$\|\pi_n\|^2_{d\sigma_\gamma} = \pi\cdot 2^{-2n+1}\frac{\sin^2 n\theta_\nu\cos^2\theta_\nu}{\sin^2(n-1)\theta_\nu}, \qquad n \geq 2. \tag{3.8'}$$

With (3.7), (3.8') inserted in (3.6), one obtains

$$\sigma_\nu^{(n)} = \frac{\pi}{2}\frac{\sin^2 n\theta_\nu}{n - \sin 2n\theta_\nu/\sin 2\theta_\nu}, \qquad \nu = 1,2,\ldots,n; \tag{3.9}$$

$$n \geq 2, \quad \nu \neq \frac{n+1}{2} \text{ if } n \text{ is odd.}$$

From this, the positivity $\sigma_\nu > 0$ follows once again, since $U_{n-1}(\cos 2\theta) = \sin 2n\theta/\sin 2\theta < n$ for $0 < \theta < \pi$, $\theta \neq \pi/2$.

It remains to consider the case $\tau_\nu = 0$, i.e., in the ordering (1.3), $\nu = (n+1)/2$, where $n \geq 1$ is odd. By (3.8), and calculating $\pi^*_{n+1}(0)$ and $\pi'_n(0)$ directly, from (3.6) one readily finds

$$(3.9') \qquad \sigma_1^{(1)} = \frac{\pi}{2}\frac{1+\gamma}{2+\gamma}; \quad \sigma^{(n)}_{(n+1)/2} = \frac{\pi}{2}\frac{1+\gamma}{1-\gamma+n(1+\gamma)}, \quad n(\text{odd}) \geq 3.$$

The positivity $\sigma^*_\mu > 0$ is a consequence of the interlacing property proved in Section 2. It is of interest, however, to produce formulae similar to (3.9), (3.9') for σ^*_μ. To do so, write $\tau^*_\mu = \cos\theta^*_\mu$ and use [cf. (1.6*)]

$$\gamma = \frac{\cos(n+1)\theta^*_\mu}{\cos(n-1)\theta^*_\mu}, \qquad n \geq 2, \quad \theta^*_\mu \neq \pi/2 \text{ if } n \text{ is even.}$$

Then a computation very similar to the one above for σ_ν, using the known formula (Monegato [4])

$$(3.10) \qquad \sigma^*_\mu = \frac{\|\pi_n\|^2_{d\sigma_\gamma}}{\pi_n(\tau^*_\mu)\pi^{*\prime}_{n+1}(\tau^*_\mu)}, \qquad \mu = 1, 2, \ldots, n+1,$$

in place of (3.2), yields

$$(3.11) \qquad \sigma^{*(n)}_\mu = \frac{\pi}{2}\frac{\cos^2 n\theta^*_\mu}{n + \sin 2n\theta^*_\mu / \sin 2\theta^*_\mu}, \qquad \mu = 1, 2, \ldots, n+1;$$

$$n \geq 2, \quad \mu \neq \frac{n+2}{2} \text{ if } n \text{ is even,}$$

and

$$(3.11') \qquad \sigma_1^{*(1)} = \sigma_2^{*(1)} = \frac{\pi}{4}\frac{(1+\gamma)^2}{2+\gamma};$$

$$\sigma^{*(n)}_{(n+2)/2} = \frac{\pi}{2}\frac{1+\gamma}{1-\gamma+n(1+\gamma)}, \quad n(\text{even}) \geq 2.$$

If the points τ_ν in (1.1) are augmented by ± 1, they become the Lobatto points with respect to the measure $d\tilde{\sigma}_\gamma(t) = (1-t^2)^{-1}d\sigma_\gamma(t)$, $-1 < \gamma < 1$, and together with the nodes τ^*_μ, one obtains in

$$(3.12) \qquad \int_{-1}^{1} f(t)d\tilde{\sigma}_\gamma(t) = \tilde{\sigma}_{n+1}f(-1) + \sum_{\nu=1}^{n}\tilde{\sigma}_\nu f(\tau_\nu) + \tilde{\sigma}_0 f(1) + \sum_{\mu=1}^{n+1}\tilde{\sigma}^*_\mu f(\tau^*_\mu) + \tilde{R}_n(f)$$

the Kronrod extension of the $(n+2)$-point Gauss-Lobatto formula for the measure $d\tilde{\sigma}_\gamma$ (cf. [1, Example 2.3]). Here,

$$(3.13) \qquad \tilde{\sigma}_\nu = \frac{\sigma_\nu}{1-\tau_\nu^2}, \qquad \nu = 1, 2, \ldots, n; \qquad \tilde{\sigma}^*_\mu = \frac{\sigma^*_\mu}{1-\tau^{*2}_\mu}, \qquad \mu = 1, 2, \ldots, n+1;$$

and by a formula analogous to (3.2),

$$(3.14) \qquad \tilde{\sigma}_0^{(1)} = \tilde{\sigma}_2^{(1)} = \frac{\pi}{4}\frac{(1+\gamma)^2}{(1-\gamma)(2-\gamma)},$$

$$\tilde{\sigma}_0^{(n)} = \tilde{\sigma}_{n+1}^{(n)} = \frac{\pi}{4}\frac{(1+\gamma)^2}{(1-\gamma)(1+\gamma+n(1-\gamma))}, \qquad n \geq 2.$$

Hence, all weights in (3.12) are positive for $-1 < \gamma < 1$ and all $n \geq 1$.

We conclude by noting that the Gauss nodes $\tau_\nu^{(n)}$ for the measure (1.5) can be computed most conveniently as eigenvalues of the symmetric tridiagonal $n \times n$-matrix having zeros on the diagonal and the quantities $\sqrt{\beta_1} = \frac{1}{2}\sqrt{1+\gamma}$, $\sqrt{\beta_2} = \cdots = \sqrt{\beta_{n-1}} = \frac{1}{2}$ on the two side diagonals, if $n \geq 2$. (If $n = 1$ then $\tau_1^{(1)} = 0$.) Likewise, $\tau_\mu^{*(n)}$, $n \geq 1$, are computable as eigenvalues of the symmetric tridiagonal $(n+1) \times (n+1)$-matrix with zero diagonal and $\sqrt{\beta_1^*} = \sqrt{\frac{1}{2}(1+\gamma)}$, $\sqrt{\beta_2^*} = \frac{1}{2}\sqrt{1-\gamma}, \sqrt{\beta_3^*} = \cdots = \sqrt{\beta_n^*} = \frac{1}{2}$ on the side diagonals, if $n \geq 2$, and $\sqrt{\beta_1^*} = \frac{1}{2}\sqrt{2+\gamma}$ on the side diagonals, if $n = 1$.

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Gauss–Kronrod quadrature formulae for weight functions of Bernstein–Szegö type *

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Abstract: We study the Kronrod extensions of Gaussian quadrature rules whose weight functions on $[-1, 1]$ consist of any one of the four Chebyshev weights divided by an arbitrary quadratic polynomial that remains positive on $[-1, 1]$. We show that in almost all cases these extended "Gauss–Kronrod" quadrature rules have all the desirable properties: Kronrod nodes interlacing with Gauss nodes, all nodes contained in $[-1, 1]$, and all weights positive and representable by semiexplicit formulas. Exceptions to these properties occur only for small values of n (the number of Gauss nodes), namely $n \leq 3$, and are carefully identified. The precise degree of exactness of each of these Gauss–Kronrod formulae is determined and shown to grow like $4n$, rather than $3n$, as is normally the case. Our findings are the result of a detailed analysis of the underlying orthogonal polynomials and "Stieltjes polynomials". The paper concludes with a study of the limit case of a linear divisor polynomial in the weight function.

Keywords: Gauss–Kronrod quadrature formulae, weight functions of Bernstein–Szegö type, orthogonal polynomials, Stieltjes polynomials.

1. Introduction

The idea of embedding Gaussian quadrature formulae in higher-order quadrature rules to improve upon their accuracy, or estimating their errors, was advanced in 1964 by Kronrod [8]. Kronrod proposed to insert $n+1$ nodes into an n-point Gauss–Legendre formula and to determine them, and the weights of the resulting $(2n+1)$-point formula, in such a way as to achieve maximum degree of exactness. He showed that the nodes to be inserted are the zeros of a polynomial of degree $n+1$—now called the Stieltjes polynomial—that is orthogonal to all lower-degree polynomials with respect to a sign-changing weight function, the Legendre polynomial of degree n. He computed these zeros, and all weights involved, to 16 decimal digits for $n = 1(1)40$. Mysovskih [13] noted that the same kind of orthogonality has previously been studied by Szegö [14], independently of its application to quadrature. Szegö indeed followed up on an

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idea already expressed in 1894 by Stieltjes in his last letter to Hermite [1, Vol. II, pp. 439–441]. Szegö proved that the zeros in question are all real, are contained in the interval $(-1, 1)$, and interlace with the zeros of the Legendre polynomial. He showed this to be true not only for the Legendre weight (constant weight function), but also for a subclass of Gegenbauer weights. For a further subclass of these, including, however, Legendre's weight function, Monegato [10] in 1978 established positivity of all quadrature weights, a result that was suggested by Kronrod's numerical tables. The interlacing and inclusion properties of the nodes, and positivity of all weights, for Gegenbauer and Jacobi weights are further studied in [3].

During the last ten years, interest in such quadrature rules has intensified, in part because of their potential use in automatic quadrature routines, but also, undoubtedly, because of the intriguing mathematical problems they pose. Recent surveys on the subject can be found in [11] and [2]. Nevertheless, relatively little has been rigorously proved in this area. Apart from the early examples of Gauss–Kronrod quadratures for Chebyshev weights [13] and Gegenbauer weights [14,9,10], only one additional family of weight functions is presently known for which the existence of Gauss–Kronrod quadrature rules with the properties mentioned, and indeed semi-explicit formulae for them, have been established; these are the symmetric weight functions considered in [4] consisting of the Chebyshev weight of the second kind divided by an even quadratic polynomial.

In the following, we substantially enlarge this class of weight functions by considering Chebyshev weight functions of any of the four kinds and dividing them by an arbitrary quadratic polynomial that remains positive on the interval $[-1, 1]$. Such weight functions, even for divisor polynomials of arbitrary degree, have been studied by Bernstein and Szegö (see, e.g., [15, §2.6]). We develop the Gauss–Kronrod formulae in these cases and provide semiexplicit formulae for them analogous to those obtained in [4]. We also prove that the desirable properties of the interlacing of nodes, their containment in the interval $[-1, 1]$, and positivity of all quadrature weights, hold true in almost all cases, exceptions occurring only for small values of n. We begin in Section 2 with identifying explicitly the class of quadratic polynomials that are positive on the interval $[-1, 1]$. We also compute the integrals of the weight functions they generate. In Section 3 we develop the relevant orthogonal polynomials and establish some of their properties. The corresponding Stieltjes polynomials are derived in Section 4. The core of the paper is Section 5 and 6. In Section 5 we study the respective Gauss–Kronrod formulae and establish the interlacing and inclusion properties of the nodes. We also determine the precise polynomial degree of exactness for each one of these quadrature formulae. Section 6 is devoted to explicit formulae for the quadrature weights and their positivity. Finally, in Section 7, we specialize the results to weight functions in which the divisor polynomial is linear, rather than quadratic.

2. The weight functions

We shall be interested in weight functions on $(-1, 1)$ of the form

$$w^{(\pm 1/2)}(t) = (1-t^2)^{\pm 1/2}/\rho(t) \tag{2.1}$$

and

$$w^{(\pm 1/2, \mp 1/2)}(t) = (1-t)^{\pm 1/2}(1+t)^{\mp 1/2}/\rho(t), \tag{2.2}$$

where $\rho(t)$ is a polynomial of exact degree 2 which remains positive on $[-1, 1]$. Our first concern is to find the explicit form of the quadratic polynomial ρ having the stated positivity property.

Proposition 2.1. *A real polynomial ρ of exact degree 2 satisfies $\rho(t) > 0$ for $-1 \leq t \leq 1$ if and only if it has the form*

$$\rho(t) = \rho(t;\ \alpha, \beta, \delta) = \beta(\beta - 2\alpha)t^2 + 2\delta(\beta - \alpha)t + \alpha^2 + \delta^2 \tag{2.3}$$

with

$$0 < \alpha < \beta, \quad \beta \neq 2\alpha, \quad |\delta| < \beta - \alpha. \tag{2.4}$$

Remark. Proposition 2.1 has previously been stated without proof in [12, p. 497].

Proof. Letting

$$\rho(t) = at^2 + bt + c, \quad a, b, c \in \mathbb{R}, \quad a \neq 0, \tag{2.5}$$

we have that $\rho(\cos\theta)$ is a cosine polynomial of degree 2 with real coefficients which is positive for all real values of θ. By [15, Theorem 1.2.2] there then exists a unique polynomial h of exact degree 2, with real coefficients, satisfying

$$h(z) \neq 0 \quad \text{in } |z| \leq 1, \quad h(0) > 0, \tag{2.6}$$

and such that

$$\rho(\cos\theta) = |h(e^{i\theta})|^2. \tag{2.7}$$

Writing

$$h(z) = pz^2 + qz + r, \quad p, q, r \in \mathbb{R}, \quad p \neq 0, \tag{2.8}$$

one finds by an elementary computation that

$$|h(e^{i\theta})|^2 = 4pr\cos^2\theta + 2q(p + r)\cos\theta + q^2 + (p - r)^2,$$

hence, by (2.7) and (2.5),

$$a = 4pr, \qquad b = 2q(p + r), \qquad c = q^2 + (p - r)^2. \tag{2.9}$$

On the other hand, all zeros of h are outside the closed unit disc $|z| \leq 1$ (the first condition in (2.6)) if and only if

$$(Th)(0) > 0, \qquad (T^2h)(0) > 0, \tag{2.10}$$

where $(Th)(\cdot)$ is the Schur transform of h and $(T^2h)(\cdot)$ its first iterate (see, e.g., [7, Theorem 6.8b]). One easily calculates $(Th)(z) = q(r - p)z + r^2 - p^2$, $(T^2h)(z) = (r - p)^2[(r + p)^2 - q^2]$. Therefore, (2.10), together with the last conditions in (2.6) and (2.8), is equivalent to

$$r > |p|, \quad r + p > |q|, \qquad p \neq 0. \tag{2.11}$$

Letting $\alpha = r - p$, $\beta = 2r$, $\delta = q$, or equivalently,

$$p = \tfrac{1}{2}\beta - \alpha, \qquad q = \delta, \qquad r = \tfrac{1}{2}\beta, \tag{2.12}$$

we obtain from (2.9) and (2.11)

$$a = \beta(\beta - 2\alpha), \qquad b = 2\delta(\beta - \alpha), \qquad c = \alpha^2 + \delta^2$$

with

$$\beta > |\beta - 2\alpha|, \qquad \beta - \alpha > |\delta|, \qquad \beta \neq 2\alpha. \tag{2.13}$$

It remains to observe that (2.13) is equivalent to (2.4). □

We will call the parameters α, β, δ *admissible*, if they satisfy (2.4).

The discriminant of the polynomial (2.3) computes to $4\alpha^2(\delta^2-\beta^2+2\alpha\beta)$, so that ρ has a pair of conjugate complex zeros if $\delta^2<\beta(\beta-2\alpha)$ (which implies $\beta>2\alpha$), and two real zeros if $\delta^2\geqslant\beta(\beta-2\alpha)$. If $\beta-2\alpha>0$, the real zeros are both negative (hence less than -1) if $\delta>0$ and both positive (hence larger than 1) if $\delta<0$ ($\delta=0$ is not possible in this case); if $\beta-2\alpha<0$, they are on opposite sides of $[-1,1]$.

We note from (2.7) that

$$\rho\left(\tfrac{1}{2}(u+u^{-1})\right)=0,\quad u\in\mathbb{C},\quad |u|>1 \text{ implies } h(u)=0. \tag{2.14}$$

Indeed, if u_1, u_2 denote the zeros of h (both larger than 1 in modules by (2.6)), then (2.7) can be written as

$$\rho\left(\tfrac{1}{2}(e^{i\theta}+e^{-i\theta})\right)=p^2(e^{i\theta}-u_1)(e^{-i\theta}-\bar{u}_1)(e^{i\theta}-u_2)(e^{-i\theta}-\bar{u}_2),$$

an identity valid for all real θ. By the Identity Theorem for holomorphic functions, the same relation holds for complex θ as well, which, letting $u=e^{i\theta}$ (θ complex), yields (2.14).

The polynomial ρ and the weight functions (2.1), (2.2) become particularly simple when $\delta=0$. In this case we write

$$\alpha/\beta=\tfrac{1}{2}(\gamma+1),\quad -1<\gamma<1, \tag{2.15}$$

and obtain by a simple computation

$$\rho(t;\,\alpha,\,\beta,\,0)=\alpha^2\left[1-\left(4\gamma/(\gamma+1)^2\right)t^2\right]. \tag{2.16}$$

Thus, apart from a constant factor, we are led to the weight functions

$$w_0^{(\pm 1/2)}(t)=(1-t^2)^{\pm 1/2}/(1-\mu t^2), \tag{2.1}$$

$$w_0^{(\pm 1/2,\mp 1/2)}(t)=\frac{(1-t)^{\pm 1/2}(1+t)^{\mp 1/2}}{1-\mu t^2},\quad -\infty<\mu=\frac{4\gamma}{(\gamma+1)^2}<1. \tag{2.2}$$

The Gauss–Kronrod quadrature rules for $w_0^{(1/2)}$ have been studied in [4].

It is of interest to compute the integrals of the weight functions (2.1), (2.2). We begin with $w^{(-1/2)}$. Letting $a=\beta(\beta-2\alpha)$ and denoting the zeros of the polynomial ρ in (2.3) by z_1, z_2, we have

$$\beta_0^{(-1/2)}=\int_{-1}^{1}w^{(-1/2)}(t)\,dt=\frac{1}{a(z_1-z_2)}\left\{\int_{-1}^{1}\frac{(1-t^2)^{-1/2}}{t-z_1}\,dt-\int_{-1}^{1}\frac{(1-t^2)^{-1/2}}{t-z_2}\,dt\right\}. \tag{2.17}$$

It is known (see, e.g., Gradshteyn and Ryzhik [6, Eq. 3.613.2]) that

$$\int_{-1}^{1}\frac{T_n(t)}{z-t}(1-t^2)^{-1/2}\,dt=\frac{2\pi}{(u-u^{-1})u^n}, \tag{2.18}$$

where T_n is the Chebyshev polynomial of degree n and

$$z=\tfrac{1}{2}(u+1/u),\quad |u|>1. \tag{2.19}$$

The relationship between u and z represents a well-known conformal map which transforms the

exterior of the unit circle, $|u| > 1$, into the whole z-plane cut along $[-1, 1]$, concentric circles going into confocal ellipses. Letting

$$z_i = \tfrac{1}{2}(u_i + 1/u_i), \quad |u_i| > 1, \qquad i = 1, 2, \tag{2.20}$$

one finds from (2.17), (2.18) (with $n = 0$) by a simple computation that

$$\beta_0^{(-1/2)} = \frac{4\pi}{a}\,\frac{u_1u_2 + 1}{u_1u_2 - 1}\,\frac{u_1u_2}{(u_1^2 - 1)(u_2^2 - 1)}, \qquad a = \beta(\beta - 2\alpha). \tag{2.21}$$

Since, by (2.20) and (2.14), u_1, u_2 are zeros of h, the symmetric functions of u_1, u_2 in (2.21) can be expressed rationally in terms of the coefficients of h, hence by (2.12) in terms of α, β and δ. One finds

$$\begin{aligned} &u_1u_2 = \frac{\beta}{\beta - 2\alpha}, \qquad u_1u_2 + 1 = \frac{2(\beta - \alpha)}{\beta - 2\alpha}, \qquad u_1u_2 - 1 = \frac{2\alpha}{\beta - 2\alpha}, \\ &(u_1^2 - 1)(u_2^2 - 1) = (u_1u_2 + 1)^2 - (u_1 + u_2)^2 = \frac{4\left[(\beta - \alpha)^2 - \delta^2\right]}{(\beta - 2\alpha)^2}. \end{aligned} \tag{2.22}$$

Substituted in (2.21), this yields

$$\beta_0^{(-1/2)} = \pi\,\frac{\beta - \alpha}{\alpha\left[(\beta - \alpha)^2 - \delta^2\right]}. \tag{2.23}$$

We proceed to the weight function $w^{(1/2)}$ and the integral

$$\beta_0^{(1/2)} = \int_{-1}^{1} w^{(1/2)}(t)\,dt. \tag{2.24}$$

A decomposition analogous to the one in (2.17), and using (cf. [6, Eq. 3.613.3])

$$\int_{-1}^{1} \frac{U_n(t)}{z - t}(1 - t^2)^{1/2}\,dt = \frac{\pi}{u^{n+1}} \tag{2.25}$$

in place of (2.18), yields

$$\beta_0^{(1/2)} = \frac{2\pi}{a}\,\frac{1}{u_1u_2 - 1}, \tag{2.26}$$

with u_i defined as in (2.20), hence, by the third relation in (2.22),

$$\beta_0^{(1/2)} = \pi/\alpha\beta. \tag{2.27}$$

Interestingly, the integral in (2.24) does not depend on the parameter δ.

Finally, for the integral

$$\beta_0^{(1/2,-1/2)} = \int_{-1}^{1} w^{(1/2,-1/2)}(t)\,dt, \tag{2.28}$$

we use (cf. [5, §5.2], where the case $(1 - t)^{-1/2}(1 + t)^{1/2}$ is treated, which is easily transformed to the present case)

$$\int_{-1}^{1} \frac{(1 - t)^{1/2}(1 + t)^{-1/2}}{z - t}\,dt = \frac{2\pi}{u + 1} \tag{2.29}$$

and find

$$\beta_0^{(1/2,-1/2)} = \frac{4\pi}{a} \frac{u_1 u_2}{(u_1 u_2 - 1)(u_1 + 1)(u_2 + 1)},$$

which by (2.22) and

$$(u_1 + 1)(u_2 + 1) = 2(\beta - \alpha - \delta)/(\beta - 2\alpha)$$

becomes

$$\beta_0^{(1/2,-1/2)} = \pi/\alpha(\beta - \alpha - \delta). \tag{2.30}$$

For the remaining weight function, $w^{(-1/2,1/2)}$, see (3.24) below.

In the following, for ease of readability, we shall often drop the superscripts $\pm 1/2$ in the notation for weight functions and related quantities, when there is no danger of ambiguity.

3. The orthogonal polynomials

In the limiting case $\rho(t) \equiv 1$ (corresponding to $\alpha = 1$, $\beta \to 2$, $\delta = 0$ in (2.3)), the orthogonal polynomials associated with (2.1) are the Chebyshev polynomials $T_n(t)$, $U_n(t)$ of the first and second kind (corresponding, respectively, to the minus and plus sign in (2.1)), whereas those associated with (2.2) are similarly the Chebyshev polynomials $V_n(t)$, $W_n(t)$ of the "third and fourth kind" (corresponding, again, to the minus and plus sign, respectively). These are characterized by the well-known formulae

$$T_n(\cos\theta) = \cos n\theta, \qquad U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta} \tag{3.1}$$

and

$$V_n(\cos\theta) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}, \qquad W_n(\cos\theta) = \frac{\sin(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta}. \tag{3.2}$$

They all satisfy the same recurrence relation,

$$y_{k+1} = 2ty_k - y_{k-1}, \quad k = 1, 2, 3, \ldots, \tag{3.3}$$

where

$$\begin{aligned} &y_0 = 1, \quad y_1 = t && \text{for } T_n(t), \\ &y_0 = 1, \quad y_1 = 2t && \text{for } U_n(t), \\ &y_0 = 1, \quad y_1 = 2t - 1 && \text{for } V_n(t), \\ &y_0 = 1, \quad y_1 = 2t + 1 && \text{for } W_n(t). \end{aligned} \tag{3.4}$$

It is natural to expect that the orthogonal polynomials for the more general weight functions (2.1), (2.2), with ρ as given in (2.3), can be expressed in a simple manner in terms of these same Chebyshev polynomials. This is indeed the case, and the respective expressions will be derived in this section.

We will denote the (monic) orthogonal polynomials relative to the weight functions (2.1), (2.2) by

$$\pi_n^{(\pm 1/2)}(t) = \pi_n(t;\, w^{(\pm 1/2)}), \quad \pi_n^{(\pm 1/2,\mp 1/2)}(t) = \pi_n(t;\, w^{(\pm 1/2,\mp 1/2)}), \quad n = 0, 1, 2, \ldots, \tag{3.5}$$

and shall drop superscripts when their values are clear from the context. With $h(z)$ the unique polynomial in (2.7), let $h(e^{i\theta}) = c(\theta) + is(\theta)$ where $c(\theta)$, $s(\theta)$ are real. Then, by [15, Theorem 2.6], we have, up to constant factors,

$$\begin{aligned}
\pi_n^{(-1/2)}(\cos\theta) &= \text{const} \cdot [c(\theta)\cos n\theta + s(\theta)\sin n\theta], \\
\pi_n^{(1/2)}(\cos\theta) &= \text{const} \cdot \left[c(\theta)\,\frac{\sin(n+1)\theta}{\sin\theta} - s(\theta)\frac{\cos(n+1)\theta}{\sin\theta}\right], \\
\pi_n^{(1/2,-1/2)}(\cos\theta) &= \text{const} \cdot \left[c(\theta)\frac{\sin(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta} - s(\theta)\frac{\cos(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta}\right].
\end{aligned} \tag{3.6}$$

From (2.8) and (2.12) we find that

$$c(\theta) = (\beta - 2\alpha)\cos^2\theta + \delta\cos\theta + \alpha, \qquad s(\theta) = \sin\theta[(\beta - 2\alpha)\cos\theta + \delta]. \tag{3.7}$$

Writing $\cos\theta = t$ in (3.7), we get in view of (3.1),

$$\begin{aligned}
\pi_n^{(-1/2)}(t) &= \text{const} \cdot \{[(\beta - 2\alpha)t^2 + \delta t + \alpha]T_n(t) + (1-t^2)[(\beta - 2\alpha)t + \delta]U_{n-1}(t)\} \\
&= \text{const} \cdot \{[t(\beta - 2\alpha) + \delta][tT_n(t) + (1-t^2)U_{n-1}(t)] + \alpha T_n(t)\}.
\end{aligned}$$

Since $tT_n + (1-t^2)U_{n-1} = T_{n-1}$, as follows easily from (3.1), this yields, if $n \geq 2$,

$$\begin{aligned}
\pi_n^{(-1/2)}(t) &= \text{const} \cdot [(\beta - 2\alpha)tT_{n-1}(t) + \delta T_{n-1}(t) + \alpha T_n(t)] \\
&= \text{const} \cdot \{(\beta - 2\alpha) \cdot \tfrac{1}{2}[T_n(t) + T_{n-2}(t)] + \delta T_{n-1}(t) + \alpha T_n(t)\} \\
&= \text{const} \cdot [\tfrac{1}{2}\beta T_n(t) + \delta T_{n-1}(t) + \tfrac{1}{2}(\beta - 2\alpha)T_{n-2}(t)].
\end{aligned}$$

As the leading coefficient of the expression in brackets is $2^{n-1} \cdot \frac{1}{2}\beta$, we obtain

$$\pi_n^{(-1/2)}(t) = \frac{1}{2^{n-1}}\left[T_n(t) + \frac{2\delta}{\beta}T_{n-1}(t) + \left(1 - \frac{2\alpha}{\beta}\right)T_{n-2}(t)\right], \quad n \geq 2. \tag{3.8}$$

When $n = 1$, one finds

$$\pi_1^{(-1/2)}(t) = t + \delta/(\beta - \alpha). \tag{3.8$'$}$$

In a similar way one computes

$$\pi_n^{(1/2)}(t) = \frac{1}{2^n}\left[U_n(t) + \frac{2\delta}{\beta}U_{n-1}(t) + \left(1 - \frac{2\alpha}{\beta}\right)U_{n-2}(t)\right], \quad n \geq 1, \tag{3.9}$$

where $U_{-1}(t) = 0$ when $n = 1$.

To obtain $\pi_n^{(1/2,-1/2)}$, we use (3.2) and (3.7) in the last equation of (3.6) and find

$$\pi_n^{(1/2,-1/2)}(t) = \text{const} \cdot \{[(\beta - 2\alpha)t + \delta][tW_n(t) - (1+t)V_n(t)] + \alpha W_n(t)\}.$$

Noting that $tW_n - (1+t)V_n = W_{n-1}$ and, for $n \geq 2$, by (3.3), $tW_{n-1} = \frac{1}{2}(W_n + W_{n-2})$, we obtain

$$\pi_n^{(1/2,-1/2)}(t) = \text{const} \cdot [\tfrac{1}{2}\beta W_n(t) + \delta W_{n-1}(t) + \tfrac{1}{2}(\beta - 2\alpha)W_{n-2}(t)].$$

Since W_n has leading coefficient 2^n (cf. (3.3), (3.4)), this yields

$$\pi_n^{(1/2,-1/2)}(t) = \frac{1}{2^n}\left[W_n(t) + \frac{2\delta}{\beta}W_{n-1}(t) + \left(1 - \frac{2\alpha}{\beta}\right)W_{n-2}(t)\right], \quad n \geq 2. \tag{3.10}$$

For $n = 1$ one finds, by virtue of (3.4),

$$\pi_1^{(1/2,-1/2)}(t) = t + (\alpha + \delta)/\beta. \tag{3.10}'$$

Denoting the polynomials (3.5) more precisely by $\pi_n^{(\pm 1/2)}(t;\ \alpha,\ \beta,\ \delta)$, and $\pi_n^{(\pm 1/2,\mp 1/2)}(t;\ \alpha,\ \beta,\ \delta)$, if we want to stress their dependence on the parameters α, β, δ, then a simple argument will show that

$$\pi_n^{(-1/2,1/2)}(t;\ \alpha,\ \beta,\ \delta) = (-1)^n \pi_n^{(1/2,-1/2)}(-t;\ \alpha,\ \beta,\ -\delta). \tag{3.11}$$

There is an alternative derivation of (3.8), (3.9) and (3.10), which explains why the coefficients on the right are the same in all three formulae, and in fact equal to $-(u_1 + u_2)/(u_1 u_2)$ and $1/(u_1 u_2)$, respectively (cf. (2.20)). We explain the method for the case of (3.8). Expand $\pi_n^{(-1/2)}$ in Chebyshev polynomials of the first kind, $2^{n-1}\pi_n^{(-1/2)}(t) = \sum_{k=0}^{n} c_k T_k(t)$, $c_n = 1$. It is easily seen that $c_k = 0$ for $k < n - 2$. To obtain the desired orthogonality

$$\int_{-1}^{1} \pi_n^{(-1/2)}(t) \frac{p(t)}{\rho(t)} (1 - t^2)^{-1/2}\, dt = 0, \quad \text{all } p \in \mathbb{P}_{n-1},$$

write

$$p(t) = \rho(t) q(t) + r(t), \qquad q \in \mathbb{P}_{n-3}, \quad r \in \mathbb{P}_1$$

to see that it suffices to make $\pi_n^{(-1/2)}$ orthogonal (with respect to $w^{(-1/2)}$) to linear functions. Choosing in $\mathbb{P}_1$ the basis functions $z_1 - t$ and $z_2 - t$ (where z_i are the zeros of ρ, assumed distinct), one arrives at the system of equations

$$c_{n-1} \int_{-1}^{1} \frac{T_{n-1}(t)}{z_i - t} (1 - t^2)^{-1/2}\, dt + c_{n-2} \int_{-1}^{1} \frac{T_{n-2}(t)}{z_i - t} (1 - t^2)^{-1/2}\, dt$$

$$= -\int_{-1}^{1} \frac{T_n(t)}{z_i - t} (1 - t^2)^{-1/2}\, dt, \quad i = 1, 2,$$

which, by virtue of (2.18), reduces to

$$u_1 c_{n-1} + u_1^2 c_{n-2} = -1, \qquad u_2 c_{n-1} + u_2^2 c_{n-2} = -1,$$

and has the solution $c_{n-1} = -(u_1 + u_2)/(u_1 u_2)$, $c_{n-2} = 1/(u_1 u_2)$, as claimed. If ρ has a double root, the result follows by continuity. The same argument goes through for the other weight functions.

Proposition 3.1. *We have, for* $n \geq 1$,

$$\pi_n^{(1/2)}(t) \pi_{n+1}^{(-1/2)}(t) = \pi_{2n+1}^{(1/2)}(t) + (\delta/\beta) \pi_{2n}^{(1/2)}(t) + \tfrac{1}{4}(1 - 2\alpha/\beta) \pi_{2n-1}^{(1/2)}(t). \tag{3.12}$$

Proof. We first note from (3.1) that

$$T_m(t) U_n(t) = \begin{cases} \tfrac{1}{2}\left[U_{m+n}(t) + U_{n-m}(t)\right], & m \leq n, \\ \tfrac{1}{2} U_{2n+1}(t), & m = n + 1, \\ \tfrac{1}{2}\left[U_{m+n}(t) - U_{m-n-2}(t)\right], & m > n + 1. \end{cases} \tag{3.13}$$

From (3.9) and (3.8) we thus obtain for the product in (3.12), if $n \geq 1$,

$$\frac{1}{2^{2n}}\left[U_n + \frac{2\delta}{\beta}U_{n-1} + \left(1 - \frac{2\alpha}{\beta}\right)U_{n-2}\right]\left[T_{n+1} + \frac{2\delta}{\beta}T_n + \left(1 - \frac{2\alpha}{\beta}\right)T_{n-1}\right]$$
$$= \frac{1}{2^{2n+1}}\left\{U_{2n+1} + \frac{2\delta}{\beta}U_{2n} + \left(1 - \frac{2\alpha}{\beta}\right)U_{2n-1}\right.$$
$$+ \frac{2\delta}{\beta}\left[U_{2n} + \frac{2\delta}{\beta}U_{2n-1} + \left(1 - \frac{2\alpha}{\beta}\right)U_{2n-2}\right]$$
$$\left.+\left(1 - \frac{2\alpha}{\beta}\right)\left[U_{2n-1} + \frac{2\delta}{\beta}U_{2n-2} + \left(1 - \frac{2\alpha}{\beta}\right)U_{2n-3}\right]\right\},$$

which, by (3.9), is precisely the right-hand side of (3.12). □

Proposition 3.2. *We have, for* $n \geq 2$,

$$\pi_n^{(1/2,-1/2)}(t)\pi_n^{(-1/2,1/2)}(t) = \pi_{2n}^{(1/2)}(t) + (\delta/\beta)\pi_{2n-1}^{(1/2)}(t) + \tfrac{1}{4}(1 - 2\alpha/\beta)\pi_{2n-2}^{(1/2)}(t). \tag{3.14}$$

Proof. From (3.2) and elementary trigonometric identities one gets

$$V_m(t)W_n(t) = \begin{cases} U_{m+n}(t) + U_{n-m-1}(t), & m < n, \\ U_{2n}(t), & m = n, \\ U_{m+n}(t) - U_{m-n-1}(t), & m > n. \end{cases} \tag{3.15}$$

Furthermore, replacing θ by $\theta + \pi$ in (3.2) gives

$$W_n(-t) = (-1)^n V_n(t). \tag{3.16}$$

Using (3.10) and (3.11), the product in (3.14) is then computed similarly as in the proof of Proposition 3.1 to be equal to the right-hand side of (3.14). □

The formulae (3.8), (3.9) and (3.10), in conjunction with (3.3), (3.4), immediately yield the recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \tag{3.17}$$

for the respective orthogonal polynomials. One finds for $w^{(-1/2)}$:

$$\alpha_0^{(-1/2)} = -\frac{\delta}{\beta - \alpha}, \qquad \alpha_1^{(-1/2)} = \frac{\alpha\delta}{\beta(\beta - \alpha)}, \qquad \alpha_k^{(-1/2)} = 0 \quad \text{for } k \geq 2;$$
$$\beta_1^{(-1/2)} = \alpha\frac{(\beta - \alpha)^2 - \delta^2}{\beta(\beta - \alpha)^2}, \qquad \beta_2^{(-1/2)} = \frac{\beta - \alpha}{2\beta}, \qquad \beta_k^{(-1/2)} = \tfrac{1}{4} \quad \text{for } k \geq 3; \tag{3.18}$$

for $w^{(1/2)}$:

$$\alpha_0^{(1/2)} = -\frac{\delta}{\beta}, \qquad \alpha_k^{(1/2)} = 0 \quad \text{for } k \geq 1;$$
$$\beta_1^{(1/2)} = \frac{\alpha}{2\beta}, \qquad \beta_k^{(1/2)} = \tfrac{1}{4} \quad \text{for } k \geq 2; \tag{3.19}$$

and for $w^{(1/2,-1/2)}$:

$$\alpha_0^{(1/2,-1/2)} = -\frac{\alpha+\delta}{\beta}, \qquad \alpha_1^{(1/2,-1/2)} = \frac{2\alpha-\beta}{2\beta}, \qquad \alpha_k^{(1/2,-1/2)} = 0 \quad \text{for } k \geq 2;$$
$$\beta_1^{(1/2,-1/2)} = \frac{\alpha(\beta-\alpha-\delta)}{\beta^2}, \qquad \beta_k^{(1/2,-1/2)} = \tfrac{1}{4} \quad \text{for } k \geq 2. \tag{3.20}$$

Accordingly, for the norms

$$\|\pi_n\|^2 = \int_{-1}^{1} \pi_n^2(t) w(t)\, dt = \beta_0\beta_1 \cdots \beta_n,$$

with β_0 given in (2.23), (2.27), and (2.30), one obtains

$$\|\pi_1^{(-1/2)}\|^2 = \frac{\pi}{\beta(\beta-\alpha)}, \qquad \|\pi_n^{(-1/2)}\|^2 = \frac{\pi}{2^{2n-3}\beta^2} \quad \text{for } n \geq 2; \tag{3.21}$$

$$\|\pi_n^{(1/2)}\|^2 = \frac{\pi}{2^{2n-1}\beta^2} \quad \text{for } n \geq 1; \tag{3.22}$$

$$\|\pi_n^{(1/2,-1/2)}\|^2 = \frac{\pi}{2^{2n-2}\beta^2} \quad \text{for } n \geq 1. \tag{3.23}$$

None of these norms, remarkably enough, depends on δ.

The analogous results for the remaining weight function, $w^{(-1/2,1/2)}$, can be obtained from those for $w^{(1/2,-1/2)}$ by means of (3.11), giving

$$\alpha_k^{(-1/2,1/2)}(\alpha, \beta, \delta) = -\alpha_k^{(1/2,-1/2)}(\alpha, \beta, -\delta),$$
$$\beta_k^{(-1/2,1/2)}(\alpha, \beta, \delta) = \beta_k^{(1/2,-1/2)}(\alpha, \beta, -\delta), \qquad k = 0, 1, 2, \ldots; \tag{3.24}$$

$$\|\pi x_n^{(-1/2,1/2)}\|^2 = \|\pi_n^{(1/2,-1/2)}\|^2, \quad n \geq 1. \tag{3.25}$$

The recursion coefficients in (3.18)–(3.20) allow us to compute the zeros of the orthogonal polynomials (3.5), as well as the zeros of the corresponding Stieltjes polynomials (except for the first few, cf. (4.2), (4.5) and (4.8)) efficiently as eigenvalues of symmetric tridiagonal matrices.

4. The Stieltjes polynomials

Given an orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; w)$ of degree n with respect to a weight function w on $[-1, 1]$, there is associated with it a unique (monic) polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; w)$ of degree $n+1$, called *Stieltjes polynomial*, which satisfies the orthogonality relation (see, e.g., [2, §1])

$$\int_{-1}^{1} \pi_{n+1}^*(t)\pi_n(t)p(t)w(t)\, dt = 0, \quad \text{all } p \in \mathbb{P}_n. \tag{4.1}$$

In this section we express the Stieltjes polynomials $\pi_{n+1}^{(\pm 1/2)*}(\cdot) = \pi_{n+1}^*(\cdot; w^{(\pm 1/2)})$, $\pi_{n+1}^{(\pm 1/2,\mp 1/2)*}(\cdot) = \pi_{n+1}^*(\cdot; w^{(\pm 1/2,\mp 1/2)})$ for the weight functions (2.1), (2.2) in terms of the orthogonal polynomials of Section 3 and determine the respective products $\pi_{n+1}^*(\cdot)\pi_n(\cdot)$ appearing in the integrand of (4.1).

Proposition 4.1. *We have*

$$\pi_{n+1}^{(-1/2)^*}(t) = (t^2-1)\pi_{n-1}^{(1/2)}(t), \quad n \geq 4, \tag{4.2}$$

and

$$\pi_{n+1}^{(-1/2)^*}(t)\pi_n^{(-1/2)}(t) = (t^2-1)\left[\pi_{2n-1}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-2}^{(1/2)}(t) + \frac{1}{4}\left(1-\frac{2\alpha}{\beta}\right)\pi_{2n-3}^{(1/2)}(t)\right], \quad n \geq 4. \tag{4.3}$$

Furthermore, for $n = 1$, 2, *and* 3,

$$\pi_2^{(-1/2)^*}(t) = t^2 + \frac{\delta}{\beta}t - \frac{1}{2}\left(1+\frac{\alpha}{\beta}\right), \tag{4.2}^1$$

$$\pi_2^{(-1/2)^*}(t)\pi_1^{(-1/2)}(t) = \pi_3^{(-1/2)}(t) + \frac{\delta}{\beta-\alpha}\pi_2^{(-1/2)}(t); \tag{4.3}^1$$

$$\pi_3^{(-1/2)^*}(t) = t^3 + \frac{\delta}{\beta}t^2 - \frac{1}{4}\left(3+\frac{2\alpha}{\beta}\right)t - \frac{3}{4}\frac{\delta}{\beta}, \tag{4.2}^2$$

$$\pi_3^{(-1/2)^*}(t)\pi_2^{(-1/2)}(t) = \pi_5^{(-1/2)}(t) + \frac{\delta}{\beta}\pi_4^{(-1/2)}(t) + \frac{1}{4}\left(1-\frac{4\alpha}{\beta}\right)\pi_3^{(-1/2)}(t); \tag{4.3}^2$$

$$\pi_4^{(-1/2)^*}(t) = t^4 + \frac{\delta}{\beta}t^3 - \left(1+\frac{\alpha}{2\beta}\right)t^2 - \frac{\delta}{\beta}t + \frac{1}{16}\left(1+\frac{6\alpha}{\beta}\right), \tag{4.2}^3$$

$$\pi_4^{(-1/2)^*}(t)\pi_3^{(-1/2)}(t) = \pi_7^{(-1/2)}(t) + \frac{\delta}{\beta}\pi_6^{(-1/2)}(t) - \frac{\alpha}{2\beta}\pi_5^{(-1/2)}(t) - \frac{\delta}{4\beta}\pi_4^{(-1/2)}(t). \tag{4.3}^3$$

Proof. Define $q_{n+1}(t) = (t^2-1)\pi_{n-1}^{(1/2)}(t)$. Clearly, q_{n+1} is monic of degree $n+1$, and using Proposition 3.1 (with n replaced by $n-1$), we find (for $n \geq 2$)

$$q_{n+1}(t)\pi_n^{(-1/2)}(t) = (t^2-1)\pi_{n-1}^{(1/2)}(t)\pi_n^{(-1/2)}(t) = (t^2-1)\left[\pi_{2n-1}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-2}^{(1/2)}(t) + \frac{1}{4}\left(1-\frac{2\alpha}{\beta}\right)\pi_{2n-3}^{(1/2)}(t)\right]. \tag{4.4}$$

Consequently, if $n \geq 4$, using $(t^2-1)w^{(-1/2)}(t) = -w^{(1/2)}(t)$, we get

$$\int_{-1}^{1} q_{n+1}(t)\pi_n^{(-1/2)}(t)p(t)w^{(-1/2)}(t)\,dt = -\int_{-1}^{1}\left[\pi_{2n-1}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-2}^{(1/2)}(t) + \frac{1}{4}\left(1-\frac{2\alpha}{\beta}\right)\pi_{2n-3}^{(1/2)}(t)\right]p(t)w^{(1/2)}(t)\,dt = 0, \quad \text{all } p \in \mathbb{P}_n,$$

by the orthogonality of the $\pi_m^{(1/2)}$, since $2n-3 > n$ for $n \geq 4$. Thus, q_{n+1} has the orthogonality property (4.1) required for $\pi_{n+1}^{(-1/2)^*}$, and by uniqueness, $q_{n+1} \equiv \pi_{n+1}^{(-1/2)^*}$. This proves (4.2), and (4.3) follows from (4.4).

To prove the special cases $n = 1$, 2 and 3, first write the polynomials $\pi_{n+1}^{(-1/2)^*}$ in (4.2)^n in terms of the U's and then verify (4.3)^n by expressing the product $\pi_{n+1}^{(-1/2)^*}\pi_n^{(-1/2)}$ in terms of the U's, using (3.8) and (3.13), and finally simplify by making use of the relations obtained by multiplying (3.8) by U_0 (thereby expressing $\pi_n^{(-1/2)}$ in terms of the U's). The computations are elementary, but tedious, and will not be reproduced here. □

Proposition 4.2. *We have*

$$\pi_{n+1}^{(1/2)^*}(t) = \pi_{n+1}^{(-1/2)}(t), \quad n \geq 2, \tag{4.5}$$

and

$$\pi_{n+1}^{(1/2)^*}(t)\pi_n^{(1/2)}(t) = \pi_{2n+1}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n}^{(1/2)}(t) + \frac{1}{4}\left(1 - \frac{2\alpha}{\beta}\right)\pi_{2n-1}^{(1/2)}(t), \quad n \geq 2. \tag{4.6}$$

Furthermore, for $n = 1$,

$$\pi_2^{(1/2)^*}(t) = t^2 + (\delta/\beta)t - \tfrac{1}{4}(1 + 2\alpha/\beta), \tag{4.5}$$

$$\pi_2^{(1/2)^*}(t)\pi_1^{(1/2)}(t) = \pi_3^{(1/2)}(t) + (\delta/\beta)\pi_2^{(1/2)}(t). \tag{4.6}$$

Proof. Let $q_{n+1}(t) = \pi_{n+1}^{(-1/2)}(t)$. Then by Proposition 3.1, for $n \geq 1$,

$$\begin{aligned} q_{n+1}(t)\pi_n^{(1/2)}(t) &= \pi_{n+1}^{(-1/2)}(t)\pi_n^{(1/2)}(t) \\ &= \pi_{2n+1}^{(1/2)}(t) + (\delta/\beta)\pi_{2n}^{(1/2)}(t) + \tfrac{1}{4}(1 - 2\alpha/\beta)\pi_{2n-1}^{(1/2)}(t), \end{aligned} \tag{4.7}$$

from which there follows, if $n \geq 2$,

$$\int_{-1}^{1} q_{n+1}(t)\pi_n^{(1/2)}(t)p(t)w^{(1/2)}(t)\,dt = 0, \quad \text{all } p \in \mathbb{P}_n,$$

by virtue of $2n - 1 > n$. Hence, $q_{n+1} \equiv \pi_{n+1}^{(1/2)^*}$, which together with (4.7) proves (4.5) and (4.6). The case $n = 1$ can be verified directly. □

Proposition 4.3. *We have*

$$\pi_{n+1}^{(1/2,-1/2)^*}(t) = (t+1)\pi_n^{(-1/2,1/2)}(t), \quad n \geq 3, \tag{4.8}$$

and

$$\begin{aligned} &\pi_{n+1}^{(1/2,-1/2)^*}(t)\pi_n^{(1/2,-1/2)}(t) \\ &\quad = (t+1)\left[\pi_{2n}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-1}^{(1/2)}(t) + \frac{1}{4}\left(1 - \frac{2\alpha}{\beta}\right)\pi_{2n-2}^{(1/2)}(t)\right], \quad n \geq 3. \end{aligned} \tag{4.9}$$

Furthermore, for $n = 1$ *and* 2,

$$\pi_2^{(1/2,-1/2)^*}(t) = t^2 + \frac{1}{2}\left(1 + \frac{2\delta}{\beta}\right)t - \frac{1}{4}\left(1 - \frac{2\delta - 2\alpha}{\beta}\right), \tag{4.8}$$

$$\pi_2^{(1/2,-1/2)^*}(t)\pi_1^{(1/2,-1/2)}(t) = \pi_3^{(1/2,-1/2)}(t) + \frac{\alpha+\delta}{\beta}\pi_2^{(1/2,-1/2)}(t); \tag{4.9}$$

$$\pi_3^{(1/2,-1/2)^*}(t) = t^3 + \frac{1}{2}\left(1 + \frac{2\delta}{\beta}\right)t^2 - \frac{1}{2}\left(1 - \frac{\delta - \alpha}{\beta}\right)t - \frac{1}{8}\left(1 + \frac{2\alpha + 4\delta}{\beta}\right), \tag{4.8}$$

$$\pi_3^{(1/2,-1/2)^*}(t)\pi_2^{(1/2,-1/2)}(t) = \pi_5^{(1/2,-1/2)}(t) + \frac{1}{2}\left(1 + \frac{2\delta}{\beta}\right)\pi_4^{(1/2,-1/2)}(t) + \frac{1}{4}\left(1 + \frac{2\delta - 2\alpha}{\beta}\right)\pi_3^{(1/2,-1/2)}(t). \tag{4.9}^2$$

Proof. Let $q_{n+1}(t) = (t+1)\pi_n^{(-1/2,1/2)}(t)$. Then, by Proposition 3.2, for $n \geqslant 2$,

$$\begin{aligned} q_{n+1}(t)\pi_n^{(1/2,-1/2)}(t) &= (t+1)\pi_n^{(-1/2,1/2)}(t)\pi_n^{(1/2,-1/2)}(t) \\ &= (t+1)\left[\pi_{2n}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-1}^{(1/2)}(t) + \frac{1}{4}\left(1 - \frac{2\alpha}{\beta}\right)\pi_{2n-2}^{(1/2)}(t)\right]. \end{aligned} \tag{4.10}$$

Using $(t+1)w^{(1/2,-1/2)}(t) = w^{(1/2)}(t)$, one thus gets, if $n \geqslant 3$,

$$\begin{aligned} &\int_{-1}^{1} q_{n+1}(t)\pi_n^{(1/2,-1/2)}(t)p(t)w^{(1/2,-1/2)}(t)\,dt \\ &= \int_{-1}^{1}\left[\pi_{2n}^{(1/2)}(t) + \frac{\delta}{\beta}\pi_{2n-1}^{(1/2)}(t) + \frac{1}{4}\left(1 - \frac{2\alpha}{\beta}\right)\pi_{2n-2}^{(1/2)}(t)\right]p(t)w^{(1/2)}(t)\,dt = 0, \\ &\text{all } p \in \mathbb{P}_n, \end{aligned}$$

since $2n - 2 > n$. This proves (4.8), and (4.9) follows from (4.10).

To verify the special cases $n = 1$ and 2, it is convenient to first express $\pi_{n+1}^{(1/2,-1/2)^*}$ in $(4.8)^n$ in terms of the T's, then compute the products in $(4.9)^n$ as linear combinations of the W's, using

$$T_m(t)W_n(t) = \begin{cases} \frac{1}{2}[W_{m+n}(t) + W_{n-m}(t)], & m < n, \\ \frac{1}{2}[W_{2n}(t) + W_0(t)], & m = n, \\ \frac{1}{2}[W_{m+n}(t) - W_{m-n-1}(t)], & m > n, \end{cases} \tag{4.11}$$

and finally simplify the results by using (3.10). The details of the computations are left to the reader. □

Proposition 4.4. *We have*

$$\pi_{n+1}^{(-1/2,1/2)^*}(t;\,\alpha,\,\beta,\,\delta) = (-1)^{n+1}\pi_{n+1}^{(1/2,-1/2)^*}(-t;\,\alpha,\,\beta,\,-\delta), \quad n \geqslant 1. \tag{4.12}$$

Proof. We verify that the polynomial on the right has the required orthogonality property (4.1). Using $\rho(-t;\,\alpha,\,\beta,\,\delta) = \rho(t;\,\alpha,\,\beta,\,-\delta)$, we find by the substitution of variables $t \mapsto -t$,

$$\begin{aligned} &(-1)^{n+1}\int_{-1}^{1} \pi_{n+1}^{(1/2,-1/2)^*}(-t;\,\alpha,\,\beta,\,-\delta)\pi_n^{(-1/2,1/2)}(t;\,\alpha,\,\beta,\,\delta)p(t) \\ &\qquad \times w^{(-1/2,1/2)}(t;\,\alpha,\,\beta,\,\delta)\,dt \\ &= (-1)^{n+1}\int_{-1}^{1} \pi_{n+1}^{(1/2,-1/2)^*}(t;\,\alpha,\,\beta,\,-\delta)\pi_n^{(-1/2,1/2)}(-t;\,\alpha,\,\beta,\,\delta)p(-t) \\ &\qquad \times w^{(1/2,-1/2)}(t;\,\alpha,\,\beta,\,-\delta)\,dt, \end{aligned}$$

since $w^{(-1/2,1/2)}(-t;\,\alpha,\,\beta,\,\delta) = w^{(1/2,-1/2)}(t;\,\alpha,\,\beta,\,-\delta)$, which by (3.11) is equal to

$$-\int_{-1}^{1} \pi_{n+1}^{(1/2,-1/2)*}(t;\,\alpha,\,\beta,\,-\delta)\pi_n^{(1/2,-1/2)}(t;\,\alpha,\,\beta,\,-\delta)p(-t) \times w^{(1/2,-1/2)}(t;\,\alpha,\,\beta,\,-\delta)\,dt.$$

This is zero for each $p \in \mathbb{P}_n$ by definition of $\pi_{n+1}^{(1/2,-1/2)*}$. □

Proposition 4.5. *Let τ_ν be the zeros of $\pi_n(\cdot;\,w)$. Then*

$$\pi_{n+1}(\tau_\nu;\,w) = \tfrac{1}{2}\pi_{n+1}^{*}(\tau_\nu;\,w), \quad \nu = 1, 2, \ldots, n, \tag{4.13}$$

for all $n \geqslant 2$ if $w = w^{(1/2)}$, for all $n \geqslant 4$ if $w = w^{(-1/2)}$, and for all $n \geqslant 3$ if $w = w^{(\pm 1/2, \mp 1/2)}$

Proof. Consider first $w = w^{(1/2)}$. By (3.9) we have

$$\pi_n^{(1/2)}(t) = \frac{1}{2^n}\left[U_n(t) + \frac{2\delta}{\beta}U_{n-1}(t) + \left(1 - \frac{2\alpha}{\beta}\right)U_{n-2}(t)\right]. \tag{4.14}$$

Here, $U_{n-1}(\tau_\nu) \neq 0$. In fact, if we had $U_{n-1}(\tau_\nu) = 0$, then, by (4.14), since τ_ν is a zero of $\pi_n^{(1/2)}$, we would obtain

$$U_n(\tau_\nu) + \left(1 - \frac{2\alpha}{\beta}\right)U_{n-2}(\tau_\nu) = 0,$$

and by the recurrence relation (3.3), $(2\alpha/\beta)U_{n-2}(\tau_\nu) = 0$, i.e., $U_{n-2}(\tau_\nu) = 0$, since $\alpha > 0$. This is impossible, since two consecutive orthogonal polynomials cannot vanish at the same point. We therefore obtain

$$\frac{\delta}{\beta} = \frac{\alpha}{\beta}\frac{U_{n-2}(\tau_\nu)}{U_{n-1}(\tau_\nu)} - \frac{1}{2}\frac{U_n(\tau_\nu) + U_{n-2}(\tau_\nu)}{U_{n-1}(\tau_\nu)}.$$

Letting $\tau_\nu = \cos\theta_\nu$, $0 < \theta_\nu < \pi$, this yields, in view of (3.1),

$$\frac{\delta}{\beta} = \frac{\alpha}{\beta}\frac{\sin(n-1)\theta_\nu}{\sin n\theta_\nu} - \cos\theta_\nu. \tag{4.15}$$

Setting $t = \cos\theta_\nu$ in (4.14), after replacing n by $n+1$, and then substituting for δ/β from (4.15), one obtains, after some elementary computation,

$$\pi_{n+1}^{(1/2)}(\tau_\nu) = -\frac{\alpha}{2^n\beta}\frac{\sin\theta_\nu}{\sin n\theta_\nu}. \tag{4.16}$$

A similar substitution in (4.5), if $n \geqslant 2$, using (3.8) (with n replaced by $n+1$), gives

$$\pi_{n+1}^{(1/2)*}(\tau_\nu) = -\frac{\alpha}{2^{n-1}\beta}\frac{\sin\theta_\nu}{\sin n\theta_\nu}. \tag{4.17}$$

Comparing (4.16) with (4.17) immediately yields (4.13).

For $w = w^{(-1/2)}$ and $n \geqslant 4$, one obtains in the same manner

$$\pi_{n+1}^{(-1/2)}(\tau_\nu) = -\frac{\alpha}{2^{n-1}\beta}\frac{\sin^2\theta_\nu}{\cos(n-1)\theta_\nu} = \tfrac{1}{2}\pi_{n+1}^{(-1/2)*}(\tau_\nu) \tag{4.18}$$

$$\left(\pi_n^{(-1/2)}(\tau_\nu) = 0, \quad \tau_\nu = \cos\theta_\nu\right),$$

and for $w = w^{(1/2,-1/2)}$, $n \geq 3$,

$$\pi_{n+1}^{(1/2,-1/2)}(\tau_\nu) = -\frac{\alpha}{2^n\beta}\frac{\sin^2\theta_\nu}{\sin\frac{1}{2}\theta_\nu \sin(n-\frac{1}{2})\theta_\nu} = \tfrac{1}{2}\pi_{n+1}^{(1/2,-1/2)*}(\tau_\nu) \tag{4.19}$$
$$\left(\pi_n^{(1/2,-1/2)}(\tau_\nu) = 0, \quad \tau_\nu = \cos\theta_\nu\right).$$

The analogous result for $w^{(-1/2,1/2)}$ follows easily from (3.11) and (4.12). □

5. Interlacing, inclusion, and exactness properties

If $\tau_\nu = \tau_\nu^{(n)}$ denote the zeros of the orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; w)$, and $\tau_\mu^* = \tau_\mu^{(n)*}$ those of the polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; w)$ satisfying (4.1), then, if they are distinct among themselves and between one another, one calls the (interpolatory) quadrature rule

$$\int_{-1}^{1} f(t)w(t)\,dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f) \tag{5.1}$$

the $(2n+1)$-point *Gauss–Kronrod quadrature rule*, or the *Kronrod extension* of the n-point Gauss rule, relative to the weight function w. The formula (5.1) is known to have precise degree of exactness $d = 2n + k$, where k is the unique integer satisfying

$$\int_{-1}^{1} \pi_{n+1}^*(t)\pi_n(t)p(t)w(t)\,dt \begin{cases} = 0 & \text{for all } p \in \mathbb{P}_{k-1}, \\ \neq 0 & \text{for some } p \in \mathbb{P}_k \end{cases} \tag{5.2}$$

(see, e.g., [2, §2]). By (4.1) clearly $k \geq n+1$, hence $d \geq 3n+1$.

We say that (5.1) has the *interlacing* property if all nodes τ_ν, τ_μ^* are real and satisfy, when ordered decreasingly,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*. \tag{5.3}$$

We say that (5.1) has the *inclusion* property if all nodes τ_ν, τ_μ^* are contained in the closed interval $[-1, 1]$, i.e.,

$$-1 \leq \tau_{n+1}^* \quad \text{and} \quad \tau_1^* \leq 1, \tag{5.4}$$

if (5.3) holds.

In this section we show that, with a few exceptions for small n, the Gauss–Kronrod formula (5.1) enjoys the interlacing property when $w(t) = w^{(\pm 1/2)}(t;\ \alpha,\ \beta,\ \delta)$ and $w(t) = w^{(\pm 1/2, \mp 1/2)}(t;\ \alpha,\ \beta,\ \delta)$ and the parameters α, β, δ are admissible. In addition, we state conditions under which the inclusion property holds, and we determine the precise degree of exactness for all Gauss–Kronrod quadrature formulae in this class. As mentioned at the end of Section 2, superscripts $\pm\frac{1}{2}$ will be deleted when there is no danger of confusion.

Theorem 5.1. *Consider the weight function $w(t) = w^{(-1/2)}(t;\ \alpha,\ \beta,\ \delta)$, with α, β, δ admissible.*

(a) *The Gauss–Kronrod rule* (5.1) *has the interlacing property for all $n \geq 1$, except when $n = 3$ and $\beta > 2\alpha$, in which case* (5.3) *holds if*

$$\delta^2 < \delta_0^2, \qquad \delta_0^2 = \frac{1}{32}\frac{(3\beta - 2\alpha)^2(\beta + 6\alpha)}{\beta + 2\alpha}. \tag{5.5}$$

(b) *The inclusion property holds for all* $n \geq 4$. *For* $n = 3$ (*assuming interlacing*; cf. (a)), *it holds precisely if* $\beta > 2\alpha$; *for* $n = 2$ *precisely if* $\beta > 2\alpha$ *and* $|\delta| \leq \beta - 2\alpha$; *and for* $n = 1$ *precisely if* $|\delta| \leq \frac{1}{2}(\beta - \alpha)$.

(c) *The precise degree of exactness* d *of* (5.1) *is equal to* $4n - 3$ *if* $n \geq 4$. *If* $n = 3$, *then* $d = 10$ *unless* $\delta = 0$, *in which case* $d = 11$. *If* $n = 2$, *then* $d = 7$ *if* $\beta \neq 4\alpha$, $d = 8$ *if* $\beta = 4\alpha$ *and* $\delta \neq 0$, *and* $d = 9$ *if* $\beta = 4\alpha$ *and* $\delta = 0$. *If* $n = 1$, *then* $d = 4$ *if* $\delta \neq 0$ *and* 5 *otherwise*.

Proof. (a) If $n = 1$, we have by $(3.8)^1$ that $\tau_1 = -\delta/(\beta - \alpha)$, hence by $(4.2)^1$,

$$\pi_2^*(\tau_1) = \frac{1}{2\beta(\beta-\alpha)^2}\left[2\alpha\delta^2 - (\alpha+\beta)(\beta-\alpha)^2\right]$$
$$< \frac{\alpha}{\beta} - \frac{\alpha+\beta}{2\beta} = \frac{1}{2}\left(\frac{\alpha}{\beta} - 1\right) < 0,$$

by virtue of (2.4). This proves (5.3) for $n = 1$.

If $n = 2$, we have by (3.8) and $(4.2)^2$

$$\pi_2(t) = t^2 + \frac{\delta}{\beta}t - \frac{\alpha}{\beta},$$
$$\pi_3^*(t) = t^3 + \frac{\delta}{\beta}t^2 - \frac{1}{4} + \left(3 + \frac{2\alpha}{\beta}\right)t - \frac{3}{4}\frac{\delta}{\beta}. \tag{5.6}$$

The interlacing property holds when $\delta = 0$, since then $\tau_{1,2}^2 = \alpha/\beta$ and π_3^* has a zero at $t = 0$ and two other zeros $\tau_{1,3}^*$ with $\tau_{1,3}^{*2} = \frac{1}{4}(3 + 2\alpha/\beta) > \alpha/\beta$. Upon varying $|\delta|$ from 0 to $\beta - \alpha$, interlacing can only break down when π_2 and π_3^* have a common zero, t_0, for some δ in that range. If that is the case, then by (5.6)

$$t_0^2 + \frac{\delta}{\beta}t_0 = \frac{\alpha}{\beta}, \qquad t_0 \cdot \frac{\alpha}{\beta} - \frac{1}{4}\left(3 + \frac{2\alpha}{\beta}\right)t_0 - \frac{3}{4}\frac{\delta}{\beta} = 0,$$

which, upon eliminating t_0, yields

$$\delta^2 = \tfrac{1}{8}(3\beta - 2\alpha)^2.$$

It is elementary to see that the right-hand side is larger than $(\beta - \alpha)^2$ for admissible α, β. Consequently, the interlacing property holds for all admissible α, β, δ.

We now discuss the case $n = 3$. One shows, similarly as in the case $n = 2$, that (5.3) is true when $\delta = 0$. As in the previous case, we determine the first value of $|\delta|$ for which the polynomials

$$\pi_3(t) = t^3 + \frac{\delta}{\beta}t^2 - \frac{1}{2}\left(1 + \frac{\alpha}{\beta}\right)t - \frac{1}{2}\frac{\delta}{\beta},$$
$$\pi_4^*(t) = t^4 + \frac{\delta}{\beta}t^3 - \left(1 + \frac{\alpha}{2\beta}\right)t^2 - \frac{\delta}{\beta}t + \frac{1}{16}\left(1 + \frac{6\alpha}{\beta}\right) \tag{5.7}$$

(cf. (3.8) and $(4.2)^3$) have a common zero t_0. Writing

$$\pi_4^*(t) = t\left[t^3 + \frac{\delta}{\beta}t^2 - \frac{1}{2}\left(1 + \frac{\alpha}{\beta}\right)t\right] - \tfrac{1}{2}t^2 - \frac{\delta}{\beta}t + \frac{1}{16}\left(1 + \frac{6\alpha}{\beta}\right)$$

and using

$$\pi_3(t_0) = 0, \tag{5.8}$$

the fact that $\pi_4^*(t_0) = 0$ yields

$$t_0^2 + \frac{\delta}{\beta} t_0 - \frac{1}{8}\left(1 + \frac{6\alpha}{\beta}\right) = 0,$$

which, upon reusing (5.8), simplifies to

$$\frac{1}{8}\left(1 + \frac{6\alpha}{\beta}\right) t_0 - \frac{1}{2}\left(1 + \frac{\alpha}{\beta}\right) t_0 - \frac{1}{2}\frac{\delta}{\beta} = 0,$$

that is, to

$$t_0 = 4\delta/(2\alpha - 3\beta).$$

Inserting this into (5.8) one finds, after a little computation, $\delta^2 = \delta_0^2$ with δ_0^2 as given in (5.5). Hence, for all values of $|\delta|$ smaller than $|\delta_0|$ we are assured of the interlacing property. An elementary computation shows that

$$\delta_0^2 \gtrless (\beta - \alpha)^2 \quad \text{iff } 40r^3 - 28r^2 - 42r + 23 \lessgtr 0, \quad r = \alpha/\beta. \tag{5.9}$$

Since $0 < r < 1$ by (2.4), and the cubic in (5.9) has a zero at $r = \frac{1}{2}$ and two other zeros outside, and on either side, of [0, 1], we have $|\delta_0| \geqslant \beta - \alpha$ (for admissible α, β) precisely if $\frac{1}{2} \leqslant r < 1$, i.e., $\beta \leqslant 2\alpha$, where equality is excluded by (2.4). Therefore, if $\beta < 2\alpha$, the interlacing property holds; if $\beta > 2\alpha$, it holds when $\delta^2 < \delta_0^2$ as claimed.

Finally, for $n \geqslant 4$, the assertion follows immediately from $\pi_n^{(-1/2)}(t) = \pi_n^{(1/2)*}(t)$ (cf. (4.5)) and $\pi_{n+1}^{(-1/2)*}(t) = (t^2 - 1)\pi_{n-1}^{(1/2)}(t)$ (cf. (4.2)), and the fact that the interlacing property holds for the weight function $w^{(1/2)}$ (cf. Theorem 5.2(a) below).

(b) For $n \geqslant 4$, the inclusion property (5.4) follows immediately from (4.2). For $n = 3$, assuming interlacing, (5.4) is equivalent to $\pi_4^*(\pm 1) \geqslant 0$, hence, by $(4.2)^3$, to $\beta \geqslant 2\alpha$. Since $\beta \neq 2\alpha$, we have inclusion precisely for $\beta > 2\alpha$. If $n = 2$, we have (5.4) if and only if $\pi_3^*(1) \geqslant 0$ and $\pi_3^*(-1) \leqslant 0$. By $(4.2)^2$, this is the same as $\delta \geqslant 2\alpha - \beta$ and $\delta \leqslant \beta - 2\alpha$. These conditions are incompatible when $\beta < 2\alpha$, and equivalent to $|\delta| \leqslant \beta - 2\alpha$ when $\beta > 2\alpha$. Finally, when $n = 1$, using $(4.2)^1$, we have by a similar argument as before that (5.4) holds precisely when $\delta \geqslant -\frac{1}{2}(\beta - \alpha)$ and $\delta \leqslant \frac{1}{2}(\beta - \alpha)$, i.e., $|\delta| \leqslant \frac{1}{2}(\beta - \alpha)$.

(c) We have $d = 2n + k$, with k determined as in (5.2). If $n \geqslant 4$, then (4.3), in view of $(1 - t^2)w^{(-1/2)}(t) = w^{(1/2)}(t)$, yields $k = 2n - 3$, since $\beta \neq 2\alpha$, hence $d = 4n - 3$. The remaining assertions follow similarly from $(4.3)^n$, $n = 3$, 2, and 1. □

Theorem 5.2. *Consider the weight function* $w(t) = w^{(1/2)}(t;\ \alpha, \beta, \delta)$, *with* α, β, δ *admissible.*

(a) *The Gauss–Kronrod rule* (5.1) *has the interlacing property for all* $n \geqslant 1$.

(b) *The inclusion property holds for all* $n \geqslant 1$, *except when* $n = 1$ *and* $\beta > 2\alpha$, *in which case* (5.4) *holds precisely when* $|\delta| \leqslant \frac{1}{4}(3\beta - 2\alpha)$.

(c) *The precise degree of exactness d of* (5.1) *is equal to* $4n - 1$ *if* $n \geqslant 2$; *if* $n = 1$, *then* $d = 4$ *if* $\delta \neq 0$ *and* $d = 5$ *if* $\delta = 0$.

Proof. (a) We first note that interlacing holds when $\delta = 0$. Indeed, we are then in the case of the weight function $w_0^{(1/2)}$ of $(2.1)^0$ for which the interlacing property (5.3), including (5.4), is known

from the work in [4]. Moving δ away from 0, either to the left or to the right, within the allowable range $|\delta| < \beta - \alpha$, the interlacing property ceases to hold only if for some δ_0 in this range the polynomials π_n and π_{n+1}^* have a common zero, t_0. Proposition 4.5, if $n \geq 2$, would then imply $\pi_{n+1}(t_0) = \pi_n(t_0) = 0$, which is impossible, and (3.9), $(4.5)^1$, if $n = 1$, would imply $\beta + 2\alpha = 0$, contradicting (2.4). Hence, interlacing prevails for all admissible, α, β, δ.

(b) The inclusion property (5.4) follows immediately from (4.5) when $n \geq 2$. If $n = 1$, we have (5.4) precisely when $\pi_2^*(\pm 1) \geq 0$, which, on using $(4.5)^1$ is equivalent to $|\delta| \leq \frac{1}{4}(3\beta - 2\alpha)$. Here, the bound is larger than $\beta - \alpha$ if $\beta < 2\alpha$, so that the constraint is active only if $\beta > 2\alpha$. (The case $\beta = 2\alpha$ is excluded by (2.4).)

(c) If $n \geq 2$, then (4.6) shows, since $\beta \neq 2\alpha$, that (5.2) holds with $k = 2n - 1$, so that $d = 2n + k = 4n - 1$. The assertion for $n = 1$ follows from $(4.6)^1$ by a similar argument. □

Theorem 5.3. *Consider the weight function $w(t) = w^{(1/2,-1/2)}(t;\ \alpha, \beta, \delta)$, with α, β, δ admissible.*

(a) *The Gauss–Kronrod rule* (5.1) *has the interlacing property for all $n \geq 1$, except when $n = 2$ and $\beta > 2\alpha$, in which case* (5.3) *holds if*

$$-(\beta - \alpha) < \delta < \delta_1, \quad \delta_1 = \frac{\beta^2 + 8\alpha\beta - 4\alpha^2}{8\alpha + 4\beta}. \tag{5.10}$$

(b) *The inclusion property holds for all $n \geq 3$. For $n = 2$ (assuming interlacing; cf. (a)), it holds precisely if*

$$\beta > 2\alpha \quad \text{and} \quad -\frac{7\beta - 6\alpha}{8} \leq \delta < \beta - \alpha, \tag{5.11}$$

and for $n = 1$ if both inequalities

$$6\delta + 5\beta - 2\alpha \geq 0 \quad \text{and} \quad 2\delta + 2\alpha - \beta \leq 0 \tag{5.12}$$

are satisfied.

(c) *The precise degree of exactness d of* (5.1) *is equal to $4n - 2$ if $n \geq 3$. If $n = 2$, then $d = 7$, unless $2\delta - 2\alpha + \beta = 0$, in which case $d = 8$. If $n = 1$, then $d = 4$ if $\alpha + \delta \neq 0$ and $d = 5$ otherwise.*

Proof. (a) It is elementary to show, using $(3.10)^1$ and $(4.8)^1$, that $\pi_2^*(\tau_1) < 0$, which implies (5.3) for $n = 1$. For $n = 2$, an argument similar to the one in the proof of Theorem 5.1(a) will show that the interlacing property holds if $\beta < 2\alpha$, and if $\beta > 2\alpha$ provided that (5.10) is satisfied. If $n \geq 3$, the assertion follows from Proposition 4.5, which, since the zeros of π_n interlace with those of π_{n+1}, implies that sign $\pi_{n+1}(\tau_\nu;\ w) = (-1)^\nu = \text{sign}\ \pi_{n+1}^*(\tau_\nu;\ w)$, $\nu = 1, 2, \ldots, n$, which in turn implies (5.3).

(b) For $n \geq 3$, the inclusion property follows trivially from (4.8). For $n = 2$ and $n = 1$, the conditions stated in (5.11) and (5.12) express $\pi_3^*(1) \geq 0$, $\pi_3^*(-1) \leq 0$ and $\pi_2^*(\pm 1) \geq 0$, respectively.

(c) The formulae for the precise degree of exactness follow in the usual way from (4.9), when $n \geq 3$, and from $(4.9)^2$, $(4.9)^1$ when $n = 2$ and 1, noting, in the case of $(4.9)^2$, that the coefficients of π_3 and π_4 in $(4.9)^2$ cannot vanish simultaneously because of $\alpha > 0$. □

The discussion for the remaining weight function $w^{(-1/2,1/2)}$ can be reduced, with the help of (3.11) and (4.12), to the one just completed for $w^{(1/2,-1/2)}$.

6. Quadrature weights, positivity, and explicit formulae

In terms of the polynomials $\pi_n(\cdot) = \pi_n(\cdot; w)$ and $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; w)$, the weights $\sigma_\nu = \sigma_\nu^{(n)}$ and $\sigma_\mu^* = \sigma_\mu^{(n)*}$ in the Gauss–Kronrod formula (5.1) admit the following representations (Monegato [9]),

$$\sigma_\nu = \lambda_\nu + \frac{\|\pi_n\|^2}{\pi_{n+1}^*(\tau_\nu)\pi_n'(\tau_\nu)}, \quad \nu = 1, 2, \ldots, n, \tag{6.1}$$

$$\sigma_\mu^* = \frac{\|\pi_n\|^2}{\pi_n(\tau_\mu^*)\pi_{n+1}^{*\prime}(\tau_\mu^*)}, \quad \mu = 1, 2, \ldots, n+1, \tag{6.2}$$

where $\lambda_\nu = \lambda_\nu^{(n)}$ are the Christoffel numbers—the weights of the Gaussian quadrature rule—relative to the weight function w. These in turn can be represented in the form (see, e.g., [15, Eq. (3.4.7)])

$$\lambda_\nu = -\frac{\|\pi_n\|^2}{\pi_{n+1}(\tau_\nu)\pi_n'(\tau_\nu)}, \quad \nu = 1, 2, \ldots, n, \tag{6.3}$$

and are known to be positive. We show in this section that also the weights $\sigma_\nu^{(n)}$ and $\sigma_\mu^{(n)*}$, with a few exceptions for small n, are all positive when $w(t) = w^{(\pm 1/2)}(t; \alpha, \beta, \delta)$ and $w(t) = w^{(\pm 1/2, \mp 1/2)}(t; \alpha, \beta, \delta)$, for arbitrary admissible parameters α, β, δ. The positivity of σ_μ^* actually follows from the interlacing property (Monegato [9]). Moreover, we give explicit formulae for the σ_ν and σ_μ^*.

If the interlacing property holds, the second term in (6.1) is always negative, whereas the first is positive. Thus, in view of (6.3), we have $\sigma_\nu > 0$ if and only if $|\pi_{n+1}^*(\tau_\nu)| > |\pi_{n+1}(\tau_\nu)|$, or, since the zeros of π_n interlace with those of π_{n+1},

$$\sigma_\nu > 0 \quad \text{iff } \pi_{n+1}^*(\tau_\nu) \lesseqgtr \pi_{n+1}(\tau_\nu) \quad \text{for } \nu = \begin{cases} \text{odd}, \\ \text{even} \end{cases} \tag{6.4}$$

(assuming the interlacing property).

We begin with the case $w = w^{(1/2)}$, which is simpler and appears to be more fundamental.

Theorem 6.1. *Consider the weight function $w(t) = w^{(1/2)}(t; \alpha, \beta, \delta)$, with α, β, δ admissible. Then all weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{(n)*}$ in (5.1) are positive for each $n \geq 1$. Specifically, when $n = 1$,*

$$\sigma_1^{(1)} = \frac{\pi}{\alpha(2\alpha+\beta)}, \qquad \sigma_1^{(1)*} = \frac{\pi}{\omega(\omega+\delta)}, \qquad \sigma_2^{(1)*} = \frac{\pi}{\omega(\omega-\delta)}, \tag{6.5}$$

where $\omega = \sqrt{\delta^2 + \beta(2\alpha+\beta)}$. For $n \geq 2$, letting $\tau_\nu^{(n)} = \cos\theta_\nu$ and $\tau_\mu^{(n)*} = \cos\theta_\mu^*$, one has for $\nu = 1, 2, \ldots, n$,

$$\sigma_\nu^{(n)} = \frac{\pi}{2\alpha^2} \frac{\sin^2 n\theta_\nu}{n - \dfrac{\sin n\theta_\nu \cos(n-1)\theta_\nu}{\sin\theta_\nu} + \dfrac{\beta}{\alpha}\sin^2 n\theta_\nu}, \tag{6.6}$$

and for $\mu = 1, 2, \ldots, n+1$,

$$\sigma_\mu^{(n)*} = \frac{\pi}{2\alpha^2} \frac{\cos^2 n\theta_\mu^*}{n + \dfrac{\sin(n-1)\theta_\mu^* \cos n\theta_\mu^*}{\sin\theta_\mu^*} + \dfrac{\beta}{\alpha}\cos^2 n\theta_\mu^*}. \tag{6.7}$$

Remark. Alternative forms of (6.6), (6.7), assuming $\theta_\nu \neq \frac{1}{2}\pi$, $\theta_\mu^* \neq \frac{1}{2}\pi$, are

$$\sigma_\nu^{(n)} = \frac{\pi}{2\alpha^2} \frac{\sin^2 n\theta_\nu}{n - \left\{\sin 2n\theta_\nu + \frac{2\delta}{\beta}\sin n\theta_\nu \cos(n-1)\theta_\nu\right\} / \left\{\sin 2\theta_\nu + \frac{2\delta}{\beta}\sin\theta_\nu\right\}}, \tag{6.6'}$$

$$\sigma_\mu^{(n)*} = \frac{\pi}{2\alpha^2} \frac{\cos^2 n\theta_\mu^*}{n + \left\{\sin 2n\theta_\mu^* + \frac{2\delta}{\beta}\sin(n-1)\theta_\mu^* \cos n\theta_\mu^*\right\} / \left\{\sin 2\theta_\mu^* + \frac{2\delta}{\beta}\sin\theta_\mu^*\right\}}. \tag{6.7'}$$

These, as $\delta \to 0$, reduce in view of (2.16) to the formulae (3.9), (3.11) obtained in [4]. We note, however, that (6.6) remains valid as $\delta \to 0$ also in the case n (odd) $\geqslant 3$, $\nu = \frac{1}{2}(n+1)$, and reduces to [4, Eq. (3.9′)]. Likewise, (6.7) in the limit $\delta = 0$ reduces to [4, Eq. (3.11′)] when n (even) $\geqslant 2$ and $\mu = \frac{1}{2}(n+2)$.

Proof. The formulae (6.5) for $n = 1$, which clearly imply the positivity of all weights, are easily obtained from (6.1), (6.2), and (6.3), using the expressions (3.9) for π_1 and π_2, (4.5)[1] for π_2^*, and (3.22) for $\|\pi_1\|^2$.

Thus assume $n \geqslant 2$. Substituting $\pi_{n+1}^*(\tau_\nu)$ from (4.13) into (6.1), we get $\sigma_\nu = \frac{1}{2}\lambda_\nu$, which proves positivity of σ_ν. Positivity of σ_μ^*, as already mentioned, follows from the interlacing property, which holds according to Theorem 5.2 (a).

We proceed to derive the explicit expressions in (6.6) and (6.7). First note that, by what has just been shown,

$$\sigma_\nu = \tfrac{1}{2}\lambda_\nu = -\|\pi_n\|^2 / \pi_{n+1}^*(\tau_\nu)\pi_n'(\tau_\nu). \tag{6.8}$$

Putting $t = \cos\theta$ in (3.9) and differentiating gives

$$2^n\left[\cos\theta \cdot \pi_n(\cos\theta) - \sin^2\theta \cdot \pi_n'(\cos\theta)\right]$$
$$= (n+1)\cos(n+1)\theta + \frac{2\delta}{\beta} n \cos n\theta + \left(1 - \frac{2\alpha}{\beta}\right)(n-1)\cos(n-1)\theta.$$

Now put $\theta = \theta_\nu$ and substitute δ/β from (4.15); then, after a short calculation, one finds

$$\pi_n'(\tau_\nu) = \frac{\alpha}{2^{n-1}\beta} \frac{1}{\sin\theta_\nu \sin n\theta_\nu}\left\{n - \frac{\sin n\theta_\nu \cos(n-1)\theta_\nu}{\sin\theta_\nu} + \frac{\beta}{\alpha}\sin^2 n\theta_\nu\right\}.$$

Multiplying this by $\pi_{n+1}^*(\tau_\nu)$ from (4.17), inserting the result in (6.8), and recalling (3.22) immediately yields the desired formula (6.6).

To derive (6.7), we let $\tau_\mu^* = \cos\theta_\mu^*$ (which is possible by virtue of (4.5)) and find from (4.5) and (3.8), similarly as in the proof of Proposition 4.5 (cf. (4.15)), that

$$\frac{\delta}{\beta} = \frac{\alpha}{\beta}\frac{\cos(n-1)\theta_\mu^*}{\cos n\theta_\mu^*} - \cos\theta_\mu^*, \tag{6.9}$$

and from (3.9) that

$$\pi_n(\tau_\mu^*) = \frac{\alpha}{2^{n-1}\beta}\frac{1}{\cos n\theta_\mu^*}.$$

Furthermore,

$$\pi_{n+1}^{*\prime}(\tau_\mu^*) = \frac{\alpha}{2^{n-1}\beta}\frac{1}{\cos n\theta_\mu^*}\left\{n + \frac{\sin(n-1)\theta_\mu^*\cos n\theta_\mu^*}{\sin\theta_\mu^*} + \frac{\beta}{\alpha}\cos^2 n\theta_\mu^*\right\},$$

from which as before, using (6.2) and (3.22), one obtains (6.7).

The alternative formulae (6.6′) and (6.7′) follow from those just derived by expressing β/α (under the assumptions made on θ_ν and θ_μ^*) in terms of δ/β by means of (4.15) and (6.9), respectively, and using elementary trigonometric identities. □

Theorem 6.2. *Consider the weight function $w(t) = w^{(-1/2)}(t;\ \alpha, \beta, \delta)$, with α, β, δ admissible. Then all weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{(n)*}$ in (5.1) are positive for each $n \geq 1$, except when $n = 3$ and $\beta > 2\alpha$, in which case positivity holds if $\delta^2 < \beta(\beta + 2\alpha)/8$.*

If $\{\bar\tau_\mu\}_{\mu=1}^{n-1}$, $\{\bar\tau_\nu^*\}_{\nu=1}^{n}$ denote the Gauss and Kronrod nodes, respectively, of the $(2n-1)$-point Gauss–Kronrod formula for the weight function $w = w^{(1/2)}$, and $\bar\sigma_\mu$, $\bar\sigma_\nu^*$ the respective weights, then for $n \geq 4$ one has

$$\sigma_\nu^{(n)} = \frac{\bar\sigma_\nu^*}{1-\tau_\nu^2}, \quad \nu = 1, 2, \ldots, n; \qquad \sigma_\mu^{(n)*} = \frac{\bar\sigma_{\mu-1}}{1-\tau_\mu^{*2}}, \quad \mu = 2, 3, \ldots, n, \tag{6.10}$$

while

$$\begin{aligned}\sigma_1^{(n)*} &= \frac{\pi}{4(\beta-\alpha+\delta)[(\beta-\alpha+\delta)n+2\alpha-\beta-\delta]},\\ \sigma_{n+1}^{(n)*} &= \frac{\pi}{4(\beta-\alpha-\delta)[(\beta-\alpha-\delta)n+2\alpha-\beta+\delta]}.\end{aligned} \tag{6.11}$$

Remark. Explicit formulae could easily be obtained for $\sigma_\nu^{(1)}$, $\sigma_\nu^{(2)}$ and $\sigma_\mu^{(1)*}$, but we refrain from writing them down here.

Proof. We begin with the cases $n = 1, 2, 3$, which require special treatment. We verify the conditions in (6.4).

For $n = 1$, the condition in (6.4) is immediate from $(4.2)^1$ and (5.6), since $\alpha < \beta$. For $n = 2$, the two inequalities in (6.4), by $(4.2)^2$ and (5.7), amount to $\tau_1 > -\delta/\beta$, $\tau_2 < -\delta/\beta$, which are true since $\pi_2(-\delta/\beta) = -\alpha/\beta < 0$ by (5.6). When $n = 3$, the three inequalities in (6.4), by (5.7) and (3.8), are equivalent to

$$\tau_\nu^2 + \frac{\delta}{\beta}\tau_\nu \gtrless \frac{1}{4}\left(1 + \frac{2\alpha}{\beta}\right), \qquad \nu = \begin{cases}1 \text{ and } 3,\\ 2,\end{cases} \tag{6.12}$$

where τ_ν as a zero of π_3 satisfies (cf. (5.7))

$$\tau_\nu\left(\tau_\nu^2 + \frac{\delta}{\beta}\tau_\nu\right) - \frac{1}{2}\left(1 + \frac{\alpha}{\beta}\right)\tau_\nu - \frac{1}{2}\frac{\delta}{\beta} = 0. \tag{6.13}$$

Consider first the case $\delta = 0$. Then, by symmetry, $\tau_3 < \tau_2 = 0 < \tau_1$, and (6.12) is trivially true for $\nu = 2$ and easily seen true for $\nu = 1, 3$ in view of (6.13) (for $\delta = 0$). Now moving $|\delta|$ continuously away from zero, positivity ceases to hold the first time we have equality in (6.12) for some ν. Combining this equality with (6.13) then yields $\tau_\nu = -2\delta/\beta$ for some ν, which, reinserted in

(6.13), yields $\delta^2 = \beta(\beta + 2\alpha)/8 =: \delta_2^2$. Thus, positivity holds for all δ with $\delta^2 < \delta_2^2$. Since $\delta_2^2 \geq (\beta - \alpha)^2$ precisely for $\beta \leq 2\alpha$ (assuming α, β admissible), positivity holds for all admissible α, β, δ when $\beta < 2\alpha$, since then the interlacing property holds by Theorem 5.1(a). In the remaining case, $\beta > 2\alpha$, we have positivity if $\delta^2 < \delta_2^2$, which can be verified to be a subregion of the region $\delta^2 < \delta_0^2$ (cf. (5.5)) in which interlacing holds.

Assume now $n \geq 4$. It follows from (4.2) and Theorem 5.1(c) that the Gauss–Kronrod formula under study has the form

$$\int_{-1}^{1} f(t) w^{(-1/2)}(t)\, dt = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sigma_1^* f(1) + \sum_{\mu=2}^{n} \sigma_\mu^* f(\tau_\mu^*) + \sigma_{n+1}^* f(-1),$$

all $f \in \mathbb{P}_{4n-3}$.

Putting here $f(t) = (1 - t^2)g(t)$, and taking note of (4.2) and (4.5), this yields

$$\begin{aligned}\int_{-1}^{1} g(t) w^{(1/2)}(t)\, dt &= \sum_{\nu=1}^{n} \sigma_\nu (1 - \tau_\nu^2) g(\tau_\nu) + \sum_{\mu=2}^{n} \sigma_\mu^* (1 - \tau_\mu^{*2}) g(\tau_\mu^*) \\ &= \sum_{\mu=1}^{n-1} \sigma_{\mu+1}^* (1 - \tau_{\mu+1}^{*2}) g(\bar{\tau}_\mu) + \sum_{\nu=1}^{n} \sigma_\nu (1 - \tau_\nu^2) g(\bar{\tau}_\nu^*),\end{aligned}$$

all $g \in \mathbb{P}_{4n-5}$,

which is precisely the $(2n-1)$-point Gauss–Kronrod formula for $w = w^{(1/2)}$. By uniqueness, (6.10) follows immediately.

To prove (6.11), it suffices to apply (6.2) for $\mu = 1$ and $\mu = n + 1$, noting that $\tau_1^* = 1$, $\tau_{n+1}^* = -1$, making use of (3.8) to evaluate $\pi_n(\pm 1)$, and of (4.2) to obtain $\pi_{n+1}^{*\prime}(\pm 1) = \pm 2\pi_{n-1}^{(1/2)}(\pm 1)$, and finally using (3.9) to evaluate $\pi_{n-1}^{(1/2)}(\pm 1)$ and recalling (3.21). The fact that both σ_1^* and σ_{n+1}^* are positive follows from $|\delta| < \beta - \alpha$ and from

$$\begin{aligned}n(\beta - \alpha \pm \delta) + 2\alpha - \beta \mp \delta &\geq 4(\beta - \alpha \pm \delta) + 2\alpha - \beta \mp \delta \\ &= 3\beta - 2\alpha \pm 3\delta > 3(\beta - \alpha \pm \delta) > 0. \qquad \square\end{aligned}$$

Theorem 6.3. *Consider the weight function $w(t) = w^{(1/2,-1/2)}(t;\ \alpha, \beta, \delta)$, with α, β, δ admissible. Then all weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{(n)*}$ in (5.1) are positive for each $n \geq 1$, except when $n = 2$ and $\beta > 2\alpha$, in which case they are positive if $-(\beta - \alpha) < \delta < \alpha$.*

Specifically, for $n \geq 3$, letting $\tau_\nu^{(n)} = \cos\theta_\nu$ and $\tau_\mu^{(n)*} = \cos\theta_\mu^*$, one has for $\nu = 1, 2, \ldots, n$,

$$\sigma_\nu^{(n)} = \frac{\pi}{2\alpha^2} \frac{\sin^2(n - \frac{1}{2})\theta_\nu}{(1 + \cos\theta_\nu)\left[n - \frac{1}{2} - \frac{\sin(n - \frac{1}{2})\theta_\nu \cos(n - \frac{3}{2})\theta_\nu}{\sin\theta_\nu} + \frac{\beta}{\alpha}\sin^2(n - \frac{1}{2})\theta_\nu\right]}, \tag{6.14}$$

for $\mu = 1, 2, \ldots, n$,

$$\sigma_\mu^{(n)*} = \frac{\pi}{2\alpha^2} \frac{\cos^2(n - \frac{1}{2})\theta_\mu^*}{(1 + \cos\theta_\mu^*)\left[n - \frac{1}{2} + \frac{\sin(n - \frac{3}{2})\theta_\mu^* \cos(n - \frac{1}{2})\theta_\mu^*}{\sin\theta_\mu^*} + \frac{\beta}{\alpha}\cos^2(n - \frac{1}{2})\theta_\mu^*\right]}, \tag{6.15}$$

and for $\mu = n+1$,

$$\sigma_{n+1}^{(n)*} = \frac{\pi}{(\beta-\alpha-\delta)[2n(\beta-\alpha-\delta)+3\alpha-\beta+\delta]}. \tag{6.16}$$

Remark. It is possible to obtain explicit formulae for $\sigma_\nu^{(1)}$, $\sigma_\nu^{(2)}$, and $\sigma_\mu^{(1)*}$, but we will not bother writing them down here.

Proof. For $n = 1, 2$, we verify the conditions in (6.4). When $n = 1$, the inequality in (6.4) follows readily from (4.8)[1] and (3.10). When $n = 2$, we must discuss

$$\pi_3^*(\tau_\nu) \lesseqgtr \pi_3(\tau_\nu), \quad \nu = \begin{cases} 1, \\ 2, \end{cases} \tag{6.17}$$

where τ_ν satisfies $\pi_2(\tau_\nu) = 0$ with (cf. (3.10))

$$\pi_2(t) = t^2 + \tfrac{1}{2}(1+2\delta/\beta)t + \tfrac{1}{2}(\delta-\alpha)/\beta. \tag{6.18}$$

The top inequality in (6.17), by (4.8)[2] and (3.10), turns out to be equivalent to

$$\tau_1 > -\tfrac{1}{2}(1+2\delta/\beta), \tag{6.19}$$

which, by virtue of

$$\pi_2\big(-\tfrac{1}{2}(1+2\delta/\beta)\big) = (\delta-\alpha)/2\beta, \tag{6.20}$$

is certainly true if $\delta = 0$. Assume first $\beta < 2\alpha$, in which case interlacing holds by Theorem 5.3(a). Since the value of π_2 in (6.20) is negative when $\delta < \alpha$, and $\alpha > \beta - \alpha$, we have (6.19), hence $\sigma_1^{(2)} > 0$, for all admissible α, β, δ. The discussion of the lower inequality in (6.17) (for $\nu = 2$) is analogous and leads to the same conclusion. If $\beta > 2\alpha$, one needs to distinguish the cases $\delta > \alpha$ and $\delta < \alpha$. In the former case, since $\delta > 0$, both zeros τ_1 and τ_2 of π_2 are negative and sum up to $-\frac{1}{2}(1+2\delta/\beta)$, by (6.18). Therefore, (6.19) holds for both τ_1 and τ_2, hence $\sigma_1^{(2)} > 0$, but $\sigma_2^{(2)} < 0$. If $\delta < \alpha$, then (6.20) implies as before that $\sigma_1^{(2)} > 0$, $\sigma_2^{(2)} > 0$. Thus we have positivity of both weights if $-(\beta-\alpha) < \delta < \alpha$, which is easily seen to be a subinterval of the interval in (5.10) in which the interlacing property holds.

Positivity for $n \geq 3$ follows as in the proof of Theorem 6.1, and the explicit formulae (6.14), (6.15) are obtained by a procedure entirely analogous to the one used to derive (6.6), (6.7), using the appropriate polynomials π_{n+1}^*, π_n in (4.8) and (3.10), respectively, and such properties as (3.11), (3.2) and (3.16). The expression (6.16) for σ_{n+1}^*, and its positivity, follow similarly as in the proof of (6.11). □

7. Linear divisors

Up until now, we assumed that the divisor ρ in (2.1), (2.2) is a polynomial of *exact* degree 2. We now relax this condition and allow the case of *linear* divisors. Formally, this case is obtained in the limit as $\beta \to 2\alpha$, which yields

$$\rho(t) = \rho(t;\, \alpha, 2\alpha, \delta) = \alpha^2(2\mu t + \mu^2 + 1),$$
$$\mu = \delta/\alpha, \quad \alpha > 0, \quad |\mu| < 1. \tag{7.1}$$

Table 1
Gauss–Kronrod quadrature for the weight functions (7.2).

w	$2^n\pi_n$	π_{n+1}^*	Interlacing	Inclusion	Degree of exactness	
					$\mu \neq 0$	$\mu = 0$
$v^{(-1/2)}$	$2(T_n + \mu T_{n-1})$	$(t^2-1)\pi_{n-1}^{(1/2)}$ $(n \geq 3)$	$n \geq 1$	$n \geq 3$	$4n-2$ $(n \geq 3)$	$4n-1$ $(n \geq 2)$
		$t(t^2-1)+\frac{1}{2}\mu\left(t^2-\frac{3}{4}\right)$ $(n=2)$		$n=2$ and $\mu=0$	7 $(n=2)$	
		$t^2-\frac{3}{4}+\frac{1}{2}\mu t$ $(n=1)$		$n=1$ and $\lvert\mu\rvert \leq \frac{1}{2}$	4 $(n=1)$	5 $(n=1)$
$v^{(1/2)}$	$U_n + \mu U_{n-1}$	$\pi_{n+1}^{(-1/2)}$	$n \geq 1$	$n \geq 1$	$4n$	$4n+1$
$v^{(1/2,-1/2)}$	$W_n + \mu W_{n-1}$	$(t+1)\pi_n^{(-1/2,1/2)}$ $(n \geq 2)$	$n \geq 1$	$n \geq 2$	$4n-1$ $(n \geq 2)$	$4n$ $(n \geq 2)$
		$(t+1)\left(t-\frac{1}{2}\right)+\frac{1}{2}\mu\left(t+\frac{1}{2}\right)$ $(n=1)$		$n=1$ and $\mu \leq 0$	4 $(n=1)$	4 $(n=1)$
$v^{(-1/2,1/2)}$	$V_n + \mu V_{n-1}$	$(t-1)\pi_n^{(1/2,-1/2)}$ $(n \geq 2)$	$n \geq 1$	$n \geq 2$	$4n-1$ $(n \geq 2)$	$4n$ $(n \geq 2)$
		$(t-1)\left(t+\frac{1}{2}\right)+\frac{1}{2}\mu\left(t-\frac{1}{2}\right)$ $(n=1)$		$n=1$ and $\mu \geq 0$	4 $(n=1)$	4 $(n=1)$

Apart from a constant factor, we are thus led to the weight functions

$$v^{(\pm 1/2)}(t) = v^{(\pm 1/2)}(t;\ \mu) = \frac{(1-t^2)^{\pm 1/2}}{2\mu t + \mu^2 + 1},$$
$$v^{(\pm 1/2, \mp 1/2)}(t) = v^{(\pm 1/2, \mp 1/2)}(t;\ \mu) = \frac{(1-t)^{\pm 1/2}(1+t)^{\mp 1/2}}{2\mu t + \mu^2 + 1}. \tag{7.2}$$

The case $\mu = 0$ corresponds to the classical Chebyshev weight functions.

The results of the previous sections, and their proofs, are easily specialized to the case $\beta = 2\alpha$. The resulting orthogonal polynomials, Stieltjes polynomials, interlacing and inclusion properties, and (sharp) degrees of exactness are summarized in Table 1, in this order.

All weights $\sigma_\mu^{(n)*}$ are positive, without exceptions, because of the interlacing property holding for all $n \geqslant 1$. The same turns out to be true for the weights $\sigma_\nu^{(n)}$. The explicit formulae given in Section 6 simplify somewhat (note that they are to be multiplied by α^2 on account of (7.1)); for $w = v^{(1/2)}$ and $n \geqslant 2$ one obtains

$$\sigma_\nu^{(n)} = \frac{\pi}{2} \frac{\sin^2 n\theta_\nu}{n - \dfrac{\sin n\theta_\nu}{\sin \theta_\nu} \cos(n+1)\theta_\nu}, \quad \nu = 1, 2, \ldots, n, \tag{7.3}$$

$$\sigma_\mu^{(n)*} = \frac{\pi}{2} \frac{\cos^2 n\theta_\mu^*}{n + \dfrac{\sin(n+1)\theta_\mu^*}{\sin \theta_\mu^*} \cos n\theta_\mu^*}, \quad \mu = 1, 2, \ldots, n+1, \tag{7.4}$$

whereas for $w = v^{(1/2, -1/2)}$ and $n \geqslant 3$,

$$\sigma_\nu^{(n)} = \frac{\pi}{2} \frac{\sin^2(n-\frac{1}{2})\theta_\nu}{(1+\cos\theta_\nu)\left[n - \frac{1}{2} - \dfrac{\sin(n-\frac{1}{2})\theta_\nu}{\sin\theta_\nu} \cos(n+\frac{1}{2})\theta_\nu\right]}, \quad \nu = 1, 2, \ldots, n, \tag{7.5}$$

$$\sigma_\mu^{(n)*} = \frac{\pi}{2} \frac{\cos^2(n-\frac{1}{2})\theta_\mu^*}{(1+\cos\theta_\mu^*)\left[n - \frac{1}{2} + \dfrac{\sin(n+\frac{1}{2})\theta_\mu^*}{\sin\theta_\mu^*} \cos(n-\frac{1}{2})\theta_\mu^*\right]}, \quad \mu = 1, 2, \ldots, n,$$

$$\sigma_{n+1}^{(n)*} = \frac{\pi}{(1-\mu)[2(1-\mu)n + 1 + \mu]}, \tag{7.6}$$

where θ_ν, θ_μ^* are as defined in Theorems 6.1 and 6.3, respectively. For $w = v^{(-1/2)}$ and $n \geqslant 4$, the weights are obtained as in Theorem 6.2 in terms of the weights $\sigma_\nu^{(n-1)}$, $\sigma_\mu^{(n-1)*}$ in (7.3), (7.4).

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QUADRATURE FORMULAE ON HALF-INFINITE INTERVALS*

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Abstract.

We develop two classes of quadrature rules for integrals extended over the positive real axis, assuming given algebraic behavior of the integrand at the origin and at infinity. Both rules are expressible in terms of Gauss-Jacobi quadratures. Numerical examples are given comparing these rules among themselves and with recently developed quadrature formulae based on Bernstein-type operators.

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1. Introduction.

For integrals extended over the whole real line, whose integrands go to zero like $|x|^{-\beta}$ when $|x| \to \infty$, special (symmetric) quadrature rules have been developed by W. M. Harper [6] and S. Haber [5] some time ago that integrate exactly the product of $(1 + x^2)^{-\beta/2}$ with certain rational functions. Here we treat in a similar spirit integrals over the half-infinite interval $[0, \infty)$ and integrands that have an algebraic singularity at the origin of type x^α, $\alpha > -1$, and behave like $x^{-\beta}$, $\beta > 1$, as $x \to \infty$. We develop two types of quadrature formulae – one having maximum polynomial degree of exactness, the other maximum "rational" degree of exactness. The former, already considered by R. Kumar and M. K. Jain [7], are subject to a severe limitation on the number of quadrature points allowed, whereas the latter are free from any such limitation. We show that both types of formulae can be reduced to Gaussian quadratures relative to appropriate Jacobi weight functions, and hence can be generated by standard mathematical software. Numerical examples are given, comparing these quadrature rules among themselves, and also with alternative rules based on Bernstein-type operators, recently developed by B. Della Vecchia [3].

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2. Formulae of maximum algebraic degree of exactness.

The object in this section is to find a quadrature formula

$$\int_0^\infty f(x)\frac{x^\alpha}{(1+x)^\beta}dx = \sum_{k=1}^n a_k f(x_k) + r_n(f) \tag{2.1}$$

of Gaussian type, that is, such that $r_n(f) = 0$ whenever $f \in \boldsymbol{P}_{2n-1}$, the class of polynomials of degree $\leq 2n-1$. To assure integrability, one has to assume that

$$\alpha > -1, \quad 2n < \beta - \alpha. \tag{2.2}$$

Thus, the formula (2.1) will be applicable only if $\beta > 0$ is relatively large.

The requirement that (2.1) be exact for $f(x) = x^\lambda$, $\lambda = 0, 1, \ldots, 2n-1$, translates, via the transformation of variables

$$\frac{1-x}{1+x} = t, \quad x = \frac{1-t}{1+t}, \tag{2.3}$$

into the condition that

$$\int_{-1}^1 \left[\frac{1-t}{1+t}\right]^{\lambda+\alpha}\left[\frac{1+t}{2}\right]^\beta \frac{2dt}{(1+t)^2} = \sum_{k=1}^n a_k x_k^\lambda, \quad \lambda = 0, 1, \ldots, 2n-1,$$

or, equivalently, that

$$\int_{-1}^1 (1-t)^\lambda (1+t)^{2n-1-\lambda}\cdot(1-t)^\alpha(1+t)^{\beta-\alpha-2n-1}dt \tag{2.4}$$

$$= 2^{\beta-1}\sum_{k=1}^n [a_k(1+t_k)^{1-2n}]\cdot(1-t_k)^\lambda(1+t_k)^{2n-1-\lambda}, \quad \lambda = 0, 1, \ldots, 2n-1.$$

Here we have set, in conformity with (2.3),

$$\frac{1-x_k}{1+x_k} = t_k, \quad x_k = \frac{1-t_k}{1+t_k}. \tag{2.5}$$

Since $\{(1-t)^\lambda(1+t)^{2n-1-\lambda}: \lambda = 0, 1, \ldots, 2n-1\}$ forms a basis in $\boldsymbol{P}_{2n-1}$, it follows from (2.4) that

$$t_k = \tau_k^J, \quad 2^{\beta-1}(1+t_k)^{1-2n}a_k = \omega_k^J, \quad k = 1, 2, \ldots, n, \tag{2.6}$$

where

$$\tau_k^J = \tau_k^{(n)}(\alpha, \beta-\alpha-2n-1), \quad \omega_k^J = \omega_k^{(n)}(\alpha, \beta-\alpha-2n-1) \tag{2.7}$$

are the n-point Gaussian nodes and weights relative to the Jacobi weight function with parameters α and $\beta - \alpha - 2n - 1$. Note, by assumption (2.2), that both parameters are larger than -1, as required by the theory of Gauss-Jacobi quadrature. (This is not the case with another relationship to Jacobi polynomials, noted in [7,

Eq. (12)], which involves parameters $-\beta$ and α.) Thus, combining (2.5) and (2.6), we obtain

$$x_k = \frac{1-\tau_k^J}{1+\tau_k^J}, \quad a_k = \frac{(1+\tau_k^J)^{2n-1}}{2^{\beta-1}}\omega_k^J, \quad k = 1,2,\ldots,n, \tag{2.8}$$

for the desired abscissae and weights in the quadrature formula (2.1).

3. Formulae of maximum "rational" degree of exactness.

For a more viable alternative to (2.1), not subject to the second condition in (2.2), we now require the quadrature rule

$$\int_0^\infty f(x)x^\alpha dx = \sum_{k=1}^n A_k f(X_k) + R_n(f) \tag{3.1}$$

to be exact (i.e., $R_n(f) = 0$) whenever

$$f(x) = \frac{1}{(1+x)^{\beta+\lambda}}, \quad \lambda = 0,1,\ldots,2n-1. \tag{3.2}$$

Here the only assumptions needed for integrability are

$$\alpha > -1, \quad \beta - \alpha > 1. \tag{3.3}$$

In the case $\alpha = 0$, $\beta = 2$, such a quadrature rule has already been suggested in [8, p. 52]; see also [2, pp. 225–226].

It is easy to see that exactness of (3.1) for the "rational" functions (3.2) is equivalent to

$$\int_0^\infty \frac{g(x)x^\alpha}{(1+x)^{\beta+2n-1}}dx = \sum_{k=1}^n A_k \frac{g(X_k)}{(1+X_k)^{\beta+2n-1}} \tag{3.4}$$

for

$$g(x) = x^\lambda, \quad \lambda = 0,1,\ldots,2n-1. \tag{3.5}$$

Indeed, putting $f(x) = g(x)/(1+x)^{\beta+2n-1}$ in (3.1), our exactness requirement implies (3.4) for $g(x) = (1+x)^{2n-\lambda-1}$, $\lambda = 0,1,\ldots,2n-1$, which is equivalent to (3.4), (3.5). Conversely, if (3.4), (3.5) holds, it suffices to put $g(x) = (1+x)^{2n-\lambda-1}$ in (3.4) to get exactness of (3.1) for (3.2).

Now using again the transformation of variables (2.3), and

$$\frac{1-X_k}{1+X_k} = T_k, \quad X_k = \frac{1-T_k}{1+T_k} \tag{3.6}$$

in place of (2.5), we get from (3.4), (3.5)

$$\int_{-1}^{1}\left[\frac{1-t}{1+t}\right]^{\lambda+\alpha}\left[\frac{1+t}{2}\right]^{\beta+2n-1}\frac{2}{(1+t)^2}\,dt$$

$$=\sum_{k=1}^{n}A_k\frac{X_k^{\lambda}}{(1+X_k)^{\beta+2n-1}},\quad \lambda=0,1,\ldots,2n-1,$$

that is,

$$\int_{-1}^{1}(1-t)^{\lambda}(1+t)^{2n-1-\lambda}\cdot(1-t)^{\alpha}(1+t)^{\beta-\alpha-2}dt$$

$$=\sum_{k=1}^{n}\tfrac{1}{2}A_k(1+T_k)^{\beta}\cdot(1-T_k)^{\lambda}(1+T_k)^{2n-1-\lambda},\quad \lambda=0,1,\ldots,2n-1.$$

As before in §2, this implies

$$T_k=T_k^J,\quad \tfrac{1}{2}A_k(1+T_k)^{\beta}=\Omega_k^J, \tag{3.7}$$

where

$$T_k^J=\tau_k^{(n)}(\alpha,\beta-\alpha-2),\quad \Omega_k^J=\omega_k^{(n)}(\alpha,\beta-\alpha-2) \tag{3.8}$$

are the n-point Jacobi nodes and weights corresponding to parameters α and $\beta-\alpha-2$. Hence, in (3.1),

$$X_k=\frac{1-T_k^J}{1+T_k^J},\quad A_k=\frac{2\Omega_k^J}{(1+T_k^J)^{\beta}}. \tag{3.9}$$

In contrast to the quadrature rule of §2, it is now meaningful to discuss convergence of the rule (3.1) as $n\to\infty$. To do this, let R_n^J denote the remainder term in the Gauss-Jacobi formula with parameters α and $\beta-\alpha-2$,

$$\int_{-1}^{1}g(t)(1-t)^{\alpha}(1+t)^{\beta-\alpha-2}dt=\sum_{k=1}^{n}\Omega_k^J g(T_k^J)+R_n^J(g). \tag{3.10}$$

Then an easy calculation shows that the remainder R_n in (3.1) is given by

$$R_n(f)=2R_n^J(h),\quad h(t)=(1+t)^{-\beta}f\left[\frac{1-t}{1+t}\right]. \tag{3.11}$$

Now typically,

$$f(x)=(1+x)^{-\beta}F(x), \tag{3.12}$$

where F is a "nice" function. In this case,

$$h(t)=2^{-\beta}F\left[\frac{1-t}{1+t}\right],\quad -1<t<1. \tag{3.13}$$

Therefore, convergence $R_n^J(h)\to 0$ in (3.10), hence $R_n(f)\to 0$ in (3.1), is assured

if h in (3.13) is continuous – in fact, bounded Riemann-integrable – on the interval $[-1,1]$, i.e., F is continuous on the closed interval $[0,\infty]$. Moreover, if $h(t)$ is analytic in a disk $|t|<r$, where $r>1$, hence F analytic outside the disk with center at $-\dfrac{r^2+1}{r^2-1}$ and radius $\dfrac{2r}{r^2-1}$, then convergence is exponentially fast, the rate of convergence being larger the larger $r>1$ (cf. [4, Eq. (A.1)].

It is also possible to combine the two approaches in §§2–3 and seek a quadrature formula

$$\int_0^\infty f(x)\frac{x^\alpha}{(1+x)^\beta}dx = \sum_{k=1}^{n} b_k f(y_k) + s_n(f) \tag{3.14}$$

for which, given an integer m with $0 \le m < 2n$, one has $s_n(f)=0$ whenever

$$f(x) = \begin{cases} x^\lambda, & \lambda = 0,1,\dots,2n-m-1, \\ \dfrac{1}{(1+x)^{\lambda+1}}, & \lambda = 0,1,\dots,m-1. \end{cases} \tag{3.15}$$

Here one needs to assume $\alpha > -1$ and $2n < \beta - \alpha + m$. To construct such formulae, however, seems to require different techniques (the solution of nonlinear equations), and we will not pursue this further. Note that the limit cases $m=0$ and $m=2n-1$ correspond to the quadrature rules (2.1) and (3.1), respectively.

4. Formulae based on Bernstein-type operators.

The linear positive operator of Bernstein type,

$$(L_n f)(x) = (1+x)^{-n}\sum_{k=0}^{n}\binom{n}{k}x^k f\left[\frac{k}{n-k+1}\right], \tag{4.1}$$

was introduced by G. Bleimann, P. L. Butzer and L. Hahn [1] for approximating continuous functions on $[0,\infty)$, and was used by B. Della Vecchia [3] to construct a quadrature rule which is exact for the function $(1+x)^{-\beta}$, $\beta>1$. Slightly generalizing her approach, we integrate $(L_n g)(x)\cdot x^\alpha(1+x)^{-\beta}$ from 0 to ∞, where $g(x)=f(x)(1+x)^\beta$, to get a quadrature rule for $\int_0^\infty x^\alpha f(x)dx$. This rule is again exact when f is the function $(1+x)^{-\beta}$, since it then takes the form $\int_0^\infty (L_n 1)(x)\cdot x^\alpha(1+x)^{-\beta}dx = \int_0^\infty x^\alpha(1+x)^{-\beta}dx$. As before, we assume that

$$\alpha > -1, \quad \beta - \alpha > 1. \tag{4.2}$$

To conform with the formulae obtained in the previous sections, we replace n in (4.1) by $n-1$, and denote the quadrature nodes by

$$\xi_k = \frac{k-1}{n-k+1}, \quad k = 1,2,\dots,n. \tag{4.3}$$

The quadrature rule then becomes

$$\int_0^\infty x^\alpha f(x)dx = \sum_{k=1}^{n} \alpha_k f(\xi_k) + \rho_n(f), \tag{4.4}$$

$$\alpha_k = \binom{n-1}{k-1}\left[\frac{n}{n-k+1}\right]^\beta \frac{\Gamma(n+\beta-\alpha-k-1)}{\Gamma(n+\beta-1)}\Gamma(\alpha+k).$$

The weights α_k are easily generated recursively by

$$\alpha_1 = \frac{\Gamma(n+\beta-\alpha-2)}{\Gamma(n+\beta-1)}\Gamma(\alpha+1), \tag{4.5}$$

$$\alpha_k = \frac{1+\dfrac{\alpha}{k-1}}{1+\dfrac{\beta-\alpha-2}{n-k+1}}\left[\frac{n-k+2}{n-k+1}\right]^\beta \alpha_{k-1}, \quad k = 2,3,\ldots,n,$$

where, for large n, one first computes $\ln \alpha_1$, and then α_1 by exponentiation, to avoid machine overflow.

The principal virtue of the quadrature rule (4.4) seems to be its simplicity and explicit form, its major drawback slow convergence. Known error estimates (for $\alpha = 0$) due to B. Della Vecchia [3] indeed exhibit a convergence order of $O(n^{-1})$ at best, and so do our examples in §5.

5. Examples.

In this section we illustrate the performance of the three quadrature schemes of §§2–4 on a number of examples. All computations were carried out in double precision (ca. 29 decimal digits) on the Cyber 205.

EXAMPLE 1. $\displaystyle\int_0^\infty \frac{x^{1/2}\tanh x}{(1+x)^{12.5}}dx = .00340388967504569561787042285.$

Here $\alpha = \frac{1}{2}$, $\beta = 12.5$, so that by (2.2) the Gauss formula (2.1) exists only for $n = 1(1)5$. The associated relative errors are shown in the second column of Table 5.1. (Integers in parentheses denote decimal exponents.)

TABLE 5.1. *Relative errors of the quadrature rules* (2.1), (3.1), (4.4) *for Example* 1.

n	(2.1)	n	(3.1)	n	(3.1)	n	(4.4)
1	2.79(−2)	5	1.38(−6)	30	1.06(−21)	200	2.12(−3)
2	2.35(−3)	10	5.08(−11)	35	2.10(−23)	400	1.06(−3)
3	1.64(−4)	15	2.63(−15)	40	3.32(−25)	800	5.26(−4)
4	9.14(−5)	20	7.98(−18)	45	1.10(−26)	1600	2.62(−4)
5	3.91(−5)	25	1.94(−19)	–	–	3200	1.31(−4)

Since $F(x) = \tanh x$ (cf. (3.12)) is continuous on the closed interval $[0, \infty]$, the quadrature formula (3.1) converges as $n \to \infty$, and Table 5.1 shows a rather satisfactory speed of convergence. The numerical value of the integral shown above indeed is the numerical limit observed as (3.1) is applied with increasing values of n.

As expected, the quadrature rule (4.4) based on a Bernstein-type operator converges rather slowly, with order $O(n^{-1})$, as is evident from the last column of Table 5.1. Applying the ε-algorithm to the first 200 approximations reduces the error by only one decimal order of accuracy.

We have repeated Example 1 with $\alpha = 0$, $\beta = 1.1$ and obtained similar results for (3.1) except that convergence is considerably slower. It now takes $n = 120$ in (3.1) to get a 16S value 9.539866086478899 for the integral; the smallest error in (4.4) is 3.57(−5) (for $n = 3200$).

EXAMPLE 2. $I(r) = \int_0^\infty \frac{x^{-1/2}}{(x - c_r)^4 - d_r^4} \frac{dx}{(1+x)^{12.5}}$, where $c_r = -(r^2 + 1)/(r^2 - 1)$, $d_r = 2r/(r^2 - 1)$, $r > 1$.

This example is chosen to illustrate how the rate of convergence of (3.1) depends on the analyticity properties of the function F in (3.12), that is, in our case, of the function

$$F(x) = \frac{1}{(x - c_r)^4 - d_r^4}. \tag{5.1}$$

This function has exactly four poles, respectively at $c_r \pm d_r$ and $c_r \pm id_r$, so that F is analytic outside the circle with center at c_r and radius $d_r (< |c_r|)$. According to the discussion following Eq. (3.13), the rate of convergence of (3.1) should therefore increase with r. This is confirmed in Table 5.2, where comparison is made also with the other two quadrature schemes, (2.1) and (4.4). Table 5.3 gives the exact values of $I(r)$ to 26 significant digits, as determined by the quadrature rule (3.1).

TABLE 5.2. *Relative errors of* (2.1), (3.1), (4.4) *for Example* 2 *with* $r = 1.1, 1.5, 2, 5$.

r	n	(2.1)	n	(3.1)	n	(4.4)	r	n	(2.1)	n	(3.1)	n	(4.4)
1.1	1	2.38(−1)	10	1.49(−5)	100	2.89(−2)	2.0	1	3.31(−2)	6	1.53(−9)	100	3.49(−3)
	2	9.90(−2)	20	1.48(−9)	200	1.46(−2)		2	3.44(−3)	9	2.85(−13)	200	1.75(−3)
	3	5.54(−2)	30	1.80(−13)	400	7.31(−3)		3	7.49(−4)	12	6.85(−17)	400	8.79(−4)
	4	3.80(−2)	40	2.33(−17)	800	3.66(−3)		4	2.76(−4)	15	1.88(−20)	800	4.40(−4)
	5	3.06(−2)	50	3.10(−21)	1600	1.83(−3)		5	1.56(−4)	18	5.57(−24)	1600	2.20(−4)
	6	2.86(−2)	60	4.23(−25)	3200	9.17(−4)		6	1.30(−4)	21	2.89(−27)	3200	1.10(−4)
1.5	1	5.45(−2)	5	1.80(−6)	100	5.65(−3)	5.0	1	2.81(−2)	2	3.00(−5)	100	3.03(−3)
	2	9.05(−3)	10	4.76(−11)	200	2.84(−3)		2	1.90(−3)	4	5.76(−10)	200	1.52(−3)
	3	2.75(−3)	15	2.02(−15)	400	1.43(−3)		3	2.67(−4)	6	2.83(−14)	400	7.60(−4)
	4	1.27(−3)	20	1.03(−19)	800	7.14(−4)		4	7.02(−5)	8	1.33(−18)	800	3.81(−4)
	5	8.15(−4)	25	5.70(−24)	1600	3.57(−4)		5	3.22(−5)	10	7.22(−23)	1600	1.90(−4)
	6	7.06(−4)	30	1.28(−27)	3200	1.79(−4)		6	2.50(−5)	12	6.05(−27)	3200	9.52(−5)

TABLE 5.3. *Exact values of the integral in Example 2.*

r	$I(r)$
1.1	.00156342765157602865464464288
1.5	.03460731089175967793658123 24
2.0	.09842746016775243696422787 5
5.0	.33387359634951902103279770 4

EXAMPLE 3. $\int_0^\infty \frac{x^{-1/2}}{(1+x)^{5/4}} e^{-x}\cos x\,dx = 1.13781186339938588294558 28.$

The function $F(x) = e^{-x}\cos x$ of this example is no longer analytic at ∞, as was the case in Example 2, and the singularities at $x = 0$ and $x = -1$ are more severe than those in Example 1. These are probably the reasons why (3.1) now converges much more slowly than in the previous examples. The relative errors of (3.1), along with those of (4.4), are shown in Table 5.4.

TABLE 5.4. *Relative errors of* (3.1), (4.4) *for Example* 3.

n	(3.1)	n	(4.4)
40	8.34(−9)	100	7.40(−3)
80	9.90(−14)	200	3.69(−3)
120	8.94(−17)	400	1.85(−3)
160	3.04(−20)	800	9.23(−4)
200	6.99(−23)	1600	4.61(−4)
240	8.60(−26)	3200	2.31(−4)

Since $\alpha = -\frac{1}{2}$, $\beta = \frac{5}{4}$, the second inequality in (2.2) is violated for $n \geq 1$, so that there are no Gaussian rules (2.1) for this example.

EXAMPLE 4. $I(\omega) = \frac{\pi}{\omega}\int_0^\infty \frac{x^{-1/2}}{(1+x)^{5/4}} \frac{dx}{1+\omega^2(x-1)^2}, \quad \omega > 0.$

The function

$$F(x) = \frac{\pi}{\omega}\frac{1}{1+\omega^2(x-1)^2} \tag{5.2}$$

in this example has poles at $x = 1 \pm i/\omega$, which approach the point 1 on the real axis as $\omega \to \infty$. (The function is normalized to have unit integral over the whole real line; since it has a sharp peak at $x = 1$ when ω is large, it may be thought of as an approximation to the Dirac delta function centered at 1.) Naturally, our quadrature rule (3.1) will have increasing difficulty converging, as ω becomes large. This can be seen from the relative errors displayed in Table 5.5. Strangely enough, the convergence of (4.4) – slow, to be sure – is relatively unaffected by the value of ω and indeed

accelerates a little bit as ω increases! The true answers for $\omega = .5, 1, 2.5, 5$, furnished by (3.1) for n sufficiently large, are shown in Table 5.6.

TABLE 5.5. *Relative errors of* (3.1), (4.4) *for Example* 4.

ω	n	(3.1)	n	(4.4)	ω	n	(3.1)	n	(4.4)
.5	10	4.97(−6)	100	4.22(−3)	2.5	30	1.02(−5)	100	2.07(−3)
	20	1.49(−10)	200	2.10(−3)		60	3.63(−11)	200	1.03(−3)
	30	9.75(−15)	400	1.05(−3)		90	1.58(−15)	400	5.16(−4)
	40	3.55(−19)	800	5.24(−4)		120	1.71(−20)	800	2.58(−4)
	50	1.03(−23)	1600	2.62(−4)		150	7.43(−26)	1600	1.29(−4)
1.0	15	3.25(−6)	100	3.25(−3)	5.0	60	2.63(−6)	100	1.72(−3)
	30	2.19(−11)	200	1.62(−3)		120	7.16(−11)	200	8.58(−4)
	45	3.80(−16)	400	8.09(−4)		180	5.14(−16)	400	4.28(−4)
	60	2.96(−21)	800	4.04(−4)		240	8.14(−22)	800	2.14(−4)
	75	4.91(−27)	1600	2.02(−4)		300	2.45(−26)	1600	1.07(−4)

TABLE 5.6. *Exact values of the integral in Example* 4.

ω	$I(\omega)$
.5	10.7185761829848814375380337
1.0	3.9449597795274933486744356
2.5	.7424115778662792308324285 2
5.0	.1821547990990704851166885 65

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On the computation of generalized Fermi–Dirac and Bose–Einstein integrals *

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Gauss-type quadrature formulae based on rational functions are proposed to evaluate generalized Fermi–Dirac and Bose–Einstein integrals to high accuracy. The method is compared with recent quadrature methods of B. Pichon and R.P. Sagar.

1. Introduction

The computation of the generalized Fermi–Dirac integrals

$$F_k(\eta, \theta) = \int_0^\infty \frac{x^k \sqrt{1 + \frac{1}{2}\theta x}}{e^{-\eta + x} + 1}\, dx,$$
$$\theta \geqslant 0, \quad \eta \in \mathbb{R}, \tag{1.1}$$

where $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, has been the subject of two recent communications [1,2]. The former proposes Gauss–Laguerre quadrature (with weight function $x^k e^{-ax}$) after dividing and multiplying the integrand by e^{-ax} with $a > 0$ suitably chosen, the latter a "Gauss–Fermi" quadrature (with weight function $x^k(e^x + 1)^{-1}$), after dividing and multiplying by $(e^x + 1)^{-1}$. Both methods disregard the major obstacle to rapid convergence (when θ is relatively small), namely the poles at

$$x = \eta \pm (2\nu - 1)i\pi, \quad \nu = 1, 2, 3, \ldots. \tag{1.2}$$

In this note we write

$$F_k(\eta, \theta) = \int_0^\infty f(x)\, x^k\, e^{-x}\, dx, \tag{1.3}$$

with

$$f(x) = \frac{\sqrt{1 + \frac{1}{2}\theta x}}{e^{-\eta} + e^{-x}}, \tag{1.4}$$

and propose a quadrature rule of the form

$$\int_0^\infty g(x)\, x^k\, e^{-x}\, dx \approx \sum_{r=1}^{n} w_r g(x_r), \tag{1.5}$$

which is exact for the n pairs of rational functions

$$g(x) = (1 + \zeta_\nu x)^{-1}, \qquad g(x) = (1 + \xi_\nu^* x)^{-1},$$
$$\nu = 1, 2, \ldots, n, \tag{1.6}$$

where

$$\zeta_\nu = -\frac{1}{\eta + (2\nu - 1)i\pi} \tag{1.7}$$

and the asterisk means complex conjugation. In this way, we take into account the first n paris of

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(conjugate complex) poles in eq. (1.2). Thus,

$$F_k(\eta, \theta) \approx \sum_{r=1}^{n} w_r f(x_r), \tag{1.8}$$

where the quadrature nodes and weights depend on n, k and η,

$$x_r = x_r^{(n)}(k, \eta), \qquad w_r = w_r^{(n)}(k, \eta). \tag{1.9}$$

An integral similar to (1.1), but arising from Bose–Einstein distributions, is

$$G_k(\eta, \theta) = \int_0^\infty \frac{x^k \sqrt{1 + \frac{1}{2}\theta x}}{e^{-\eta + x} - 1}\, dx, \quad \theta \geq 0, \quad \eta \leq 0, \tag{1.10}$$

for which analytic methods of evaluation, again for $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, were discussed in the appendix of ref. [1]. Here we develop a quadrature method analogous to the one proposed above for $F_k(\eta, \theta)$ and compare it with other quadrature methods in the spirit of refs. [1,2].

It will be seen that the choice of quadratures proposed here significantly improves the accuracy of the results at the expense of requiring a sequence of quadrature rules to be generated for each k and η. Methods for generating such "rational Gauss" formulae will be briefly described in section 2. In section 3 we present numerical results and compare our method with those in refs. [1,2].

2. Gauss formulae for rational functions

2.1. Fermi–Dirac integrals

Let $\zeta_\nu = \xi_\nu + i\eta_\nu$, that is (cf. (1.7)),

$$\begin{aligned} \xi_\nu &= -\frac{\eta}{\eta^2 + (2\nu - 1)^2 \pi^2}, \\ \eta_\nu &= \frac{(2\nu - 1)\pi}{\eta^2 + (2\nu - 1)^2 \pi^2}, \\ \nu &= 1, \ldots, n, \end{aligned} \tag{2.1}$$

and define

$$\omega_{2n}(x) = \prod_{\nu=1}^{n} \left[(1 + \xi_\nu x)^2 + \eta_\nu^2 x^2 \right]. \tag{2.2}$$

Then (1.5) is exact for the rational functions in (1.6) precisely if

$$x_r = x_r^G, \qquad w_r = w_r^G \omega_{2n}(x_r^G), \tag{2.3}$$

where x_r^G, w_r^G are the Gauss nodes and weights for the weight function $x^k e^{-x}/\omega_{2n}(x)$:

$$\begin{aligned} &\int_0^\infty p(x) \frac{x^k e^{-x}}{\omega_{2n}(x)}\, dx \\ &\quad = \sum_{r=1}^{n} w_r^G p(x_r^G), \quad \text{all } p \in \mathbb{P}_{2n-1} \end{aligned} \tag{2.4}$$

(cf., e.g., ref. [3, Theorem 1.1 with $m = 2n$]). The orthogonal polynomials required for (2.4) can be generated, similarly as in ref. [2], by a discretized Stieltjes procedure. It is generally more efficient, however, to use a partial fraction decomposition of $[\omega_{2n}(x)]^{-1}$ and construct special Gauss formulae for each partial fraction prior to using the Stieltjes algorithm. This results in a finite algorithm, whereas the discretized Stieltjes procedure requires iteration. On the other hand, it may happen that the partial fractions involve large coefficients with varying signs, which will cause serious cancellation errors in the generation of the desired (rational) Gauss formulae. For details we refer to ref. [3].

2.2. Bose–Einstein integrals

For the integral (1.10), it is convenient to write

$$G_k(\eta, \theta) = \int_0^\infty f(x)\, x^{k-1} e^{-x}\, dx, \tag{2.5}$$

with

$$f(x) = \frac{x}{e^{-\eta} - e^{-x}} \sqrt{1 + \tfrac{1}{2}\theta x}\,. \tag{2.6}$$

By splitting off a factor x, we insure that $f(x)$ remains regular as $x \to 0$ even when $\eta = 0$. The poles of f are now at

$$x = \eta \pm 2\nu i\pi, \quad \nu = 0, 1, 2, \ldots, \tag{2.7}$$

which suggests letting

$$\zeta_\nu = -\frac{1}{\eta + 2\nu i\pi} \tag{2.8}$$

and proceeding similarly as in (1.5)–(1.7), except that k is to be replaced by $k-1$ in (1.5). The appropriate rational Gauss formulae (cf. ref. [3, Theorem 1.1 with $m = 2n-1$]) are then constructed similarly as in section 2.1, with

$$\xi_\nu = -\frac{\eta}{\eta^2 + 4\nu^2\pi^2}, \qquad \eta_\nu = \frac{2\nu\pi}{\eta^2 + 4\nu^2\pi^2}, \quad \nu = 0, 1, 2, \ldots, n-1, \tag{2.9}$$

and (2.4) replaced by

$$\int_0^\infty p(x)\,\frac{x^{k-1}\,e^{-x}}{\omega_{2n-1}(x)}\,dx = \sum_{r=1}^{n} w_r^G p(x_r^G), \quad \text{all } p \in \mathbb{P}_{2n-1}, \tag{2.10}$$

where ω_{2n-1} is defined by

$$\omega_{2n-1}(x) = (1+\xi_0 x)\prod_{\nu=1}^{n-1}\left[(1+\xi_\nu x)^2 + \eta_\nu^2 x^2\right]. \tag{2.11}$$

3. Numerical results

All computations reported in this section were carried out in both single and double precision on the Cyber 205, which allows for precisions of approximately 14 and 28 decimal digits, respectively. Unless stated otherwise, our goal was to produce results with relative errors $\le \frac{1}{2}\times 10^{-10}$ in single precision, and $\le \frac{1}{2}\times 10^{-25}$ in double precision.

3.1. Fermi–Dirac integrals

For purposes of identification, we denote our method (1.8), (1.4), (2.3) by GR(n) (n-point Gauss Rational). The method in ref. [2], i.e.,

$$F_k(\eta,\theta) = \int_0^\infty f_1(x)\,\frac{x^k}{e^x+1}\,dx \approx \sum_{r=1}^{n} w_r^F f_1(x_r^F),$$

$$f_1(x) = \frac{\sqrt{1+\frac{1}{2}\theta x}}{e^{-\eta+x}+1}(e^x+1), \tag{3.1}$$

we denote by GF(n) (n-point Gauss–Fermi), while GL(n) (n-point Gauss–Laguerre) will refer to

$$F_k(\eta,\theta) = \int_0^\infty f(x)\,x^k\,e^{-x}\,dx \approx \sum_{r=1}^{n} w_r^L f(x_r^L) \tag{3.2}$$

(with f as in (1.4)), which is the case $a=1$ of ref. [1]. The first 40 recursion coefficients for the orthogonal polynomials required in (3.1) are tabulated to 19 significant digits in ref. [2, table 1] for $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$. We have recomputed them to 25 digits and observed complete agreement to 19 digits (with the exception of occasional discrepancies of one unit in the last digit). Contrary to ref. [2], we computed the Gauss formulae from the respective Jacobi matrix via eigenvalue techniques (cf. refs. [4; 5, §6]).

All numerical examples in ref. [2] use $\theta = 1\times 10^{-4}$, a comfortably small value that puts the square root singularity of the integrand in (1.1) at -2×10^4, sufficiently far away from the interval of integration to have any appreciable effect on the convergence properties of quadrature schemes. For ease of comparison, we use the

Table 1
Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = -1$ and $\theta = 1\times 10^{-4}$.

k	n	GR(n)	GF(n)	GL(n)
$\frac{1}{2}$	5	8.1 (−9)	8.4(−5)	5.6(−5)
	10	5.9(−18)	2.7(−7)	1.6(−7)
	15	1.5(−25)	6.5(−9)	4.1(−9)
$\frac{3}{2}$	5	2.5 (−8)	1.3(−4)	9.5(−5)
	10	3.1(−17)	8.2(−7)	5.6(−7)
	15	1.6(−27)	1.5(−8)	1.1(−8)
$\frac{5}{2}$	5	5.6 (−8)	9.8(−5)	7.3(−5)
	10	1.1(−16)	7.7(−7)	5.7(−7)
	15	3.2(−25)	9.9(−9)	7.8(−9)

Table 2
Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = 1$ and $\theta = 1 \times 10^{-4}$.

k	n	GR(n)	GF(n)	GL(n)
$\frac{1}{2}$	5	2.1 (−8)	3.7(−4)	6.3(−4)
	10	1.7(−17)	7.4(−6)	1.5(−5)
	15	1.2(−25)	4.4(−7)	7.7(−7)
$\frac{3}{2}$	5	5.6 (−8)	4.7(−4)	9.5(−4)
	10	7.7(−17)	4.4(−6)	4.8(−6)
	15	2.4(−25)	2.7(−7)	6.7(−7)
$\frac{5}{2}$	5	1.1 (−7)	1.9(−5)	1.6(−4)
	10	2.5(−16)	1.3(−5)	2.4(−5)
	15	5.0(−26)	5.2(−7)	8.3(−7)

same value of θ in most of our examples, but experiment also with significantly larger values. Tables 1 and 2 are the analogues of tables 3 and 4 of ref. [2], showing relative errors of the three above quadrature methods for $\eta = -1$ and $\eta = 1$, respectively. As can be seen, GF and GL are very comparable in accuracy, in contrast to GR, which converges incomparably faster. The accuracy obtained with 15 quadrature points in the two former schemes is almost (if $\eta = -1$) or actually (if $\eta = 1$) achieved with 5 points in the latter, and considerably surpassed (not shown in the tables) when $n = 6$.

Table 3
Exact values of Fermi–Dirac integrals.

k	η	$F_k(\eta, 10^{-4})$
$\frac{1}{2}$	−1	0.29051241701949266261676 42
$\frac{3}{2}$	−1	0.46087845417799195535347 58
$\frac{5}{2}$	−1	1.18607350107575578398272 6
$\frac{1}{2}$	1	1.39644182034911533960636 2
$\frac{3}{2}$	1	2.66187327910715013811245 6
$\frac{5}{2}$	1	7.62725609565344763290499 8

The exact values to 25 digits (taken to be the limit values observed with our method) are given in table 3.

For convenience to the reader, and to illustrate the differences in the three quadrature rules, we list these in table 4 for $n = 5$, $k = \frac{1}{2}$ and $\eta = -1$. It can be seen that GR(5) has significantly smaller nodes than either of GL(5) and GF(5), presumably because of the "pull" exerted by the poles (1.2) in the complex plane located on the vertical line with real part $\eta = -1$. As this line is moved to the right, the nodes of GR(5) follow along and indeed become all larger than those of GL(5) and GF(5) by the time $\eta = 15$.

Convergence of the quadrature rule (1.8) speeds up as η is made larger negative, since the

Table 4
Nodes and weights of the three quadrature rules GF(n), GL(n), GR(n) for $n = 5$, $k = \frac{1}{2}$ and $\eta = -1$.

	nodes	weights
GF(5)	4.85328285405254890204160 7(−1)	2.52809318263459080871402 7(−1)
	1.87396691632534234315904 4 (0)	3.33446223446954928545794 5(−1)
	4.21586238502131046221617 5 (0)	8.69187357847713414475412 0(−2)
	7.84656073687659968502251 7 (0)	4.88428503383712745161271 2(−3)
	1.35530574790110437510801 6 (1)	3.53326240785289959577356 3(−5)
GL(5)	4.31398807147851484447134 2(−1)	3.70450570007458506324368 5(−1)
	1.75975369842369642857390 3 (0)	4.12584373769452882100027 0(−1)
	4.10446536282831498999195 3 (0)	9.77798200531807029913924 9(−2)
	7.74670377954255707088229 2 (0)	5.37341534117198651399474 4(−3)
	1.34576783520575800261047 2 (1)	3.87462814939357193010687 3(−5)
GR(5)	3.12639858745048921232677 4(−1)	2.55607580790689403284817 8(−1)
	1.25582574383047931396594 8 (0)	4.05916167492284748338682 0(−1)
	2.90086600433533730205035 6 (0)	1.92457758693324545374355 2(−1)
	5.48165947377484347146421 5 (0)	3.11315809868256673061915 7(−2)
	9.62440682964173576740457 3 (0)	1.11382962779749884911700 4(−3)

poles (1.2) then move further away from the interval of integration. For example, when $k = \frac{1}{2}$, double-precision accuracy $\approx 10^{-25}$ is attained with $n = 14$ for $\eta = -10$, with $n = 11$ for $\eta = -50$, and with $n = 9$ for $\eta = -100$. It is important, however, that the discretized Stieltjes procedure be used for constructing the quadrature rules in question, since the method of partial fraction decomposition gradually loses accuracy because of the cancellation problem mentioned at the end of section 2.1.

The case of large positive η is considerably more difficult: Not only is it harder to generate the rational Gauss formulae, but their convergence also slows down. When $\eta = 10$ (and $k = \frac{1}{2}$), double-precision accuracy 10^{-25} can still be attained with $n = 17$, but for $\eta = 50$, we obtain only 12 decimal places when $n = 17$, and the generation of n-point rational Gauss rules for larger values of n becomes increasingly subject to cancellation errors. Still, the results are far more accurate than those with Gauss–Fermi and Gauss–Laguerre quadrature, which for $n = 17$ yield about 3 respectively 2 correct decimal digits when $\eta = 10$ and $\eta = 50$, respectively.

We also experimented with larger values of θ, and $\eta = \pm 1$, $k = \frac{1}{2}$, to observe the damaging effect of the square root singularity at $x = -2/\theta$ as it moves toward the interval of integration $[0, \infty]$ (i.e., as θ increases). Interestingly, GF and GL seem to be less affected by this singularity than GR. For $\theta = 0.01$ and $\theta = 0.1$, the results are very similar to those in tables 1 and 2; for $\theta = 1$, they are shown in table 5.

Table 5
Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = \pm 1$, $k = \frac{1}{2}$ and $\theta = 1$.

η	n	GR(n)	GF(n)	GL(n)
−1.0	5	8.6 (−8)	4.8(−5)	2.0 (−5)
	10	1.8(−10)	8.8(−8)	7.4 (−8)
	15	1.2(−12)	1.6(−9)	1.3(−10)
1.0	5	1.4 (−8)	2.7(−4)	4.0 (−4)
	10	1.6(−10)	9.5(−6)	1.8 (−5)
	15	1.1(−12)	3.8(−7)	6.1 (−7)

Table 6
Relative errors of three quadrature schemes for Bose–Einstein integrals with $\eta = -1$ and $\theta = 1 \times 10^{-4}$.

k	n	GR(n)	GE(n)	GL(n)
$\frac{1}{2}$	5	5.4(−8)	1.6(−3)	6.6(−3)
	10	4.1(−17)	4.3(−5)	2.0(−4)
	15	7.5(−26)	2.6(−6)	1.3(−5)
$\frac{3}{2}$	5	1.6(−7)	7.6(−4)	3.2(−3)
	10	2.3(−15)	2.3(−5)	1.1(−4)
	15	1.5(−25)	1.5(−6)	7.0(−6)
$\frac{5}{2}$	5	3.3(−7)	3.2(−4)	1.4(−3)
	10	8.1(−16)	9.5(−6)	4.6(−5)
	15	1.1(−24)	6.1(−7)	3.0(−6)

3.2. *Bose–Einstein integrals*

In analogy to Fermi–Dirac integrals, we consider three quadrature methods for evaluating the Bose–Einstein integral (2.5), (2.6), namely the n-point Gauss Rational formula GR(n) with weight function $x^{k-1}\,e^{-x}$ (cf. section 2.2), the n-point "Gauss–Einstein" formula GE(n),

$$G_k(n, \theta) = \int_0^\infty f(x)\,\frac{1-e^{-x}}{x}\,\frac{x^k}{e^x-1}\,dx$$

$$\approx \Sigma_{r=1}^{n} w_r^{\mathrm{E}} f\left(x_r^{\mathrm{E}}\right)\frac{1-e^{-x_r^{\mathrm{E}}}}{x_r^{\mathrm{E}}}, \qquad (3.3)$$

and the n-point Gauss–Laguerre formula GL(n),

$$G_k(\eta, \theta) = \int_0^\infty f(x)\,x^{k-1}\,e^{-x}\,dx$$

$$\approx \sum_{r=1}^{n} w_r^{\mathrm{L}} f\left(x_r^{\mathrm{L}}\right), \qquad (3.4)$$

Table 7
Exact values of Bose–Einstein integrals.

k	η	$G_k(\eta, 10^{-4})$
$\frac{1}{2}$	−1	0.37970886599807399070148 02
$\frac{3}{2}$	−1	0.52608888707964629059191 74
$\frac{5}{2}$	−1	1.26656912654311754693224 6

where f in (3.3) and (3.4) is given by (2.6). The results for $\eta = -1$ and $\theta = 1 \times 10^{-4}$ are shown in table 6. They are similar to those for Fermi–Dirac integrals in table 1, except that GR is now slightly less accurate and GE, GL both considerably less accurate. Exact values are shown in table 7.

As η decreases from -1 to larger negative values, convergence of all three quadrature schemes speeds up, particularly so for GE and GL. The opposite is true when η increases from -1 to 0: convergence slows down, particularly for GE and GL, but much less so for GR. On the other hand, GR becomes harder to generate, although there is no loss of accuracy as in the case of Fermi–Dirac integrals.

An increase of θ affects convergence similarly as in the case of Fermi–Dirac integrals. For $k = \frac{1}{2}$, $\eta = -1$, and $\theta = 1$, the results are shown in table 8.

Table 8
Relative errors of three quadrature schemes for Bose–Einstein integrals with $\eta = -1$, $k = \frac{1}{2}$ and $\theta = 1$.

n	GR(n)	GE(n)	GL(n)
5	5.5(−7)	3.7(−3)	8.8(−4)
10	3.2(−10)	1.1(−4)	2.4(−5)
15	1.9(−12)	6.9(−6)	1.4(−6)

4. Conclusions

We have shown that Gauss-type quadrature formulae based on rational functions are capable of producing very accurate approximations to generalized Fermi–Dirac and Bose–Einstein integrals, provided the poles of the rational functions are suitably matched with those exhibited by the integrals in question. The use of these formulae is costly in as much as they are parameter-dependent. This probably rules them out for purposes of large-scale production, but makes them eminently suitable for isolated high-precision calculation of generalized (as well as ordinary) Fermi–Dirac and Bose–Einstein integrals. Indeed, any integral whose integrand has sufficiently many poles (outside the interval of integration) is a natural candidate for evaluation by rational Gauss-type quadrature rules.

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STIELTJES POLYNOMIALS AND RELATED QUADRATURE FORMULAE FOR A CLASS OF WEIGHT FUNCTIONS

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ABSTRACT. Consider a (nonnegative) measure $d\sigma$ with support in the interval $[a, b]$ such that the respective orthogonal polynomials, above a specific index ℓ, satisfy a three-term recurrence relation with constant coefficients. We show that the corresponding Stieltjes polynomials, above the index $2\ell - 1$, have a very simple and useful representation in terms of the orthogonal polynomials. As a result of this, the Gauss-Kronrod quadrature formulae for $d\sigma$ have all the desirable properties, namely, the interlacing of nodes, their inclusion in the closed interval $[a, b]$ (under an additional assumption on $d\sigma$), and the positivity of all weights. Furthermore, the interpolatory quadrature formulae based on the zeros of the Stieltjes polynomials have positive weights, and both of these quadrature formulae have elevated degrees of exactness.

1. INTRODUCTION

Consider a (nonnegative) measure $d\sigma$ with support in the interval $[a, b]$, and let $\pi_n(\cdot) = \pi_n(\cdot\,; d\sigma)$ be the respective monic orthogonal polynomial of degree n. The corresponding monic Stieltjes polynomial $\pi^*_{n+1}(\cdot) = \pi^*_{n+1}(\cdot\,; d\sigma)$, of degree $n+1$, can be uniquely defined by the orthogonality condition

$$\int_a^b \pi^*_{n+1}(t) t^k \pi_n(t) d\sigma(t) = 0, \quad k = 0, 1, \ldots, n \tag{1.1}$$

(see [2, §4]), that is, π^*_{n+1} is orthogonal to all polynomials of lower degree relative to the variable-sign distribution $d\sigma^*(t) = \pi_n(t) d\sigma(t)$.

Related to π^*_{n+1} is the Gauss-Kronrod quadrature formula for $d\sigma$,

$$\int_a^b f(t) d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma^*_\mu f(\tau^*_\mu) + R^K_n(f), \tag{1.2}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of π_n, and the nodes $\tau^*_\mu = \tau_\mu^{*(n)}$ and all weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma^*_\mu = \sigma_\mu^{*(n)}$ are chosen such that (1.2) has maximum degree of exactness (at least) $3n+1$, i.e., $R^K_n(f) = 0$ for all $f \in \mathbb{P}_{3n+1}$. A necessary and sufficient condition for this is that the τ^*_μ be the zeros of π^*_{n+1} (see [5, Corollary]).

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Also connected with π_{n+1}^* is the interpolatory quadrature formula

$$\int_a^b f(t)d\sigma(t) = \sum_{\mu=1}^{n+1} w_\mu^* f(\tau_\mu^*) + R_n^S(f), \tag{1.3}$$

where $\tau_\mu^* = \tau_\mu^{*(n)}$ are the zeros of π_{n+1}^*. This kind of quadrature formula was first considered by Monegato in [10, Part II.1] for the Legendre measure $d\sigma(t) = dt$ on $[-1,1]$; he conjectured, in this case, that the w_μ^* are all positive.

We now assume that the orthogonal polynomials relative to $d\sigma$ satisfy a three-term recurrence relation of the following kind,

$$\begin{gathered}\pi_{n+1}(t) = (t-\alpha_n)\pi_n(t) - \beta_n\pi_{n-1}(t), \ n = 0,1,2,\dots, \\ \alpha_n = \alpha, \ \beta_n = \beta \text{ for } n \geq \ell,\end{gathered} \tag{1.4}$$

where $\alpha_n \in \mathbb{R}$, $\beta_n > 0$, $\ell \in \mathbb{N}$, and $\pi_0(t) = 1$, $\pi_{-1}(t) = 0$. Thus, the coefficients α_n and β_n are constant equal, respectively, to some $\alpha \in \mathbb{R}$ and $\beta > 0$ for $n \geq \ell$. Any such measure $d\sigma$ is known to be supported on a finite interval [8, Theorem 10], say $[a,b]$, and we indicate this, together with the property (1.4), by writing $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. We show in §2 that, if $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$, then $\pi_{n+1}^*(\,\cdot\,;d\sigma)$ has a very simple and convenient representation (see (2.13)) in terms of $\pi_{n+1}(\,\cdot\,;d\sigma)$ and $\pi_{n-1}(\,\cdot\,;d\sigma)$, provided that $n \geq 2\ell - 1$. Subsequently in § 3, this representation is used to derive a number of properties for the Gauss-Kronrod formula (1.2), namely that the nodes τ_μ^* interlace with the nodes τ_ν, all nodes τ_ν, τ_μ^* are contained in $[a,b]$ (under an additional assumption on $d\sigma$), all weights σ_ν, σ_μ^* are positive, and the degree of exactness is at least $4n - 2\ell + 2$. Moreover, in § 4 we show that the interpolatory formula (1.3) has positive weights and degree of exactness $2n-1$.

Among the many orthogonal polynomials satisfying (1.4) we mention the four Chebyshev-type polynomials and their modifications discussed in Allaway's thesis [1, Ch. 4], as well as those associated with the Bernstein-Szegö measures. For many of these, the Stieltjes polynomials have previously been expressed explicitly in terms of Chebyshev polynomials, and the corresponding Gauss-Kronrod formulae have been shown to possess the desirable properties mentioned above (see [6, 7, 10, 11, 12]). In addition, it has been shown in [12] that, for a class of Bernstein-Szegö measures, the weights in the interpolatory formula (1.3) are all positive.

2. The Stieltjes polynomials

We now present, assuming $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$, the explicit formula for $\pi_{n+1}^*(\,\cdot\,;d\sigma)$ in terms of the respective orthogonal polynomials $\pi_m(\,\cdot\,) = \pi_m(\,\cdot\,;d\sigma)$. We begin with two preliminary lemmas, which play an important role in the subsequent development. Both make reference to the expansion of $t^k\pi_n(t)$ for $k = 0,1,\dots,n$ in terms of the π_m's, which we write in the form

$$t^k\pi_n(t) = \sum_{i=-k}^{k} c_{i,k}^n \pi_{n+i}(t), \ k = 0,1,\dots,n; \ n \geq 1. \tag{2.1}$$

Note that the terms π_{n+i} with $i < -k$ are absent in (2.1) because of orthogonality of the π_m.

Lemma 2.1. *Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. For a given $n \geq \ell$, the corresponding Stieltjes polynomial has the form*

$$\pi_{n+1}^*(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t) \tag{2.2}$$

if and only if in (2.1) *we have*

$$c_{-1,k}^n = \beta c_{1,k}^n, \quad k = 1, 2, \ldots, n. \tag{2.3}$$

Proof. `Sufficiency`. Assume that (2.3) holds. To prove (2.2), it suffices to show, by virtue of (1.1), that

$$\int_a^b [\pi_{n+1}(t) - \beta\pi_{n-1}(t)]t^k\pi_n(t)d\sigma(t) = 0, \quad k = 0, 1, \ldots, n. \tag{2.4}$$

For $k = 0$, this is true by orthogonality. When $k = 1, 2, \ldots, n$, we obtain from (2.1), (2.3) and orthogonality

(2.5)

$$\int_a^b [\pi_{n+1}(t) - \beta\pi_{n-1}(t)]t^k\pi_n(t)d\sigma(t)$$

$$= \int_a^b [\pi_{n+1}(t) - \beta\pi_{n-1}(t)][\cdots + c_{1,k}^n\pi_{n+1}(t) + c_{0,k}^n\pi_n(t) + \beta c_{1,k}^n\pi_{n-1}(t) + \cdots]d\sigma(t)$$

$$= c_{1,k}^n \left[\int_a^b \pi_{n+1}^2(t)d\sigma(t) - \beta^2 \int_a^b \pi_{n-1}^2(t)d\sigma(t)\right]$$

$$= c_{1,k}^n \left(\|\pi_{n+1}\|^2 - \beta^2\|\pi_{n-1}\|^2\right),$$

where $\|\cdot\|$ is the L_2-norm. Since $n \geq \ell$, there follows from (1.4) that $\beta_n = \beta_{n+1} = \beta$, or equivalently,

$$\frac{\|\pi_n\|^2}{\|\pi_{n-1}\|^2} = \frac{\|\pi_{n+1}\|^2}{\|\pi_n\|^2} = \beta \tag{2.6}$$

(cf. [4, Eq. (5.3)]). This yields

$$\frac{\|\pi_{n+1}\|^2}{\|\pi_{n-1}\|^2} = \beta^2,$$

which, inserted in the last equality of (2.5), proves (2.4) for $k = 1, 2, \ldots, n$.

`Necessity`. Assume that the Stieltjes polynomial is given by (2.2). Then we have, by virtue of (1.1) and (2.1),

$$\int_a^b [\pi_{n+1}(t) - \beta\pi_{n-1}(t)][\cdots + c_{1,k}^n\pi_{n+1}(t) + c_{0,k}^n\pi_n(t) + c_{-1,k}^n\pi_{n-1}(t) + \cdots]d\sigma(t) = 0,$$
$$k = 1, 2, \ldots, n,$$

which by orthogonality gives

$$c_{1,k}^n \int_a^b \pi_{n+1}^2(t)d\sigma(t) - \beta c_{-1,k}^n \int_a^b \pi_{n-1}^2(t)d\sigma(t) = 0, \quad k = 1, 2, \ldots, n,$$

or equivalently,

$$c_{1,k}^n\|\pi_{n+1}\|^2 - \beta c_{-1,k}^n\|\pi_{n-1}\|^2 = 0, \quad k = 1, 2, \ldots, n.$$

In view of (2.6), this yields

$$\|\pi_n\|^2(\beta c_{1,k}^n - c_{-1,k}^n) = 0, \quad k = 1, 2, \dots, n,$$

and since $\|\pi_n\|^2 \neq 0$, there follows (2.3). □

Lemma 2.2. *Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$ with $\ell = 1$. Then in (2.1) there holds*

$$c_{-i,k}^n = \beta^i c_{i,k}^n \tag{2.7}$$

for $i = 0, 1, \dots, k$, and all $k = 0, 1, \dots, n$, $n \geq 1$.

Proof. We apply induction on n. For $n = 1$, the induction claim holds trivially when $k = 0$, and by means of (1.4) when $k = 1$, since

$$t\pi_1(t) = \pi_2(t) + \alpha\pi_1(t) + \beta\pi_0(t),$$

that is, $c_{1,1}^1 = 1$, $c_{-1,1}^1 = \beta$.

Assume now that the claim is true for some index n, that is,

(2.8)
$$\begin{aligned} t^k\pi_n(t) = {} & c_{k,k}^n\pi_{n+k}(t) + c_{k-1,k}^n\pi_{n+k-1}(t) + \cdots + c_{i,k}^n\pi_{n+i}(t) + \cdots + c_{0,k}^n\pi_n(t) \\ & + \cdots + \beta^i c_{i,k}^n\pi_{n-i}(t) + \cdots + \beta^{k-1}c_{k-1,k}^n\pi_{n-(k-1)}(t) \\ & + \beta^k c_{k,k}^n\pi_{n-k}(t), \quad k = 0, 1, \dots, n; \end{aligned}$$

we want to prove it for the index $n+1$. The expansion of $t^k\pi_n(t)$ in terms of the π_m's results from applying k times (1.4), solved for the term $t\pi_n$. Since (1.4) is assumed to hold with $\ell = 1$, we have

$$t\pi_m(t) = \pi_{m+1}(t) + \alpha\pi_m(t) + \beta\pi_{m-1}(t) \tag{2.9}$$

for all $m \geq 1$. It follows that the coefficients in (2.8) depend only on α, β and k, and not on n. Therefore, replacing n in π_n by $n+1$ gives the corresponding expansion for $t^k\pi_{n+1}(t)$, $k = 0, 1, \dots, n$, that is,

(2.10)
$$\begin{aligned} t^k\pi_{n+1}(t) = {} & c_{k,k}^n\pi_{n+1+k}(t) + c_{k-1,k}^n\pi_{n+1+k-1}(t) + \cdots + c_{i,k}^n\pi_{n+1+i}(t) \\ & + \cdots + c_{0,k}^n\pi_{n+1}(t) + \cdots + \beta^i c_{i,k}^n\pi_{n+1-i}(t) \\ & + \cdots + \beta^{k-1}c_{k-1,k}^n\pi_{n+1-(k-1)}(t) + \beta^k c_{k,k}^n\pi_{n+1-k}(t), \\ & \qquad k = 0, 1, \dots, n. \end{aligned}$$

This proves the induction claim for the index $n+1$ when $k = 0, 1, \dots, n$. It remains to show the claim for $k = n+1$. The expansion for $t^{n+1}\pi_{n+1}(t)$ is obtained by multiplying the expansion for $t^n\pi_{n+1}(t)$ by t, and then applying (2.9) to each term in the expansion. This yields, in the notation of (2.1),

(2.11)
$$c_{i,n+1}^{n+1} = \begin{cases} \beta c_{i+1,n}^{n+1} + \alpha c_{i,n}^{n+1} + c_{i-1,n}^{n+1}, & i = 1, 2, \dots, n-1, \\ \alpha c_{n,n}^{n+1} + c_{n-1,n}^{n+1}, & i = n, \\ c_{n,n}^{n+1}, & i = n+1 \end{cases}$$

and

(2.12)
$$c_{-i,n+1}^{n+1} = \begin{cases} \beta c_{-(i-1),n}^{n+1} + \alpha c_{-i,n}^{n+1} + c_{-(i+1),n}^{n+1}, & i = 0, 1, \dots, n-1, \\ \beta c_{-(n-1),n}^{n+1} + \alpha c_{-n,n}^{n+1}, & i = n, \\ \beta c_{-n,n}^{n+1}, & i = n+1. \end{cases}$$

From (2.10), with $k = n$, there follows

$$c_{-i,n}^{n+1} = \beta^i c_{i,n}^{n+1}, \quad i = 0, 1, \dots, n,$$

which, combined with (2.11) and (2.12), gives

$$c_{-i,n+1}^{n+1} = \beta^i c_{i,n+1}^{n+1}, \quad i = 0, 1, \dots, n+1.$$

This proves the induction claim for $k = n+1$, and completes the induction. □

Theorem 2.3. *Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. Then the corresponding Stieltjes polynomials are given by*

$$\pi_{n+1}^*(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t) \quad \textit{for } n \geq 2\ell - 1. \tag{2.13}$$

Proof. In order to prove (2.13), it suffices to show, in view of Lemma 2.1, that if (1.4) holds for all $n \geq \ell$, then so does (2.3) for all $n \geq 2\ell - 1$. To this end we apply induction on ℓ. This requires us to compare the coefficients in the expansion (2.1) in the orthogonal polynomials associated with a $d\sigma_\ell \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$ with those of the analogous expansion in the (different) orthogonal polynomials associated with a $d\sigma_{\ell+1} \in \mathcal{M}_{\ell+1}^{(\alpha,\beta)}[a',b']$. This we do by starting from the trivial identity $\pi_n(t) = \pi_n(t)$ for the polynomial in question and then multiplying both sides repeatedly by t, whereby on the right we continuously use (2.9) or the analogous relation from (1.4) (whichever is appropriate) to express the result in terms of higher- and lower-degree polynomials π_r.

The induction claim for $\ell = 1$ follows from Lemma 2.2 with $i = 1$. Assume now that the claim is true for some index ℓ; we want to prove it for the index $\ell + 1$. Replacing ℓ in (1.4) by $\ell + 1$ has the effect that the recursion coefficients α_ℓ and β_ℓ may no longer be equal to α and β, respectively. As a consequence, the coefficients $c_{\pm i,k}^n$ in (2.1) generated by the above procedure will eventually change as well. In order to prove the induction claim for the index $\ell + 1$, we must show that for all $n \geq 2\ell + 1$, the coefficients $c_{\pm 1,k}^n$ that evolve are not affected by the replacement of ℓ in (1.4) by $\ell + 1$, i.e., α_ℓ and β_ℓ do not become involved in determining these coefficients. This will be the case for all $k = 0, 1, \dots, n - \ell$ since (2.9) still holds for $m \geq \ell + 1$. When $k = n - \ell + 1$, then α_ℓ and β_ℓ enter the picture for the first time as parts of the coefficients of $\pi_\ell, \pi_{\ell-1}$, and they, as well as lower-order coefficients α_λ, β_λ with $\lambda < \ell$, continue to be involved for the remaining values of $k = n - \ell + 2, n - \ell + 3, \dots, n$. When $k = n$, then α_λ, β_λ with $\lambda \leq \ell$ are involved in the expansion coefficients of $\pi_{2\ell-1}, \pi_{2\ell-2}, \dots, \pi_0$. Since the highest-degree polynomial so affected is $\pi_{2\ell-1}$, it is clear that when $n \geq 2\ell + 1$, the expansion coefficients associated with π_{n-1} and π_{n+1}, that is, $c_{\pm 1,k}^n$, $1 \leq k \leq n$, are independent of α_λ, β_λ with $\lambda \leq \ell$. This proves the induction claim for the index $\ell + 1$, and completes the induction. □

The following proposition will be useful in the development of §3.

Proposition 2.4. *Consider a measure* $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$ *and let* τ_ν *be the zeros of the corresponding orthogonal polynomial* π_n. *Then*

$$\pi_{n+1}(\tau_\nu) = \frac{1}{2}\pi_{n+1}^*(\tau_\nu), \quad \nu = 1,2,\dots,n, \tag{2.14}$$

for all $n \geq 2\ell - 1$.

Proof. Let $n \geq 2\ell - 1$. First, (2.13) gives

$$\pi_{n+1}^*(\tau_\nu) = \pi_{n+1}(\tau_\nu) - \beta\pi_{n-1}(\tau_\nu). \tag{2.15}$$

Since τ_ν is a zero of π_n, we have by (1.4) that

$$\beta\pi_{n-1}(\tau_\nu) = -\pi_{n+1}(\tau_\nu),$$

which, inserted into (2.15), yields (2.14). □

3. Gauss-Kronrod quadrature formulae

The Gauss-Kronrod formula (1.2) is said to have the interlacing property if the nodes τ_ν, τ_μ^* are real and satisfy, when ordered decreasingly,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*. \tag{3.1}$$

Formula (1.2) is said to have the inclusion property if all nodes τ_ν, τ_μ^* are contained in the closed interval $[a,b]$. Clearly, if (3.1) holds, the inclusion property is equivalent to

$$a \leq \tau_{n+1}^* \quad \text{and} \quad \tau_1^* \leq b. \tag{3.2}$$

If $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$, then trivially $\alpha_n \to \alpha$, $\beta_n \to \beta$ as $n \to \infty$, and it follows [3, p. 121] that

$$[\alpha - 2\sqrt{\beta}, \alpha + 2\sqrt{\beta}\,] \tag{3.3}$$

is the "limiting spectral interval" of $d\sigma$. It may well be, however, that $d\sigma$ has support points outside the interval (3.3) (cf. [3, Exercise 4.6, p. 128]), but for inclusion results we will assume the following property.

Property A. The measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$ is such that

$$a = \alpha - 2\sqrt{\beta}, \quad b = \alpha + 2\sqrt{\beta}. \tag{3.4}$$

Before we state and prove the properties of the quadrature formula (1.2) announced in §1, we add another lemma in the spirit of Lemma 2.2 and Theorem 2.3.

Lemma 3.1. *Consider a measure* $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. *Then in* (2.1) *there holds, for all* $n \geq 2\ell - 1$,

$$c_{-i,n}^n = \beta^i c_{i,n}^n, \quad i = 0,1,\dots,n - 2\ell + 2. \tag{3.5}$$

Proof. For $\ell = 1$, this is Lemma 2.2 with $k = n$. The proof for general ℓ is again by induction, very much along the lines of the proof of Theorem 2.3. The details are left to the reader. □

Theorem 3.2. *Consider a measure* $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. *Then the following holds* :

(a) *The Gauss-Kronrod formula* (1.2) *has the interlacing property for all* $n \geq 2\ell - 1$.

(b) *If* $d\sigma$ *has Property A, then the inclusion property holds for all* $n \geq 2\ell - 1$.

(c) *All weights* σ_ν, σ_μ^* *in* (1.2) *are positive for each* $n \geq 2\ell - 1$.

(d) *The formula* (1.2) *has degree of exactness (at least)* $4n - 2\ell + 2$ *if* $n \geq 2\ell - 1$.

Remark. In part (b) of this theorem, Property A can be replaced by assuming the two inequalities in (3.8).

Proof. (a) Let $n \geq 2\ell - 1$. Proposition 2.4, in view of the separation property for the zeros of π_n and π_{n+1} (see [13, Theorem 3.3.2]), implies

$$\text{sign } \pi_{n+1}^*(\tau_\nu) = \text{sign } \pi_{n+1}(\tau_\nu) = (-1)^\nu, \quad \nu = 1, 2, \dots, n. \tag{3.6}$$

In addition, it is clear that

$$\begin{aligned} \lim_{t\to\infty} \pi_{n+1}^*(t) &= \infty, \\ \lim_{t\to-\infty} \pi_{n+1}^*(t) &= (-1)^{n+1}\infty. \end{aligned} \tag{3.7}$$

From (3.6) and (3.7) there follows that the τ_μ^* are real and satisfy (3.1). This proves the interlacing property.

(b) Let $n \geq 2\ell - 1$. Since (3.1) is true, the inclusion property comes down to showing that (3.2) holds. A necessary and sufficient condition for that is

$$(-1)^{n+1}\pi_{n+1}^*(a) \geq 0 \quad \text{and} \quad \pi_{n+1}^*(b) \geq 0,$$

which, on account of (2.13), is equivalent to

$$\beta \leq \frac{\pi_{n+1}(a)}{\pi_{n-1}(a)} \quad \text{and} \quad \beta \leq \frac{\pi_{n+1}(b)}{\pi_{n-1}(b)}. \tag{3.8}$$

Assuming Property A, we now prove both these inequalities. Beginning with the second, we set $t = b$ in (1.4), to get, using the second relation in (3.4),

$$\pi_{n+1}(b) = 2\sqrt{\beta}\pi_n(b) - \beta\pi_{n-1}(b), \quad n \geq \ell. \tag{3.9}$$

Dividing both sides of (3.9) by $\pi_n(b)$, and letting $q_n = \pi_n(b)/\pi_{n-1}(b)$, we obtain

$$q_{n+1} = 2\sqrt{\beta} - \frac{\beta}{q_n}, \quad n \geq \ell.$$

Subtracting q_n from both sides gives

$$q_{n+1} - q_n = -\frac{(q_n - \sqrt{\beta})^2}{q_n}, \quad n \geq \ell. \tag{3.10}$$

Since $q_n > 0$ for $n \geq 1$, there follows from (3.10) that q_n is a decreasing sequence for $n \geq \ell$ and hence converges to, say, q as $n \to \infty$. Thus, $q_n \geq q$ for $n \geq \ell$. Multiplying both sides of (3.10) by q_n, and then taking the limit as $n \to \infty$, we immediately obtain $q = \sqrt{\beta}$, hence

$$q_n \geq \sqrt{\beta}, \quad n \geq \ell. \tag{3.11}$$

Now,

$$\frac{\pi_{n+1}(b)}{\pi_{n-1}(b)} = \frac{\pi_{n+1}(b)}{\pi_n(b)} \cdot \frac{\pi_n(b)}{\pi_{n-1}(b)} = q_{n+1}q_n,$$

which by (3.11) yields the second inequality in (3.8).

For the first inequality, the proof is analogous. One now defines q_n by $q_n = \pi_n(a)/\pi_{n-1}(a)$ and shows that q_n for $n \geq \ell$ is a (negative) increasing sequence converging to $-\sqrt{\beta}$, hence,

$$q_n \leq -\sqrt{\beta}, \quad n \geq \ell,$$

from which the first inequality in (3.8) follows as before.

(c) The weights σ_ν are given by the formula

$$\sigma_\nu = \lambda_\nu + \frac{\|\pi_n\|^2}{\pi_n'(\tau_\nu)\pi_{n+1}^*(\tau_\nu)}, \quad \nu = 1, 2, \dots, n \tag{3.12}$$

(see [9, Theorem 2]), where $\lambda_\nu = \lambda_\nu^{(n)}$ are the weights of the n-point Gauss formula relative to $d\sigma$, known to be all positive, and $\|\cdot\|$ denotes the L_2-norm. Also, the λ_ν can be represented by

$$\lambda_\nu = -\frac{\|\pi_n\|^2}{\pi_n'(\tau_\nu)\pi_{n+1}(\tau_\nu)}, \quad \nu = 1, 2, \dots, n \tag{3.13}$$

(see [13, Eq. (3.4.7)]). Let $n \geq 2\ell - 1$. Then (3.12), by virtue of (2.14) and (3.13), yields

$$\sigma_\nu = \frac{1}{2}\lambda_\nu, \quad \nu = 1, 2, \dots, n, \tag{3.14}$$

from which the positivity of the σ_ν follows immediately.

The positivity of the σ_μ^* is equivalent to the interlacing property (see [9, Theorem 1]) already proved in (a).

(d) Let $n \geq 2\ell - 1$. To prove that the degree of exactness is (at least) $4n - 2\ell + 2$, it suffices to show

$$\int_a^b \pi_{n+1}^*(t) t^k \pi_n(t) d\sigma(t) = 0, \quad k = 0, 1, \dots, 2n - 2\ell + 1 \tag{3.15}$$

(see [5, Corollary]). By (1.1), this is true for $k = 0, 1, \dots, n$. For the remaining values $k = n+1, n+2, \dots, 2n - 2\ell + 1$ we can write (3.15) in view of (2.13) as

$$\int_a^b t^k [\pi_{n+1}(t) - \beta\pi_{n-1}(t)] t^n \pi_n(t) d\sigma(t) = 0, \quad k = 0, 1, \dots, n - 2\ell + 1. \tag{3.16}$$

By Lemma 3.1, we can write

$$\begin{aligned} t^n \pi_n(t) = {} & c_{n,n}^n \pi_{2n}(t) + \cdots + c_{n-2\ell+2,n}^n \pi_{2n-2\ell+2}(t) + \cdots + c_{i,n}^n \pi_{n+i}(t) \\ & + \cdots + c_{0,n}^n \pi_n(t) + \cdots + \beta^i c_{i,n}^n \pi_{n-i}(t) \\ & + \cdots + \beta^{n-2\ell+2} c_{n-2\ell+2,n}^n \pi_{2\ell-2}(t) + \cdots + c_{-n,n}^n \pi_0(t), \\ & \qquad\qquad\qquad\qquad\qquad\qquad n \geq 2\ell - 1. \end{aligned} \tag{3.17}$$

Similarly, in the expansion

$$t^k [\pi_{n+1}(t) - \beta\pi_{n-1}(t)] = \sum_{i=-(k+1)}^{k+1} d_{i,k+1}^n \pi_{n+i}$$

we have $d_{0,k+1}^n = 0$, and $d_{-i,k+1}^n = -\beta^i d_{i,k+1}^n$ for each $i = 1, 2, \dots, k+1$, and for all $k = 0, 1, \dots, n - 2\ell + 1$, $n \geq 2\ell - 1$. The proof goes by induction on ℓ. Let

$\ell = 1$. First, we have from Lemma 2.2

(3.18)
$$\begin{aligned} t^k\pi_{n-1}(t) &= c_{k,k}^{n-1}\pi_{n-1+k}(t) + c_{k-1,k}^{n-1}\pi_{n-1+k-1}(t) + \cdots + c_{i+1,k}^{n-1}\pi_{n-1+i+1}(t) \\ &\quad + c_{i,k}^{n-1}\pi_{n-1+i}(t) + c_{i-1,k}^{n-1}\pi_{n-1+i-1}(t) + \cdots + c_{2,k}^{n-1}\pi_{n+1}(t) \\ &\quad + c_{1,k}^{n-1}\pi_n(t) + c_{0,k}^{n-1}\pi_{n-1}(t) + \beta c_{1,k}^{n-1}\pi_{n-2}(t) + \beta^2 c_{2,k}^{n-1}\pi_{n-3}(t) \\ &\quad + \cdots + \beta^{i-1}c_{i-1,k}^{n-1}\pi_{n-1-(i-1)}(t) + \beta^i c_{i,k}^{n-1}\pi_{n-1-i}(t) \\ &\quad + \beta^{i+1}c_{i+1,k}^{n-1}\pi_{n-1-(i+1)}(t) + \cdots + \beta^{k-1}c_{k-1,k}^{n-1}\pi_{n-1-(k-1)}(t) \\ &\quad + \beta^k c_{k,k}^{n-1}\pi_{n-1-k}(t), \quad k = 0, 1, \ldots, n-1, \quad n \geq 1. \end{aligned}$$

Since (1.4), with $\ell = 1$, holds for all $n \geq 1$, the coefficients in this expansion are given in terms of α, β and k only. Therefore, replacing $n-1$ in π_{n-1} by $n+1$ gives the corresponding expansion for $t^k\pi_{n+1}(t)$, $k = 0, 1, \ldots, n-1$, that is,

(3.19)
$$\begin{aligned} t^k\pi_{n+1}(t) &= c_{k,k}^{n-1}\pi_{n+1+k}(t) + c_{k-1,k}^{n-1}\pi_{n+1+k-1}(t) + \cdots + c_{i+1,k}^{n-1}\pi_{n+1+i+1}(t) \\ &\quad + c_{i,k}^{n-1}\pi_{n+1+i}(t) + c_{i-1,k}^{n-1}\pi_{n+1+i-1}(t) + \cdots + c_{2,k}^{n-1}\pi_{n+3}(t) \\ &\quad + c_{1,k}^{n-1}\pi_{n+2}(t) + c_{0,k}^{n-1}\pi_{n+1}(t) + \beta c_{1,k}^{n-1}\pi_n(t) + \beta^2 c_{2,k}^{n-1}\pi_{n-1}(t) \\ &\quad + \cdots + \beta^{i-1}c_{i-1,k}^{n-1}\pi_{n+1-(i-1)}(t) + \beta^i c_{i,k}^{n-1}\pi_{n+1-i}(t) \\ &\quad + \beta^{i+1}c_{i+1,k}^{n-1}\pi_{n+1-(i+1)}(t) + \cdots + \beta^{k-1}c_{k-1,k}^{n-1}\pi_{n+1-(k-1)}(t) \\ &\quad + \beta^k c_{k,k}^{n-1}\pi_{n+1-k}(t), \quad k = 0, 1, \ldots, n-1, \quad n \geq 1 \end{aligned}$$

(see also the proof of Lemma 2.2). Adding (3.18) multiplied by $-\beta$ to (3.19), we get

$$\begin{aligned} t^k[\pi_{n+1}(t) - \beta\pi_{n-1}(t)] &= c_{k,k}^{n-1}\pi_{n+k+1}(t) + c_{k-1,k}^{n-1}\pi_{n+k}(t) \\ &\quad + \cdots + (c_{i-1,k}^{n-1} - \beta c_{i+1,k}^{n-1})\pi_{n+i}(t) + \cdots + (c_{0,k}^{n-1} - \beta c_{2,k}^{n-1})\pi_{n+1}(t) \\ &\quad + (\beta c_{1,k}^{n-1} - \beta c_{1,k}^{n-1})\pi_n(t) + (\beta^2 c_{2,k}^{n-1} - \beta c_{0,k}^{n-1})\pi_{n-1}(t) \\ &\quad + \cdots + (\beta^{i+1}c_{i+1,k}^{n-1} - \beta^i c_{i-1,k}^{n-1})\pi_{n-i}(t) + \cdots - \beta^k c_{k-1,k}^{n-1}\pi_{n-k}(t) \\ &\quad - \beta^{k+1}c_{k,k}^{n-1}\pi_{n-(k+1)}(t), \end{aligned}$$

or equivalently,

$$\begin{aligned} t^k[\pi_{n+1}(t) - \beta\pi_{n-1}(t)] &= c_{k,k}^{n-1}\pi_{n+k+1}(t) + c_{k-1,k}^{n-1}\pi_{n+k}(t) \\ &\quad + \cdots + (c_{i-1,k}^{n-1} - \beta c_{i+1,k}^{n-1})\pi_{n+i}(t) + \cdots + (c_{0,k}^{n-1} - \beta c_{2,k}^{n-1})\pi_{n+1}(t) \\ &\quad - \beta(c_{0,k}^{n-1} - \beta c_{2,k}^{n-1})\pi_{n-1}(t) - \beta^i(c_{i-1,k}^{n-1} - \beta c_{i+1,k}^{n-1})\pi_{n-i}(t) \\ &\quad - \cdots - \beta^k c_{k-1,k}^{n-1}\pi_{n-k}(t) - \beta^{k+1}c_{k,k}^{n-1}\pi_{n-(k+1)}(t), \\ &\qquad k = 0, 1, \ldots, n-1, \quad n \geq 1, \end{aligned}$$

which proves the induction claim for $\ell = 1$.

Assume that the claim is true for some index ℓ, that is,

(3.20)
$$t^k[\pi_{n+1}(t) - \beta\pi_{n-1}(t)] = d^n_{k+1,k+1}\pi_{n+k+1}(t) + \cdots + d^n_{i,k+1}\pi_{n+i}(t) + \cdots + d^n_{1,k+1}\pi_{n+1}(t) - \beta d^n_{1,k+1}\pi_{n-1}(t) - \cdots - \beta^i d^n_{i,k+1}\pi_{n-i}(t) - \cdots - \beta^{k+1} d^n_{k+1,k+1}\pi_{n-(k+1)}(t),$$
$$k = 0, 1, \ldots, n - 2\ell + 1, \ n \geq 2\ell - 1;$$

we want to prove it for the index $\ell+1$. Replacing ℓ in (1.4) by $\ell+1$ has the effect of making the recursion coefficients α_ℓ and β_ℓ in general different from α and β, respectively. As a consequence, the coefficients in the expansion of $t^k[\pi_{n+1}(t) - \beta\pi_{n-1}(t)]$ change as well, and α_ℓ and β_ℓ enter these coefficients as k advances. Indeed, for $k = 0, 1, \ldots, n - \ell - 1$, the coefficients are the same as before the replacement. When $k = n - \ell$, then α_ℓ and β_ℓ enter the scene for the first time as parts of the coefficients of π_ℓ, $\pi_{\ell-1}$ (see also the proof of Theorem 2.3). However, $n - \ell > n - 2\ell + 1$ for $\ell > 1$. Hence, the expansion coefficients in (3.20) are independent of α_ℓ and β_ℓ, and therefore the coefficients in the expansion of $t^k[\pi_{n+1}(t) - \beta\pi_{n-1}(t)]$, $k = 0, 1, \ldots, n - 2\ell - 1$, $n \geq 2\ell + 1$, are the same as before the replacement of ℓ in (1.4) by $\ell + 1$. This proves the induction claim for index $\ell + 1$, and completes the induction.

Now, (3.16) can be verified by multiplying together the expansions (3.17) and (3.20), and by using orthogonality and the fact that

$$\|\pi_{n+i}\|^2 - \beta^{2i}\|\pi_{n-i}\|^2 = 0, \quad i = 0, 1, \ldots, n - \ell + 1, \quad n \geq \ell - 1$$

(cf. [4, Eq. (5.3)]). □

4. Interpolatory quadrature formulae

In this section we show that, under the assumption $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a, b]$, formula (1.3) has real nodes, all included in the closed interval $[a, b]$ (if $d\sigma$ has Property A), and positive weights for all $n \geq 2\ell - 1$. In addition, we determine the precise degree of exactness of (1.3).

Theorem 4.1. *Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a, b]$. Then the following holds :*

(a) *The interpolatory formula* (1.3) *has real nodes which, if $d\sigma$ has Property A, are all contained in the closed interval $[a, b]$, for each $n \geq 2\ell - 1$.*

(b) *All weights w^*_μ in* (1.3) *are positive for each $n \geq 2\ell - 1$.*

(c) *The precise degree of exactness of* (1.3) *is $2n - 1$ if $n \geq 2\ell - 1$.*

Proof. (a) The assertions follow from Theorem 3.2 (a), (b).

(b) Setting $f(t) = \pi^*_{n+1}(t)/(t - \tau^*_\mu)$ in the interpolatory formula (1.3), we get

$$w^*_\mu = \frac{1}{\pi^{*\prime}_{n+1}(\tau^*_\mu)} \int_a^b \frac{\pi^*_{n+1}(t)}{t - \tau^*_\mu} d\sigma(t), \ \mu = 1, 2, \ldots, n + 1. \tag{4.1}$$

That same substitution in the Gauss-Kronrod formula (1.2) and in the n-point Gauss formula relative to $d\sigma$,

$$\int_a^b f(t)d\sigma(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R^G_n(f),$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of π_n and $\lambda_\nu = \lambda_\nu^{(n)}$ the Christoffel numbers, gives

$$\int_a^b \frac{\pi_{n+1}^*(t)}{t-\tau_\mu^*} d\sigma(t) = \sum_{\nu=1}^n \sigma_\nu \frac{\pi_{n+1}^*(\tau_\nu)}{\tau_\nu - \tau_\mu^*} + \sigma_\mu^* \pi_{n+1}^{*\prime}(\tau_\mu^*) \tag{4.2}$$

and

$$\int_a^b \frac{\pi_{n+1}^*(t)}{t-\tau_\mu^*} d\sigma(t) = \sum_{\nu=1}^n \lambda_\nu \frac{\pi_{n+1}^*(\tau_\nu)}{\tau_\nu - \tau_\mu^*}, \tag{4.3}$$

respectively. Let $n \geq 2\ell - 1$. Equating the right sides of (4.2) and (4.3), we find, in view of (3.14),

$$\sum_{\nu=1}^n \sigma_\nu \frac{\pi_{n+1}^*(\tau_\nu)}{\tau_\nu - \tau_\mu^*} = \sigma_\mu^* \pi_{n+1}^{*\prime}(\tau_\mu^*),$$

which, inserted into (4.2), yields

$$\int_a^b \frac{\pi_{n+1}^*(t)}{t-\tau_\mu^*} d\sigma(t) = 2\sigma_\mu^* \pi_{n+1}^{*\prime}(\tau_\mu^*). \tag{4.4}$$

Now, (4.1), by virtue of (4.4), implies

$$w_\mu^* = 2\sigma_\mu^*, \quad \mu = 1, 2, \ldots, n+1. \tag{4.5}$$

By Theorem 3.2 (c), the positivity of w_μ^* follows.

(c) The precise degree of exactness of (1.3) is $n+k$, where k is the unique integer satisfying

$$\int_a^b \pi_{n+1}^*(t) p(t) d\sigma(t) \begin{cases} = 0 & \text{for all } p \in \mathbb{P}_{k-1}, \\ \neq 0 & \text{for some } p \in \mathbb{P}_k \end{cases}$$

(see [4, §1.3]). Now, for $n \geq 2\ell - 1$, we have by orthogonality, in view of (2.13),

$$\int_a^b \pi_{n+1}^*(t) p(t) d\sigma(t)$$

$$= \int_a^b [\pi_{n+1}(t) - \beta \pi_{n-1}(t)] p(t) d\sigma(t) \begin{cases} = 0 & \text{for all } p \in \mathbb{P}_{n-2}, \\ = -\|\pi_n\|^2 \neq 0 & \text{for } p = \pi_{n-1}. \end{cases}$$

Thus, the precise degree of exactness of (1.3) is $2n-1$. □

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ADAPTIVE QUADRATURE—REVISITED *

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Dedicated to Cleve B. Moler on his 60th birthday

Abstract.

First, the basic principles of adaptive quadrature are reviewed. Adaptive quadrature programs being recursive by nature, the choice of a good termination criterion is given particular attention. Two Matlab quadrature programs are presented. The first is an implementation of the well-known adaptive recursive Simpson rule; the second is new and is based on a four-point Gauss–Lobatto formula and two successive Kronrod extensions. Comparative test results are described and attention is drawn to serious deficiencies in the adaptive routines **quad** and **quad8** provided by Matlab.

AMS subject classification: 65D30, 65D32.

Key words: Adaptive quadrature, Gauss quadrature, Kronrod rules.

1 The basic idea of adaptive quadrature.

Let $[a, b]$ be the interval of integration, assumed to be bounded, and f a real integrable function. To compute

$$I = \int_a^b f(x)\,dx,$$

one generally proceeds as follows (see also, e.g., [2, Ch. 6]). First one integrates f using two different numerical integration methods, thus obtaining the approximations I_1 and I_2. Typically, one, say I_1, is more accurate than the other. If the relative difference of the two approximations is smaller than some prescribed tolerance, one accepts I_1 as the value of the integral. Otherwise the interval $[a, b]$ is divided, e.g., in two equal parts $[a, m]$ and $[m, b]$, where $m = (a + b)/2$, and the two respective integrals are computed independently:

$$I = \int_a^m f(x)\,dx + \int_m^b f(x)\,dx.$$

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One now again computes recursively two approximations for each integral and, if necessary, continues to subdivide the smaller intervals.

As is well known, it is impossible to construct a program that is foolproof, i.e., that correctly integrates any given function [1]. It is easy to construct a function f which a given program will not integrate correctly [10]. Our task is therefore to design an algorithm that works well for as many functions as possible.

M.T. Heath writes in his recent textbook [9]:

> "If the integrand is noisy, or if the error tolerance is unrealistically tight relative to the machine precision, then an adaptive quadrature routine may be unable to meet the error tolerance and will likely expend a large number of function evaluations only to return a warning message that its subdivision limit was exceeded. Such a result should not be regarded as a fault of the adaptive routine but as a reflection of the difficulty of the problem or unrealistic expectations on the part of the user, or both."

This is true for the two adaptive quadrature functions `quad` and `quad8` provided by Matlab. However, our routines will show that Heath's assessment is overly pessimistic in general—we can do much better than he says.

2 Termination criterion.

If I_1 and I_2 are two estimates for the integral, a conventional stopping criterion is

(2.1) `if abs(i1-i2) < tol*abs(i1),`

where *tol* is some prescribed error tolerance. This criterion by itself is not sufficient. Consider for example $f(x) = \sqrt{x}$, the integration interval $[0, 1]$, I_2: Simpson's rule using the step size h, I_1: Simpson's rule for the step size $h/2$ and $tol = 10^{-4}$. If implemented in Matlab, this procedure terminates fatally with the error message `Segmentation fault`. In this example the two Simpson values never agree to 4 decimals in the first interval containing 0.

The function `quad` in Matlab is based on an adaptive recursive Simpson's rule. The stopping criterion (2.1) is supplemented by a limitation on the number of recursion levels. This prevents failure in the example above. However, it is not clear how many recursion levels should be allowed, and the value `LEVMAX = 10` used in `quad` is often inadequate. A warning error message is given if the recursion level limit is reached. In case of $f(x) = \sqrt{x}$ and $[a, b] = [0, 1]$ we obtain with the call `quad('f',0,1,1e-12)` the warning `Recursion level limit reached 1024 times` and the value 0.666665790717630 is returned, which is correct to only 6 digits instead of the requested 12 digits.

We somehow have to terminate the recursion if the magnitude of the partial integral I_1 or I_2 is negligible compared to the whole integral (see [4, p. 209], [3]). Therefore, we have to add the criterion

(2.2) $$|I_1| < \eta \left| \int_a^b f(x)\,dx \right|,$$

where η is another prescribed tolerance and where we have to use an estimate for the unknown integral. With both criteria (2.1) and (2.2) used together, and with some reasonable choices of *tol* and η, a working algorithm can be obtained. If, e.g., for the above example we use

(2.3) `if (abs(i1-i2) < 1e-4*abs(i1)) | (abs(i1<1e-4))`

as stopping criterion, we obtain $I = 0.666617217$ in 41 function evaluations.

The stopping criterion (2.3), however, is still not satisfactory because the user has to choose *tol* and η, which depend on the machine and on the problem. A wrong selection is easily possible.

To improve the criterion, we first need a rough estimate

(2.4) `is, is` $\neq 0$,

of the modulus of the integral I. The stopping criterion (2.2) would then be $|I_1| < \eta \cdot is$. In order to eliminate η, we stop the recursion machine-independently by

(2.5) `if is + i1 == is.`

In the same spirit we may as well replace the criterion (2.1) by

(2.6) `if is + (i1-i2) == is.`

The criterion (2.6) will in general be met before the criterion (2.5) and therefore we shall require only (2.6). There are cases, e.g., $\int_0^1 1/\sqrt{1-x^2}\,dx$, where, when ignoring the singularity, the subdivision will continue until an interval contains no machine number other than the end points. In this case we also need to terminate the recursion. Thus, our termination criterion is

(2.7) `if (is + (i1-i2) == is) | (m <= a) | (b<=m),`

where $m = (a+b)/2$. This, in particular, guarantees termination of the program, and an explicit limitation on the number of recursion levels is no longer necessary.

Using the stopping criterion (2.7), we attempt to compute the integral to machine precision. If we wish to compute the integral with less accuracy, say within the tolerance *tol* , it suffices to magnify the estimated value *is*:

`is = is*tol/eps,`

where `eps` denotes the machine precision.

3 Adaptive Simpson quadrature.

The idea of adaptive Simpson quadrature is old [12]. However, in order to obtain good performance, a careful implementation is necessary. The Matlab function `quad` compares two successive Simpson values (relative and absolute difference) and has a limitation on the number of recursion steps. If we compute $\int_0^1 \sqrt{x}\,dx$ with $tol = 10^{-8}$ we obtain the message "`Warning: Recursion level`

`limit reached in quad. Singularity likely.`". The routine returns 0.6666657907152264 (a value correct to only 6 digits) and needs 800 function evaluations.

First, we propose to use for is a Monte Carlo estimate which also uses the function values in the middle and at the end points of the interval (those values are used for Simpson's rule):

$$is = \frac{b-a}{8}\Big(f(a) + f(m) + f(b) + \sum_{i=1}^{5} f(\xi_i)\Big). \tag{3.1}$$

Here $m = (a+b)/2$ and $\xi = a + [0.9501\ 0.2311\ 0.6068\ 0.4860\ 0.8913](b-a)$ is a vector of random numbers in (a,b). If by accident we get $is = 0$, then we use the value $is = b - a$.

With this choice of is, we adopt the stopping criterion (2.7). Furthermore, we do not compare successive Simpson values $i1 = S(h)$ and $i2 = S(h/2)$ but overwrite $i1$ with one step of Romberg extrapolation:

```
i1 = (16*i2 - i1)/15.
```

In order to avoid recomputation of function values, we pass $fa = f(a)$, $fm = f((a+b)/2)$ and $fb = f(b)$ as parameters. In every recursion step, only two new function evaluations are necessary to compute the approximations $i1$ and $i2$. The following Matlab function `adaptsim` has the same structure as `quad`. For $\int_0^1 \sqrt{x}\,dx$ with $tol = 10^{-8}$ we obtain with `adaptsim` the value 0.6666666539870345 (correct to almost 8 digits) using only 126 function evaluations.

```
function Q = adaptsim(f,a,b,tol,trace,varargin)
%ADAPTSIM  Numerically evaluate integral using adaptive
%   Simpson rule.
%
%   Q = ADAPTSIM('F',A,B) approximates the integral of
%   F(X) from A to B to machine precision.  'F' is a
%   string containing the name of the function. The
%   function F must return a vector of output values if
%   given a vector of input values.
%
%   Q = ADAPTSIM('F',A,B,TOL) integrates to a relative
%   error of TOL.
%
%   Q = ADAPTSIM('F',A,B,TOL,TRACE) displays the left
%   end point of the current interval, the interval
%   length, and the partial integral.
%
%   Q = ADAPTSIM('F',A,B,TOL,TRACE,P1,P2,...) allows
%   coefficients P1,... to be passed directly to the
%   function F:  G = F(X,P1,P2,...). To use default values
```

```
%   for TOL or TRACE, one may pass the empty matrix ([]).
%
%   See also ADAPTSIMSTP.
%
%   Walter Gander, 08/03/98
%   Reference: Gander, Computermathematik, Birkhaeuser, 1992.

global termination2

  termination2 = 0;
  if (nargin < 4), tol = []; end;
  if (nargin < 5), trace = []; end;
  if (isempty(tol)), tol = eps; end;
  if (isempty(trace)), trace = 0; end;
  if tol<eps
      tol= eps;
  end
  x = [a (a+b)/2 b];
  y = feval(f, x, varargin{:});
  fa = y(1); fm = y(2); fb = y(3);
  yy = feval(f, a+[.9501 .2311 .6068 .4860 .8913]*(b-a),...
       varargin{:});
  is = (b - a)/8*(sum(y)+sum(yy));
  if is==0, is = b-a; end;
  is = is*tol/eps;
  Q = adaptsimstp(f,a,b,fa,fm,fb,is,trace,varargin{:});


function Q = adaptsimstp (f,a,b,fa,fm,fb,is,trace,varargin)
%ADAPTSIMSTP  Recursive function used by ADAPTSIM.
%
%   Q = ADAPTSIMSTP('F',A,B,FA,FM,FB,IS,TRACE) tries to
%   approximate the integral of F(X) from A to B to
%   an appropriate relative error. The argument 'F' is
%   a string containing the name of f. The remaining
%   arguments are generated by ADAPTSIM or by recursion.
%
%   See also ADAPTSIM.
%
%   Walter Gander, 08/03/98

global termination2

  m = (a + b)/2; h = (b - a)/4;
  x = [a + h, b - h];
```

```
y = feval(f, x, varargin{:});
fml = y(1); fmr = y(2);
i1 = h/1.5 * (fa + 4*fm + fb);
i2 = h/3 * (fa + 4*(fml + fmr) + 2*fm + fb);
i1 = (16*i2 - i1)/15;
if (is + (i1-i2) == is) | (m <= a) | (b<=m),
  if ((m <= a) | (b<=m)) & (termination2==0);
     warning(['Interval contains no more machine number.',...
              'Required tolerance may not be met.']);
     termination2 =1;
  end;
  Q = i1;
  if (trace), disp([a b-a Q]), end;
else
  Q = adaptsimstp (f,a,m,fa,fml,fm,is,trace,varargin{:}) + ...
      adaptsimstp (f,m,b,fm,fmr,fb,is,trace,varargin{:});
end;
```

The minimal number of function evaluations is 10, which is attained if the error test is met in the very first call to `adaptsimstp`.

Discontinuous functions are integrated quite well by `adaptsim`. For example, if we integrate

$$f(x) = \begin{cases} x+1, & x < 1 \\ 3-x, & 1 \le x \le 3 \\ 2, & x > 3 \end{cases} \tag{3.2}$$

on $[0,5]$ with `adaptsim('f',0,5,1e-6)`, i.e., with $tol = 10^{-6}$, we obtain instead of the exact value 7.5 the value 7.49996609147638 with 98 function evaluations. Using quad with the same tolerance $tol = 10^{-6}$, one obtains the value 7.50227769215902 (correct to only 3 digits) with 88 function evaluations. The difference in performance is due to the different termination criteria and the artificial limitation to 10 recursion levels used in quad.

4 Adaptive Lobatto quadrature.

4.1 The basic quadrature rule.

As basic quadrature rule we use the Gauss–Lobatto rule with two (symmetric) interior nodes. On the canonical interval $[-1,1]$, the two interior nodes are the zeros of $\pi_2(x)$, where

$$\int_{-1}^{1} (1-x^2)\pi_2(x)p(x)\,dx = 0 \quad \text{for all} \quad p \in \mathbb{P}_1.$$

Thus, up to a constant factor, π_2 is the Jacobi polynomial $P_2^{(\alpha,\beta)}$ of degree 2 corresponding to parameters $\alpha = \beta = 1$. Since $P_2^{(1,1)}(x) = \text{const} \cdot (x^2 - \frac{1}{5})$, the

interior nodes are $x_{\pm 1} = \pm\frac{1}{\sqrt{5}}$. By symmetry, the formula has the form

$$\int_{-1}^{1} f(x)\,dx = a[f(-1)+f(1)] + b\Big[f(-\tfrac{1}{\sqrt{5}}) + f(\tfrac{1}{\sqrt{5}})\Big] + R^{GL}(f),$$

where

$$R^{GL}(f) = 0 \quad \text{for} \quad f \in \mathbb{P}_5.$$

Exactness for $f(x) = 1$ and $f(x) = x^2$ yields

$$\left.\begin{array}{rcl} 2a + 2b &=& 2 \\ 2a + \frac{2}{5}b &=& \frac{2}{3} \end{array}\right\} \quad \text{hence} \quad a = \tfrac{1}{6},\ b = \tfrac{5}{6}.$$

Thus, the basic quadrature rule on $[-1,1]$ is

$$\int_{-1}^{1} f(x)\,dx = \tfrac{1}{6}[f(-1)+f(1)] + \tfrac{5}{6}\Big[f(-\tfrac{1}{\sqrt{5}}) + f(\tfrac{1}{\sqrt{5}})\Big] + R^{GL}(f). \tag{4.1}$$

We note that using Maple one can compute the basic quadrature rule directly by means of the ansatz $a(f(-1)+f(1)) + b(f(-x1)+f(x1))$ and requiring that it be exact for $f(x) = 1, x^2$ and x^4:

```
u1 := 2*a +2*b:
u2 := 2*a + 2*b*x1^2:
u3 :=  2*a + 2*b*x1^4:
solve({u1=2, u2=2/3, u3=2/5},{a,b,x1});
```

The result is:

$$\left\{x1 = RootOf(5\_Z^2 - 1),\ a = 1/6,\ b = 5/6\right\},$$

in agreement with (4.1).

4.2 Kronrod extension of the Gauss–Lobatto formula.

To estimate the error of (4.1) we construct the Kronrod extension of (4.1). (For background information and history on Gauss–Kronrod extensions see, e.g., [7].) By a well-known theorem on quadrature rules of maximum algebraic degree of exactness (cf. [8, Theorem 3.2.1]), the three Kronrod points are the zeros of $\pi_3^*(x)$, a (monic) polynomial of degree 3 satisfying

$$\int_{-1}^{1} (1-x^2)\pi_2(x)\pi_3^*(x)p(x)\,dx = 0 \quad \text{for all} \quad p \in \mathbb{P}_2.$$

Here, $\pi_2(x) = x^2 - \frac{1}{5} =: \pi_1(x^2)$, and by symmetry

$$\pi_3^*(x) = x\pi_1^*(x^2)$$

for some $\pi_1^* \in \mathbb{P}_1$. It suffices, therefore, to choose $\pi_1^*(x^2)$ such that

$$\int_{-1}^{1} (1-x^2)\pi_1(x^2)\pi_1^*(x^2)x^2\,dx = 0.$$

Putting $x^2 = t$ yields

$$\int_0^1 (1-t)\pi_1(t)\pi_1^*(t)t^{\frac{1}{2}}dt = 0,$$

and, with $\pi_1^*(t) = t - c$, we obtain

$$\int_0^1 (1-t)(t-\tfrac{1}{5})(t-c)t^{\frac{1}{2}}dt = 0,$$

that is,

$$c\int_0^1 t^{\frac{1}{2}}(t^2 - \tfrac{6}{5}t + \tfrac{1}{5})dt = \int_0^1 t^{\frac{3}{2}}(t^2 - \tfrac{6}{5}t + \tfrac{1}{5})dt,$$

giving $32c = \frac{64}{3}$, or $c = \frac{2}{3}$. The three Kronrod points, therefore, are

$$x_{\pm 1}^* = \pm\sqrt{\tfrac{2}{3}}, \qquad x_0^* = 0.$$

By symmetry, the Kronrod extension has the form

$$\int_{-1}^1 f(x)\,dx = A[f(-1) + f(1)] + B\left[f\Big(-\sqrt{\tfrac{2}{3}}\Big) + f\Big(\sqrt{\tfrac{2}{3}}\Big)\right] + C\left[f(-\tfrac{1}{\sqrt{5}}) + f(\tfrac{1}{\sqrt{5}})\right] + Df(0) + R^{GLK}(f),$$

where

$$R^{GLK}(f) = 0 \quad \text{for} \quad f \in \mathbb{P}_9.$$

Exactness for $f(x) = 1, x^2, x^4, x^6$ yields

$$\begin{aligned}
2A \quad &+2B \quad &+2C &+D &= 2,\\
2A &+2\cdot\tfrac{2}{3}B &+2\cdot\tfrac{1}{5}C & &= \tfrac{2}{3},\\
2A &+2\cdot\tfrac{4}{9}B &+2\cdot\tfrac{1}{25}C & &= \tfrac{2}{5},\\
2A &+2\cdot\tfrac{8}{27}B &+2\cdot\tfrac{1}{125}C & &= \tfrac{2}{7}.
\end{aligned}$$

Gauss elimination gives

$$A = \tfrac{11}{210}, \quad B = \tfrac{72}{245}, \quad C = \tfrac{125}{294}, \quad D = \tfrac{16}{35}.$$

Thus,

$$\int_{-1}^1 f(x)\,dx = \tfrac{11}{210}[f(-1) + f(1)] + \tfrac{72}{245}\left[f(-\sqrt{\tfrac{2}{3}}) + f(\sqrt{\tfrac{2}{3}})\right] + \tfrac{125}{294}\left[f(-\tfrac{1}{\sqrt{5}}) + f(\tfrac{1}{\sqrt{5}})\right] + \tfrac{16}{35}f(0) + R^{GLK}(f). \tag{4.2}$$

Again, we can compute this extension directly, using Maple and the ansatz

$$A[f(-1) + f(1)] + B[f(-x1) + f(x1)] + C[f(-1/\sqrt{5}) + f(1/\sqrt{5})] + Df(0),$$

requiring exactness for $f(x) = 1, x^2, x^4, x^6$ and x^8:

```
x2 := 1/sqrt(5);
u1 := 2*A + 2*B +2*C +D = 2;
u2 := 2*A + 2*B*x1^2 + 2*C*x2^2 = 2/3;
u3 := 2*A + 2*B*x1^4 + 2*C*x2^4 = 2/5;
u4 := 2*A + 2*B*x1^6 + 2*C*x2^6 = 2/7;
u5 := 2*A + 2*B*x1^8 + 2*C*x2^8 = 2/9;
solve({u1,u2,u3,u4,u5},{A,B,C,D,x1});
```

The result, as above, is:

$$\{B = \tfrac{72}{245},\ A = \tfrac{11}{210},\ D = \tfrac{16}{35},\ C = \tfrac{125}{294},\ x1 = RootOf(3\_Z^2 - 2)\}.$$

4.3 Kronrod extension of (4.2).

It will be desirable to estimate how much more accurate (4.2) is compared to (4.1). We try to estimate the respective errors by constructing a Kronrod extension of (4.2), hoping that one exists with real nodes and positive weights. There will be six symmetrically located Kronrod points $\pm x_1, \pm x_2, \pm x_3$, which, it is hoped, interlace with the nodes of (4.2). Again, on the basis of [8, Theorem 3.2.1], with $n = 13$ and

$$\omega_n(x) = (x^2 - 1)\big(x^2 - \tfrac{2}{3}\big)\big(x^2 - \tfrac{1}{5}\big)x\pi_6^*(x),$$
$$\pi_6^*(x) = (x^2 - x_1^2)(x^2 - x_2^2)(x^2 - x_3^2),$$

the 13-point quadrature rule to be constructed will have degree of exactness $d = 12 + k$ provided that π_6^* is chosen to satisfy the "orthogonality" condition

$$\int_{-1}^{1} (x^2 - 1)(x^2 - \tfrac{2}{3})(x^2 - \tfrac{1}{5})x\pi_6^*(x)p(x)\,dx = 0 \quad \text{for all } \ p \in \mathbb{P}_{k-1}.$$

The optimal value of k is $k = 6$, yielding a formula of degree $d = 18$ (actually, $d = 19$ because of symmetry). If we let

$$\alpha_i = x_i^2, \quad i = 1, 2, 3,$$

and make the substitution $x^2 = t$, $\pi_6^*(x) = \pi_3^*(x^2)$, the orthogonality relation becomes

$$\int_0^1 (t - 1)(t - \tfrac{2}{3})(t - \tfrac{1}{5})\sqrt{t}\pi_3^*(t)p(t)dt = 0 \quad \text{for all } \ p \in \mathbb{P}_2,$$

where

$$\pi_3^*(t) = (t - \alpha_1)(t - \alpha_2)(t - \alpha_3) = t^3 - at^2 + bt - c.$$

Putting $p(t) = 1, t, t^2$ in this relation, one finds, after some tedious calculations, that the coefficients a, b, c must satisfy

$$\begin{aligned} 30a \quad -13b \quad\quad\ \ &= 35, \\ 595a \quad -510b \quad +221c \ &= 588, \\ 11172a \ -11305b \ +9690c \ &= 10395. \end{aligned}$$

Solving for a, b, c gives

$$a = \tfrac{37975}{27987}, \quad b = \tfrac{4095}{9329}, \quad c = \tfrac{9737}{475779},$$

and then solving the cubic equation $\pi_3^*(t) = 0$ yields, with the help of Maple, to 38 decimal digits,

$$\begin{aligned}
\alpha_1 &= .88902724982774341965844097377815423496,\\
\alpha_2 &= .41197571308045073755318461761021278774,\\
\alpha_3 &= .05587701708251581527560062078156901902 6,
\end{aligned}$$

and hence

$$\begin{aligned}
x_1 &= \sqrt{\alpha_1} = .94288241569547971905635175843185720232,\\
x_2 &= \sqrt{\alpha_2} = .64185334234578130578123554132903188354,\\
x_3 &= \sqrt{\alpha_3} = .23638319966214988028222377349205292599.
\end{aligned}$$

It is a fortunate circumstance that the α_i turn out to be all positive, hence also the x_i, and moreover the $\pm x_i$ interlace with the nodes of (4.2).

Alternatively, Maple can be used to compute the zeros of π_3^* directly as follows:

```
restart;
Digits :=40;
pis := t->(t-a1)*(t-a2)*(t-a3);
sols := solve({int((t-1)*(t-2/3)*(t-1/5)*sqrt(t)*pis(t),t=0..1)=0,
       int((t-1)*(t-2/3)*(t-1/5)*sqrt(t)*pis(t)*t,t=0..1)=0,
       int((t-1)*(t-2/3)*(t-1/5)*sqrt(t)*pis(t)*t^2,t=0..1)=0},
       {a1,a2,a3}):
evalf(sols);
```

The desired Kronrod extension has the form

$$\begin{aligned}
\int_{-1}^{1} f(x)\,dx = {} & A[f(-1)+f(1)] + B[f(-x_1)+f(x_1)] + C\left[f\Big(-\sqrt{\tfrac{2}{3}}\Big) + f\Big(\sqrt{\tfrac{2}{3}}\Big)\right]\\
& + D[f(-x_2)+f(x_2)] + E\left[f(-\tfrac{1}{\sqrt{5}}) + f(\tfrac{1}{\sqrt{5}})\right]\\
& + F[f(-x_3)+f(x_3)] + Gf(0) + R^{GLKK}(f), \quad R^{GLKK}(\mathbb{P}_{19}) = 0. \qquad (4.3)
\end{aligned}$$

Exactness for the first seven powers of x^2 yields, after division by 2, the system

$$\begin{aligned}
A \quad &+B \quad &&+C \quad &&+D \quad &&+E \quad &&+F &&+\tfrac{1}{2}G &&= 1,\\
A &+\alpha_1 B &&+\tfrac{2}{3}C &&+\alpha_2 D &&+\tfrac{1}{5}E &&+\alpha_3 F &&&&= \tfrac{1}{3},\\
A &+\alpha_1^2 B &&+\tfrac{4}{9}C &&+\alpha_2^2 D &&+\tfrac{1}{25}E &&+\alpha_3^2 F &&&&= \tfrac{1}{5},\\
A &+\alpha_1^3 B &&+\tfrac{8}{27}C &&+\alpha_2^3 D &&+\tfrac{1}{125}E &&+\alpha_3^3 F &&&&= \tfrac{1}{7},\\
A &+\alpha_1^4 B &&+\tfrac{16}{81}C &&+\alpha_2^4 D &&+\tfrac{1}{625}E &&+\alpha_3^4 F &&&&= \tfrac{1}{9},\\
A &+\alpha_1^5 B &&+\tfrac{32}{243}C &&+\alpha_2^5 D &&+\tfrac{1}{3125}E &&+\alpha_3^5 F &&&&= \tfrac{1}{11},\\
A &+\alpha_1^6 B &&+\tfrac{64}{729}C &&+\alpha_2^6 D &&+\tfrac{1}{15625}E &&+\alpha_3^6 F &&&&= \tfrac{1}{13}.
\end{aligned}$$

The solution is, to 38 digits,

$$
\begin{aligned}
A &= .01582719197348018308716998633305510591,\\
B &= .09427384021885004553128250507710817196 0,\\
C &= .15507198733658539625363597980210298680,\\
D &= .18882157396018245442000533937297167125,\\
E &= .19977340522685852679206802206648840246,\\
F &= .22492646533333952701601768799639508076,\\
G &= .24261107190140773379964095790325635233.
\end{aligned}
$$

By good fortune, it consists of entirely positive entries.

Note that even here we can use Maple to obtain the result by "brute force". Using the ansatz (4.3) with unknown knots a_1, a_2 and a_3, and requiring that it be exact for the monomials $1, x^2, x^4, \ldots, x^{18}$, we obtain 10 nonlinear equations in 10 unknowns:

```
x1:=sqrt(2/3); x2:=sqrt(1/5);
u1:=2*A+2*B+2*C+2*D+2*E+2*F+G = 2;
u2:=2*A+2*B*a1^2+2*C*x1^2+2*D*a2^2+2*E*x2^2+2*F*a3^2 = 2/3;
u3:=2*A+2*B*a1^4+2*C*x1^4+2*D*a2^4+2*E*x2^4+2*F*a3^4 = 2/5;
u4:=2*A+2*B*a1^6+2*C*x1^6+2*D*a2^6+2*E*x2^6+2*F*a3^6 = 2/7;
u5:=2*A+2*B*a1^8+2*C*x1^8+2*D*a2^8+2*E*x2^8+2*F*a3^8 = 2/9;
u6:=2*A+2*B*a1^10+2*C*x1^10+2*D*a2^10+2*E*x2^10+2*F*a3^10 = 2/11;
u7:=2*A+2*B*a1^12+2*C*x1^12+2*D*a2^12+2*E*x2^12+2*F*a3^12 = 2/13;
u8:=2*A+2*B*a1^14+2*C*x1^14+2*D*a2^14+2*E*x2^14+2*F*a3^14 = 2/15;
u9:=2*A+2*B*a1^16+2*C*x1^16+2*D*a2^16+2*E*x2^16+2*F*a3^16 = 2/17;
u10:=2*A+2*B*a1^18+2*C*x1^18+2*D*a2^18+2*E*x2^18+2*F*a3^18 = 2/19;
sols:=solve({u1,u2,u3,u4,u5,u6,u7,u8,u9,u10},
            {A,B,C,D,E,F,G,a1,a2,a3});
```

Maple solves this system in 7 minutes on a SUN Sparcstation 20/514 (50 MHz SuperSparc processor) and gives a solution containing very complicated expressions (several pages long). However, evaluating the expressions as floating point numbers (`Digits:=15; evalf(sols);`) yields (rounded to 10 digits)

```
{a1 = -.2363831997, a2 = -.6418533423, E = .1997734052,
 a3 = -.9428824157, D = .1888215742, F = .09427384020,
 G = .2426110719, B = .2249264653, C = .1550719873,
 A = .01582719197},
```

a permutation of the solution given above.

4.4 The adaptive procedure.

For an arbitrary interval $[a, b]$, the formulae (4.1) and (4.2) can be written respectively as

$$
\int_a^b f(x)\,dx \approx \frac{h}{6}\{f(a)+f(b)+5[f(m-\beta h)+f(m+\beta h)]\} \tag{4.4}
$$

and

$$\int_a^b f(x)\,dx \approx \frac{h}{1470}\{77[f(a)+f(b)]+432[f(m-\alpha h)+f(m+\alpha h)]$$
$$+625[f(m-\beta h)+f(m+\beta h)]+672f(m)\}, \tag{4.5}$$

where

$$h=\frac{1}{2}(b-a), \qquad m=\frac{1}{2}(a+b), \qquad \alpha=\frac{\sqrt{2}}{\sqrt{3}}, \qquad \beta=\frac{1}{\sqrt{5}}.$$

A similar reformulation holds for (4.3).

The adaptive Lobatto procedure is similar to the adaptive Simpson procedure of Section 3, with the second Kronrod extension (i.e., the formula (4.3) relative to the initial interval $[a,b]$) providing the estimate is, and (4.4) and (4.5) playing the roles of $i2$ and $i1$, respectively. There are three additional features, however:

(i) If the ratio ρ of the error of (4.5) and the error of (4.4), as determined for the initial interval $[a,b]$ by comparison with is, is less than 1, then the basic error tolerance tol is relaxed to tol/ρ, since we always accept the more accurate approximation (4.5). (A similar relaxation of the tolerance has already been suggested by Lyness in [12, Modification 1].)

(ii) At each recursive level, the current interval $[a,b]$ is subdivided into six subintervals when the error tolerance is not met, namely the intervals $[a,m-\alpha h]$, $[m-\alpha h,m-\beta h]$, $[m-\beta h,m]$, $[m,m+\beta h]$, $[m+\beta h,m+\alpha h]$, and $[m+\alpha h,b]$ determined by (4.4) and (4.5). In this way, all function values computed are being reused.

(iii) Consistent with (ii), the termination criterion (2.7) is modified by replacing the last two conditions by $m-\alpha h \le a$ and $b \le m+\alpha h$, respectively.

The adaptive Lobatto procedure requires five new values of f to be computed at each level of the recursion.

4.5 Matlab code.

The adaptive Lobatto procedure is implemented by the recursive Matlab program below.

```
function Q=adaptlob(f,a,b,tol,trace,varargin)
%ADAPTLOB  Numerically evaluate integral using adaptive
%   Lobatto rule.
%
%   Q=ADAPTLOB('F',A,B) approximates the integral of
%   F(X) from A to B to machine precision.  'F' is a
%   string containing the name of the function. The
%   function F must return a vector of output values if
%   given a vector of input values.
```

```
%
%   Q=ADAPTLOB('F',A,B,TOL) integrates to a relative
%   error of TOL.
%
%   Q=ADAPTLOB('F',A,B,TOL,TRACE) displays the left
%   end point of the current interval, the interval
%   length, and the partial integral.
%
%   Q=ADAPTLOB('F',A,B,TOL,TRACE,P1,P2,...) allows
%   coefficients P1,... to be passed directly to the
%   function F:  G=F(X,P1,P2,...). To use default values
%   for TOL or TRACE, one may pass the empty matrix ([]).
%
%   See also ADAPTLOBSTP.

%   Walter Gautschi, 08/03/98
%   Reference: Gander, Computermathematik, Birkhaeuser, 1992.

global termination2

  termination2 = 0;
  if(nargin<4), tol=[]; end;
  if(nargin<5), trace=[]; end;
  if(isempty(tol)), tol=eps; end;
  if(isempty(trace)), trace=0; end;
  if tol < eps
    tol = eps;
  end
  m=(a+b)/2; h=(b-a)/2;
  alpha=sqrt(2/3); beta=1/sqrt(5);
  x1=.942882415695480; x2=.641853342345781;
  x3=.236383199662150;
  x=[a,m-x1*h,m-alpha*h,m-x2*h,m-beta*h,m-x3*h,m,m+x3*h,...
    m+beta*h,m+x2*h,m+alpha*h,m+x1*h,b];
  y=feval(f,x,varargin{:});
  fa=y(1); fb=y(13);
  i2=(h/6)*(y(1)+y(13)+5*(y(5)+y(9)));
  i1=(h/1470)*(77*(y(1)+y(13))+432*(y(3)+y(11))+ ...
     625*(y(5)+y(9))+672*y(7));
  is=h*(.0158271919734802*(y(1)+y(13))+.0942738402188500 ...
     *(y(2)+y(12))+.155071987336585*(y(3)+y(11))+ ...
     .188821573960182*(y(4)+y(10))+.199773405226859 ...
     *(y(5)+y(9))+.224926465333340*(y(6)+y(8))...
     +.242611071901408*y(7));
  s=sign(is); if(s==0), s=1; end;
```

```
  erri1=abs(i1-is);
  erri2=abs(i2-is);
  R=1; if(erri2~=0), R=erri1/erri2; end;
  if(R>0 & R<1), tol=tol/R; end;
  is=s*abs(is)*tol/eps;
  if(is==0), is=b-a, end;
  Q=adaptlobstp(f,a,b,fa,fb,is,trace,varargin{:});


function Q=adaptlobstp(f,a,b,fa,fb,is,trace,varargin)
%ADAPTLOBSTP  Recursive function used by ADAPTLOB.
%
%   Q = ADAPTLOBSTP('F',A,B,FA,FB,IS,TRACE) tries to
%   approximate the integral of F(X) from A to B to
%   an appropriate relative error. The argument 'F' is
%   a string containing the name of f.  The remaining
%   arguments are generated by ADAPTLOB or by recursion.
%
%   See also ADAPTLOB.

%   Walter Gautschi, 08/03/98

global termination2

  h=(b-a)/2; m=(a+b)/2;
  alpha=sqrt(2/3); beta=1/sqrt(5);
  mll=m-alpha*h; ml=m-beta*h; mr=m+beta*h; mrr=m+alpha*h;
  x=[mll,ml,m,mr,mrr];
  y=feval(f,x,varargin{:});
  fmll=y(1); fml=y(2); fm=y(3); fmr=y(4); fmrr=y(5);
  i2=(h/6)*(fa+fb+5*(fml+fmr));
  i1=(h/1470)*(77*(fa+fb)+432*(fmll+fmrr)+625*(fml+fmr) ...
     +672*fm);
  if(is+(i1-i2)==is) | (mll<=a) | (b<=mrr),
   if ((m <= a) | (b<=m)) & (termination2==0);
       warning(['Interval contains no more machine number. ',...
                'Required tolerance may not be met.']);
       termination2 =1;
    end;
    Q=i1;
    if(trace), disp([a b-a Q]), end;
  else
    Q=adaptlobstp(f,a,mll,fa,fmll,is,trace,varargin{:})+...
      adaptlobstp(f,mll,ml,fmll,fml,is,trace,varargin{:})+...
      adaptlobstp(f,ml,m,fml,fm,is,trace,varargin{:})+...
```

```
    adaptlobstp(f,m,mr,fm,fmr,is,trace,varargin{:})+...
    adaptlobstp(f,mr,mrr,fmr,fmrr,is,trace,varargin{:})+...
    adaptlobstp(f,mrr,b,fmrr,fb,is,trace,varargin{:});
end;
```

The minimal number of function evaluations is 18 and occurs if the error test is met in the very first call to `adaptlobstp`. This can be expected only in cases where f is very regular on $[a, b]$ and the tolerance *tol* is not too stringent. Discontinuities of f in the interior of $[a, b]$, on the other hand, cannot be expected to be handled efficiently by our routine; but the routine has been observed to cope rather efficiently with other difficult behavior, as long as f remains bounded on the interval $[a, b]$ and smooth in its interior.

5 Test results.

In comparing adaptive quadrature routines, one must take into account a number of characteristics, of which the more important ones are:

(i) *efficiency*, as measured by the number of function evaluations required to meet a given error tolerance;

(ii) *reliability*, the extent to which the requested error tolerance is achieved; and

(iii) *tolerance responsiveness*, the extent to which the efficiency is sensitive to changes in the error tolerance.

We will try to convey these characteristics graphically by displaying a histogram over four tolerances: $tol = eps$ (the machine precision[1]), $tol = 10^{-9}$, $tol = 10^{-6}$, and $tol = 10^{-3}$, the height of each of the four bars in the histogram indicating the number of function evaluations in a logarithmic scale. A bar that is completely white signifies that the requested tolerance has been attained; a shaded bar means that the result produced has a relative error that exceeds the tolerance by a factor larger than 1 but less than or equal to 10. A black bar indicates a discrepancy by a factor larger than 10. Thus, a white bar identifies a routine that is reliable for the tolerance in question, a shaded bar one that is slightly unreliable, and a black bar one that might be severely unreliable. The tolerance responsiveness can be seen from how rapidly the histogram falls off with decreasing tolerance. A histogram that is flat (or partially flat) at relatively high numbers of function evaluations indicates poor tolerance responsiveness.

We compared our routines `adaptsim` and `adaptlob` with the worst and best routines in the IMSL library (`DQDAG`, `DQDAGS`), the worst and best routines of the NAG library (`D01AHF`, `D01AJF`, `D01AKF`), and with the routines `quad` and `quad8` from Matlab. The results are displayed in the 23 histograms of Table 2 in [5, pp. 17–20], of which the first 21 refer to Kahaner's collection of test functions [11] and the last two to functions taken from [6]. Here, in Figure 5.1 we present

[1]The choice $tol = eps$ makes our routines, especially `adaptsim`, work much harder than necessary, without yielding any noticeable gain in accuracy compared to, say, $tol = 10 \cdot eps$.

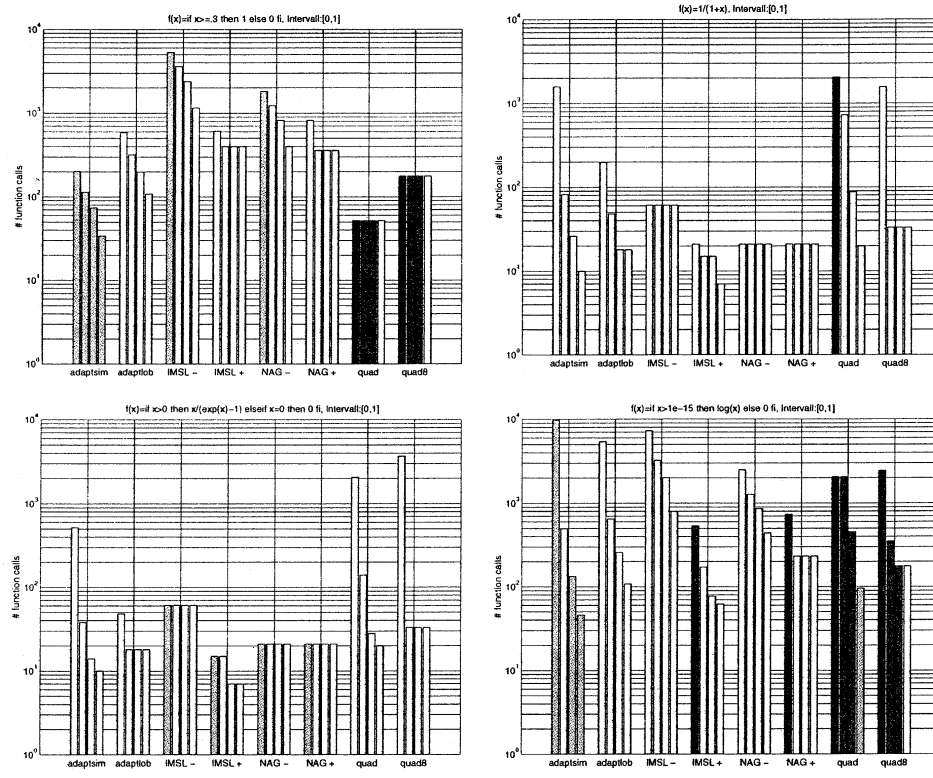

Figure 5.1: Comparison with other adaptive quadrature routines.

four typical examples. The tests were conducted on three different machines with four different versions of Matlab: SGI 02 R5000 (Matlab 5.0 and 5.1), HP A 9000/770 (Matlab 5.0), and SUN SPARCstation 20 (Matlab 5.0, 5.1, 5.2, and 5.2.1). The results were nearly identical. (The only significant difference was observed in connection with function #22, for which the routine `adaptsim` with *tol* = *eps*—and only for this tolerance—on the machine SGI 02 returns a totally false answer with the minimum number 10 of function evaluations, whereas on the SUN SPARCstation it integrates the function correctly in 49926 function calls.) The graphics shown is based on the results obtained on the SUN SPARCstation with Matlab version 5.0. The tests of the NAG and IMSL routines were carried out in fortran on the HP/Convex Exemplar SPP2000/X-32 machine.

The following observations can be made.

- In terms of efficiency, the routine `adaptlob` performs distinctly better than `adaptsim` when the accuracy requirement is high. For machine precision *eps* it outperforms `adaptsim` in all but one example, and often significantly so. (The one exception is the discontinuous function #2, for which, however, `adaptsim` is slightly unreliable.) For the accuracy tolerance 10^{-9}, it

does so in about half the cases. For lower tolerances, `adaptsim` is generally (but not always) more efficient than `adaptlob`, but less reliable.

- Compared with the other routines, those of the IMSL and NAG libraries are the most serious competitors. The best of them performs distinctly better than our routines in about one-third of the cases.

- In terms of reliability, the routine `adaptlob` is by far the best, exhibiting only one serious failure out of the $4 \cdot 23 = 92$ individual runs. It is followed by the IMSL and NAG library routines, which failed 6 or 7 times. The routines `quad` and `quad8` are by far the least reliable, having seriously failed in 30 resp. 15 cases. It is perhaps of interest to note that the second half of the termination criterion (2.7) for `adaptsim` and the analogous one for `adaptlob` has never been invoked in any of the 23 test cases. As already observed in Section 2, there are cases, however, for example the function $f(x) = \frac{1}{\sqrt{1-x^2}}$ for $0 \le x < 1$ and $f(1) = 0$, where for $tol = eps$ that part of the stopping criterion is indeed activated, both in `adaptsim` and `adaptlob`. Also for the example (3.2) and $tol = eps$, one of our routines, `adaptlob` (but not the other), terminates in this manner.

- Both of our routines show excellent response to changes in the tolerance, in contrast to some of the other routines, where the response is more sluggish.

In view of these (admittedly limited) test results it would appear that the routines `adaptsim` and `adaptlob` are worthy contenders for inclusion in software libraries.

Acknowledgments.

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19.13. [166] "COMPUTING THE HILBERT TRANSFORM OF THE GENERALIZED LAGUERRE AND HERMITE WEIGHT FUNCTIONS"

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COMPUTING THE HILBERT TRANSFORM OF THE GENERALIZED LAGUERRE AND HERMITE WEIGHT FUNCTIONS *

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Abstract.

Explicit formulae are given for the Hilbert transform $\int_{\mathbb{R}} w(t)dt/(t-x)$, where w is either the generalized Laguerre weight function $w(t) = 0$ if $t \leq 0$, $w(t) = t^{\alpha}e^{-t}$ if $0 < t < \infty$, and $\alpha > -1$, $x > 0$, or the Hermite weight function $w(t) = e^{-t^2}$, $-\infty < t < \infty$, and $-\infty < x < \infty$. Furthermore, numerical methods of evaluation are discussed based on recursion, contour integration and saddle-point asymptotics, and series expansions. We also study the numerical stability of the three-term recurrence relation satisfied by the integrals $\int_{\mathbb{R}} \pi_n(t;w)w(t)dt/(t-x)$, $n = 0, 1, 2, \ldots$, where $\pi_n(\,\cdot\,;w)$ is the generalized Laguerre, resp. the Hermite, polynomial of degree n.

AMS subject classification: 65D30, 65D32, 65R10.

Key words: Hilbert transform, classical weight functions, computational methods.

1 Introduction.

In [5], the Hilbert transform of the Jacobi weight function is considered and a combination of analytic and numerical methods for its evaluation set forth. In this paper we consider the Hilbert transform of the remaining classical weight functions, namely the generalized Laguerre, and the Hermite, weight function. For the former, unlike the Jacobi weight, no analytic results seem to exist in the literature (except for the ordinary Laguerre weight). Here we express it in terms of Tricomi's incomplete gamma function and also propose numerical methods using a recurrence relation, contour integration and saddle-point asymptotics, and series expansions. For the Hermite weight, the Hilbert transform is expressed in terms of Dawson's integral. A similar expression holds for the generalized Laguerre weight with parameter $\alpha = -\frac{1}{2}$.

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2 The generalized Laguerre weight.

The problem we wish to consider is to evaluate

$$I_\alpha(x) = \fint_0^\infty \frac{t^\alpha e^{-t}}{t-x}\,dt, \quad \alpha > -1, \quad x > 0, \tag{2.1}$$

where the integral is taken in the sense of the Cauchy principal value. For $\alpha = 0$, the result is expressible in terms of an exponential integral (cf. [1, Ch. 5]),

$$I_0(x) = -e^{-x} \fint_{-\infty}^x \frac{e^t}{t}\,dt = -e^{-x}\,\mathrm{Ei}(x), \tag{2.2}$$

and for general α, as will be shown in Section 2.3, in terms of Tricomi's incomplete gamma function.

2.1 Recurrence relation.

In principle it suffices to know $I_\alpha(x)$ for $0 < \alpha \le 1$, since there is a simple relationship between $I_\alpha(x)$ and $I_{\alpha-1}(x)$. Indeed, from (2.1), writing

$$\frac{t^\alpha}{t-x} = \frac{t}{t-x}\,t^{\alpha-1} = \left(1 + \frac{x}{t-x}\right) t^{\alpha-1},$$

one obtains the recurrence relation

$$I_\alpha(x) = \Gamma(\alpha) + xI_{\alpha-1}(x). \tag{2.3}$$

If $0 < \alpha \le 1$ and the left side is known, we can solve for the last term on the right and obtain $I_{\alpha-1}(x)$ for $-1 < \alpha - 1 \le 0$. For $\alpha = 1$, we simply have $I_1(x) = 1 + xI_0(x) = 1 - xe^{-x}\,\mathrm{Ei}(x)$. To compute $I_{\alpha+n}(x)$ for $0 < \alpha \le 1$ and $n = 1, 2, \ldots$, let

$$y_n = \frac{I_{\alpha+n}(x)}{\Gamma(\alpha+n)}, \quad n = 0, 1, 2, \ldots, \quad 0 < \alpha \le 1. \tag{2.4}$$

Then (2.3) yields the first-order inhomogeneous difference equation

$$\begin{aligned} y_n &= 1 + \frac{x}{\alpha+n-1}\,y_{n-1}, \quad n = 1, 2, 3, \ldots, \\ y_0 &= I_\alpha(x)/\Gamma(\alpha). \end{aligned} \tag{2.5}$$

This recursion is quite stable, as can be seen from the behavior of the "amplification factors"

$$\rho_n = \frac{y_0 h_n}{y_n}, \quad h_n = \frac{x^n \Gamma(\alpha)}{\Gamma(\alpha+n)}, \tag{2.6}$$

which measure the amplification of relative errors, assuming $y_n \neq 0$. More precisely (cf. [6]), ρ_t/ρ_s measures the amplification (or damping, as it were) at $n = t$ of a small relative error committed at $n = s$. The quantity h_n in (2.6) is the

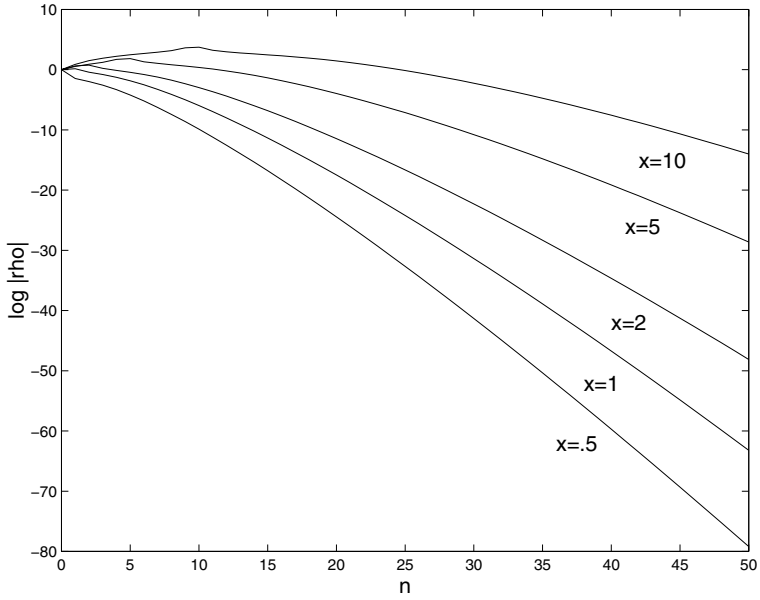

Figure 2.1: Amplification factors for the recursion (2.5).

solution, with $h_0 = 1$, of the homogeneous recurrence relation associated with (2.5).

Figure 2.1 displays $|\rho_n|$ on a logarithmic scale for $\alpha = \frac{1}{2}$ and $x = 0.5, 1, 2, 5, 10$. The value $\alpha = \frac{1}{2}$ is representative for all other values of α in the interval $(0, 1]$, even very small ones. Although ρ_n is defined only for nonnegative integer values of n, the plots are drawn continuously by linear interpolation between consecutive integer arguments. If y_n happens to be zero, or almost zero, then $|\rho_n|$ is infinite or very large, which, however, should not be taken too seriously, since for such values of n it is normally the absolute error that matters, not the relative error. An instance of this is visible for the curve $x = 10$ near $n = 10$.

2.2 Contour integration.

Closely related to the integral $I_\alpha(x)$, but in some sense more fundamental than $I_\alpha(x)$, is the contour integral

$$G_\alpha(x) = \frac{1}{2\pi i} \int_C \frac{(-t)^\alpha e^{-t}}{t - x} dt, \tag{2.7}$$

where the contour C starts at $+\infty + i\varepsilon$, $\varepsilon > 0$, encircles the origin once counterclockwise, and returns to $+\infty - i\varepsilon$. In order to compute this integral, we decompose the path of integration into $C = C_0 \cup C_1 \cup \cdots \cup C_6$ as shown in Figure 2.2. For brevity we write

$$f(t) = f_\alpha(t) = \frac{1}{2\pi i} \frac{(-t)^\alpha e^{-t}}{t - x}, \quad t \in \mathbb{C} \setminus \mathbb{R}_+ \tag{2.8}$$

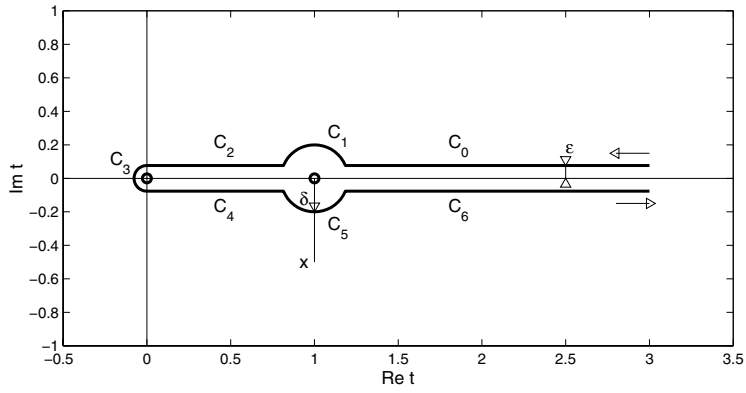

Figure 2.2: Path C of integration (for $x = 1$).

(suppressing in the notation the dependence on x) and restrict t to the cut plane as indicated in (2.8). The αth power is understood in the sense of the principal value. We then have the following limit relations, as ε and δ tend to zero in an appropriate manner, assuming $\alpha > -1$:

$$\lim \int_{C_0 \cup C_2} f(t)dt = -\frac{1}{2\pi i} e^{-i\alpha\pi} I_\alpha(x),$$

$$\lim \int_{C_4 \cup C_6} f(t)dt = \frac{1}{2\pi i} e^{i\alpha\pi} I_\alpha(x),$$

$$\lim \int_{C_3} f(t)dt = 0,$$

$$\lim \int_{C_1} f(t)dt = \tfrac{1}{2} e^{-i\alpha\pi} x^\alpha e^{-x},$$

$$\lim \frac{1}{2\pi i} \int_{C_5} f(t)dt = \tfrac{1}{2} e^{i\alpha\pi} x^\alpha e^{-x}.$$

Adding up all contributions yields

$$G_\alpha(x) = \frac{\sin \alpha\pi}{\pi} I_\alpha(x) + \cos \alpha\pi \cdot x^\alpha e^{-x}. \tag{2.9}$$

We remark that the definition (2.7) of $G_\alpha(x)$ makes sense for arbitrary $\alpha \in \mathbb{C}$. Moreover, the path C may be deformed to any path $\tilde{C}$ in $\mathbb{C} \setminus \mathbb{R}_+$ without changing the value of $G_\alpha(x)$ as long as $\tilde{C}$ enters through the first quadrant and leaves the fourth (with $\operatorname{Re} t \to \infty$). Therefore, the variable x need not be confined to $\mathbb{R}_+$ but can be arbitrary complex, provided the path $\tilde{C}$ is chosen to leave x on its left as it is run through. Consequently, $G_\alpha(x)$ is an entire function in both variables α and x. It will be identified in the next subsection.

Equation (2.9) may serve to define the analytic continuation of $I_\alpha(x)$ to every $x \in \mathbb{C}$ and $\alpha \in \mathbb{C} \setminus \mathbb{Z}$, by solving (2.9) for $I_\alpha(x)$:

$$I_\alpha(x) = \frac{\pi}{\sin \alpha\pi} \left[G_\alpha(x) - \cos \alpha\pi \cdot x^\alpha e^{-x} \right]. \tag{2.10}$$

When $\alpha \to n$, $n \in \mathbb{N}_0$, since $I_\alpha(x)$ remains finite, one needs to use the rule of Bernoulli–L'Hospital, with

$$\frac{\partial}{\partial \alpha} G_\alpha(x)\Big|_{\alpha=n} = \frac{1}{2\pi i}\int_{\tilde{C}} f_n(t)\log(-t)dt. \tag{2.11}$$

2.3 Closed-form expression for $G_\alpha(x)$.

We now show that

$$G_\alpha(x) = e^{-x}\gamma^*(-\alpha, -x), \tag{2.12}$$

that is, by (2.10),

$$I_\alpha(x) = \frac{\pi}{\sin \alpha\pi} e^{-x}\left[\gamma^*(-\alpha, -x) - x^\alpha \cos \alpha\pi\right], \tag{2.13}$$

where γ^* is the incomplete gamma function as defined by Tricomi (cf. [7]), an entire function in both of its variables. It has the power series expansion

$$e^z\gamma^*(a, z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(a + k + 1)}, \quad a \in \mathbb{C},\ z \in \mathbb{C}. \tag{2.14}$$

We choose a contour $C = \tilde{C}$ in (2.7) such that the geometric series

$$\frac{1}{t - x} = \sum_{k=0}^{\infty} x^k t^{-(1+k)}$$

converges for every $t \in \tilde{C}$. Substitution in (2.7) yields

$$G_\alpha(x) = \sum_{k=0}^{\infty}(-x)^k \cdot \frac{-1}{2\pi i}\int_{\tilde{C}} (-t)^{\alpha-k-1}e^{-t}dt.$$

The integral on the right can be evaluated by the same integration technique as employed in Section 2.2. Using, in addition, the reflection formula for the gamma function,

$$\Gamma(z)\Gamma(1 - z) = \frac{\pi}{\sin \pi z} \tag{2.15}$$

with $z = k - \alpha + 1$, we find

$$-\frac{1}{2\pi i}\int_{\tilde{C}} (-t)^{\alpha-k-1}e^{-t}dt = \Gamma(\alpha - k)\frac{1}{\pi}\sin(k - \alpha + 1)\pi = \frac{1}{\Gamma(k - \alpha + 1)},$$

and thus

$$G_\alpha(x) = \sum_{k=0}^{\infty} \frac{(-x)^k}{\Gamma(k - \alpha + 1)}.$$

Comparison with (2.14) shows the validity of (2.12).

For $\alpha = n$, $n \in \mathbb{N}_0$, the function $\gamma^*(-\alpha, -x)$ is elementary (cf. [7, Eq. (2.2)]), namely

$$G_n(x) = (-x)^n e^{-x}.$$

2.4 The case $\alpha = -\frac{1}{2}$.

Here, we get from (2.13)

$$I_{-\frac{1}{2}}(x) = -\pi e^{-x}\gamma^*(\tfrac{1}{2}, -x).$$

Since (cf. [7, Eqs. (2.1),(1.6)])

$$\begin{aligned}\gamma^*(\tfrac{1}{2}, -x) &= \frac{1}{i\sqrt{\pi x}}\gamma(\tfrac{1}{2}, -x) = \frac{-i}{\sqrt{x}}\operatorname{erf}(i\sqrt{x}) \\ &= -\frac{i}{\sqrt{x}} \cdot \frac{2}{\sqrt{\pi}} \int_0^{i\sqrt{x}} e^{-t^2} dt = \frac{2}{\sqrt{\pi x}} \int_0^{\sqrt{x}} e^{t^2} dt,\end{aligned}$$

we find

$$I_{-\frac{1}{2}}(x) = -2\sqrt{\frac{\pi}{x}} F(\sqrt{x}), \tag{2.16}$$

where F is Dawson's integral

$$F(x) = e^{-x^2} \int_0^x e^{t^2} dt. \tag{2.17}$$

3 Numerical examples.

3.1 Contour integration.

The formula (2.10) lends itself to efficient numerical evaluation. Assuming $x > 0$, $\alpha > -1$, we take the path $C = \tilde{C}$ in (2.7) to be a parabola with focus at $t = 0$ opening in the direction of the positive real axis. Reversing the direction of integration (and hence changing the sign of the integral), we accomplish this by introducing the new variable of integration $s = i\sqrt{-t}$, i.e., $t = s^2$, and letting s vary on a horizontal line $s = \sigma + i\tau$, $-\infty < \sigma < \infty$, from left to right, where $\tau > 0$ is a constant. The integral (2.7) then becomes

$$G_\alpha(x) = \int g(s)ds, \quad g(s) = -\frac{1}{\pi i} \frac{s(-s^2)^\alpha e^{-s^2}}{s^2 - x}. \tag{3.1}$$

It is conveniently approximated by the rectangular (or trapezoidal) rule with stepsize $h > 0$,

$$T(h) := h \sum_{k=-\infty}^{\infty} g(kh + i\tau) = G_\alpha(x) + R(h). \tag{3.2}$$

According to general theory (cf., e.g. [4, Eq. 3.4.12]), the error $R(h)$ tends to zero exponentially fast in h^{-1} as $h \to 0$, i.e.,

$$R(h) = O(e^{-\gamma/h}), \quad h \to 0, \tag{3.3}$$

for some $\gamma > 0$.

In the following we estimate $\tau = \tau_0$ and $h = h_0$ in such a way that, approximately, $|R(h_0)| = \varepsilon$, where $\varepsilon > 0$ is a given error tolerance. To do this, we first

apply the Poisson summation formula (see, e.g., [8, p. 29]) to express $T(h)$ in terms of the Fourier transform

$$\hat{g}(\omega) = \int_{-\infty}^{\infty} g(s)e^{-i\omega s}ds, \quad \omega \in \mathbb{R}, \tag{3.4}$$

of g (where the path of integration is actually slightly above the real line to avoid the poles of g). The result is

$$T(h) = \sum_{\ell=-\infty}^{\infty} \hat{g}\left(\ell \cdot \frac{2\pi}{h}\right) \exp\left(-\ell \cdot \frac{2\pi}{h}\tau\right). \tag{3.5}$$

Since $G_\alpha(x) = \hat{g}(0)$, we obtain from (3.2) and (3.5)

$$R(h) = \sum_{\ell\neq 0} \hat{g}\left(\ell \cdot \frac{2\pi}{h}\right) \exp\left(-\ell \cdot \frac{2\pi}{h}\tau\right). \tag{3.6}$$

For small $h > 0$ we can estimate $R(h)$ by taking only the terms with $\ell = \pm 1$,

$$R(h) \simeq \hat{g}\left(-\frac{2\pi}{h}\right) \exp\left(\frac{2\pi}{h}\tau\right) + \hat{g}\left(\frac{2\pi}{h}\right) \exp\left(-\frac{2\pi}{h}\tau\right). \tag{3.7}$$

The values of $\hat{g}(\omega)$ for large positive and negative ω, on the other hand, can be approximated asymptotically by applying the saddle point method to the integral in (3.4). The "saddles" are the critical points for (3.4), i.e., the zeros of $(d/ds)(\log g(s) - i\omega s)$. There are four of them, namely the four roots of the equation

$$i\omega + 2s - \frac{2\alpha+1}{s} + \frac{2s}{s^2 - x} = 0. \tag{3.8}$$

Since the path of integration in (3.1) is lying in the upper half-plane, we are interested only in critical points in that half-plane, in particular those with smallest "strength" $|g(s)|$.

In order to find asymptotic expansions of the four zeros of (3.8) for large $|\omega|$, it suffices to find values of s such that the constant term $i\omega$ in (3.8) is asymptotically compensated as $|\omega| \to \infty$ by a single one of the remaining terms. In each of the three cases, the solution, s_0, may be found as a Laurent series in ω.

Case I. $i\omega + 2s = O(1)$. Here,

$$s_0 = i\left[-\frac{\omega}{2} + \frac{2\alpha - 1}{\omega} + \frac{8x + 2(2\alpha-1)^2}{\omega^3} + O(\omega^{-5})\right].$$

Case II. $i\omega - \dfrac{2\alpha+1}{s} = O(1)$. In this case,

$$s_0 = \frac{i\beta}{\omega}\left[1 - \frac{2\beta(1 - x^{-1})}{\omega^2} + O(\omega^{-4})\right],$$

where $\beta := -(2\alpha+1)$.

Case III. $i\omega + \dfrac{2s}{s^2-x} = O(1)$. Here,

$$s_0 = \pm\sqrt{x} + \frac{i}{\omega} \pm \frac{2\alpha + \frac{1}{2} - 2x}{\omega^2\sqrt{x}} + O(\omega^{-3}).$$

The saddle of Case I is in the upper half-plane only if $\omega \to -\infty$, whereas both saddles of Case III are in the upper half-plane if $\omega \to +\infty$. The saddle of Case II is seen to contribute only if $\omega \to +\infty$ and $\beta > 0$. (If $\beta = 0$ or $\beta < 0$, the saddle is not present at all, or is irrelevant, respectively.)

The saddle point method calls for evaluating the integrand (of (3.4)),

$$E(s) := \exp(\log g(s) - i\omega s), \tag{3.9}$$

at the relevant saddles and for adding up the contributions of all saddles on the deformed path of integration. To first order, the contribution of a saddle s_0 can be obtained by expanding the exponent in (3.9) about s_0 to second-order terms and integrating. The result is

$$\sqrt{\pi} E(s_0)[c(s_0)]^{-\frac{1}{2}} \quad \text{with } c(s) := -\frac{1}{2}\frac{d^2}{ds^2}\log E(s).$$

Thus, for $\omega \to +\infty$, we obtain

$$\hat{g}(\omega) = \hat{g}_+(\omega) := \sqrt{\frac{2}{\pi}}\left[e^{1-x}x^\alpha \cos(\omega\sqrt{x} + \alpha\pi) + \frac{e^\beta}{x}\omega^{\beta-1}(\beta^{\frac{1}{2}-\beta})_+\right](1 + O(\omega^{-1}), \tag{3.10}$$

where $(f(\beta))_+$ is the positive part of $f(\beta)$, i.e., $(f(\beta))_+ = f(\beta)$ or 0 according as $\beta > 0$ or $\beta \le 0$. The first term in brackets comes from the saddles in Case III, the second from the one in Case II. For $\omega \to -\infty$, we obtain analogously from the saddle in Case I

$$\hat{g}(\omega) = \hat{g}_-(\omega) := \frac{1}{\sqrt{\pi}}\left(-\frac{\omega}{2}\right)^{2\alpha-1}\exp(-\frac{\omega^2}{4})(1 + O(\omega^{-2})). \tag{3.11}$$

Inserting (3.10) and (3.11) into (3.7), one obtains the estimate

$$\begin{aligned} R(h) \simeq \sqrt{\frac{2}{\pi}}\Bigg\{ &\frac{1}{\sqrt{2}}\left(\frac{\pi}{h}\right)^{2\alpha-1}\exp\left[\frac{2\pi}{h}\tau - \frac{1}{4}\left(\frac{2\pi}{h}\right)^2\right] + \exp\left(-\frac{2\pi}{h}\tau\right) \\ &\times\left[e^{1-x}x^\alpha\cos\left(\frac{2\pi}{h}\sqrt{x} + \alpha\pi\right) + \frac{e^\beta}{x}\left(\frac{2\pi}{h}\right)^{\beta-1}(\beta^{\frac{1}{2}-\beta})_+\right]\Bigg\}. \end{aligned} \tag{3.12}$$

A natural choice of τ_0 and h_0 is one that makes both terms in (3.12) of about equal magnitude ε, i.e., using the exponential factors only,

$$\tau_0 = \sqrt{\frac{\ln\frac{1}{\varepsilon}}{8}}, \quad h_0 = \frac{2\pi}{\sqrt{8\ln\frac{1}{\varepsilon}}}. \tag{3.13}$$

This results in an error slightly larger than ε,

$$|R(h_0)| \simeq \varepsilon\sqrt{\frac{2}{\pi}}\left\{\frac{1}{\sqrt{2}}\left(2\ln\frac{1}{\varepsilon}\right)^{\alpha-\frac{1}{2}} + e^{1-x}x^{\alpha} + \frac{e^{\beta}}{x}(\beta^{\frac{1}{2}-\beta})_{+}\cdot\left(8\ln\frac{1}{\varepsilon}\right)^{-\alpha-1}\right\}. \tag{3.14}$$

With regard to the summation in (3.2), note that only terms with $k \geq 0$ need to be computed since $g(-\sigma+i\tau) = \overline{g(\sigma+i\tau)}$. Moreover, the summation can be truncated at $k = N_0$, where N_0 is such that $|h_0 g(N_0 h_0 + i\tau_0)|$ is approximately equal to ε. This yields

$$N_0 \simeq \frac{1}{h_0}\sqrt{\ln\frac{1}{\varepsilon} + \tau_0^2} = \frac{3}{2\pi}\ln\frac{1}{\varepsilon}. \tag{3.15}$$

The number of evaluations of g, therefore, is roughly 1.1 ($= 3\ln 10/2\pi$) times the precision measured in decimal digits.

To provide a numerical example, we take $\alpha = 1.25$, $x = 2$, and $\varepsilon = 10^{-d}$. In Table 3.1 we illustrate for various values of d the accuracy (number of decimal digits) actually achieved (the last column) when N_0 is taken as estimated in (3.15). Also shown are the values of τ_0 and of h_0^* (the value of h_0 approximately expressed as a rational number with the denominator an appropriate power of 2 to reduce the effects of rounding errors). In the penultimate column the number of function evaluations needed to achieve the desired accuracy is given. The loss

Table 3.1: Numerical example for the summation in (3.2).

d	τ_0	h_0^*	N_0	#eval	#dec
9	1.61	62/128	10	11	6.6
19	2.34	42/128	21	22	15.7
28	2.84	35/128	31	33	23.4
38	3.31	30/128	42	44	31.9
48	3.72	27/128	53	54	40.6

of accuracy observed in the last column is due to internal cancellation in the summation of (3.2). It may be reduced by using slightly smaller values of τ and h, say $\tau = \frac{3}{4}\tau_0$, $h = \frac{3}{4}h_0^*$.

3.2 Series expansions.

A possible implementation of the explicit formula (2.13) for $0 < \alpha < 1$ consists in evaluating the function γ^* either by a power series for small and moderately large values of x, or by an asymptotic expansion valid for large positive x.

From the second series in [1, 6.5.29] (the first is subject to internal cancellation problems in our application) and the reflection formula (2.15) for the gamma function, one indeed obtains

$$\gamma^*(-\alpha,-x) = \frac{1}{\Gamma(-\alpha)}\sum_{n=0}^{\infty}\frac{x^n}{(n-\alpha)n!} = -\Gamma(1+\alpha)\frac{\sin\pi\alpha}{\pi}\sum_{n=0}^{\infty}\frac{x^n}{(n-\alpha)n!},$$

so that by (2.13)

$$I_\alpha(x) = -e^{-x}\left[\Gamma(1+\alpha)\sum_{n=0}^{\infty}\frac{x^n}{(n-\alpha)n!} + x^\alpha \pi\cot\alpha\pi\right]. \tag{3.16}$$

When α is very close to 0 or 1, the expression in brackets is computationally problematic. If it is written as

$$\Gamma(1+\alpha)\left(-\frac{1}{\alpha}+\frac{x}{1-\alpha}+\frac{x^\alpha\pi\cot\alpha\pi}{\Gamma(1+\alpha)}+\sum_{n=2}^{\infty}\frac{x^n}{(n-\alpha)n!}\right),$$

the sum of the first three terms in parentheses should be computed either in very high precision or by appropriate power series expansions in α near $\alpha = 0$ and $\alpha = 1$.

Likewise, from the asymptotic expansion [1, 6.5.32] for $\Gamma(a,x)$, the relation $\gamma^*(a,x) = \frac{x^{-a}}{\Gamma(a)}[\Gamma(a) - \Gamma(a,x)]$, and again the reflection formula for the gamma function, one finds

$$I_\alpha(x) \sim -\frac{\Gamma(1+\alpha)}{x}\left[1+\frac{\alpha+1}{x}+\frac{(\alpha+1)(\alpha+2)}{x^2}+\cdots\right], \quad x\to\infty. \tag{3.17}$$

Numerical experimentation reveals that for $0 < \alpha < 1$ the asymptotic expansion (3.17) can be used for $x \geq 26$ in IEEE single precision, and for $x \geq 39$ in IEEE double precision, whereas the power series (3.16) works well for the remaining positive values of x. Respective double-precision results are shown in Table 3.2, where the penultimate column indicates the number n_s of terms in (3.16) resp. (3.17) required for the series to yield full machine single precision, and the last column the analogous number n_d for double precision.

4 The Hermite weight.

The problem now is to compute

$$I(x) = \int_{-\infty}^{\infty}\frac{e^{-t^2}}{t-x}\,dt, \quad x\in\mathbb{R}. \tag{4.1}$$

Since $I(-x) = -I(x)$, it suffices to consider positive values of x.

The desired result can be obtained from (2.16) if in (2.1) we let $\alpha = -\frac{1}{2}$ and make the change of variables $t \mapsto t^2$,

$$\begin{aligned} I_{-\frac{1}{2}}(x) &= 2\int_0^\infty \frac{e^{-t^2}}{t^2-x}dt = \int_{-\infty}^{\infty}\frac{e^{-t^2}}{t^2-x}dt \\ &= \frac{1}{2\sqrt{x}}\int_{-\infty}^{\infty}\left(\frac{1}{t-\sqrt{x}}-\frac{1}{t+\sqrt{x}}\right)e^{-t^2}dt \\ &= \frac{1}{\sqrt{x}}I(\sqrt{x}). \end{aligned}$$

Table 3.2: Numerical results for $I_\alpha(x)$.

x	α	Hilbert	n_s	n_d
1.00	0.10	−0.56265102861247D+00	9	17
1.00	0.30	−0.33268825757247D+00	10	18
1.00	0.50	−0.13498833733624D+00	11	18
1.00	0.70	0.45225853622100D−01	10	17
1.00	0.90	0.21746191635749D+00	9	17
5.00	0.10	−0.26572309225656D+00	21	33
5.00	0.30	−0.26628521400850D+00	20	32
5.00	0.50	−0.27836545370654D+00	20	32
5.00	0.70	−0.30070906239231D+00	20	32
5.00	0.90	−0.33337268126874D+00	20	32
25.00	0.10	−0.39890144312158D−01	55	76
25.00	0.30	−0.37965005424693D−01	55	76
25.00	0.50	−0.37825484314284D−01	55	76
25.00	0.70	−0.39133270868438D−01	55	76
25.00	0.90	−0.41800307309395D−01	55	76
26.00	0.10	−0.38281378089155D−01	10	78
26.00	0.30	−0.36420147248551D−01	10	78
26.00	0.50	−0.36272343011410D−01	11	78
26.00	0.70	−0.37511689663752D−01	12	78
26.00	0.90	−0.40052135177656D−01	12	78
38.00	0.10	−0.25803986182139D−01	7	99
38.00	0.30	−0.24479334077100D−01	8	99
38.00	0.50	−0.24309277722928D−01	8	99
38.00	0.70	−0.25065763527742D−01	8	99
38.00	0.90	−0.26683118958861D−01	9	99
39.00	0.10	−0.25121984527160D−01	7	39
39.00	0.30	−0.23828694168664D−01	8	39
39.00	0.50	−0.23659490306967D−01	8	39
39.00	0.70	−0.24391927507379D−01	8	39
39.00	0.90	−0.25961679225431D−01	8	39
70.00	0.10	−0.13811002568837D−01	6	16
70.00	0.30	−0.13067331213346D−01	6	17
70.00	0.50	−0.12941885974893D−01	6	17
70.00	0.70	−0.13308644423984D−01	6	18
70.00	0.90	−0.14128818114899D−01	6	18
100.00	0.10	−0.96204249748500D−02	5	13
100.00	0.30	−0.90941541677365D−02	5	14
100.00	0.50	−0.89986485040109D−02	5	14
100.00	0.70	−0.92451885752255D−02	5	14
100.00	0.90	−0.98059106000491D−02	6	14
1000.00	0.10	−0.95239946017470D−03	3	7
1000.00	0.30	−0.89864010054248D−03	3	7
1000.00	0.50	−0.88755960087627D−03	3	7
1000.00	0.70	−0.91018760485528D−03	3	7
1000.00	0.90	−0.96359850708701D−03	3	7

Thus, replacing $\sqrt{x}$ by x and using (2.16), we get

$$I(x) = -2\sqrt{\pi}F(x), \tag{4.2}$$

where F is Dawson's integral (2.17).

From the series [1, Eq. 7.1.5] and the asymptotic expansion [1, Eq. 7.1.23] of the error function one finds, since $F(x) = -i\frac{\sqrt{\pi}}{2}e^{-x^2}\operatorname{erf}(ix)$, that

$$\begin{aligned} I(x) &= -\sqrt{\pi}x\sum_{k=0}^{\infty}\frac{1}{k+\frac{1}{2}}\frac{x^{2k}}{k!}, \\ I(x) &\sim -\frac{\sqrt{\pi}}{x}\left(1+\sum_{k=1}^{\infty}\frac{1\cdot 3\cdots(2k-1)}{(2x^2)^k}\right) \quad \text{as } x\to\infty. \end{aligned} \tag{4.3}$$

For computation, one can use the series expansion when x is small or moderately large, and the asymptotic expansion when x is large. For single-precision accuracy, $x = 5$ may be taken as the separation point, for double precision $x = 7.5$. Results thus obtained are displayed in Table 4.1. The last two columns

Table 4.1: Numerical results for $I(x)$.

x	Hilbert	n_s	n_d
0.50	−0.15045878048051D+01	6	12
1.00	−0.19074421882418D+01	10	17
2.00	−0.10682238655627D+01	18	29
5.00	−0.36205586704396D+00	8	76
7.50	−0.23848654284464D+00	5	17
10.00	−0.17814524994095D+00	5	12
50.00	−0.35456171091663D−01	3	6
100.00	−0.17725424868948D−01	2	5
200.00	−0.88623800370477D−02	2	4

show the number of terms required in single resp. double precision for the series to yield full machine precision.

There are also rational approximations for $F(x)$ that could be used, e.g., those in [3].

5 The Hilbert transform of the generalized Laguerre and Hermite polynomials; pseudo-stability of the three-term recurrence relation.

Let $\{\pi_n(t;w)\}$ denote the (monic) orthogonal polynomials relative to the weight function w, and x be a point in the interior of the support of w. The Cauchy principal value integrals

$$\rho_n(x) = \fint_{\mathbb{R}}\frac{\pi_n(t;w)}{t-x}\,w(t)dt, \quad n = 0,1,2,\ldots, \tag{5.1}$$

are of interest in connection with singular integral equations. They satisfy the same three-term recurrence relation as the orthogonal polynomials themselves, namely

$$y_{k+1} = (x - \alpha_k)y_k - \beta_k y_{k-1}, \quad k = 0, 1, 2, \ldots, \tag{5.2}$$

but with initial values

$$y_{-1} = -1, \quad y_0 = \int_{\mathbb{R}} \frac{w(t)}{t - x}\, dt. \tag{5.3}$$

(It is assumed in (5.2) that $\beta_0 = \int_{\mathbb{R}} w(t)dt$.) Let $\{z_k\}$ be a second solution of (5.2) defined by

$$z_{-1} = y_0, \quad z_0 = 1. \tag{5.4}$$

It is shown in [5, Section 4] that the amplification of relative error in y_k, if $y_k \neq 0$, due to small relative errors in y_0 and y_1 can be measured by the quantity

$$\omega_k = \frac{|z_1/y_1 - z_k/y_k| + |z_0/y_0 - z_k/y_k|}{|z_1/y_1 - z_0/y_0|}. \tag{5.5}$$

In this section, we wish to observe the behavior of $\{\omega_k\}$ in the two cases of the generalized Laguerre weight and the Hermite weight.

For the weight $w(t) = t^\alpha e^{-t}$, $0 < t < \infty$, it appears that serious growth of ω_k is most likely to occur when $x > 0$ in (5.1) is small and α large. We illustrate this by computing ω_k for $1 \leq k \leq 50$ in the case $\alpha = 10$ for selected values of x. The results, for $x = 0.5, 1, 2$, and 5, are plotted in the left frame of Figure 5.1 with a logarithmic scale on the vertical axis. (The remarks made in connection with Figure 2.1 apply also to Figure 5.1.) It would appear that ω_k remains finite, in

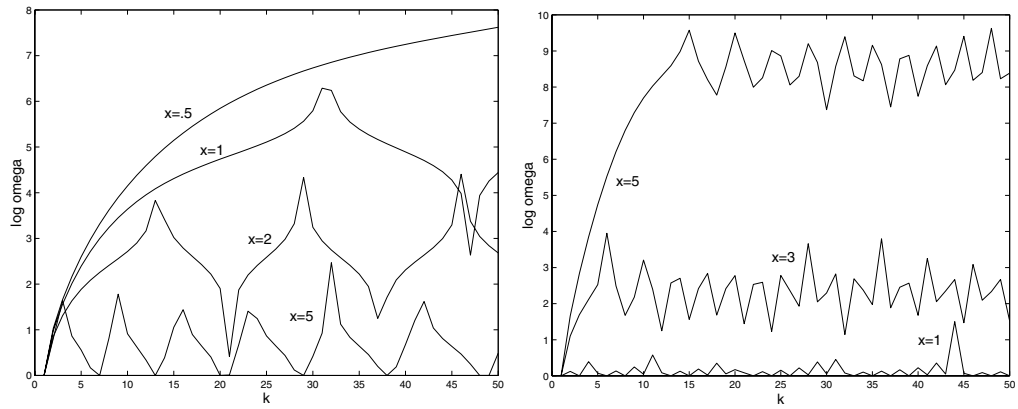

Figure 5.1: Amplification factors ω_k for generalized Laguerre and Hermite weights.

general, as $k \to \infty$. Yet, Figure 5.1 shows that it can assume rather large values—many decimal orders of magnitude—a phenomenon called pseudo-stability in [5]. A similar phenomenon takes place for the Hermite weight function $w(t) = e^{-t^2}$, $-\infty < t < \infty$, as is shown in the right frame of Figure 5.1 for $x = 1, 3$, and 5. Here, it is large absolute values of x that give rise to pseudo-stability.

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ORIGINAL PAPER

Numerical integration over the square in the presence of algebraic/logarithmic singularities with an application to aerodynamics

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Abstract Tensor-product formulae based on one-dimensional Gaussian quadratures are developed for evaluating double integrals of the type indicated in the title. If the singularities occur only along the diagonal and the regular part of the integrand is a polynomial of total degree d, the formulae can be made exact by choosing the number of quadrature points larger than, or equal to, $1 + d/2$. Numerical examples are given as well as an application to a problem in aerodynamics.

Keywords Numerical integration over the square · Algebraic/logarithmic singular lines along the diagonal and the sides of the square · Gaussian quadrature · Aerodynamical drag coefficient

Mathematics Subject Classification (2010) 65D32

1 Introduction

We are interested in computing double integrals of the form

$$I = \int_0^L \int_0^L F(X, Y)|X - Y|^\alpha \ln|X - Y| dX dY, \quad L > 0, \ \alpha > -1, \qquad (1.1)$$

Dedicated to Claude Brezinski and Sebastiano Seatzu on the occasion of their 70th birthdays.

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and

$$I^* = \int_0^L \int_0^L F(X, Y)(XY)^\beta [(L - X)(L - Y)]^\alpha \ln|X - Y| dX dY, \quad L > 0, \ \alpha > -1, \ \beta > -1, \tag{1.2}$$

where F is a smooth function. It is convenient to transform these integrals to the canonical unit square $[0, 1] \times [0, 1]$ by letting $X = Lx$, $Y = Ly$ and denoting $F(Lx, Ly) = f(x, y)$. Thus,

$$I = L^{\alpha+2} \left(\ln L \int_0^1 \int_0^1 f(x, y)|x - y|^\alpha dxdy + \int_0^1 \int_0^1 f(x, y)|x - y|^\alpha \ln|x - y| dxdy \right)$$

and

$$I^* = L^{2(\alpha+\beta+1)} \left(\ln L \int_0^1 \int_0^1 f(x, y)(xy)^\beta [(1 - x)(1 - y)]^\alpha dxdy + \int_0^1 \int_0^1 f(x, y)(xy)^\beta [(1 - x)(1 - y)]^\alpha \ln|x - y| dxdy \right).$$

We are led to consider the integrals

$$I_{\text{alg}} = \int_0^1 \int_0^1 f(x, y)|x - y|^\alpha dxdy,$$

$$I_{\log} = \int_0^1 \int_0^1 f(x, y)|x - y|^\alpha \ln|x - y| dxdy \tag{1.3}$$

for I, and

$$I^*_{\text{alg}} = \int_0^1 \int_0^1 f(x, y)(xy)^\beta [(1 - x)(1 - y)]^\alpha] dxdy,$$

$$I^*_{\log} = \int_0^1 \int_0^1 f(x, y)(xy)^\beta [(1 - x)(1 - y)]^\alpha \ln|x - y| dxdy \tag{1.4}$$

for I^*, in terms of which

$$I = L^{\alpha+2}\big(I_{\text{alg}} \ln L + I_{\log}\big), \quad I^* = L^{2(\alpha+\beta+1)}\big(I^*_{\text{alg}} \ln L + I^*_{\log}\big). \tag{1.5}$$

Both integrals in (1.3) are singular along the diagonal (if α is nonintegral), the first having an algebraic singularity, the other both an algebraic and a logarithmic singularity. The integrals in (1.4) are algebraically singular along the sides of the square, the second having an additional logarithmic singularity along the diagonal.

In what follows, we use two Gaussian quadrature rules: the classical Gauss–Jacobi rule on [0, 1],

$$\int_0^1 g(x)(1 - x)^\alpha x^\beta dx = \sum_{\nu=1}^n \omega_\nu^{(\alpha,\beta)} g\big(\xi_\nu^{(\alpha,\beta)}\big), \quad \alpha, \beta > -1, \ g \in \mathbb{P}_{2n-1}, \tag{1.6}$$

and a nonclassical Gaussian rule in which the Jacobi weight is multiplied by a logarithmic term,

$$\int_0^1 g(x)(1-x)^\alpha x^\beta \ln(1/x)dx = \sum_{\nu=1}^{n} w_\nu^{(\alpha,\beta)} g\big(x_\nu^{(\alpha,\beta)}\big), \quad \alpha,\beta > -1, \quad g \in \mathbb{P}_{2n-1}, \tag{1.7}$$

where $\mathbb{P}_{2n-1}$ denotes the set of polynomials of degree $\le 2n-1$. Both can be generated numerically, the latter from appropriate modified moments, with software for them being available (cf. Section 4 and [2, Section 2.1.7], [3]).

The approach described allows us to calculate both double integrals (1.3) and I_{alg}^* in (1.4) (but not $I_{\log}^*$) exactly whenever the function $f(x,y)$ is a polynomial of total degree $d \le 2n-2$ resp. $d \le 2n-1$. This is shown in Sections 2 and 3.1. The evaluation of the integrals (1.3), (1.4) is discussed in Sections 2 and 3. In Section 4 we provide examples, and in Section 5 give an application to a classical problem in aerodynamics.

2 The integrals I_{alg} and $I_{\log}$

2.1 The integral I_{alg}

In this subsection we will use exclusively the Gauss–Jacobi quadrature rule (1.6) with Jacobi parameters $\alpha_J = 0, \beta_J = \alpha$. For simplicity we shall denote the corresponding nodes and weights by

$$\xi_\nu = \xi_\nu^{(0,\alpha)}, \quad \omega_\nu = \omega_\nu^{(0,\alpha)}, \tag{2.1}$$

not indicating their dependence on n.

In order to compute I_{alg} in (1.3), we first integrate with respect to x for fixed y, $0 < y < 1$:

$$\int_0^1 f(x,y)|x-y|^\alpha dx = \int_0^y f(x,y)(y-x)^\alpha dx + \int_y^1 f(x,y)(x-y)^\alpha dx.$$

In the first integral on the right we make the change of variables $x = (1-t)y$ and get, using (1.6),

$$\int_0^y f(x,y)(y-x)^\alpha dx = y^{\alpha+1}\int_0^1 f((1-t)y,y)t^\alpha dt \approx y^{\alpha+1}\sum_{\nu=1}^{n}\omega_\nu f((1-\xi_\nu)y,y).$$

In the second integral, the change of variables $x = y + t(1-y)$ similarly yields

$$\begin{aligned}\int_y^1 f(x,y)(x-y)^\alpha dx &= (1-y)^{\alpha+1}\int_0^1 f(y+t(1-y),y)t^\alpha dt \\ &\approx (1-y)^{\alpha+1}\sum_{\nu=1}^{n}\omega_\nu f(y+\xi_\nu(1-y),y).\end{aligned}$$

Therefore,

$$\int_0^1 f(x, y)|x - y|^\alpha dx \approx y^\alpha F_1(y) + (1 - y)^\alpha F_2(y), \tag{2.2}$$

where

$$F_1(y) = y \sum_{\nu=1}^{n} \omega_\nu f((1 - \xi_\nu)y, y),$$

$$F_2(y) = (1 - y) \sum_{\nu=1}^{n} \omega_\nu f(y + \xi_\nu(1 - y), y). \tag{2.3}$$

Now, integrating (2.2) with respect to y gives

$$I_{\text{alg}} \approx \int_0^1 F_1(y) y^\alpha dy + \int_0^1 F_2(y)(1 - y)^\alpha dy.$$

Letting $1 - y = s$ in the second integral and then writing again y in place of s yields, once again using (1.6),

$$I_{\text{alg}} \approx \int_0^1 [F_1(y) + F_2(1 - y)] y^\alpha dy \approx \sum_{\mu=1}^{n} \omega_\mu [F_1(\xi_\mu) + F_2(1 - \xi_\mu)].$$

Substituting from (2.3), we obtain the desired approximation

$$I_{\text{alg}} \approx \sum_{\mu=1}^{n} \sum_{\nu=1}^{n} A_{\mu\nu} [f((1 - \xi_\nu)\xi_\mu, \xi_\mu) + f(1 - (1 - \xi_\nu)\xi_\mu, 1 - \xi_\mu)], \tag{2.4}$$

where

$$A_{\mu\nu} = \omega_\mu \xi_\mu \omega_\nu. \tag{2.5}$$

If f is a polynomial of total degree d, then from the way the approximation (2.2) was derived, it follows that (2.2) is an equality whenever $2n - 1 \geq d$, i.e., $n \geq (d + 1)/2$. Consequently, since F_1 and F_2 are polynomials of degree $d + 1$, the approximation (2.4) is an equality whenever $2n - 1 \geq d + 1$, i.e., $n \geq 1 + d/2$.

2.2 The integral $I_{\log}$

Here again, we use the same Gauss–Jacobi quadrature rule as in the previous subsection, with the nodes and weights in (2.1). In addition, we need the

logarithmic companion rule (1.7) with the same Jacobi parameters, whose nodes and weights will be denoted by

$$x_\nu = x_\nu^{(0,\alpha)}, \quad w_\nu = w_\nu^{(0,\alpha)}. \tag{2.6}$$

The computation of $I_{\log}$ proceeds along lines analogous to those in Section 2.1. We omit details and state only the final result:

$$I_{\log} \approx -\sum_{\mu=1}^{n}\sum_{\nu=1}^{n}\big\{B_{\mu\nu}[f((1-\xi_\nu)x_\mu, x_\mu) + f(1-(1-\xi_\nu)x_\mu, 1-x_\mu)] + C_{\mu\nu}[f((1-x_\nu)\xi_\mu, \xi_\mu) + f(1-(1-x_\nu)\xi_\mu, 1-x_\mu)]\big\}, \tag{2.7}$$

where

$$B_{\mu\nu} = w_\mu x_\mu \omega_\nu, \quad C_{\mu\nu} = \omega_\mu \xi_\mu w_\nu. \tag{2.8}$$

An argument similar to the one at the end of Section 2.1 will show that we have equality in (2.7) if $n \geq 1 + d/2$ when f is a polynomial of total degree d.

The tensor-product approximation (2.7) with $\alpha = 0$ finds good use in Section 5.2 (cf. (5.6)).

3 The integrals I^*_{alg} and $I^*_{\log}$

3.1 The integral I^*_{alg}

Here we use the quadrature rule (1.6) in its full generality and denote the respective nodes and weights by

$$\xi_\nu^* = \xi_\nu^{(\alpha,\beta)}, \quad \omega_\nu^* = \omega_\nu^{(\alpha,\beta)}. \tag{3.1}$$

The procedure used previously then yields the approximation

$$I^*_{\text{alg}} \approx \sum_{\mu=1}^{n}\sum_{\nu=1}^{n}\omega_\mu^*\omega_\nu^* f(\xi_\nu^*, \xi_\mu^*). \tag{3.2}$$

If $f(x, y)$ is a polynomial of degree d in x and y, we have equality in (3.2) if $n \geq (d+1)/2$.

3.2 The integral $I^*_{\log}$

This integral, compared to all the others, is by far the most challenging one to compute. Even in the case $f(x, y) = 1$, for example, it defies exact evaluation. For numerical evaluation we require four cases of the Gauss–Jacobi rule (1.6) and four cases of the logarithmic companion rule (1.7). Their weight functions and corresponding quadrature nodes and weights are displayed respectively in Tables 1 and 2. Thus, in the notation used in (1.6),

$$\xi_\nu^\alpha = \xi_\nu^{(\alpha,0)}, \quad \xi_\nu^\beta = \xi_\nu^{(\beta,0)}, \quad \xi_\nu = \xi_\nu^{(\alpha,2\beta+1)}, \quad \overline{\xi}_\nu = \xi_\nu^{(\beta,2\alpha+1)}$$

Table 1 The Gauss–Jacobi quadrature rules required for $I^*_{\log}$

Weight function	Nodes	Weights
$(1-t)^\alpha$	ξ_ν^α	ω_ν^α
$(1-t)^\beta$	ξ_ν^β	ω_ν^β
$(1-t)^\alpha t^{2\beta+1}$	ξ_ν	ω_ν
$(1-t)^\beta t^{2\alpha+1}$	$\overline{\xi}_\nu$	$\overline{\omega}_\nu$

and similarly for the weights. Likewise, in the notation of (1.7),

$$x_\nu^\alpha = x_\nu^{(\alpha,0)}, \quad x_\nu^\beta = x_\nu^{(\beta,0)}, \quad x_\nu = x_\nu^{(\alpha,2\beta+1)}, \quad \overline{x}_\nu = x_\nu^{(\beta,2\alpha+1)},$$

and similarly for the weights.

Although the derivation of a suitable approximation to $I^*_{\log}$ in principle uses the same technique as before, the effectiveness of the procedure is now compromised by the fact that the integrals arising after the first integration with respect to x, if α and/or β are not integers, have not only the endpoint singularities that, as before, can be handled by Gaussian quadrature, but also algebraic singularities outside the interval of integration but close to their endpoints if y is near 0 or 1. The approximation so obtained,

$$\begin{aligned} I^*_{\log} = -\sum_{\mu=1}^{n}\sum_{\nu=1}^{n} \{ & w_\mu \omega_\nu^\beta f\big((1-\xi_\nu^\beta)x_\mu, x_\mu\big)\big(1-x_\mu+\xi_\nu^\beta x_\mu\big)^\alpha \\ & + \overline{w}_\mu \omega_\nu^\alpha f\big(1-\overline{x}_\mu+\xi_\nu^\alpha \overline{x}_\mu, 1-\overline{x}_\mu\big)\big(1-\overline{x}_\mu+\xi_\nu^\alpha \overline{x}_\mu\big)^\beta \\ & + \omega_\mu w_\nu^\beta f\big((1-x_\nu^\beta)\xi_\mu, \xi_\mu\big)\big(1-\xi_\mu+x_\nu^\beta \xi_\mu\big)^\alpha \\ & + \overline{\omega}_\mu w_\nu^\alpha f\big(1-\overline{\xi}_\mu+x_\nu^\alpha \overline{\xi}_\mu, 1-\overline{\xi}_\mu\big)\big(1-\overline{\xi}_\mu+x_\nu^\alpha \overline{\xi}_\mu\big)^\beta \}, \end{aligned} \tag{3.3}$$

therefore, contrary to $I_{\log}$, is no longer exact for polynomials of low degree, not even for a constant, unless α and β are nonnegative integers. In that case, if f has total degree d, the formula (3.3) is exact if $n \geq (d+\max(\alpha,\beta)+1)/2$.

For applications of (3.3), see Section 5.1.

Table 2 The logarithmic Gauss–Jacobi quadrature rules required for $I^*_{\log}$

Weight function	Nodes	Weights
$(1-t)^\alpha \ln(1/t)$	x_ν^α	w_ν^α
$(1-t)^\beta \ln(1/t)$	x_ν^β	w_ν^β
$(1-t)^\alpha t^{2\beta+1} \ln(1/t)$	x_ν	w_ν
$(1-t)^\beta t^{2\alpha+1} \ln(1/t)$	$\overline{x}_\nu$	$\overline{w}_\nu$

4 Numerical examples

All computations that we report on in this and the following section are done in Matlab. The main programs—the Matlab functions `Ial.m` and `Istaral.m` implementing our procedures for computing the integrals in (1.3) and (1.4)—as well as all other programs required can be downloaded from the website http://www.cs.purdue.edu/archives/2002/wxg/codes/NUMINT.html.

4.1 The integrals in (1.3)

We first describe some preliminary testing for the program `Ial.m`.

Preliminary tests We take $f(x, y) = 1$ and run the program for $n = 1 : 3$ and a few selected values of α. The results are compared with the known answers $I_{\text{alg}} = 2/((\alpha + 1)(\alpha + 2))$, $I_{\log} = -2(2\alpha + 3)/((\alpha + 1)^2(\alpha + 2)^2)$. They should agree with these for each $n \geq 1$, in particular for $n = 1 : 3$. It is found that this indeed is the case; cf. the routine `test_Ial.m` (with `fxy_test.m` appended to `Ial.m`).

Example 1 Let f be the Matlab `peaks` function shown in Fig. 1.

The function f involves exponential functions of linear up to fifth-degree polynomials in x and y; see `fxy_peaks`. Rather remarkably, small values of n suffice to obtain accurate results. Indeed, the driver program `Ex1_Ial.m` (with `fxy_peaks.m` appended to `Ial.m`), for $\alpha = -.8 : .2 : 1$, produces the following output, where n is the number of quadrature points required for two

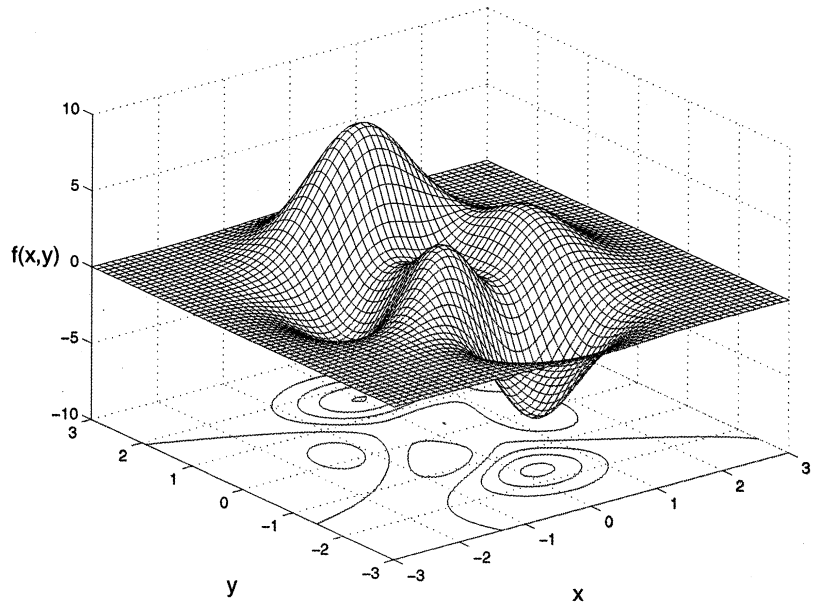

Fig. 1 The Matlab `peaks` function

successive approximations, either to `Ialg` or to `Ilog`, to agree to within 14 significant digits.

```
>> Ex1_Ial
       n  alpha          Ialg                  Ilog
      11  -0.80   7.7862415770711e+000 -4.3175624314696e+001
      12  -0.60   3.5500666273105e+000 -1.0261166207151e+001
      12  -0.40   2.2112271140758e+000 -4.3416287631133e+000
      11  -0.20   1.5726159079911e+000 -2.3416027595378e+000
      11   0.00   1.2040904162894e+000 -1.4478417538807e+000
      11   0.20   9.6604605547011e-001 -9.7764032583602e-001
      11   0.40   8.0032912619267e-001 -7.0189412848092e-001
      11   0.60   6.7865912572909e-001 -5.2707477472028e-001
      11   0.80   5.8572367008314e-001 -4.0953706593989e-001
      11   1.00   5.1254422335153e-001 -3.2681197757723e-001
>>
```

4.2 The integrals in (1.4)

Preliminary tests For the second program `Istaral.m`, we also take $f(x, y) = 1$, in which case $I^*_{\text{alg}} = [\Gamma(\alpha+1)\Gamma(\beta+1)/\Gamma(\alpha+\beta+2)]^2$, but for $I^*_{\log}$ no explicit answers are known except for $I^*_{\log} = -3/2$ when $\alpha = \beta = 0$. However, we know (cf. the statement following (3.3)) that the answers must be exact if α, β are nonnegative integers and $n \geq \frac{1}{2}(\max(\alpha, \beta) + 1)$. All this has been checked successfully; cf. `test_Istaral` (with `fxy_test.m` appended to `Istaral.m`).

Example 2 Accuracy of $I^*_{\log}$.

We examine the accuracy of the quadrature approximation $I^*_{\log}(n)$ for $n = 50$ when $f(x, y) = 1$ and α, β vary in the square $(-1, 1) \times (-1, 1)$. Because of symmetry with respect to the line $\alpha = \beta$, it suffices to consider $\beta \geq \alpha$. For each α, β in this half of the square we compute $I^*_{\log}(n)$ and $I^*_{\log}(n-1)$ and take

$$-\log_{10}\left(|(I^*_{\log}(n) - I^*_{\log}(n-1))/I^*_{\log}(n)|\right)$$

to indicate approximately the number of correct decimal digits. The results for $\alpha = -.9 : .1 : .9$, $\beta = \alpha : .1 : .9$ are plotted in Fig. 2, which was produced by the program `Ex2_Istaral.m` (with `fxy_test.m` still appended to `Istaral.m`); it calls on `acc_Istaral.m` and may take awhile to run.

It is seen from the plot that the accuracy is lowest near the lines $\alpha = -1$ and $\beta = -1$ and raises steadily as the point (α, β) moves toward the upper right corner $(1, 1)$ of the square $\{(\alpha, \beta) : -1 < \alpha \leq 1, -1 < \beta \leq 1\}$. There are narrow ridges of increasingly higher accuracy along the lines $\beta = 0, 0 < \alpha \leq 1$ and $\alpha = 0, 0 < \beta \leq 1$ and a conspicuous peak at $\alpha = \beta = 0$, where of course we have exactness for all $n \geq 1$.

We expect this pattern of accuracy to extend to more general functions f, as long as they are smooth. The next example is intended to lend support to this expectation.

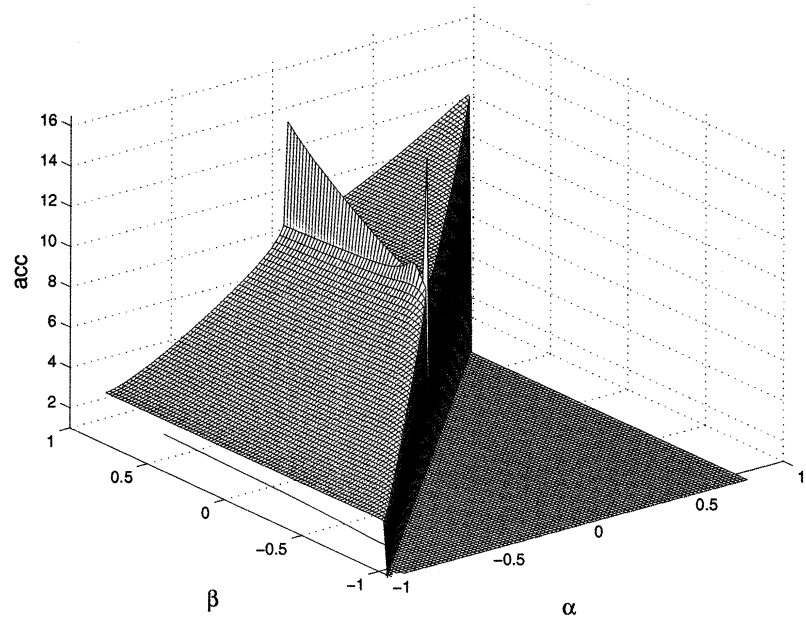

Fig. 2 The accuracy of $I^*_{\log}(n), n = 50$

Example 3 Let f be the Matlab `peaks` function (as in Example 1).

The accuracy plot in this case, produced by the same program (but with the subfunction `fxy_peaks.m` appended to `Istaral.m`) looks almost identical to the one in Fig. 2.

5 Applications to a problem in aerodynamcis

The integral $I_{\log}$ in (1.3), where $\alpha = 0$, and $I^*_{\log}$ in (1.4), where $\alpha = \beta = -1/2$, are of interest in the linear theory of the aerodynamics of slender bodies of revolution. Let the body be of length 1 and $x, 0 \le x \le 1$, measuring the distance of a point on the axis of the body from its left end point. Denote by $S(x)$ the cross-sectional area of the body as a function of x. Then the wave drag of the body due to volume can be expressed approximately, up to a constant factor, by the integral

$$D = -\int_0^1 \int_0^1 S''(x)S''(y) \ln|x - y| dxdy. \tag{5.1}$$

We first show how D can be computed in the case of two special bodies of interest in supersonic flow problems. We then consider a problem of minimizing D over a class of functions S having prescribed values and derivatives at $x = 0$ and $x = 1$.

5.1 The Sears–Haack and von Kármán bodies

The *Sears–Haack body* corresponds to (see, e.g., [1, eq.(9–34)], where $\cos\theta = 1 - 2x$)

$$S(x) = \frac{4}{3}[x(1-x)]^{3/2},$$

for which

$$S''(x) = [x(1-x)]^{-1/2}(1 - 8x + 8x^2).$$

Thus, the integral (5.1) becomes $I^*_{\log}$ of (1.4), with

$$\alpha = \beta = -1/2, \quad f(x, y) = (1 - 8x + 8x^2)(1 - 8y + 8y^2).$$

We can see from Fig. 2 that the point $(\alpha, \beta) = (-1/2, -1/2)$ is located near the lower front tip of the surface depicted there, that is, in an area of low accuracy. Therefore, to compute D, we need high-order quadrature rules, and even then can only achieve a modest degree of accuracy. Taking n quadrature points, $n = 50 : 50 : 250$, we obtain the results shown in Table 3, using the program `SearsKarman_Istaral.m` (with `fxy_Sears.m` appended to `Istaral.m`). We see that even with 250 quadrature points, we can get only about five correct decimal digits.

The integral I^*_{alg}, incidentally, happens to be zero, as can easily be shown.

The *von Kármán body* has the cross-sectional distribution (see [1, eq. (9–30)]),

$$S(x) = \frac{1}{\pi}\left(\arccos(1-2x) - 2(1-2x)\sqrt{x(1-x)}\right),$$

giving

$$S''(x) = \frac{4}{\pi}[x(1-x)]^{-1/2}(1-2x).$$

Thus again, D becomes $I^*_{\log}$ with

$$\alpha = \beta = -1/2, \quad f(x, y) = \left(\frac{4}{\pi}\right)^2 (1-2x)(1-2y).$$

Table 3 Wave drag approximations for the Sears–Haack body

n	D
50	2.462455422168
100	2.465960275731
150	2.466708069724
200	2.466990374942
250	2.467127904913

The same program (but with `fxy_Karman.m` appended to `Istaral.m`) now yields the results in Table 4. It looks like the true value might be $D = 8$. The integral I^*_{alg} is again zero.

5.2 A minimum problem for the drag

Problems of minimizing the wave drag for certain classes of functions S have been considered before, e.g. in [4], where the approach taken was via Fourier analysis. We prefer here to use algebraic polynomials rather than trigonometric polynomials since our computational procedure developed in Section 2 is capable of yielding exact answers for polynomials. But as in Fourier analysis, we use orthogonal polynomials, specifically the (monic) Legendre polynomials $\{\pi_j\}$ on [0, 1] satisfying the orthogonality relations

$$\int_0^1 \pi_k(x)\pi_\ell(x)dx = \begin{cases} 0 & \text{if } k \neq \ell, \\ \|\pi_k\|^2 & \text{if } k = \ell. \end{cases} \tag{5.2}$$

Let $\mathbb{F}$ be the space of functions p admitting a uniformly convergent Fourier expansion in the polynomials $\{\pi_k\}$,

$$\mathbb{F} = \left\{ p : p(x) = \sum_{k=0}^{\infty} c_k \pi_k(x) \text{ on } [0, 1],\ c_k = \frac{(\pi_k, p)}{(\pi_k, \pi_k)} \right\}, \tag{5.3}$$

where $(\cdot, \cdot)$ is the usual inner product $(u, v) = \int_0^1 u(x)v(x)dx$. The space $\mathbb{F}$ contains, e.g., the space $\mathbb{P}$ of polynomials. Assume that $S'' \in \mathbb{F}$ and let

$$S''(x) = \sum_{k=0}^{\infty} c_k \pi_k(x), \quad 0 \leq x \leq 1. \tag{5.4}$$

Insertion into (5.1) gives for D the quadratic form

$$D = \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} p_{kl} c_k c_\ell \tag{5.5}$$

in the variables $c_0, c_1, c_2, \ldots$ with the matrix

$$P = [p_{kl}], \quad p_{kl} = -\int_0^1 \int_0^1 \pi_k(x)\pi_\ell(y) \ln|x - y| dxdy. \tag{5.6}$$

Table 4 Wave drag approximations for the von Kármán body

n	D
50	7.991986539889
100	7.997664522215
150	7.998876564661
200	7.999334178245
250	7.999557121310

Since $f(x, y) = \pi_k(x)\pi_\ell(y)$, $0 \le k, l \le n$, is a polynomial of total degree $\le 2n$, the principal submatrix of P of order $n+1$ can be computed exactly by the method of Section 2.2 using $(n+1)$-point quadrature rules (cf. the sentence following (2.8)). Clearly, P is symmetric; from numerical computations using Cholesky decompositions, P also appears to be positive definite which, on physical grounds, is to be expected since the drag is intrinsically positive.

We now pose, and solve numerically, the following extremal problem: *Among all functions $S \in \mathbb{F}$ having prescribed values*

$$S_0 = S(0), \quad S_1 = S(1); \quad S_0' = S'(0), \quad S_1' = S'(1), \tag{5.7}$$

find the one for which D in (5.1) *is minimum.*

We begin with expressing the conditions (5.7) in terms of the coefficients c_k. Noting that $\pi_0 = 1, \pi_1(t) = t - 1/2$, we have

$$\begin{aligned} S'(x) &= S_0' + \int_0^x S''(t)dt \\ &= S_0' + c_0 x + \frac{1}{2} c_1 x(x-1) + \sum_{k=2}^{\infty} c_k \int_0^x \pi_k(t)dt. \end{aligned}$$

When $x = 1$, the integral on the far right, by orthogonality, is zero for all $k \ge 2$, so that $S'(1) = S_0' + c_0$, i.e.,

$$c_0 = S_1' - S_0'. \tag{5.8}$$

Integrating once more, we get

$$\begin{aligned} S(x) &= S_0 + \int_0^x S'(t)dt \\ &= S_0 + S_0' x + \frac{1}{2} c_0 x^2 + \frac{1}{12} c_1 x^2(2x-3) + \sum_{k=2}^{\infty} c_k \int_0^x dt \int_0^t \pi_k(\tau)d\tau. \end{aligned} \tag{5.9}$$

Here the repeated integral on the right is

$$\int_0^x dt \int_0^t \pi_k(\tau)d\tau = \int_0^x (x-t)\pi_k(t)dt, \tag{5.10}$$

which for $x = 1$, again by orthogonality, is zero for all $k \ge 2$. Therefore, by (5.9) and (5.8),

$$S(1) = S_0 + S_0' + \frac{1}{2}(S_1' - S_0') - \frac{1}{12} c_1,$$

giving

$$c_1 = 12\left[S_0 - S_1 + \frac{1}{2}(S_0' + S_1')\right]. \tag{5.11}$$

Thus, we can write

$$D = p_{00}c_0^2 + 2p_{01}c_0c_1 + p_{11}c_1^2 + 2c_0\sum_{\ell=2}^{\infty} p_{0\ell}c_\ell$$
$$+ 2c_1\sum_{\ell=2}^{\infty} p_{1\ell}c_\ell + \sum_{k=2}^{\infty}\sum_{\ell=2}^{\infty} p_{kl}c_kc_\ell.$$

Here c_0 and c_1 are prescribed (cf. (5.8) and (5.11)), the free variables thus being $c_2, c_3, \ldots$. Since one computes $p_{00} = 3/2$, $p_{01} = 0$[1], $p_{11} = 1/16$, one has

$$D = \frac{1}{16}\left(24c_0^2 + c_1^2\right) + 2c_0\sum_{\ell=2}^{\infty} p_{0\ell}c_\ell$$
$$+ 2c_1\sum_{\ell=2}^{\infty} p_{1\ell}c_\ell + \sum_{k=2}^{\infty}\sum_{\ell=2}^{\infty} p_{kl}c_kc_\ell. \tag{5.12}$$

We solve the minimization problem for D in (5.12) numerically, replacing the upper limit ∞ in the summations by a finite number, say N. The right-hand side of (5.12) then is a quadratic function in the unknowns $c_2, c_3, \ldots, c_N$. Putting the partial derivatives $\partial D/\partial c_k$, $2 \le k \le N$, equal to zero yields the system of linear equations

$$\sum_{\ell=2}^{N} p_{k\ell}c_\ell = -(c_0p_{0k} + c_1p_{1k}), \quad k = 2, 3, \ldots, N. \tag{5.13}$$

The solution of this system will yield a minimum of D since the Hessian matrix of (5.12) (with ∞ replaced by N) is positive definite, at least for the values of N being used here.

As already pointed out, the $p_{k\ell}$ can be computed from (5.6) by the procedure in Section 2.2, yielding exact answers if the number n of quadrature points is taken to be $n \ge N + 1$.

If we want the profile of the body to have pointed ends on the axis and be symmetric with respect to the vertical midplane, i.e., if $S_0 = S_1 = 0$ and $S_1' = -S_0'$, then $c_1 = 0$ by (5.11), which means that the solution of (5.13), since $c_0 = -2S_0'$, is a multiple of S_0', and the system to be solved is

$$\sum_{\ell=2}^{N} p_{k\ell}\gamma_\ell = 2p_{0k}, \quad k = 2, 3, \ldots, N, \tag{5.14}$$

whereupon

$$c_\ell = S_0'\gamma_\ell, \quad \ell = 2, 3, \ldots, N.$$

[1] Actually, the matrix P was found to have a checkerboard pattern of alternating zero and nonzero elements: $p_{k\ell} = 0$ if $k + \ell$ is odd, and nonzero otherwise.

In view of the checkerboard pattern of zero and nonzero elements of the matrix P, mentioned in footnote 1, all odd-numbered γ_k turn out to be zero,

$$\gamma_k = 0 \quad \text{if } k \text{ is odd.}$$

Once the system (5.14) is solved, the optimal value of D can be found from (5.12) to be

$$D_{\text{opt}} = (S_0')^2 \left[6 - 4 \sum_{\ell} p_{0\ell}\gamma_\ell + \sum_{k} \sum_{\ell} p_{k\ell}\gamma_k\gamma_\ell \right], \tag{5.15}$$

where the summations are over even k and ℓ from 2 to $2\lfloor N/2 \rfloor$. The optimal function S, by (5.9), (5.10), then is

$$S_{\text{opt}}(x) = S_0' \left[x(1-x) + \sum_{k} \gamma_k \int_0^x (x-t)\pi_k(t)dt \right], \tag{5.16}$$

giving the optimal profile $R_{\text{opt}}(x) = \sqrt{S_{\text{opt}}(x)/\pi}$, $0 \le x \le 1$.

To illustrate, let $N = 4 : 2 : 10$; for N odd, the results are the same as those for $N-1$ because of the special property of the matrix P stated in footnote 1. The systems (5.14) then have the following solutions, rounded to 8 decimals (only nonzero components are shown):

$$\gamma_2 = -13.714286,\ \gamma_4 = -120.00000 \ (N = 4),$$
$$\gamma_2 = -14.285714,\ \gamma_4 = -147.27273,\ \gamma_6 = -1400.0000 \ (N = 6),$$
$$\gamma_2 = -14.545455,\ \gamma_4 = -158.60140,\ \gamma_6 = -1792.0000,$$
$$\gamma_8 = -17640.000 \ (N = 8),$$
$$\gamma_2 = -14.685315,\ \gamma_4 = -164.47552,\ \gamma_6 = -1976.4706,$$
$$\gamma_8 = -23210.526,\ \gamma_{10} = -232848.00 \ (N = 10).$$

The condition numbers of the systems grow from 5.002×10^2 (for $N = 4$) to 2.072×10^{10} (for $N = 10$). From (5.15) one computes the optimal drags shown in Table 5; cf. the routine `Dopt.m` with `fxy_pkpl.m` appended to `Ial.m`.

Table 5 Optimal drags

N	$D_{\text{opt}} = (S_0')^2 \times$
4	5.60000
6	5.57619
8	5.56508
10	5.55902

Table 6 The coefficients of p_{n-2}

n	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	Div
2	1									12
4	3	−14	14							420
6	1	−12	45	−66	33					1848
8	1	−22	165	−572	1001	−858	286			25740
10	3	−104	1274	−7644	25480	−49504	55692	−33592	8398	1108536

To obtain S_{opt}, we need to evaluate the integrals in (5.16), the twice integrated Jacobi polynomials. From Rodrigues's formula, one expects these to have the form

$$\int_0^x (x-t)\pi_n(t)dt = [x(1-x)]^2 p_{n-2}(x), \tag{5.17}$$

where p_{n-2} is a polynomial of exact degree $n-2$,

$$p_{n-2}(x) = a_0 + a_1 x + \cdots + a_{n-2}x^{n-2}. \tag{5.18}$$

Using Maple, one indeed finds the coefficients $a_0, a_1, a_2, \ldots$ to be as shown in Table 6. Here the numbers in the last column are divisors by which the preceding numbers in the same row (except of course the one in column 1) have to be divided.

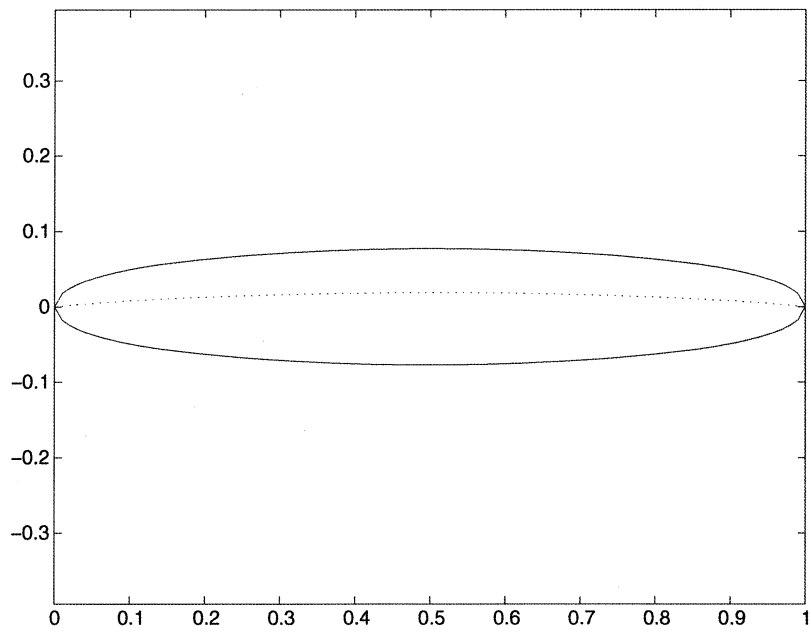

Fig. 3 Optimal cross-sectional areas (*dotted line*) and profile (*solid line*) for $N = 10$

The plots for S_{opt} and R_{opt} are practically indistinguishable when $N = 4 : 2 : 10$; they are shown in Fig. 3 for $N = 10$ and produced as part of the routine `Dopt.m`.

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20.1. [31] "Construction of Gauss–Christoffel Quadrature Formulas"

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Construction of Gauss-Christoffel Quadrature Formulas

By Walter Gautschi*

1. Introduction. Let $w(x)$ be a given function ("weight function") defined on a finite or infinite interval (a, b). Consider a sequence of quadrature rules

$$\int_a^b f(x)w(x)dx \doteq \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\xi_\nu^{(n)}), \qquad n = 1, 2, 3, \cdots. \tag{1.1}$$

Each of these rules will be called a *Gauss-Christoffel quadrature formula* if it has maximum degree of exactness, i.e. if (1.1) is an exact equality whenever f is a polynomial of degree $2n - 1$. It is a well-known fact, due to Christoffel [3], that such quadrature formulas exist uniquely, provided the weight function $w(x)$ is nonnegative, integrable with $\int_a^b w(x)dx > 0$, and such that all its moments

$$\mu_k = \int_a^b x^k w(x)dx, \qquad k = 0, 1, 2, \cdots, \tag{1.2}$$

exist. Then, moreover, $\xi_\nu^{(n)} \in (a, b)$, and $\lambda_\nu^{(n)} > 0$. If $w(x)$ is not of constant sign, Gauss-Christoffel formulas still exist if certain Hankel determinants in the moments are different from zero [21]. In this case, however, some of the abscissas $\xi_\nu^{(n)}$ may fall outside the interval (a, b); in particular, they may become complex. We shall call $\xi_\nu^{(n)}$ the *Christoffel abscissas*, and $\lambda_\nu^{(n)}$ the *Christoffel weights* associated with the weight function $w(x)$.

Gauss [7] originally considered the case $w(x) \equiv 1$ on $[-1, 1]$. Other classical cases are associated with the names of Jacobi, Laguerre, and Hermite. In more recent times, the subject has experienced a considerable resurgence, as is evidenced by the appearance of numerous numerical tables [15], [21], both relative to classical and nonclassical weight functions. The emergence of powerful high-speed computers, undoubtedly, has been a major force in this development. Curiously enough, the constructive (algorithmic) aspect of the subject, until very recently, has remained at the state of development in which it was left by Christoffel, and Stieltjes [20]. The generally recommended procedure still consists [1] in constructing the system $\{\pi_\nu\}$ of orthogonal polynomials associated with the weight function $w(x)$, and to obtain $\xi_\nu^{(n)}$ as the zeros of π_n, and $\lambda_\nu^{(n)}$, in a number of possible ways, in terms of these orthogonal polynomials. An alternative procedure, suggested by Rutishauser [19], makes use of the quotient-difference algorithm, while Golub and Welsch [11] use Francis' QR-transformations to compute $\xi_\nu^{(n)}$ as eigenvalues of a Jacobi matrix and $\lambda_\nu^{(n)}$ as the first component of the corresponding eigenvectors. These methods, as interesting as they are, appear to be computationally feasible, for large n, only if the orthogonal polynomials π_ν, or the associated Stieltjes continued fraction, are explicitly known. Otherwise, they are subject to severe numerical instability,

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making it virtually impossible to obtain meaningful answers, unless one resorts to multiple-precision work.

The reason for this is the ill-conditioned character of the problem which these methods attempt to solve. The problem, basically, is the purely algebraic one of deriving $\xi_\tau^{(n)}$, $\lambda_\tau^{(n)}$ from the first $2n$ moments of $w(x)$, i.e. of solving the algebraic system of equations

$$\sum_{\tau=1}^{n} \lambda_\tau^{(n)} [\xi_\tau^{(n)}]^k = \mu_k \qquad (k = 0, 1, 2, \cdots, 2n-1)\,. \tag{1.3}$$

It will be shown (Section 2) that for a finite interval (0, 1) the (asymptotic, relative) condition number κ_n for this problem can be estimated from below by

$$\kappa_n > \min\left(\mu_0, \frac{1}{\mu_0}\right) \max_{1\le\tau\le n} \left\{(1+\xi_\tau^{(n)}) \prod_{k=1;k\neq\tau}^{n} \left(\frac{1+\xi_k^{(n)}}{\xi_\tau^{(n)} - \xi_k^{(n)}}\right)^2\right\}. \tag{1.4}$$

Considering that the abscissas $\xi_\tau^{(n)}$, for large n, tend to cluster near the endpoints of the interval (0, 1), many of the differences $\xi_\tau^{(n)} - \xi_k^{(n)}$ will be quite small in absolute value. Consequently, some of the products in (1.4), and thus the lower bound for κ_n, are likely to be very large when n is large.

To give a more concrete idea of just how large κ_n may become, we note [22, p. 309] that for a wide class of weight functions the abscissas $\xi_\tau^{(n)}$ ultimately (as $n \to \infty$) assume an arc cos-distribution, i.e.

$$\xi_\tau^{(n)} \doteq \tfrac{1}{2}(1 + \cos\theta_\tau^{(n)})\,, \qquad \theta_\tau^{(n)} = (2\tau - 1)\pi/2n\,. \tag{1.5}$$

Replacing the $\xi_\tau^{(n)}$ in (1.4) by their approximate values in (1.5), one finds that

$$\kappa_n > \min\left(\mu_0, \frac{1}{\mu_0}\right) \frac{(17+6\sqrt{8})^n}{64n^2} > \min\left(\mu_0, \frac{1}{\mu_0}\right) \frac{(33.97)^n}{64n^2}\,. \tag{1.6}$$

Numerical values of the lower bound in (1.6), for $\mu_0 = 1$ and a few selected values of n, are shown in Table 1.

TABLE 1
Lower bound for condition number κ_n

n	$(33.97)^n/64n^2$
5	2.8×10^4
10	3.2×10^{11}
15	6.4×10^{18}
20	1.6×10^{26}

It is thus seen that in the presence of rounding errors the above-mentioned methods, if they rely on the moments, must be expected to suffer a loss of at least 11 decimal digits, if $n = 10$, and a loss of 26 digits, when $n = 20$. This is well above the attrition level one is normally willing to accept!

The lesson to be learned from this analysis is evident: the moments are not suitable, as data, for constructing Gauss-Christoffel quadrature formulas of large order n. Apart from the fact that they are not always easy to compute, small changes in the moments (due to rounding, for example) may result in very large changes in the Christoffel numbers.

In Section 3 we propose an alternative procedure for generating Gauss-Christoffel formulas, which is based on a suitable discretization of the inner product $(f, g) = \int_a^b f(x)g(x)w(x)dx$, and thus bypasses the moments altogether. As the discretization is made infinitely fine, the process converges to the desired Christoffel numbers provided the singularities of $w(x)$, if any, are located at the endpoints of the interval and are monotonic. Extensive tests have shown that the method is reasonably accurate, relatively "inexpensive," and requiring only single-precision arithmetic. A computer algorithm (in ALGOL) is to appear in [10].

Cases may arise in which our method converges very slowly. While approximate Christoffel numbers are still obtained, it may be desirable to further improve their accuracy. This can be done by applying Newton's method to a system of equations, equivalent to (1.3), using as initial approximations the approximate Christoffel numbers already obtained. An appropriate procedure for this will be described in Section 4. Unfortunately, this iterative refinement calls for the moments of the weight function, and therefore is of limited practical value, unless one is prepared to use higher-precision work in some preliminary parts of the computation.

The ability to generate Gauss-Christoffel quadrature formulas, as needed, is of considerable practical interest, not only for integrating singular functions, but also for the numerical solution of integral equations and boundary value problems. We also remark that this new capability may well be useful in future systems of "automated numerical analysis," such as the NAPSS system currently under development at Purdue University [18].

In the appendix are collected a few general properties, more or less known, of orthogonal polynomials which are relevant to our discussion in Sections 3, 4.

Extensions of our work seem possible to quadrature formulas of maximum degree of exactness, where some of the abscissas are prescribed, or the quadrature sum involves derivative values as well as function values. Such generalizations, however, will not be considered here.

2. Condition of the Classical Approach. In this section we discuss the condition of the problem of solving the system of algebraic equations (1.3). In particular we derive the estimates (1.4) and (1.6) for the asymptotic condition number, and compare them with the condition of inverting Hilbert matrices.

It will be useful, first, to consider the condition of a mapping M, say, from one normed space X into another, Y:

$$M: \quad X \to Y.$$

Following Rice [17], we define the (relative) δ-condition number $\kappa(\delta)$ of M at $x_0 \in X$ by

$$\kappa(\delta) \stackrel{\text{def}}{=} \max_{\|h\| = \delta} \frac{\|M(x_0 + h) - Mx_0\|}{\|Mx_0\|} \Big/ \frac{\delta}{\|x_0\|}. \tag{2.1}$$

Thus, $\kappa(\delta)$ represents the maximum amount by which a (relative) perturbation in the space X, as given by $\delta/\|x_0\|$, is magnified under the mapping M. Since the perturbations to be considered are small (rounding errors!) it is natural to consider the (relative) asymptotic condition number κ of M at x_0, as defined by

$$\kappa = \lim_{\delta \to 0} \kappa(\delta) , \tag{2.2}$$

where the existence of the limit, of course, is assumed.

In solving the system of equations (1.3) we are dealing with the mapping $M: X \to Y$ of a $2n$-dimensional Euclidean space into itself, if we identify X with the "moment space," and Y with the space of Christoffel numbers. This mapping is one-to-one in the neighborhood of the exact solution of (1.3). We may write (1.3) in the compact form

$$F(y) = x , \tag{2.3}$$

where $x^T = (\mu_0, \mu_1, \cdots, \mu_{2n-1})$, $y^T = (\lambda_1, \cdots, \lambda_n, \xi_1, \cdots, \xi_n)$, $F^T = (F_1, F_2, \cdots, F_{2n})$, and

$$F_k(y) = \sum_{\nu=1}^{n} \lambda_\nu \xi_\nu^{k-1} \qquad (k = 1, 2, \cdots, 2n) . \tag{2.4}$$

The (relative) asymptotic condition number $\kappa = \kappa_n$ for solving the nonlinear system of equations (2.3) at x_0 is well known to be (cf. [17])

$$\kappa_n = \frac{\|x_0\|}{\|y_0\|} \|[F_y(y_0)]^{-1}\| , \tag{2.5}$$

where y_0 is the solution of $F(y) = x_0$, and $F_y(y)$ denotes the Jacobian matrix of F. The matrix norm in (2.5) is assumed to be subordinate to the vector norm chosen in X and Y. From (2.4) we obtain by a simple computation that

$$F_y(y_0) = \Xi\Lambda , \tag{2.6}$$

where

$$\Xi = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ \xi_1 & \cdots & \xi_n & 1 & \cdots & 1 \\ \xi_1^2 & \cdots & \xi_n^2 & 2\xi_1 & \cdots & 2\xi_n \\ \cdot & & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & & \cdot \\ \xi_1^{2n-1} & \cdots & \xi_n^{2n-1} & (2n-1)\xi_1^{2n-2} & \cdots & (2n-1)\xi_n^{2n-2} \end{bmatrix} , \tag{2.7}$$

$$\Lambda = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & 1 & & \\ & & & & \lambda_1 & \\ & & & & & \lambda_2 \\ & & & & & & \ddots \\ & & & & & & & \lambda_n \end{bmatrix} .$$

(For simplicity, we have written ξ_r for $\xi_r^{(n)}$, and λ_r for $\lambda_r^{(n)}$.) Hence, by (2.5),

$$\kappa_n = \frac{\|x_0\|}{\|y_0\|} \|\Lambda^{-1}\Xi^{-1}\| . \tag{2.8}$$

We now choose our norms. We take as vector norm $\|x\| = \max_k |x_k|$, and correspondingly as matrix norm $\|A\| = \max_k \sum_r |a_{kr}|$. We further assume the basic interval to be (0, 1), and $w(x) \geqq 0$. Clearly, $\|x_0\| \geqq \mu_0$. Since $\lambda_r > 0$, and $\sum_{r=1}^{n} \lambda_r = \mu_0$, we have $\lambda_r < \mu_0$. Also, $0 < \xi_r < 1$. Therefore,

$$\|y_0\| = \max_r (\lambda_r, \xi_r) < \max (1, \mu_0) .$$

Moreover, with the matrix norm as defined,

$$\|\Lambda^{-1}\Xi^{-1}\| \geqq \min (1, 1/\mu_0) \|\Xi^{-1}\| .$$

It thus follows from (2.8), that

$$\kappa_n > \frac{\mu_0 \min (1, 1/\mu_0)}{\max (1, \mu_0)} \|\Xi^{-1}\| ,$$

or, equivalently,

$$\kappa_n > \min (\mu_0, 1/\mu_0) \|\Xi^{-1}\| . \tag{2.9}$$

Further discussion now hinges on obtaining a lower bound for $\|\Xi^{-1}\|$, where Ξ is the matrix in (2.7), a confluent Vandermonde matrix [8].

THEOREM 2.1. *Let $\xi_1, \xi_2, \cdots, \xi_n$ be mutually distinct positive numbers, and Ξ the matrix defined in* (2.7). *Then*

$$u_1 \leqq \|\Xi^{-1}\| \leqq \max (u_1, u_2) , \tag{2.10}$$

where $\|\cdot\|$ denotes the maximum row sum norm, and

$$u_i = \max_{1 \leq r \leq n} b_r^{(i)} \prod_{k=1; k \neq r}^{n} \left(\frac{1 + \xi_k}{\xi_r - \xi_k} \right)^2 \qquad (i = 1, 2) , \tag{2.11}$$

$$b_r^{(1)} = 1 + \xi_r, \quad b_r^{(2)} = \left| 1 + 2\xi_r \sum_{k=1; k \neq r}^{n} \frac{1}{\xi_r - \xi_k} \right| + 2 \left| \sum_{k=1; k \neq r}^{n} \frac{1}{\xi_r - \xi_k} \right| . \tag{2.12}$$

Proof. It was shown in [8] that

$$\Xi^{-1} = \begin{bmatrix} A \\ B \end{bmatrix},$$

where $A = (a_{rs})$, $B = (b_{rs})$ are $(n \times 2n)$-matrices satisfying

$$\sum_{s=1}^{2n} |a_{rs}| \leqq b_r^{(2)} \prod_{k \neq r} \left(\frac{1 + \xi_k}{\xi_r - \xi_k} \right)^2, \qquad \sum_{s=1}^{2n} |b_{rs}| = b_r^{(1)} \prod_{k \neq r} \left(\frac{1 + \xi_k}{\xi_r - \xi_k} \right)^2 . \tag{2.13}$$

Letting

$$\alpha = \max_{1 \leq r \leq n} \sum_{s=1}^{2n} |a_{rs}| , \qquad \beta = \max_{1 \leq r \leq n} \sum_{s=1}^{2n} |b_{rs}| ,$$

we have by (2.11) and (2.13), $\alpha \leqq u_2$, $\beta = u_1$. Now, either $\alpha \leqq \beta$, or $\alpha > \beta$. In the

first case, $\|\Xi^{-1}\| = \beta = u_1$, in the second case, $u_1 < \|\Xi^{-1}\| = \alpha \leqq u_2$. Hence, (2.10) holds in either case, and Theorem 2.1 is proved.

We remark that in the case $u_1 \geqq u_2$ we have $\|\Xi^{-1}\| = u_1$.

Applying Theorem 2.1 to (2.9), we obtain

$$\kappa_n > \min\left(\mu_0, \frac{1}{\mu_0}\right) \max_{1\leqq r\leqq n} \left\{(1+\xi_r) \prod_{k\neq r} \left(\frac{1+\xi_k}{\xi_r - \xi_k}\right)^2\right\}, \tag{2.14}$$

the result already stated in (1.4).

Using the approximations (cf. (1.5))

$$\xi_r \doteq \tfrac{1}{2}(1+x_r), \qquad x_r = \cos\theta_r, \qquad \theta_r = (2r-1)\pi/2n,$$

where x_r are the zeros of the Chebyshev polynomial $T_n(x)$, we may estimate

$$\begin{aligned}(1+\xi_r) \prod_{k\neq r} \left(\frac{1+\xi_k}{\xi_r - \xi_k}\right)^2 &\doteq \frac{1}{2}(3+x_r) \prod_{k\neq r} \left(\frac{3+x_k}{x_r - x_k}\right)^2 \\ &= \frac{1}{2(3+x_r)} \left[\frac{T_n(3)}{T_n'(x_r)}\right]^2 > \frac{1}{8}\left[\frac{T_n(3)}{T_n'(x_r)}\right]^2.\end{aligned} \tag{2.15}$$

We have

$$T_n'(x_r) = T_n'(\cos\theta_r) = n\frac{\sin(n\theta_r)}{\sin\theta_r} = (-1)^{r-1}\frac{n}{\sin\theta_r}. \tag{2.16}$$

Now the maximum in (2.14) is obviously larger than the respective expression evaluated for any fixed $r = r_0$. Choosing $r_0 = [n/2] + 1$, we obtain in view of (2.15), (2.16)

$$\kappa_n \dot{>} \frac{1}{8}\min\left(\mu_0, \frac{1}{\mu_0}\right)\left[\frac{c_n T_n(3)}{n}\right]^2, \qquad \begin{aligned} c_n &= 1 \quad (n \text{ odd}), \\ c_n &= \cos(\pi/2n) \quad (n \text{ even}).\end{aligned}$$*

Since $\cos(\pi/2n) \geqq 1/\sqrt{2}$ $(n \geqq 2)$, it follows that $c_n \geqq 1/\sqrt{2}$, and so

$$\kappa_n \dot{>} (1/16n^2)\min(\mu_0, 1/\mu_0)[T_n(3)]^2.$$

As is well known, $z_n = T_n(3)$ satisfies

$$z_{n+1} - 6z_n + z_{n-1} = 0, \qquad z_0 = 1, \qquad z_1 = 3.$$

Hence, using standard results from the theory of linear difference equations,

$$z_n = T_n(3) = \tfrac{1}{2}(t_1^n + t_2^n), \qquad t_1 = 3 + \sqrt{8}, \qquad t_2 = 3 - \sqrt{8}.$$

It follows that $T_n(3) > \frac{1}{2}t_1^n$, and we finally obtain

$$\kappa_n \dot{>} \min\left(\mu_0, \frac{1}{\mu_0}\right)\frac{(17+6\sqrt{8})^n}{64n^2}, \tag{2.17}$$

the result already stated in (1.6).

We note from (2.17) that κ_n grows at least at a rate essentially equal to $\exp[n \ln(17 + 6\sqrt{8})] = \exp(3.5255\cdots n)$. Surprisingly, this coincides with the rate of growth of the (Turing) condition number for the nth order segment of

* We use the symbol $\dot{>}$ to remind the reader that we are now dealing with an *approximate* lower bound.

the Hilbert matrix, as estimated by Todd [23]. Computing Christoffel numbers on the interval (0, 1) from given moments is therefore about as ill-conditioned as the inversion of Hilbert matrices!

3. Computation of Christoffel Numbers by Orthogonal Polynomials of a Discrete Variable. We begin with the classical construction due to Christoffel. We introduce the inner product

$$(f, g) = \int_a^b f(x)g(x)w(x)dx\,, \tag{3.1}$$

and let $\{\pi_r\}_{r=0}^{\infty}$ denote the associated orthonormal polynomials (cf. Example 1 of the appendix),

$$(\pi_r, \pi_s) = \delta_{rs}\,, \qquad \text{degree}\,(\pi_r) = r\,. \tag{3.2}$$

Let $\xi_r^{(n)}$ be the zeros of $\pi_n(x)$ in (say) increasing order. Then $\xi_r^{(n)}$ are precisely the Christoffel abscissas corresponding to the weight function $w(x)$. The Christoffel weights can be found, e.g., from

$$\lambda_r^{(n)} = \frac{1}{\sum_{k=0}^{n-1} [\pi_k(\xi_r^{(n)})]^2}\,. \tag{3.3}$$

This representation is particularly suitable for computation since it involves the summation of positive terms.

It seems appropriate, at this point, to distinguish two cases:

(a) The polynomials $\{\pi_r\}$ are known explicitly, i.e. either the coefficients of $\pi_r(x)$, or the coefficients in the three-term recurrence relation [cf. (A.7)], * are known in closed form. We may refer to this as the *classical case*, and call the corresponding weight functions "classical." In this case the approach just outlined is entirely satisfactory for computational purposes.

(b) The polynomials $\{\pi_r\}$ are not explicitly known. We refer to this as the *nonclassical case*, and call the corresponding weight functions "nonclassical." In this case it is necessary to progressively generate either the coefficients of $\pi_r(x)$, or the coefficients in the three-term recurrence relation for the π_r. This amounts to an orthogonalization of the successive powers, and hence requires knowledge of the moments of the given weight function. We are therefore in essence solving the ill-conditioned problem discussed in Section 2, and must thus be prepared to encounter severe numerical instability.

The following approach is specifically designed to handle the case of nonclassical weight functions.

Let

$$Q_N(\phi) \overset{\text{def}}{=} \sum_{k=1}^{N} w_k^{(N)}\phi(x_k^{(N)})\,, \qquad w_k^{(N)} > 0\,, \qquad N > n\,,$$

denote a sequence of auxiliary quadrature formulas with positive weights,

$$Q_N(\phi) \doteq \int_a^b \phi(x)dx\,. \tag{3.4}$$

* (A.7) refers to formula (7) of the appendix.

We assume first (a, b) a finite interval, say $(-1, 1)$ for definiteness. We define a new inner product,

$$[f, g]_N \overset{\text{def}}{=} Q_N(fgw) , \tag{3.5}$$

that is, more explicitly,

$$[f, g]_N = \sum_{k=1}^{N} W_k^{(N)} f(x_k^{(N)}) g(x_k^{(N)}) , \qquad W_k^{(N)} = w_k^{(N)} w(x_k^{(N)}) . \tag{3.5'}$$

Since $W_k^{(N)} > 0$ (we assume here that $w(x_k^{(N)}) \neq 0$ for $k = 1, 2, \cdots, N$), the inner product (3.5') gives rise to a set $\{\pi_{r,N}\}_{r=0}^{N-1}$ of orthonormal polynomials of a discrete variable (cf. Example 2 of the appendix),

$$[\pi_{r,N}, \pi_{s,N}]_N = \delta_{rs} , \qquad r, s = 0, 1, 2, \cdots, N-1 . \tag{3.6}$$

These polynomials may be generated as described in the appendix. The process requires the computation of inner products of the form (3.5'), which in turn requires only a finite summation and the evaluation of $w(x)$ at the points $x_k^{(N)}$ (no moments!).

In analogy with the classical approach we now define $\xi_{r,N}^{(n)}$ to be the zeros of $\pi_{n,N}(x)$ (known to be real), and let

$$\lambda_{r,N}^{(n)} = \frac{1}{\sum_{k=0}^{n-1} [\pi_{k,N}(\xi_{r,N}^{(n)})]^2} . \tag{3.7}$$

The $\xi_{r,N}^{(n)}$, $\lambda_{r,N}^{(n)}$, suitably ordered, are taken to approximate $\xi_r^{(n)}$, $\lambda_r^{(n)}$, respectively. These approximations depend on the parameter N, and hopefully converge to the desired Christoffel numbers as $N \to \infty$.

We may now rephrase Theorem 4 of the appendix, and its Corollary, as follows:

THEOREM 3.1. *Suppose that* $\lim_{N\to\infty} [f, g]_N = (f, g)$, *whenever* f *and* g *are polynomials. Then*

$$\lim_{N\to\infty} \pi_{r,N}(x) = \pi_r(x) , \tag{3.8}$$

and

$$\lim_{N\to\infty} \xi_{r,N}^{(n)} = \xi_r^{(n)} , \qquad \lim_{N\to\infty} \lambda_{r,N}^{(n)} = \lambda_r^{(n)} . \tag{3.9}$$

Under the assumption of Theorem 3.1, our construction thus yields a convergent process. The stated assumption, in essence, requires that the quadrature rule Q_N in (3.4) be convergent for integrands of the form $\phi(x) = p(x)w(x)$, where $p(x)$ is a polynomial, and $w(x)$ is the given weight function. Since $w(x)$ might be singular, we require, in other words, *convergence of the quadrature rule in the presence of singularities*. Fortunately, most of the common quadrature formulas do converge, even in the presence of singularities, particularly if the singularities occur at the endpoints of the interval and are monotonic [5], [16].

From the computational point of view, convergence alone, while desirable, is far from sufficient. Practical considerations lead us to impose the following additional requirements on the quadrature rules Q_N:

(i) Convergence should be reasonably fast, even in the presence of singularities;

(ii) The quadrature rule Q_N should be easy to generate for arbitrary, and especially large, values of N;

(iii) The interval $[x_1^{(N)}, x_2^{(N)}, \cdots, x_N^{(N)}]$ spanned by $x_1^{(N)}, \cdots, x_N^{(N)}$ should contain the desired Christoffel abscissas $\xi_1^{(n)}, \cdots, \xi_n^{(n)}$.

The first requirement assures that the value of N, necessary for given accuracy, is not excessively large. This is important, since the work involved in generating the discrete polynomials $\pi_{r,N}$ is proportional to N. The second requirement provides flexibility of the process, and also eliminates the need for storing a large number of high-order quadrature formulas in the computer memory. The third requirement is necessary because of the known fact that the zeros of $\pi_{n,N}(x)$ are all located in the interval $[x_1^{(N)}, \cdots, x_N^{(N)}]$. Since these zeros are supposed to approximate the abscissas $\xi_r^{(n)}$, these latter had better be contained in that interval!

These, of course, are hard criteria to accommodate. In view of the tendency of the $\xi_r^{(n)}$ to crowd near the endpoints of $(-1, 1)$, requirements (i) and (iii) suggest that we choose the abscissas $x_k^{(N)}$ to have the same property. This rules out the most common quadrature rules, such as trapezoidal, midpoint, and Simpson rules. The classical Gaussian quadrature formula, on the other hand, is in conflict with requirement (ii). A quadrature rule which comes close to satisfying all the requirements is the Newton-Cotes formula for the abscissas

$$x_k^{(N)} = \cos \theta_k^{(N)}, \qquad \theta_k^{(N)} = (2k - 1)\pi/2N, \tag{3.10}$$

the zeros of the Chebyshev polynomial $T_N(x)$. The corresponding weight factors $w_k^{(N)}$ can be written down explicitly, as was already pointed out by Fejér [6]. In fact,

$$w_k^{(N)} = \frac{2}{N}\left\{1 - 2\sum_{m=1}^{[N/2]} \frac{\cos(2m\theta_k^{(N)})}{4m^2 - 1}\right\}. \tag{3.11}$$

This takes care of the requirements (ii) and (iii), although it may be argued that (3.10), (3.11) require the evaluation of a large number of cosines. Actually, only *one* value of the cosine, viz. $\cos(\pi/2N)$, is needed, since all the others, both in (3.10) and (3.11), can be generated by well-known recurrence formulas! For best accuracy, however, it is recommended that only the cosines in (3.11) be computed recursively, especially if N is very large (say, exceeding 200).

As to requirement (i) we have recently shown [9] that the Fejér quadrature formula does indeed converge, not only for continuous functions, but also for singular functions, provided the singularities occur at the endpoints and are monotonic. The exact nature of the singularity is otherwise irrelevant. The rate of convergence, of course, depends on the type of singularity, though in a manner which is not well understood at the present time. Numerical experience indicates that convergence can be rather fast for some singularities (e.g. logarithmic singularities), but discouragingly slow for others (e.g. square-root singularities).

Another quadrature formula, which might be suitable, is the Gauss-Chebyshev formula

$$\int_{-1}^{1} \frac{\Phi(x)}{(1 - x^2)^{1/2}}\, dx \doteq \frac{\pi}{N}\sum_{k=1}^{N} \Phi(x_k^{(N)}),$$

if it is rewritten in the form

$$\int_{-1}^{1} \phi(x)dx \doteq \frac{\pi}{N}\sum_{k=1}^{N} (\sin \theta_k^{(N)})\phi(x_k^{(N)}). \tag{3.12}$$

Here we have exact equality if $\phi(x) = p_{2N-1}(x)(1 - x^2)^{-1/2}$, where $p_{2N-1}(x)$ is a polynomial of degree $2N - 1$. The formula (3.12) is therefore particularly suitable in cases where the weight function $w(x)$ has square-root singularities at the endpoints ± 1, which is one of the cases where the Fejér formula converges very slowly.

It is interesting to point out the close kinship between the Fejér formula (3.10), (3.11) and the Gauss-Chebyshev formula (3.12), noting that the right-hand side in (3.11) is nothing else but the truncated Fourier expansion of $(\pi/N) \sin \theta_k^{(N)}$, the weight factor in (3.12)!

We may also remark, at this point, that in the process of generating the polynomials $\pi_{r,N}$ $(r = 0, 1, \cdots, n)$, one needs to evaluate inner products $[f, g]_N$ only for polynomials f, g of degree $\leqq n$. Using the Fejér quadrature formula, which is of interpolatory type, it thus follows from (3.1), (3.5) that for such f and g, $[f, g]_N = (f, g)$ whenever $w(x)$ is a polynomial of degree m, and $N > 2n + m$. As a result, *our process of constructing Christoffel numbers, based on the Fejér formula* (3.10), (3.11), *is exact if* $w(x)$ *is a polynomial of degree* m *and* $N > 2n + m$. The process, in this case, converges trivially. Similarly, *our process of constructing Christoffel numbers, based on the Gauss-Chebyshev formula* (3.12), *is exact if* $w(x) = (1 - x^2)^{-1/2}$ *and* $N > n$.

Our development so far assumed $[-1, 1]$ as the basic interval. This is no restriction of generality. In fact, the case of an arbitrary finite interval $[a, b]$ is readily reduced to the case considered by a linear transformation of the independent variable. In the case of a half-infinite interval, say $(0, \infty)$, let $\phi(t)$ be any continuously differentiable monotonically increasing function mapping the interval $(-1, 1)$ onto $(0, \infty)$. Then

$$(f, g) = \int_0^\infty f(x)g(x)w(x)dx = \int_{-1}^1 f(\phi(t))g(\phi(t))w(\phi(t))\phi'(t)dt\,,$$

and we can proceed as before if we define

$$[f, g]_N = \sum_{k=1}^N W_k^{(N)} f(\phi(x_k^{(N)}))g(\phi(x_k^{(N)}))\,,$$

where now

$$W_k^{(N)} = w_k^{(N)} w(\phi(x_k^{(N)}))\phi'(x_k^{(N)})\,.$$

An analogous device applies for a doubly infinite interval $(-\infty, \infty)$, in which case $\phi(t)$ is to map $(-1, 1)$ onto $(-\infty, \infty)$. Simple transformation functions, which proved satisfactory, are $\phi(t) = (1 + t)/(1 - t)$ for $(0, \infty)$, and $\phi(t) = t/(1 - t^2)$ for $(-\infty, \infty)$.

We conclude this section with a few comments on the computation of the zeros $\xi_{r,N}^{(n)}$ of $\pi_{n,N}(x)$. We assume that the coefficients a_r, b_{r+1} in the recurrence relation (cf. (A.7*))

$$\begin{aligned} \pi_{r+1,N}(x) &= ((x - a_r)\pi_{r,N}(x) - b_r\pi_{r-1,N}(x))/b_{r+1} \\ &\qquad (r = 0, 1, \cdots, n - 1)\,, \\ \pi_{0,N}(x) &= [1, 1]_N^{-1/2}\,, \qquad \pi_{-1,N}(x) = 0\,, \end{aligned} \tag{3.13}$$

have already been obtained by the methods described in the appendix. We propose two different procedures to find the Christoffel abscissas, depending on whether the

$\xi_r^{(k)}$ are desired for all $k = 1, 2, \cdots, n$, $r = 1, 2, \cdots, k$, or $\xi_r^{(n)}$, $r = 1, 2, \cdots, n$, are desired for only one, or a few selected values of n.

In the first case we apply Newton's method to each of the equations $\pi_{k,N}(x) = 0\,(k = 2, 3, \cdots, n)$, using $(\xi_{r-1}^{(k-1)} + \xi_r^{(k-1)})/2$ as initial approximation for $\xi_r^{(k)}$. (Here, $\xi_0^{(k-1)}$ is equal to a, if a is finite, or a lower bound for $\xi_1^{(n)}$, if $a = -\infty$. Similarly $\xi_k^{(k-1)}$ is equal to b, if b is finite, or an upper bound for $\xi_n^{(n)}$, if $b = \infty$.) The choice of the initial approximation is motivated by the interlacing property of the zeros of $\pi_{r,N}$ and is normally sufficiently accurate to assure rapid convergence of Newton's iteration. Occasionally, however, because of the highly oscillatory character of the polynomials $\pi_{r,N}$, it may happen that some of the Newton iterates fall astray. For this reason it is recommended that each Newton approximation be checked upon whether or not it satisfies the interlacing property. If not, the appropriate subinterval should be examined more carefully for possible zeros, and Newton's iteration repeated with a suitably revised initial approximation.

In the second case, the zeros $\xi_r^{(n)}$ may be computed in their natural order, using Newton's method in combination with successive deflation. Thus suppose $\xi_1 = \xi_1^{(n)}$ is already obtained. We then construct the deflated polynomial (we drop the second subscripts N for notational simplicity)

$$\pi_n^{[1]}(x) = (\pi_n(x) - \pi_n(\xi_1))/(x - \xi_1) \tag{3.14}$$

and compute its smallest zero by Newton's method, using ξ_1 as initial approximation. Thereafter, we deflate again, and compute the smallest zero of the twice deflated polynomial. The process is repeated until all zeros are obtained. We note, that $\pi_n^{[1]}$ can be obtained by a recurrence relation very similar to (3.13), namely

$$\begin{aligned} &\pi_{r+1}^{[1]}(x) = (\pi_r(\xi_1) + (x - a_r)\pi_r^{[1]}(x) - b_r\pi_{r-1}^{[1]}(x))/b_{r+1} \\ &\qquad\qquad (r = 1, 2, \cdots, n-1)\,, \\ &\pi_1^{[1]}(x) = \pi_0/b_1\,, \qquad \pi_0^{[1]} = 0\,. \end{aligned} \tag{3.13^1}$$

This follows readily from (3.13), and the definition (3.14), where n is to be replaced by r. (This technique of deflation, in the context of matrices, was already described by Wilkinson [24, p. 468ff.]. He also analyzes its numerical stability.) Similarly, the m-times deflated polynomial $\pi_n^{[m]}(x)$ can be generated from

$$\begin{aligned} &\pi_{r+1}^{[m]}(x) = (\pi_r^{[m-1]}(\xi_m) + (x - a_r)\pi_r^{[m]}(x) - b_r\pi_{r-1}^{[m]}(x))/b_{r+1} \\ &\qquad\qquad (r = m, m+1, \cdots, n-1)\,, \\ &\pi_m^{[m]}(x) = \pi_{m-1}^{[m-1]}/b_m\,, \qquad \pi_{m-1}^{[m]}(x) = 0\,. \end{aligned} \tag{3.13^m}$$

To avoid undesirable accumulation of error, it is recommended that each deflation (except the first) be preceded by a "refinement" of the respective zero using Newton's iteration applied to the original (undeflated) polynomial $\pi_n(x)$.

It should be noted that the initial approximations to the zeros, if successive deflations are used, are not as accurate as those used in the first procedure (without deflation).

4. Iterative Refinement of Christoffel Numbers. We assume now that we have certain approximations ξ_r^0, λ_r^0 to the desired Christoffel numbers $\xi_r^{(n)}$, $\lambda_r^{(n)}$, which

are sufficiently accurate to attempt solving the basic system of algebraic equations by Newton's method. The approximations ξ_r^0, λ_r^0, for example, may have been obtained by the procedure discussed in Section 3.

Let $\{p_r\}_{r=0}^{2n-1}$ be a system of $2n$ linearly independent polynomials, and define the "modified moments" by

$$m_k = \int_a^b p_k(x)w(x)dx\,. \tag{4.1}$$

The basic system of equations (1.3) is obviously equivalent to

$$\sum_{r=1}^{n} \lambda_r^{(n)} p_k(\xi_r^{(n)}) = m_k \qquad (k = 0, 1, 2, \cdots, 2n-1)\,. \tag{4.2}$$

We wish to choose the polynomials p_r in such a way that the system (4.2), unlike (1.3), is well-conditioned. Ideally, this would be achieved if the Jacobian matrix $J(\lambda_1, \cdots, \lambda_n; \xi_1, \cdots, \xi_n)$ of (4.2) evaluated at the exact solution $\lambda_r = \lambda_r^{(n)}$, $\xi_r = \xi_r^{(n)}$, is orthogonal. We shall settle for the next best, which is orthogonality of $J(\lambda_1^0, \cdots, \lambda_n^0; \xi_1^0, \cdots, \xi_n^0)$. Since

$$J(\lambda_r; \xi_r) = \begin{bmatrix} p_0(\xi_1) & \cdots & p_0(\xi_n) & \lambda_1 p_0'(\xi_1) & \cdots & \lambda_n p_0'(\xi_n) \\ p_1(\xi_1) & \cdots & p_1(\xi_n) & \lambda_1 p_1'(\xi_1) & \cdots & \lambda_n p_1'(\xi_n) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ p_{2n-1}(\xi_1) & \cdots & p_{2n-1}(\xi_n) & \lambda_1 p_{2n-1}'(\xi_1) & \cdots & \lambda_n p_{2n-1}'(\xi_n) \end{bmatrix}, \tag{4.3}$$

the required orthogonality means that the rows in the matrix (4.3) be mutually orthonormal. In terms of the inner product

$$\{f, g\} = \sum_{r=1}^{n} [f(\xi_r^0)g(\xi_r^0) + (\lambda_r^0)^2 f'(\xi_r^0)g'(\xi_r^0)]\,, \tag{4.4}$$

this in turn implies that

$$\{p_r, p_s\} = \delta_{rs}\,, \qquad r, s = 0, 1, \cdots, 2n-1\,. \tag{4.5}$$

We are led to the discrete analogue of Gröbner polynomials, considered in Example 3 of the appendix.

In choosing the polynomials p_r as described, we not only are achieving a well-conditioned system of algebraic equations, (4.2), but also assure that the linear systems of equations which need to be solved in Newton's method are all well-conditioned. This is so because the first of these is exactly orthogonal, while the remaining ones are nearly orthogonal.

Unfortunately, the modified moments (4.1) are not known in advance, and must be generated, along with the polynomials p_r. As is shown in the first section of the appendix, we have for $\{p_r\}$ the recurrence relation

$$\begin{aligned} p_{r+1}(x) &= ((x - a_{r,r})p_r(x) - a_{r,r-1}p_{r-1}(x) - \cdots - a_{r,0}p_0(x))/b_{r+1} \\ &\qquad\qquad (r = 0, 1, \cdots, 2n-2)\,, \\ p_0(x) &= \{1, 1\}^{-1/2}\,, \end{aligned} \tag{4.6}$$

where the coefficients a_{rs} and b_{r+1} can be computed as described in the appendix. Let us define, then,

$$m_{rk} = \int_a^b x^k p_r(x) w(x) dx \,. \tag{4.7}$$

We have, in particular,

$$m_{0k} = p_0 \mu_k \,, \qquad m_{r0} = m_r \,, \tag{4.8}$$

where μ_k are the moments (1.2) of $w(x)$. From (4.6) and (4.7) we obtain

$$m_{r+1,k} = \left(m_{r,k+1} - \sum_{i=0}^{r} a_{ri} m_{ik} \right) / b_{r+1} \,. \tag{4.9}$$

We may consider $m_{r,k}$ as entries at grid points of the triangular region $r \geqq 0$, $k \geqq 0$, $r + k \leqq 2n - 1$ in the first quadrant of the (r, k)-plane. The entries along the vertical boundary of the triangle, by (4.8), are $p_0 \mu_k$, which we assume to be known. The relation (4.9) then permits to progressively fill in the triangle, proceeding from left to right. When completed, the entries along the horizontal boundary will be found, which by (4.8) are precisely the modified moments m_r.

Our process of iterative refinement thus consists of two parts. First, the generation of the orthonormal polynomials p_r and, along with this, the generation of the modified moments m_r. Second, the solution of the system of equations (4.2) by Newton's method. Since the whole process (starting, as it does, with the moments μ_k) is unstable, and the second part is stable, we conclude that the first part must be unstable. In practice, therefore, unless n is small, this part should be carried out with high precision.

5. Examples. We select at random some of the possible applications of our procedure to numerical integration, and also point out some of its limitations. The examples, of course, could easily be multiplied. For additional numerical examples we refer to [10].

(a) In the theory of radiative equilibrium of stellar atmospheres one encounters integrals of the form

$$J(\tau) = \frac{1}{2} \int_0^\infty f(t) E_1(|t - \tau|) dt \,,$$

$$F(\tau) = 2 \int_\tau^\infty f(t) E_2(t - \tau) dt - 2 \int_0^\tau f(t) E_2(\tau - t) dt \,,$$

to evaluate mean intensities and fluxes. Here, $f(t)$ is a known function, and $E_n(x) = \int_1^\infty e^{-xt} t^{-n} dt$, the exponential integral. After a suitable change of variables, one is thus faced with integrals of the form

$$\int_0^\infty f(x) E_n(x) dx \,, \qquad \int_0^\tau f(x) E_n(\tau - x) dx \,.$$

Since $E_n(x)$ has a logarithmic singularity at $x = 0$, and an essential singularity at $x = \infty$, it is natural to treat $E_n(x)$ and $E_n(\tau - x)$ as weight functions, and to apply the corresponding Gauss-Christoffel quadrature formulas [2, p. 65ff]. These may be constructed by our procedure of Section 3, both singularities being monotonic. A 20-point formula for $w(x) = E_1(x)$, $0 < x < \infty$, so obtained, may be found in [10].

(b) For the evaluation of Fourier coefficients it may be useful to compute

$$\frac{1}{2\pi}\int_0^{2\pi} f(x)\left(1 - \begin{matrix}\cos\\ \sin\end{matrix} \alpha x\right)dx$$

by Gaussian quadrature treating the trigonometric factor as a weight function [25].

(c) Fourier integrals, such as $\int_0^\infty f(x)\cos \alpha x\, dx$, may be treated by Gaussian quadrature, in a manner described in [14]. This calls for n-point Gauss-Christoffel formulas with weight function $w(x) = (1 + \cos x)/(1 + x)^{2n+s}$ on $(0, \infty)$, where $s > 0$ is a suitable number, depending on the behavior of $f(x)$ at $x = \infty$.

We have here a case of a nonmonotonic singularity (at $x = \infty$) and thus no theoretical justification for the process of Section 3. The process, accordingly, seems to converge very slowly, if at all. To illustrate, we display below the minimum and maximum relative errors in the abscissas $\xi_\tau^{(n)}$ and weights $\lambda_\tau^{(n)}$ for the case $s = 1$, $n = 5$, and values of N as shown.

N	min. err. $\xi_\tau^{(5)}$	max. err. $\xi_\tau^{(5)}$	min. err. $\lambda_\tau^{(5)}$	max. err. $\lambda_\tau^{(5)}$
20	.00245	.07907	.00250	.30546
40	.00354	.05818	.00372	.18464
80	.00584	.18406	.00611	.39220
160	.00025	.01658	.00021	.04318
320	.00132	.04617	.00132	.09630

(d) In an attempt to integrate numerically the remainder term in the Euler-Maclaurin sum formula [25], one might use Gauss-Christoffel formulas with weight function $w(x) = 1/x - [1/x]$ on $(0, 1)$. This function has an infinite number of discontinuities, accumulating at $x = 0$, and is all but monotonic there. Not surprisingly, our procedure of Section 3 does not seem to converge, not even for n as small as 5, as may be seen from the following results.

N	$\xi_{1,N}^{(5)}$	$\xi_{3,N}^{(5)}$	$\xi_{5,N}^{(5)}$
100	.04756	.47518	.89997
200	.04392	.47103	.89932
400	.04308	.47499	.89983
800	.04510	.47361	.89968

Appendix. Orthogonal polynomials

We collect here, for easy reference, some elementary properties, computational aspects, and examples of orthogonal polynomials which are useful in the context of Sections 3 and 4.

Consider a (real) linear function space S containing the powers x^r, $r = 0, 1, 2, \cdots, N$, where N may be finite or infinite. Designate by $(\ ,\ )$ an inner product in S. The set of orthogonal polynomials, relative to this inner product, will be denoted by $\{p_r\}_{r=0}^N$. Thus,

(1) $\qquad (p_r, p_s) = 0 \text{ for } r \neq s, \qquad \text{degree } (p_r) = r.$

These polynomials are uniquely determined if we require that each p_r has leading coefficient one. The orthonormal polynomials will be denoted by p_r^*. We have

$$p_r^*(x) = c_r p_r(x), \qquad c_r = (p_r, p_r)^{-1/2}. \tag{2}$$

1. Recurrence relations.

THEOREM 1. *The orthogonal polynomials in* (1), *having leading coefficients one, satisfy the recurrence relation*

$$p_{r+1}(x) = (x - a_{r,r})p_r(x) - a_{r,r-1}p_{r-1}(x) - \cdots - a_{r,0}p_0(x) \qquad (r = 0, 1, 2, \cdots, N-1), \tag{3}$$

where

$$a_{r,s} = (xp_r, p_s)/(p_s, p_s) \qquad (s = 0, 1, 2, \cdots, r). \tag{4}$$

Proof. It is clear that the polynomials defined by (3), and $p_0(x) = 1$, have leading coefficients one and correct degrees. A simple computation shows that orthogonality of $p_0, p_1, \cdots, p_r$ implies orthogonality of $p_0, p_1, \cdots, p_{r+1}$. Since p_0 and p_1 are orthogonal, Theorem 1 follows by induction.

A recurrence relation for the orthonormal polynomials p_r^* could be obtained in the obvious manner by substituting (2) into (3). Computationally, it is slightly more convenient to introduce

$$\tilde{p}_r(x) = c_{r-1}p_r(x) = c_{r-1}p_r^*(x)/c_r, \tag{5}$$

and to transform (3), (4) into

$$\begin{aligned} \tilde{p}_{r+1}(x) &= (x - a_{r,r}^*)p_r^*(x) - a_{r,r-1}^*p_{r-1}^*(x) - \cdots - a_{r,0}^*p_0^*(x), \\ p_{r+1}^*(x) &= \tilde{p}_{r+1}(x)/(\tilde{p}_{r+1}, \tilde{p}_{r+1})^{1/2}, \end{aligned} \tag{3*}$$

where

$$a_{r,s}^* = (xp_r^*, p_s^*) \qquad (s = 0, 1, \cdots, r).$$

THEOREM 2. *If the inner product satisfies*

$$(xf, g) = (f, xg), \tag{6}$$

then (3) *is a three-term recurrence relation, i.e.*

$$p_{r+1}(x) = (x - a_r)p_r(x) - b_r p_{r-1}(x) \qquad (r = 0, 1, \cdots, N-1), \tag{7}$$

where

$$a_r = (xp_r, p_r)/(p_r, p_r) \qquad (r = 0, 1, \cdots, N-1), \tag{8}$$

$$b_r = (xp_r, p_{r-1})/(p_{r-1}, p_{r-1}) = (p_r, p_r)/(p_{r-1}, p_{r-1}) \qquad (r = 1, 2, \cdots, N-1). \tag{9}$$

(*We adopt the convention, in* (7), *that* $p_{-1}(x) \equiv 0$.)

Proof. By (6) we have $(xp_r, p_s) = (p_r, xp_s) = 0$ if $s < r - 1$, since xp_s is a polynomial of degree $\leqq r - 1$, and p_r is orthogonal to every polynomial of degree $< r$. Consequently, by (4), $a_{r,s} = 0$ if $s < r - 1$, and Theorem 2 is a corollary of Theorem 1. The second expression for b_r is obtained by noting that $(xp_r, p_{r-1}) = (p_r, xp_{r-1}) = (p_r, p_r)$, since xp_{r-1} differs from p_r by a polynomial of degree $< r$.

We may interpret $p_r(x)$ of Theorem 2 as the characteristic polynomial $\det(xI_r - J_r)$ of the symmetric tridiagonal matrix

$$J_r = \begin{bmatrix} a_0 & \sqrt{b_1} & & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & & \\ & \cdot & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \sqrt{b_{r-1}} & a_{r-1} \end{bmatrix}.$$

Since, by the second relation in (9), $b_r > 0$, we have that J_r is a Jacobi matrix. Consequently, as is well known, the polynomials $\{p_r(x)\}_{r=0}^{N-1}$ have the Sturm sequence property (cf. [24, p. 300]). In particular, the zeros of p_r separate those of p_{r+1}.

Using (5), we obtain for the orthonormal polynomials p_r^* of Theorem 2 the recursion

$$(7^*) \quad \tilde{p}_{r+1}(x) = (x - a_r^*)p_r^*(x) - b_r^* p_{r-1}^*(x), \qquad p_{r+1}^*(x) = \tilde{p}_{r+1}(x)/b_{r+1}^*$$

where

$$a_r^* = (xp_r^*, p_r^*), \qquad b_r^* = (\tilde{p}_r, \tilde{p}_r)^{1/2}.$$

This form of the recurrence relation is particularly convenient for computation [4, p. 234].

Noting that $a_r^* = a_r$, $b_r^* = \sqrt{b_r}$, the Gershgorin circle theorem applied to the Jacobi matrix J_n permits one to find upper and lower bounds for the zeros of $p_n(x)$ in terms of the coefficients a_r^* and b_r^*.

2. Examples.

Example 1. Let $S = C[-1, 1]$, the class of continuous functions on $[-1, 1]$ (hence $N = \infty$), and let the inner product be defined by

$$(10) \qquad (f, g) = \int_{-1}^{1} f(x)g(x)w(x)dx.$$

Here, $w(x)$ is a weight function assumed to be positive for $-1 < x < 1$, and such that all its moments $\int_{-1}^{1} x^r w(x)dx$, $r = 0, 1, 2, \cdots$, exist. The inner product (10) clearly satisfies (6).

The recursion (7) can be used, in principle, to generate the orthogonal polynomials $p_r(x)$ successively for $r = 1, 2, 3, \cdots$, starting with $p_{-1}(x) \equiv 0$, $p_0(x) = 1$. In practice, this requires the computation of the inner products in (8), (9), which in view of (10) may be problematic, especially if $w(x)$ is a singular function not of the standard type $w(x) = (1 - x)^\alpha(1 + x)^\beta$, $\alpha > -1$, $\beta > -1$. In the latter case, p_r are the Jacobi polynomials, and the coefficients a_r, b_r in (7) are known explicitly [22].

Example 2. Let $N = n - 1$ be a fixed positive integer, and S the set of polynomials of degree $\leqq N$. Define

$$(f, g) = \sum_{r=1}^{n} w_r f(x_r) g(x_r) , \tag{11}$$

where w_r, x_r are fixed real numbers with $w_r > 0$, $x_r \neq x_s$ for $r \neq s$. We note that S is an inner product space, since $(f, f) = 0$ implies $f(x_r) = 0$ $(r = 1, 2, \cdots, n)$, which in turn implies $f \equiv 0$, f being a polynomial of degree $< n$.

In contrast to Example 1, we now have a finite set of orthogonal polynomials depending on a parameter, n. To different values of n correspond different sets of orthogonal polynomials. As (6) is satisfied, these polynomials again obey the relations in (7)–(9). The successive computation of the coefficients a_r, b_r is now straightforward, since the inner product (11) requires only the evaluation of a finite sum.

Example 3. Let $N = 2n - 1$ be fixed, and S the set of polynomials of degree $\leqq N$. Define

$$(f, g) = \sum_{r=1}^{n} [u_r f(x_r) g(x_r) + v_r f'(x_r) g'(x_r)] , \tag{12}$$

where u_r, v_r, x_r are fixed real numbers, with $u_r > 0$, $v_r > 0$. As in Example 2 one shows that S is an inner-product space. Unlike the previous example, however, the inner product now fails to satisfy (6). As a result, the associated orthogonal polynomials p_r obey the "long" recurrence relation (3). The coefficients $a_{r,s}$ appearing in this relation are different from zero, in general, although in special circumstances some of them may vanish (cf. Theorem 3 below).

While it is true that the recurrence relation is now more complicated, it can still be used, as in Example 2, to successively build up the coefficients $a_{r,s}$. The inner products required in (4) are readily computed by the finite summation in (12), using for the derivatives the recursion

$$p'_{r+1}(x) = p_r(x) + (x - a_{r,r}) p_r'(x) - a_{r,r-1} p'_{r-1}(x) - \cdots - a_{r,1} p_1'(x) . \tag{13}$$

We remark that the continuous analogues of the polynomials considered in Example 3 were recently studied by Gröbner [12].

3. Symmetry Properties. If $w(x)$ is an *even* function on $(-a, a)$, where $0 < a \leqq \infty$, then the associated orthogonal polynomials satisfy

$$p_r(x) = (-1)^r p_r(-x) .$$

In particular, the zeros of p_r are located symmetrically with respect to the origin, and $x = 0$ is a zero of p_r if r is odd.

This property may be used to essentially cut in half the amount of work required to construct the Christoffel numbers for an even weight function. Indeed, the polynomials $p_{n,e}(x) = p_{2n}(\sqrt{x})$ form a set of orthogonal polynomials relative to the inner product

$$(f, g)_e = \int_0^{a^2} f(x) g(x) \frac{w(\sqrt{x})}{\sqrt{x}} \, dx .$$

It follows that the Christoffel numbers $\xi_{r,e}^{(n)}$, $\lambda_{r,e}^{(n)}$ of $p_{n,e}$ are related to those of p_{2n} by

$$\xi_{r,e}^{(n)} = [\xi_r^{(2n)}]^2 , \qquad \lambda_{r,e}^{(n)} = 2\lambda_r^{(2n)} \qquad (r = 1, 2, \cdots, n) ,$$

where $\xi_r^{(2n)}$ are the *positive* zeros of p_{2n} and $\lambda_r^{(2n)}$ the corresponding weight factors.

Similarly, the polynomials $p_{n,0}(x) = (1/\sqrt{x})p_{2n+1}(\sqrt{x})$ are orthogonal with respect to the inner product

$$(f, g)_0 = \int_0^{a^2} f(x)g(x)\sqrt{x}w(\sqrt{x})dx ,$$

and their zeros and weight factors are given by

$$\xi_{r,0}^{(n)} = [\xi_r^{(2n+1)}]^2 , \qquad \lambda_{r,0}^{(n)} = 2\xi_{r,0}^{(n)}\lambda_r^{(2n+1)} \qquad (r = 1, 2, \cdots, n) .$$

Here again $\xi_r^{(2n+1)}$ denotes the *positive* zeros of p_{2n+1} and $\lambda_r^{(2n+1)}$ the corresponding weight factors. Moreover,

$$\int_{-a}^{a} w(x)dx - \sum_{r=1}^{n} \lambda_{r,0}^{(n)}/\xi_{r,0}^{(n)} = \lambda_0^{(2n+1)}$$

is the weight factor corresponding to the zero $\xi_0^{(2n+1)} = 0$ of p_{2n+1}.

The inner product (12) may be called *equilibrated* if

$$\begin{aligned} x_{n+1-r} &= x_1 + x_n - x_r \\ u_{n+1-r} &= u_r, \qquad v_{n+1-r} = v_r \end{aligned} \qquad (r = 1, 2, \cdots, n) . \tag{14}$$

THEOREM 3. *If the inner product* (12) *is equilibrated, in the sense of* (14), *then the associated orthogonal polynomials* p_r *satisfy*

$$p_r(x_1 + x_n - x) = (-1)^r p_r(x) . \tag{15}$$

Moreover, every other coefficient in the recursion (3) *is zero, i.e.*

$$a_{r,r-2s} = 0 \qquad (s = 1, 2, 3, \cdots) . \tag{16}$$

The proof of Theorem 3 is elementary, and is omitted here.

4. Discrete vs. Continuous Orthogonal Polynomials. The orthogonal polynomials of Example 2 may be considered discrete analogues of those in Example 1. It is reasonable to expect that the former approach the latter, as $n \to \infty$, if the inner product in (11) converges to the inner product in (10).

THEOREM 4. *Let* (f, g) *denote the inner product in* (10), *and let*

$$[f, g]_n = \sum_{r=1}^{n} w_r^{(n)} f(x_r^{(n)})g(x_r^{(n)}) , \tag{17}$$

where $w_r^{(n)}$ *are positive numbers and* $x_r^{(n)}$, *for each* n, *are* n *distinct numbers in* $[-1, 1]$. *Let* $\{p_r\}_{r=0}^{\infty}$ *denote the set of orthogonal polynomials associated with* (10), *and* $\{p_{r,n}\}_{r=0}^{n-1}$ *the set of orthogonal polynomials associated with* (17). *Suppose that*

$$\lim_{n\to\infty} [f, g]_n = (f, g) , \tag{18}$$

whenever f *and* g *are polynomials. Then for each* $r = 0, 1, 2, \cdots$ *we have the limit relation*

$$\lim_{n\to\infty} p_{r,n}(x) = p_r(x) \tag{19}$$

for any fixed x, *and thus uniformly for* x *in any finite interval.*

Proof. We begin with the observation that

$$|[f, g]_n| \leqq \sum_{r=1}^{n} w_r^{(n)} \max_{-1\leqq x\leqq 1} |f(x)| \cdot \max_{-1\leqq x\leqq 1} |g(x)|$$

for any continuous functions f, g, and therefore

$$|[f, g]_n| \leqq ||f||\, ||g||[1, 1]_n . \tag{20}$$

The polynomials p_r, by Theorem 2, satisfy (7)–(9), while the polynomials $p_{r,n}$, by the same theorem, satisfy

$$p_{r+1,n}(x) = (x - a_{r,n})p_{r,n}(x) - b_{r,n}p_{r-1,n}(x) , \tag{21}$$

with

$$a_{r,n} = \frac{[xp_{r,n}, p_{r,n}]_n}{[p_{r,n}, p_{r,n}]_n} , \qquad b_{r,n} = \frac{[xp_{r,n}, p_{r-1,n}]_n}{[p_{r-1,n}, p_{r-1,n}]_n} . \tag{22}$$

Suppose now that (19) is true for $r = s$ and $r = s - 1$. We want to show that (19) holds for $r = s + 1$. For this it suffices to show that

$$a_{s,n} \to a_s , \quad b_{s,n} \to b_s \qquad (n \to \infty) , \tag{23}$$

since by (21), this implies $p_{s+1,n}(x) \to (x - a_s)p_s(x) - b_s p_{s-1}(x) = p_{s+1}(x)$.

We have

$$\begin{aligned} [p_{s,n}, p_{s,n}]_n &= [p_s + (p_{s,n} - p_s), p_s + (p_{s,n} - p_s)]_n \\ &= [p_s, p_s]_n + 2[p_s, p_{s,n} - p_s]_n + [p_{s,n} - p_s, p_{s,n} - p_s]_n . \end{aligned} \tag{24}$$

The first term on the right, by (18), has the limit (p_s, p_s) as $n \to \infty$. To the second term we apply (20), with the result that

$$|[p_s, p_{s,n} - p_s]_n| \leqq ||p_s||\, ||p_{s,n} - p_s||[1, 1]_n .$$

Since $[1, 1]_n \to (1, 1)$, and $p_{s,n} \to p_s$ (by assumption), we see that the bound on the right tends to zero as $n \to \infty$. By the same reasoning, one shows that the last term in (24) also tends to zero. Consequently,

$$\lim_{n\to\infty} [p_{s,n}, p_{s,n}]_n = (p_s, p_s) .$$

In the same manner, analogous limit relations can be established for all the other inner products appearing in (22), thus proving (23).

Since, trivially, $p_{0,n} \to p_0$, $p_{-1,n} \to p_{-1}$, the assertion (19) now follows by induction.

Theorem 4 may also be obtained from a general theorem of B. R. Kripke [13] on best approximation with respect to nearby norms, if one observes that $x^r - p_{r,n}(x)$ and $x^r - p_r(x)$ are the best approximations to x^r, from polynomials of degree $r - 1$, in the norms of (17) and (10), respectively. The author is indebted to Professor J. R. Rice for this remark.

COROLLARY. *Let the zeros of $p_r(x)$, in increasing order, be denoted by $x_1^{(r)}, x_2^{(r)}, \cdots, x_r^{(r)}$, and the zeros of $p_{r,n}(x)$, in the same order, by $x_{1,n}^{(r)}, x_{2,n}^{(r)}, \cdots, x_{r,n}^{(r)}$. Under the assumptions of Theorem 4, we have*

$$\lim_{n\to\infty} x_{s,n}^{(r)} = x_s^{(r)} , \quad \lim_{n\to\infty} p_{t,n}(x_{s,n}^{(r)}) = p_t(x_s^{(r)}) \qquad (s = 1, 2, \cdots, r; t < r) . \tag{25}$$

Proof. The first relation in (25) follows from the continuity of the zeros of an algebraic equation. The second relation follows from

$$p_{t,n}(x_{s,n}^{(r)}) - p_t(x_s^{(r)}) = [p_{t,n}(x_{s,n}^{(r)}) - p_t(x_{s,n}^{(r)})] + [p_t(x_{s,n}^{(r)}) - p_t(x_s^{(r)})]$$

by observing that $|p_{t,n}(x_{s,n}^{(r)}) - p_t(x_{s,n}^{(r)})| \leqq \max_{-1\leq x\leq 1} |p_{t,n}(x) - p_t(x)| \to 0$ $(n \to \infty)$, and $p_t(x_{s,n}^{(r)}) \to p_t(x_s^{(r)})$ $(n \to \infty)$.

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On the Construction of Gaussian Quadrature Rules from Modified Moments*

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Abstract. Given a weight function $\omega(x)$ on (α, β), and a system of polynomials $\{p_k(x)\}_{k=0}^{\infty}$, with degree $p_k(x) = k$, we consider the problem of constructing Gaussian quadrature rules $\int_\alpha^\beta f(x)\omega(x)dx \doteq \sum_{\nu=1}^n \lambda_\nu^{(n)} f(\xi_\nu^{(n)})$ from "modified moments" $\nu_k = \int_\alpha^\beta p_k(x)\omega(x)dx$. Classical procedures take $p_k(x) = x^k$, but suffer from progressive ill-conditioning as n increases. A more recent procedure, due to Sack and Donovan, takes for $\{p_k(x)\}$ a system of (classical) orthogonal polynomials. The problem is then remarkably well-conditioned, at least for finite intervals $[\alpha, \beta]$. In support of this observation, we obtain upper bounds for the respective asymptotic condition number. In special cases, these bounds grow like a fixed power of n. We also derive an algorithm for solving the problem considered, which generalizes one due to Golub and Welsch. Finally, some numerical examples are presented.

1. Introduction. Let $\omega(x)$ be a weight function on the (finite or infinite) interval (α, β), i.e., measurable and nonnegative on (α, β), with all moments

$$\mu_k = \int_\alpha^\beta x^k \omega(x)\, dx, \qquad k = 0, 1, 2, \ldots, \tag{1.1}$$

finite and $\mu_0 > 0$. Given a set $\{p_k(x)\}_{k=0}^{\infty}$ of polynomials, with degree $p_k = k$, we call

$$\nu_k = \int_\alpha^\beta p_k(x)\omega(x)\, dx, \qquad k = 0, 1, 2, \ldots \tag{1.2}$$

the *modified moments* of ω. Clearly, $\nu_k = \mu_k$, if $p_k(x) = x^k$.

A *Gaussian quadrature rule* associated with the weight function ω is a functional

$$G_n f = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\xi_\nu^{(n)}), \tag{1.3}$$

which has the property that

$$G_n f = \int_\alpha^\beta f(x)\omega(x)\, dx, \quad \text{all } f \in \mathbf{P}_{2n-1}, \tag{1.4}$$

where $\mathbf{P}_{2n-1}$ is the class of polynomials of degree $\leqq 2n - 1$. As is well known, G_n exists uniquely for each $n = 1, 2, 3, \ldots$. In fact, the abscissas $\xi_\nu^{(n)}$ are the zeros of $\pi_n(x)$,

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$$\pi_n(\xi_r^{(n)}) = 0, \qquad r = 1, 2, \ldots, n, \tag{1.5}$$

where $\{\pi_k(x)\}_{k=0}^{\infty}$ is the system of orthonormal polynomials belonging to the weight function ω,

$$\text{degree } \pi_k = k, \qquad \int_\alpha^\beta \pi_r(x)\pi_s(x)\omega(x)\,dx = \delta_{rs} \begin{cases} = 0 & r \neq s, \\ = 1 & r = s. \end{cases} \tag{1.6}$$

The weights $\lambda_r^{(n)}$, too, can be expressed in terms of these polynomials, e.g., by

$$\lambda_r^{(n)} = \left(\sum_{k=0}^{n-1} [\pi_k(\xi_r^{(n)})]^2 \right)^{-1}, \qquad r = 1, 2, \ldots, n, \tag{1.7}$$

showing that $\lambda_r^{(n)} > 0$.

The problem we want to consider is the computation of the functional G_n (i.e., the computation of the abscissas $\xi_r^{(n)}$ and weights $\lambda_r^{(n)}$), given the modified moments ν_k. In view of (1.5), (1.7), the problem may be considered as solved, once the orthonormal polynomials $\{\pi_k\}$ have been obtained accurately.

We note, incidentally, that these polynomials are also useful for the construction of rules

$$\tilde{G}_n f = \tilde{\lambda}_1^{(n)} f(\xi) + \sum_{r=2}^{n} \tilde{\lambda}_r^{(n)} f(\tilde{\xi}_r^{(n)}), \tag{1.3}^{\sim}$$

where ξ is an arbitrary real number with $\pi_{n-1}(\xi) \neq 0$, and

$$\tilde{G}_n f = \int_\alpha^\beta f(x)\omega(x)\,dx, \quad \text{all } f \in \mathbf{P}_{2n-2}. \tag{1.4}^{\sim}$$

The abscissas $\tilde{\xi}_r^{(n)}$, $r \geqq 2$, are then in fact the zeros (other than ξ) of

$$\psi_n(x) = \pi_{n-1}(\xi)\pi_n(x) - \pi_n(\xi)\pi_{n-1}(x), \tag{1.5}^{\sim}$$

while the weights $\tilde{\lambda}_r^{(n)}$, $r = 1, 2, \ldots, n$, are still given by the expression on the right of (1.7), if $\xi_r^{(n)}$ is replaced by $\tilde{\xi}_r^{(n)}$ and $\tilde{\xi}_1^{(n)} = \xi$ [2, Sections I.3–4].

The problem stated, in the special case $p_k(x) = x^k$, is classical, and a number of methods are known for its solution. However, the problem becomes increasingly ill-conditioned as n increases, as we have shown in [6]. In order to obtain high-order Gaussian quadrature rules in this manner, it is therefore necessary to resort to multiple-precision computations. Alternatively, more elaborate procedures may be used, such as the one in [6], which do not rely on the moments μ_k.

The general problem was considered recently by Sack and Donovan [12], in the case of polynomials $\{p_k\}$ satisfying a recurrence relation

$$xp_j(x) = a_j p_{j+1}(x) + b_j p_j(x) + c_j p_{j-1}(x), \qquad j = 0, 1, 2, \ldots; \qquad p_{-1}(x) = 0, \tag{1.8}$$

with known coefficients $a_j \neq 0$, b_j, c_j. If $\{p_k\}$ are themselves orthogonal polynomials (e.g., Legendre polynomials, or Chebyshev polynomials of the first and second kind), and (α, β) is a finite interval, the results reported in [12] suggest that the problem is now remarkably well-conditioned. This new approach is therefore a useful alternative to the procedures mentioned above, in cases where the modified moments are accurately computable.

It seems worthwhile, therefore, to investigate the condition of the general problem in the case of polynomials $\{p_k\}$ which are orthogonal with respect to some other weight function $w(x)$ on the interval (a, b) [not necessarily equal to (α, β)],

$$\text{degree } p_k = k, \qquad \int_a^b p_r(x)p_s(x)w(x)\,dx = 0 \qquad (r \neq s). \tag{1.9}$$

Such polynomials always satisfy a recurrence relation of the form (1.8). In Section 2 we obtain upper bounds for the condition number of this problem, relative to both finite and infinite intervals (a, b). Asymptotic estimates of the condition number are given in Section 3 for certain classical weight functions on the interval $[-1, 1]$. Rather strikingly, these estimates grow only like a fixed power of n. The condition is less favorable, in general, if the interval (α, β) is infinite. In Section 4 we then derive an algorithm for solving the problem under study. The algorithm reduces to one given by Golub and Welsch [8] for the case $p_k(x) = x^k$ and is similar (although not identical) to the algorithm of Sack and Donovan [12]. Some numerical examples are presented in Section 5. In particular, we obtain Gaussian quadrature rules G_n for $n = 1(1)8, 16, 32$, relative to the weight functions

$$\omega(x) = \frac{1}{2}\left(1 + \begin{matrix}\cos \\ \sin\end{matrix} m\pi x\right), \qquad m = 1(1)12,$$

on $[-1, 1]$. Tables of the respective Gaussian abscissas and weights may be found on the microfiche card attached to this issue.

2. Condition of the Problem. In studying the condition of our problem, it is convenient to consider normalized modified moments as defined by

$$\tilde{v}_k = h_k^{-1/2} \int_\alpha^\beta p_k(x)\omega(x)\,dx, \qquad k = 0, 1, 2, \ldots, \tag{2.1}$$

where

$$h_k = \int_a^b p_k^2(x)w(x)\,dx. \tag{2.2}$$

The normalized moments $\tilde{v}_k$ are invariant under different normalizations of the orthogonal polynomials $\{p_k\}$.

The problem stated in Section 1 is then equivalent to solving the system of $2n$ (nonlinear) algebraic equations

$$h_k^{-1/2} \sum_{r=1}^{n} \lambda_r p_k(\xi_r) = \tilde{v}_k, \qquad k = 0, 1, 2, \ldots, 2n - 1, \tag{2.3}$$

for the unknowns λ_r, ξ_r. We can write these equations in vector form,

$$F(y) = \tilde{v}, \tag{2.4}$$

by letting $y^T = [\lambda_1, \ldots, \lambda_n, \xi_1, \ldots, \xi_n]$, $\tilde{v}^T = [\tilde{v}_0, \tilde{v}_1, \ldots, \tilde{v}_{2n-1}]$, $F^T = [F_0, F_1, \ldots, F_{2n-1}]$, and

$$F_k(y) = h_k^{-1/2} \sum_{r=1}^{n} \lambda_r p_k(\xi_r), \qquad k = 0, 1, \ldots, 2n - 1. \tag{2.5}$$

In conformity with (1.3), we denote the solution of (2.4) by

$$y_0^T = [\lambda_1^{(n)}, \dots, \lambda_n^{(n)}, \xi_1^{(n)}, \dots, \xi_n^{(n)}]. \tag{2.6}$$

Given a vector norm $\|\cdot\|$, and an associated matrix norm, we may define, as in [6], a (relative) asymptotic condition number κ_n for the problem (2.4), viz.

$$\kappa_n = \frac{\|\tilde{v}\|}{\|y_0\|} \|[F_y(y_0)]^{-1}\|, \tag{2.7}$$

where $F_y(y)$ denotes the Jacobian matrix of $F(y)$. An elementary computation shows that

$$F_y(y_0) = H\Xi\Lambda, \tag{2.8}$$

where

$$H = \operatorname{diag}(h_0^{-1/2}, h_1^{-1/2}, \dots, h_{2n-1}^{-1/2}), \qquad \Lambda = \operatorname{diag}(1, \dots, 1, \lambda_1, \dots, \lambda_n) \tag{2.9}$$

are diagonal matrices, and

$$\Xi = \begin{vmatrix} p_0(\xi_1) \cdots & p_0(\xi_n) & p_0'(\xi_1) \cdots & p_0'(\xi_n) \\ p_1(\xi_1) \cdots & p_1(\xi_n) & p_1'(\xi_1) \cdots & p_1'(\xi_n) \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ p_{2n-1}(\xi_1) \cdots & p_{2n-1}(\xi_n) & p_{2n-1}'(\xi_1) \cdots & p_{2n-1}'(\xi_n) \end{vmatrix}. \tag{2.10}$$

(For simplicity, we have written ξ_r for $\xi_r^{(n)}$, and λ_r for $\lambda_r^{(n)}$ in (2.9), (2.10).) Therefore,

$$\kappa_n \leqq \frac{\|\tilde{v}\|}{\|y_0\|} \|\Lambda^{-1}\| \|\Xi^{-1} H^{-1}\|. \tag{2.11}$$

For the following, it turns out to be convenient to work with the L_1-norm

$$\|y\|_1 = \sum_{k=0}^{2n-1} |y_k|, \qquad y^T = [y_0, y_1, \dots, y_{2n-1}]. \tag{2.12}$$

THEOREM 2.1. *Let $[a, b]$ be a finite interval. With $\{l_\lambda(x)\}_{\lambda=1}^n$ denoting the Lagrange interpolation polynomials associated with the abscissas $\{\xi_r^{(n)}\}_{r=1}^n$,*

$$l_\lambda(x) = \prod_{\nu=1;\nu\neq\lambda}^{n} \frac{x - \xi_\nu^{(n)}}{\xi_\lambda^{(n)} - \xi_\nu^{(n)}} = \frac{\pi_n(x)}{\pi_n'(\xi_\lambda^{(n)})(x - \xi_\lambda^{(n)})}, \tag{2.13}$$

let

$$L_n = \int_a^b \sum_{\lambda=1}^{n} l_\lambda^2(x) w(x)\, dx, \tag{2.14}$$

$$\sigma_n = \max_{1 \leqq \lambda \leqq n} |l_\lambda'(\xi_\lambda^{(n)})|. \tag{2.15}$$

Let, furthermore,

$$M_\mu = \max_{a \leqq x \leqq b} |p_\mu(x)|, \qquad h_\mu = \int_a^b p_\mu^2(x) w(x)\, dx, \tag{2.16}$$

$$\Delta_n = \max\{|\xi_\lambda^{(n)} - x| : a \leqq x \leqq b, \lambda = 1, 2, \dots, n\}. \tag{2.17}$$

Then, using the L_1-norm (2.12) *in* (2.7), *we have*

$$\kappa_n \leqq \kappa_n^{(1)}\kappa_n^{(2)}\kappa_n^{(3)}, \tag{2.18}$$

where

$$\kappa_n^{(1)} = \max(1, 1/\min \lambda_r^{(n)})[1 + (2\sigma_n + 1)\Delta_n]/\left(\mu_0 + \sum_{r=1}^{n} |\xi_r^{(n)}|\right), \tag{2.19^1}$$

$$\kappa_n^{(2)} = \max_{0 \leqq \mu \leqq 2n-1} (M_\mu/h_\mu^{1/2}), \tag{2.19^2}$$

$$\kappa_n^{(3)} = L_n \|\tilde{v}\|_1. \tag{2.19^3}$$

Remarks. 1. The quantity $\kappa_n^{(1)}$ depends only on the weight function $\omega(x)$, the quantity $\kappa_n^{(2)}$ only on $w(x)$, while $\kappa_n^{(3)}$ depends on both $\omega(x)$ and $w(x)$.

2. Normally, $[\alpha, \beta] = [a, b]$, in which case $\Delta_n \leqq b - a$.

Proof of Theorem 2.1. The key issue in the proof is a bound on the norm of $\Xi^{-1}H^{-1}$. We first determine Ξ^{-1} explicitly.

Let

$$P_\lambda(x) = l_\lambda^2(x)[1 - 2l_\lambda'(\xi_\lambda^{(n)})(x - \xi_\lambda^{(n)})], \tag{2.20}$$

$$Q_\lambda(x) = l_\lambda^2(x)(x - \xi_\lambda^{(n)}) \tag{2.21}$$

denote the fundamental Hermite interpolation polynomials belonging to the abscissas $\{\xi_r^{(n)}\}$. Let

$$P_\lambda(x) = \sum_{\mu=0}^{2n-1} a_{\lambda\mu}p_\mu(x), \qquad Q_\lambda(x) = \sum_{\mu=0}^{2n-1} b_{\lambda\mu}p_\mu(x). \tag{2.22}$$

Then, as in [4], one shows that

$$\Xi^{-1} = \begin{bmatrix} A \\ B \end{bmatrix}, \qquad A = [a_{\lambda\mu}], \qquad B = [b_{\lambda\mu}]. \tag{2.23}$$

By the orthogonality of $\{p_k(x)\}$, one obtains from (2.22)

$$a_{\lambda\mu} = \frac{1}{h_\mu}\int_a^b P_\lambda(x)p_\mu(x)w(x)\,dx, \qquad b_{\lambda\mu} = \frac{1}{h_\mu}\int_a^b Q_\lambda(x)p_\mu(x)w(x)\,dx,$$

or, in view of (2.20), (2.21),

$$a_{\lambda\mu} = \frac{1}{h_\mu}(\alpha_{\lambda\mu} - 2s_\lambda^{(n)}\beta_{\lambda\mu}), \qquad b_{\lambda\mu} = \frac{1}{h_\mu}\beta_{\lambda\mu}, \tag{2.24}$$

where

$$s_\lambda^{(n)} = l_\lambda'(\xi_\lambda^{(n)}), \tag{2.25}$$

and

$$\alpha_{\lambda\mu} = \int_a^b l_\lambda^2(x)p_\mu(x)w(x)\,dx, \qquad \beta_{\lambda\mu} = \int_a^b l_\lambda^2(x)p_\mu(x)(x - \xi_\lambda^{(n)})w(x)\,dx. \tag{2.26}$$

We are now in a position to bound the norm of $\Xi^{-1}H^{-1}$. From (2.26), we have

$$\sum_{\lambda=1}^{n} |\alpha_{\lambda\mu}| \leqq \sum_{\lambda=1}^{n} \int_a^b l_\lambda^2(x)|p_\mu(x)|w(x)\,dx \leqq M_\mu L_n, \tag{2.27}$$

$$\sum_{\lambda=1}^{n} |\beta_{\lambda\mu}| \leqq \sum_{\lambda=1}^{n} \int_a^b l_\lambda^2(x)|p_\mu(x)|\,|x - \xi_\lambda^{(n)}|w(x)\,dx \leqq M_\mu\,\Delta_n L_n. \tag{2.28}$$

Therefore, by (2.24),

$$\sum_{\lambda=1}^{n} |a_{\lambda\mu}| \leqq \frac{M_\mu}{h_\mu}(1 + 2\,\Delta_n\sigma_n)L_n, \qquad \sum_{\lambda=1}^{n} |b_{\lambda\mu}| \leqq \frac{M_\mu}{h_\mu}\Delta_n L_n.$$

Consequently,

$$\|\Xi^{-1}H^{-1}\|_1 \leqq [1 + (2\sigma_n + 1)\,\Delta_n]L_n \max_{0\leqq\mu\leqq 2n-1} M_\mu/h_\mu^{1/2}. \tag{2.29}$$

The theorem now follows from (2.11) and (2.29), by observing that

$$\|y_0\|_1 = \sum_{r=1}^{n} (\lambda_r^{(n)} + |\xi_r^{(n)}|) = \mu_0 + \sum_{r=1}^{n} |\xi_r^{(n)}|, \tag{2.30}$$

and

$$\|\Lambda^{-1}\|_1 = \max(1, 1/\min \lambda_r^{(n)}). \tag{2.31}$$

The following theorem is not restricted to finite intervals $[a, b]$.

THEOREM 2.2. *Let (a, b) be a finite or infinite interval. In addition to the notations of Theorem* 2.1, *let*

$$\begin{aligned} L_{n,1} &= \int_a^b \left[\sum_{\lambda=1}^{n} l_\lambda^2(x)\right]^2 w(x)\,dx, \\ L_{n,2} &= \int_a^b \left[\sum_{\lambda=1}^{n} l_\lambda^2(x)|x - \xi_\lambda^{(n)}|\right]^2 w(x)\,dx. \end{aligned} \tag{2.32}$$

Then, using the L_1-norm (2.12) *in* (2.7), *we have*

$$k_n \leqq k_n^{(1)} k_n^{(2)}, \tag{2.33}$$

where

$$k_n^{(1)} = \frac{\max(1, 1/\min \lambda_r^{(n)})}{\mu_0 + \sum_{r=1}^{n} |\xi_r^{(n)}|}, \tag{2.34}$$

$$k_n^{(2)} = (L_{n,1}^{1/2} + (1 + 2\sigma_n)L_{n,2}^{1/2})\|\tilde{v}\|_1. \tag{2.35}$$

Proof. The proof is virtually the same as that for Theorem 2.1, except that the sums in (2.27), (2.28) are estimated differently, using Schwarz's inequality:

$$\sum_{\lambda=1}^{n} |\alpha_{\lambda\mu}| \leqq \int_a^b \sum_{\lambda=1}^{n} l_\lambda^2(x)|p_\mu(x)|w(x)\,dx$$

$$\leqq \left\{\int_a^b \left[\sum_{\lambda=1}^{n} l_\lambda^2(x)\right]^2 w(x)\,dx \int_a^b p_\mu^2(x)w(x)\,dx\right\}^{1/2} = h_\mu^{1/2} L_{n,1}^{1/2},$$

$$\sum_{\lambda=1}^{n} |\beta_{\lambda\mu}| \leqq \int_a^b \sum_{\lambda=1}^{n} l_\lambda^2(x)|x - \xi_\lambda^{(n)}||p_\mu(x)|w(x)\,dx$$

$$\leqq \left\{\int_a^b \left[\sum_{\lambda=1}^{n} l_\lambda^2(x)|x - \xi_\lambda^{(n)}|\right]^2 w(x)\,dx \int_a^b p_\mu^2(x)w(x)\,dx\right\}^{1/2} = h_\mu^{1/2} L_{n,2}^{1/2}.$$

Hence, as previously,

$$\|\Xi^{-1}H^{-1}\|_1 \leqq L_{n,1}^{1/2} + (1 + 2\sigma_n)L_{n,2}^{1/2},$$

and Theorem 2.2 follows from (2.11), (2.30), and (2.31).

For infinite intervals (α, β) the bounds in (2.18) and (2.33) are likely to be very large, even for only moderately large n, on account of the smallness of $\min \lambda_r^{(n)}$. Severe ill-conditioning, in such cases, is therefore a potential hazard. Example (iii) of Section 5 illustrates this point.

3. Asymptotic Estimates of Condition Number. We illustrate Theorem 2.1 of the previous section by considering some special (classical) weight functions. We use the notation

$$a_n \doteq b_n \quad \text{as} \quad n \to \infty$$

to express the fact that $|a_n/b_n|$ remains between positive bounds not depending on n, as $n \to \infty$.

THEOREM 3.1. *Let* $[a, b] = [\alpha, \beta] = [-1, 1]$.

(a) *If* $\omega(x) = (1 - x^2)^\alpha$, $-\frac{1}{2} \leqq \alpha \leqq 0$, *then* $\kappa_n^{(1)} \leqq \bar{\kappa}_n^{(1)}$, *where* $\bar{\kappa}_n^{(1)} \doteq n^{2\alpha+3}$ *as* $n \to \infty$.

(b) *If* $w(x) = (1 - x)^\alpha(1 + x)^\beta$, $\alpha > -1$, $\beta > -1$, *then, as* $n \to \infty$, $\kappa_n^{(2)} \doteq n^{q+1/2}$ *if* $q \geqq -\frac{1}{2}$, *and* $\kappa_n^{(2)} \doteq 1$ *if* $q < -\frac{1}{2}$, *where* $q = \max(\alpha, \beta)$.

(c) *If* $\omega(x) = w(x)$, *then* $\kappa_n^{(3)} = \mu_0^{3/2}$.

(d) *If* $\omega(x) = (1 - x^2)^\alpha$, $-1 < \alpha \leqq 0$, *and* $w(x) = (1 - x^2)^\beta$, $\beta \geqq -\frac{1}{2}$, *then* $\kappa_n^{(3)} \leqq \bar{\kappa}_n^{(3)}$, *where, as* $n \to \infty$, $\bar{\kappa}_n^{(3)} \doteq n^{\beta+3/2}$ *if* $\alpha \neq 0$, *and* $\bar{\kappa}_n^{(3)} \doteq n^{\beta+7/2}$ *if* $\alpha = 0$.**

Proof. (a) The polynomials $\pi_k(x)$, in this case, are the ultraspherical polynomials $P_k^{(\alpha,\alpha)}(x)$, properly normalized. We assume the zeros $\xi_r = \xi_r^{(n)}$ of $P_n^{(\alpha,\alpha)}(x)$ numbered in decreasing order,

$$1 > \xi_1 > \xi_2 > \cdots > \xi_n > -1. \tag{3.1}$$

They are symmetrically distributed with respect to the origin, i.e., $\xi_r = -\xi_{n+1-r}$. It is known [14, p. 121] that for $|\alpha| \leqq \frac{1}{2}$,

$$\cos\left(r\frac{\pi}{n+1}\right) \leqq \xi_r \leqq \cos\left(r - \frac{1}{2}\right)\frac{\pi}{n}, \qquad r = 1, 2, \ldots, [n/2]. \tag{3.2}$$

From this one obtains by an elementary computation

$$\cot\frac{\pi}{2(n+1)} - 1 \leqq \sum_{r=1}^{n} |\xi_r| \leqq \frac{1}{\sin(\pi/2n)}.$$

It follows that $\sum_{r=1}^{n} |\xi_r| \doteq n$, and therefore

The result in the case $\alpha = 0$ could be sharpened to read $\bar{\kappa}_n^{(3)} \doteq n^{\beta+5/2}\ln^2 n$. See footnote *.

$$\mu_0 + \sum_{r=1}^{n} |\xi_r| \doteq n \quad \text{as } n \to \infty. \tag{3.3}$$

For the corresponding Christoffel numbers $\lambda_r^{(n)}$ we have [14, p. 350] $\min \lambda_r^{(n)} = \lambda_1^{(n)}$, whenever $\alpha \geqq -\frac{1}{2}$. (Note that for $\alpha = -\frac{1}{2}$ all $\lambda_r^{(n)}$ are equal to π/n.) Moreover [14, p. 350], $\lambda_1^{(n)} \doteq n^{-2\alpha-2}$. Therefore,

$$\max(1, 1/\min \lambda_r^{(n)}) \doteq n^{2\alpha+2} \quad \text{as } n \to \infty. \tag{3.4}$$

In order to estimate σ_n in (2.15), we recall (see, e.g., [11, p. 63]) that for $\alpha \leqq 0$,

$$v_\lambda(x) > |\alpha| \quad \text{on } -1 \leqq x \leqq 1, \tag{3.5}$$

where

$$v_\lambda(x) = 1 - 2l'_\lambda(\xi_\lambda)(x - \xi_\lambda).$$

We distinguish two cases, depending on whether $l'_\lambda(\xi_\lambda) \geqq 0$ or $l'_\lambda(\xi_\lambda) < 0$. In the first case we let $x = 1$ in (3.5), and obtain

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 - \xi_\lambda)}.$$

Using (3.1) and (3.2), we get

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 - \xi_1)} \leqq \frac{1 - |\alpha|}{2(1 - \cos(\pi/2n))} = \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)}.$$

In the second case we let $x = -1$ in (3.5) and obtain by a similar reasoning

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{2(1 + \xi_\lambda)} \leqq \frac{1 - |\alpha|}{2(1 + \xi_n)} \leqq \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)}.$$

Thus, in either case,

$$|l'_\lambda(\xi_\lambda)| < \frac{1 - |\alpha|}{4 \sin^2(\pi/4n)},$$

and it follows that

$$\sigma_n = \max_\lambda |l'_\lambda(\xi_\lambda)| \leqq \bar{\sigma}_n, \qquad \bar{\sigma}_n \doteq n^2 \quad \text{as } n \to \infty. \tag{3.6}$$

Combining (3.3), (3.4), and (3.6) gives the desired result.

(b) With $p_\mu(x) = P_\mu^{(\alpha,\beta)}(x)$, and $q = \max(\alpha, \beta)$, we have for the quantity M_μ in (2.16) [14, p. 166]

$$M_\mu = \frac{\Gamma(\mu + q + 1)}{\Gamma(q + 1)\Gamma(\mu + 1)} \doteq \mu^q \quad \text{if } q \geqq -\tfrac{1}{2}, \tag{3.7}$$

and

$$M_\mu \doteq \mu^{-1/2} \quad \text{if } q < -\tfrac{1}{2}. \tag{3.8}$$

Since

$$h_\mu^{1/2} = 2^{(\alpha+\beta+1)/2}\left[\frac{\Gamma(\mu+\alpha+1)\Gamma(\mu+\beta+1)}{(2\mu+\alpha+\beta+1)\Gamma(\mu+1)\Gamma(\mu+\alpha+\beta+1)}\right]^{1/2} \doteq \mu^{-1/2}, \quad \mu \to \infty, \tag{3.9}$$

the assertion follows.

(c) Since $\omega(x) = w(x)$, we have $L_n = \mu_0$ (see, e.g., [11, p. 52]), and $\tilde{v}_0 = \sqrt{\mu_0}$, $\tilde{v}_k = 0$ for $k > 0$, giving $\kappa_n^{(3)} = \mu_0^{3/2}$ as asserted.

(d) In the ultraspherical case $\omega(x) = (1-x^2)^\alpha$, $-1 < \alpha \leqq 0$, it is known that [14, Problems 58, 60]

$$\sum_{\lambda=1}^{n} l_\lambda^2(x) \leqq \frac{1}{|\alpha|} \quad (-1 < \alpha < 0), \qquad \sum_{\lambda=1}^{n} l_\lambda^2(x) \leqq \frac{1}{\tan^2(3\pi/4(2n+1))} \quad (\alpha = 0),$$

uniformly on $[-1, 1]$. Therefore,

$$\bar{L}_n = m_0/|\alpha| \qquad (-1 < \alpha < 0),$$

$$L_n \leqq \bar{L}_n, \tag{3.10}$$

$$\bar{L}_n = m_0/\tan^2\frac{3\pi}{4(2n+1)} \qquad (\alpha = 0),$$

where $m_0 = \int_{-1}^{1} w(x)\,dx$. In particular***,

$$\bar{L}_n \doteq 1 \qquad (-1 < \alpha < 0),$$

$$\bar{L}_n \doteq n^2 \qquad (\alpha = 0). \tag{3.11}$$

From (3.7), (3.9) (with $\alpha = \beta = q$) one finds by a simple computation that $M_k/h_k^{1/2}$ is an increasing function of k, if $\beta > -\frac{1}{2}$, and constant (for $k > 0$) equal to $2/\sqrt{\pi}$, if $\beta = -\frac{1}{2}$. Therefore,

$$\|\tilde{v}\|_1 = \sum_{k=0}^{2n-1} |\tilde{v}_k| \leqq \mu_0 \sum_{k=0}^{2n-1} M_k/h_k^{1/2} \leqq \mu_0 2n M_{2n-1}/h_{2n-1}^{1/2},$$

and using the asymptotic estimates in (3.7) and (3.9),

$$\|\tilde{v}\|_1 \leqq N_n, \qquad N_n \doteq n^{\beta+3/2}. \tag{3.12}$$

The desired result now follows from (3.10)–(3.12). Theorem 3.1 is proved.

As an example, suppose we generate the Gaussian rule G_n associated with the ultraspherical weight function $(1-x^2)^\alpha$, $-\frac{1}{2} \leqq \alpha \leqq 0$, using as $\{p_k\}$ the ultraspherical polynomials with parameter β, $-\frac{1}{2} \leqq \beta \leqq 0$. Then Theorem 3.1, together with (2.18), tells us that the associated condition number κ_n satisfies $\kappa_n \leqq \bar{\kappa}_n$, where, as $n \to \infty$,

$$\bar{\kappa}_n \doteq n^{2(\alpha+\beta)+5} \quad \text{if } \alpha \neq 0 \text{ and } \alpha \neq \beta,$$

$$\bar{\kappa}_n \doteq n^{2\beta+7} \quad \text{if } \alpha = 0 \text{ and } \beta \neq 0,$$

$$\bar{\kappa}_n \doteq n^{3\alpha+7/2} \quad \text{if } \alpha = \beta.$$

***In the case $\alpha = 0$, the sharper estimate $L_n \leqq L_n^*$, $L_n^* \doteq n \ln^2 n$ could be obtained by using an estimate for $\sum_{\lambda=1}^{n} |l_\lambda(x)|$, due to G. I. Natanson [10], in conjunction with the inequality $\sum_{\lambda=1}^{n} l_\lambda^2(x) \leqq (\sum_{\lambda=1}^{n} |l_\lambda(x)|)^2$.

Theorem 3.1, and the example just given, are presented here for the sole purpose of illustrating the magnitude of the condition number for the problem considered. It is not suggested that for such classical weight functions Gaussian quadrature rules be constructed from modified moments, since the respective orthogonal polynomials are explicitly known.

In practice, $\omega(x)$ being given, we have no control over $\kappa_n^{(1)}$. However, we may influence the magnitude of $\kappa_n^{(2)}$, and to some extent that of $\kappa_n^{(3)}$, by an appropriate choice of the polynomials $\{p_k\}$. In this connection, part (b) of Theorem 3.1 suggests the Chebyshev polynomials of the first kind, $p_k(x) = T_k(x)$, as both convenient and well-conditioned. With this choice, in fact, $\kappa_n^{(2)} = (2/\pi)^{1/2}$.

4. An Algorithm for Generating Orthonormal Polynomials. We now derive an algorithm for generating the orthonormal polynomials $\{\pi_k(x)\}_{k=0}^n$ of (1.6), given a set of polynomials $\{p_k(x)\}$ (orthogonal or not), satisfying the recurrence relation

$$xp_j(x) = a_j p_{j+1}(x) + b_j p_j(x) + c_j p_{j-1}(x), \qquad j = 0, 1, 2, \ldots; \tag{4.1}$$
$$p_{-1}(x) = 0, \quad a_j \neq 0,$$

and given the associated modified moments $\{\nu_k\}_{k=0}^{2n}$ of (1.2). Our aim is toward determining the coefficients α_j, β_j $(j = 0, 1, 2, \ldots, n-1)$ in the recurrence relation

$$x\pi_j(x) = \alpha_j \pi_{j+1}(x) + \beta_j \pi_j(x) + \alpha_{j-1}\pi_{j-1}(x), \quad j = 0, 1, 2, \ldots; \quad \pi_{-1}(x) = 0. \tag{4.2}$$

We denote by

$$(f, g) = \int_\alpha^\beta f(x)g(x)\omega(x)\,dx$$

the inner product with respect to which the $\pi_k(x)$ are orthonormal. Let $M = [m_{ij}]$ be the Gram matrix of order $n+1$, i.e.,

$$m_{ij} = (p_i, p_j) \qquad (i, j = 0, 1, \ldots, n). \tag{4.3}$$

Clearly, M is positive-definite. Let

$$M = R^T R, \qquad R = [r_{ij}] \tag{4.4}$$

be the Cholesky decomposition of M, and

$$S = R^{-1}, \qquad S = [s_{ij}]. \tag{4.5}$$

Both R and S are upper triangular matrices with positive diagonal elements. By an observation of Mysovskih [9],

$$\pi_j(x) = s_{0j}p_0(x) + s_{1j}p_1(x) + \cdots + s_{jj}p_j(x), \qquad j = 0, 1, \ldots, n. \tag{4.6}$$

Substituting (4.6) into (4.2), we can write

$$\begin{aligned} x[s_{0j}p_0 + \cdots + s_{j-1,j}p_{j-1} + s_{jj}p_j] &= \alpha_j[s_{0,j+1}p_0 + \cdots + s_{j,j+1}p_j + s_{j+1,j+1}p_{j+1}] + \beta_j[s_{0j}p_0 + \cdots + s_{jj}p_j] \\ &\quad + \alpha_{j-1}[s_{0,j-1}p_0 + \cdots + s_{j-1,j-1}p_{j-1}]. \end{aligned}$$

Each term on the left, in view of (4.1), can be expressed as a linear combination of p's. Having done this, coefficients of equal p's must agree on both sides, because of the linear independence of the system $\{p_k(x)\}$. In particular, comparing the coefficients of p_{j+1} and p_j, one gets

$$s_{jj}a_j = \alpha_j s_{j+1,j+1}, \qquad s_{jj}b_j + s_{j-1,j}a_{j-1} = \alpha_j s_{j,j+1} + \beta_j s_{jj},$$

from which

$$\alpha_j = \frac{s_{jj}}{s_{j+1,j+1}}a_j, \qquad \beta_j = b_j - \frac{s_{j,j+1}}{s_{j+1,j+1}}a_j + \frac{s_{j-1,j}}{s_{jj}}a_{j-1}.$$

Since

$$s_{jj} = \frac{1}{r_{jj}} \qquad (j = 0, 1, \ldots, n),$$

$$s_{j,j+1} = -\frac{r_{j,j+1}}{r_{jj}r_{j+1,j+1}} \qquad (j = 0, 1, \ldots, n-1),$$

one finally obtains

$$\begin{aligned} \alpha_j &= \frac{r_{j+1,j+1}}{r_{jj}}a_j, \\ \beta_j &= b_j + \frac{r_{j,j+1}}{r_{jj}}a_j - \frac{r_{j-1,j}}{r_{j-1,j-1}}a_{j-1}, \end{aligned} \qquad j = 0, 1, \ldots, n-1. \tag{4.7}$$

For $j = 0$, $r_{-1,0}$ is to be interpreted as zero, and $r_{-1,-1}$ as an arbitrary nonzero number.

We note that the formulas (4.7) reduce to those of Golub and Welsch [8], if $a_j = 1$, $b_j = c_j = 0$, i.e., $p_k(x) = x^k$. Also, of course, $M = R = I$, and thus $\alpha_j = a_j$, $\beta_j = b_j$, if $p_k(x) = \pi_k(x)$.

Once the Gram matrix M is known, the desired coefficients α_j, β_j can thus be obtained from (4.7) by a Cholesky decomposition of M.

The Gram matrix M, on the other hand, can be built up from the modified moments v_j in the following manner. Applying the recursion (4.1) twice, one has

$$\begin{aligned} m_{ij} = (p_i, p_j) &= \left(\frac{1}{a_{i-1}}[(x - b_{i-1})p_{i-1} - c_{i-1}p_{i-2}], p_j\right) \\ &= \frac{1}{a_{i-1}}[(xp_{i-1}, p_j) - b_{i-1}(p_{i-1}, p_j) - c_{i-1}(p_{i-2}, p_j)] \\ &= \frac{1}{a_{i-1}}[(p_{i-1}, xp_j) - b_{i-1}(p_{i-1}, p_j) - c_{i-1}(p_{i-2}, p_j)] \\ &= \frac{1}{a_{i-1}}[a_j(p_{i-1}, p_{j+1}) + b_j(p_{i-1}, p_j) + c_j(p_{i-1}, p_{j-1}) - b_{i-1}(p_{i-1}, p_j) \\ &\qquad - c_{i-1}(p_{i-2}, p_j)], \end{aligned}$$

that is,

$$(4.8)\quad m_{ij} = \frac{1}{a_{i-1}}\left[a_j m_{i-1,j+1} + (b_j - b_{i-1})m_{i-1,j} + c_j m_{i-1,j-1} - c_{i-1}m_{i-2,j}\right].$$

Since

$$(4.9)\qquad m_{-1,j} = 0, \qquad m_{0j} = p_0 v_j \qquad (j = 0, 1, \ldots, 2n),$$

we have in (4.8) a recursive scheme to progressively build up the matrix M, using (4.9) as initial values.

The involvement of v_{2n} in (4.9) may appear puzzling at first, the Gaussian rule G_n being determined uniquely by the first $2n$ modified moments $v_j, j = 0, 1, 2, \ldots, 2n-1$. Actually, the role of v_{2n} is just that of normalizing $\pi_n(x)$, and its value affects neither $\xi_r^{(n)}$ nor $\lambda_r^{(n)}$, in view of (1.5), (1.7).

The algorithm presented here does not compare favorably with the algorithm of Sack and Donovan [12] in terms of speed and storage requirements. Our derivation, however, appears to us more transparent than the derivation given in [12].

5. Numerical Examples. All computations described in this section were carried out on the CDC 6500 computer in single precision arithmetic.

(i) We repeat and extend some of the experiments reported by Sack and Donovan [12]. For $p_k(x)$ we choose in turn x^k, $(1+x)^k$, $P_k(x)$, $T_k(x)$, $U_k(x)$, where P_k, T_k, U_k denote, respectively, the Legendre polynomial, and the Chebyshev polynomials of the first and second kind. We apply the algorithm of Section 4 to produce the coefficients α_r, β_r, $r = 0, 1, \ldots, n-1$, in the recurrence relation for the normalized Legendre and Chebyshev polynomials, making use of the appropriate modified moments shown in Table 1. (Notations: $(2n)!! = 2\cdot 4\cdots(2n)$, $(2n+1)!! = 1\cdot 3\cdot 5\cdots(2n+1)$, $0!! = (-1)!! = 1$, $(-3)!! = -1$.)

TABLE 1. *Modified moments* ν_k

$p_k(x)$ \ $\omega(x)$		1	$(1-x^2)^{-1/2}$	$(1-x^2)^{1/2}$
x^k	k even	$2/(k+1)$	$(k-1)!!\pi/k!!$	$(k-1)!!\pi/(k+2)!!$
	k odd	0	0	0
$(1+x)^k$		$2^{k+1}/(k+1)$	$2^k(2k-1)!!\pi/(2k)!!$	$(2k+1)!!\pi/(k+2)!$
$P_k(x)$	k even		$(k!)^2\pi/(k!!)^4$	$-(k-1)!!(k-3)!!\pi/(k!!(k+2)!!)$
	k odd		0	0
$T_k(x)$	k even	$-2/((k+1)(k-1))$		$\pi/2 \quad (k=0)$ $-\pi/4 \quad (k=2)$
	k odd	0		0 (otherwise)
$U_k(x)$	k even	$2/(k+1)$	π	
	k odd	0	0	

For the first two choices of $p_k(x)$, as is to be expected, the Gram matrix M becomes increasingly ill-conditioned with n increasing, and the Cholesky decomposition of M eventually breaks down on taking the square root of a negative number. Prior to this, the errors in α_r and β_r steadily increase, except for β_r in the first case $[p_k(x) = x^k]$, where the algorithm consistently returns the correct value $\beta_r = 0$. Sample values of

errors are shown in Table 2 for the case $\omega(x) = 1$. The Cholesky decomposition, in this case, fails at $n = 23$ and $n = 12$, respectively. The situation is very similar for the other two weight functions.

TABLE 2. *Errors in the recursion coefficients for normalized Legendre polynomials.*

	$p_k(x) = x^k$	$p_k(x) = (1 + x)^k$	
	error in α_r	error in α_r	error in β_r
$r = 5$	1.9×10^{-12}	1.8×10^{-8}	1.1×10^{-8}
10	5.3×10^{-9}	2.3×10^{-2}	1.0×10^{-1}
15	1.9×10^{-5}	—	—
20	2.5×10^{-2}	—	—
25	—	—	—

No problems of any kind are encountered for the remaining three choices of $p_k(x)$, even going with n as high as 100. The coefficients α_r, β_r are obtained essentially to machine accuracy, the largest error observed being 7.1×10^{-14}.

(ii) Weight functions of interest in Fourier analysis are $\omega(x) = c_m(x)$, and $\omega(x) = s_m(x)$, where

$$\begin{aligned} c_m(x) &= \tfrac{1}{2}(1 + \cos m\pi x), \\ s_m(x) &= \tfrac{1}{2}(1 + \sin m\pi x), \end{aligned} \qquad -1 \leqq x \leqq 1; \quad m = 0, 1, 2, \ldots. \tag{5.1}$$

Writing Fourier coefficients in the form [15]

$$\begin{aligned} \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\cos mx\, dx &= \int_{-1}^{1} f(\pi x)c_m(x)\, dx - \int_{-1}^{1} f(\pi x)s_0(x)\, dx, \\ \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\sin mx\, dx &= \int_{-1}^{1} f(\pi x)s_m(x)\, dx - \int_{-1}^{1} f(\pi x)s_0(x)\, dx, \end{aligned} \tag{5.2}$$

$$m = 1, 2, 3, \ldots,$$

the first integrals on the right may be calculated by an appropriately weighted Gaussian quadrature rule, and the second integrals by classical Gaussian quadrature. To the best of our knowledge, no extensive tables exist for Gaussian rules G_n associated with the weight functions (5.1). Admittedly, their usefulness is somewhat limited, because the set of points at which f must be evaluated differs from one Fourier coefficient to another.

Our algorithm of Section 4 may be used to generate the required orthonormal polynomials. It is convenient to use it with $p_k(x) = P_k(x)$, since the modified moments can then be expressed in terms of spherical Bessel functions. In fact, using [1, p. 122]

$$\int_{-1}^{1} e^{im\pi x} P_k(x)\,dx = i^k \left(\frac{2}{m}\right)^{1/2} J_{k+1/2}(m\pi),$$

we obtain in the cosine-case

$$(5.3)\qquad \nu_0 = 1, \quad \nu_{2k} = \frac{(-1)^k}{(2m)^{1/2}} J_{2k+1/2}(m\pi) \quad (k > 0), \quad \nu_{2k+1} = 0 \quad (k \geqq 0),$$

and in the sine-case

$$(5.4)\qquad \nu_0 = 1, \quad \nu_{2k-1} = \frac{(-1)^{k+1}}{(2m)^{1/2}} J_{2k-1/2}(m\pi) \quad (k > 0), \quad \nu_{2k} = 0 \quad (k > 0).$$

To compute the Bessel functions in (5.3), (5.4), we use the procedure *Japlusn*† of [5], and the Gaussian abscissas and weights have been obtained using the relevant portions (both sequential and nonsequential) of Algorithm 331 [7]. The results are checked by having the quadrature rules regenerate the modified moments.

Table 3 of the microfiche section gives 12D values of $\xi_r^{(n)}$, $\pi\zeta_r^{(n)}$, $\lambda_r^{(n)}$ for the Gaussian rule (1.3) associated with $\omega(x) = c_m(x)$, for $n = 1(1)8, 16, 32$, $m = 1(1)12$. (Because of symmetry, only the nonnegative abscissas and corresponding weights are listed.) Table 4 contains the analogous information for $\omega(x) = s_m(x)$, $m = 0(1)12$.

(iii) To give an example for an infinite interval, we consider the "one-sided" Gauss-Hermite quadrature rules (1.3) corresponding to $\omega(x) = e^{-x^2}$ on $[0, \infty)$. Tables for such rules were recently published in [13], [3]. It seems natural, in this case, to choose $p_k(x) = H_k(x)$, the Hermite polynomials orthogonal with respect to $\omega(x)$ on $(-\infty, \infty)$. Then clearly,

$$(5.5)\qquad \nu_0 = \sqrt{\pi}/2, \qquad \nu_{2k} = 0 \qquad (k > 0).$$

To compute ν_{2k+1}, we start from the explicit representation

$$H_{2k+1}(x) = \sum_{r=0}^{k} (-1)^r \binom{2k+1}{2r} \frac{(2r)!}{2^r r!} 2^{2k+1-r} x^{2k+1-2r}.$$

Multiplying both sides by e^{-x^2}, and integrating between 0 and ∞, we obtain, in view of $\int_0^\infty e^{-x^2} x^{2k+1-2r}\,dx = \frac{1}{2}(k-r)!$,

$$\nu_{2k+1} = \int_0^\infty e^{-x^2} H_{2k+1}(x)\,dx = \sum_{r=0}^{k} (-1)^r \binom{2k+1}{2r} \frac{(2r)!}{2^r r!} 2^{2k-r}(k-r)!,$$

or, after simplification,

$$(5.6)\qquad \nu_{2k+1} = \sum_{r=0}^{k} s_r^{(k)}, \qquad s_r^{(k)} = 2^k(-1)^r \prod_{i=r+1}^{k} (2i) \prod_{i=k-r+1}^{k} (2i+1).$$

Each $s_r^{(k)}$ being an integer, the sum in (5.6) can be evaluated in integer arithmetic without loss of accuracy, as long as no overflow occurs. Even so, however, it is found that the Gauss abscissas and weights obtained by our algorithm gradually deteriorate

† This procedure calls the gamma function $\Gamma(1 + a)$. Since $a = 1/2$ in our application, we have replaced "gamma(1 + a)" by its numerical value $\sqrt{\pi}/2 = .88622692545276$ in the procedure body.

in accuracy. For $n = 6$, for example, only 9–11 correct significant digits are obtained, while for $n = 12$ only the first 2–4 significant digits are correct. It is believed that this deterioration of accuracy is a reflection of the progressive ill-conditioning of our problem. The quantity $\min \lambda_r^{(n)}$, in fact, is about 9.8×10^{-5} for $n = 6$, and 1.2×10^{-10} for $n = 12$, resulting in a value of $k_n^{(1)}$ in (2.34) of the order 10^4 and 10^{10}, respectively.

Note Added in Proof. A substantially greater loss of accuracy is observed in Example (iii) if for $p_k(x)$ one chooses the Laguerre polynomials $L_k(x)$ instead of the Hermite polynomials $H_k(x)$. It is found that the Cholesky decomposition (4.4), in this case, breaks down for $n = 7$, and the final results for $n = 6$ are correct to only 3 decimal digits (using single precision arithmetic on the CDC 6500).

It is instructive to compare the condition number κ_n for these two choices of the polynomials $p_k(x)$ on the basis of Theorem 2.2. The constant $k_n^{(1)}$ in (2.34) being the same for both choices of p_k, it suffices to compare $k_n^{(2)}$ in (2.35). Using the Gauss abscissas published in [3] to compute the Lagrange polynomials $l_\lambda(x)$, the quantities $L_{n,1}$ and $L_{n,2}$ in (2.32) may be evaluated by $2n$-point Hermite quadrature (if $p_k = H_k$) and by $2n$-point Gauss-Laguerre quadrature (if $p_k = L_k$). This will give $L_{n,1}$ exactly (apart from rounding errors), and $L_{n,2}$ at least approximately. For $n = 6$, one obtains

$$L_{n,1} = 3.25 \times 10^{10}, \quad L_{n,2} = 3.80 \times 10^{11} \quad (p_k = H_k),$$

$$L_{n,1} = 1.72 \times 10^{19}, \quad L_{n,2} = 8.42 \times 10^{21} \quad (p_k = L_k).$$

Since $\|\tilde{v}\|_1$ is of comparable magnitude in both cases (approximately .808 for $p_k = H_k$, and 1.84 for $p_k = L_k$), one concludes that $k_n^{(2)}$ has the order of magnitude 10^6 in the case of Hermite polynomials, but the order of magnitude 10^{11} in the case of Laguerre polynomials.

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20.3. [84] "HOW AND HOW NOT TO CHECK GAUSSIAN QUADRATURE FORMULAE"

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HOW AND HOW NOT TO CHECK GAUSSIAN QUADRATURE FORMULAE*

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Abstract.

We discuss characteristic difficulties inherent in the validation of Gaussian quadrature formulae, in particular the futility of moment-related tests. We propose instead more effective tests based on the recursion coefficients of the appropriate orthogonal polynomials and on the sum of the quadrature nodes.

1. Introduction.

The preparation of this note was prompted by the appearance, in the chemistry literature, of a 16-digit table of a Gaussian quadrature formula for integration with measure $d\lambda(t) = \exp(-t^3/3)dt$ on $(0, \infty)$, a table, which we suspected is accurate to only 1–2 decimal digits. How does one go about convincing a chemist, or anybody else for that matter, that his Gaussian quadrature formula is seriously defective?

The question is not as easy to answer as one might think at first, and is not without intrinsic interest, considering that the most obvious test – using the n-point quadrature rule to reproduce the first $2n$ moments of $d\lambda$ – is totally ineffective. The latter, of course, is a manifestation of the extreme ill-conditioning (if n is large) of the map from the first $2n$ moments to the n-point Gaussian quadrature rule (cf. [3, § 3.2]).

In Section 2 we present the nodes $\tau_\nu^{(n)}$ and weights $\lambda_\nu^{(n)}$ for the Gaussian formula

$$\int_0^\infty f(t)\exp(-t^3/3)dt = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f) \tag{1.1}$$

with $n = 15$, on the one hand as published in the literature, and on the other as recomputed by us. In Section 3 we discuss two tests, both ineffective, designed to determine which of the two formulae is the more trustworthy one. More conclusive tests are described in Section 4 which not only allow us to decide in favor of one of the two formulae, but also to indicate the accuracy of each.

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2. Two competing implementations of (1.1).

In Table 2.1 are listed the nodes and weights of the quadrature rule (1.1) as published in [5]. (Integers in parentheses denote decimal exponents.) They were obtained by applying a "product-difference algorithm" (a variant of Rutishauser's quotient-difference algorithm) of R. G. Gordon [4] to produce the J-fraction belonging to $d\lambda(t) = \exp(-t^3/3)dt$, starting from the moments $\mu_k = \int_0^\infty t^k d\lambda(t) = 3^{(k-2)/3} \times \Gamma((k+1)/3)$, $k = 0, 1, 2, \ldots$. The nodes $\tau_\nu^{(n)}$ can then be obtained as eigenvalues of a symmetric tridiagonal matrix (the Jacobi matrix

Table 2.1. *The Gauss formula* (1.1) *according to* [5].

ν	$\tau_\nu^{(15)}$	$\lambda_\nu^{(15)}$
1	1.457697817613696(−2)	3.805398607861561(−2)
2	8.102669876765460(−2)	9.622028412880550(−2)
3	2.081434595902250(−1)	1.572176160500219(−1)
4	3.944841255669402(−1)	2.091895332583340(−1)
5	6.315647839882239(−1)	2.377990401332924(−1)
6	9.076033998613676(−1)	2.271382574940649(−1)
7	1.210676808760832(0)	1.732845807252921(−1)
8	1.530983977242980(0)	9.869554247686019(−2)
9	1.861844587312434(0)	3.893631493517167(−2)
10	2.199712165681546(0)	9.812496327697071(−3)
11	2.543839804028289(0)	1.439191418328875(−3)
12	2.896173043105410(0)	1.088910025516801(−4)
13	3.262066731177372(0)	3.546866719463253(−6)
14	3.653371887506584(0)	3.590718819809800(−8)
15	4.102376773975577(0)	5.112611678291437(−11)

for $d\lambda$), and the weights $\lambda_\nu^{(n)}$ in terms of the first components of the associated eigenvectors. The procedure, thus, is a particular realization of the (ill-conditioned) map from the moments to the Gaussian quadrature rule. (The sensitivity to rounding errors of this procedure has been explicitly noted by Gordon, who suggests the use of double precision arithmetic or, better yet, exact integer arithmetic. It is not clearly stated by the author of [5] what computer, and what type of arithmetic, he has used.) Table 2.2 displays the same quadrature rule (1.1), produced, however, by an application of the "discretized Stieltjes procedure", in combination with a suitable partition of the interval $(0, \infty)$ into eight subintervals (cf. [3, Example 4.6]), to generate the required orthogonal polynomials. Essentially the same method as in Gordon [4] was then used to obtain the $\tau_\nu^{(n)}$ and $\lambda_\nu^{(n)}$. (The computation was carried out in double precision on the CDC 6500, using a relative error tolerance of 0.5×10^{-20} in the discretized Stieltjes procedure.) It is seen that the two tables agree only to about 1–2 decimal digits. Which one is correct?

Table 2.2. *The Gauss formula* (1.1) *recomputed.*

ν	$\tau_\nu^{(15)}$	$\lambda_\nu^{(15)}$
1	1.929765389638693(−2)	4.940830823126689(−2)
2	1.006599142226749(−1)	1.126586278069619(−1)
3	2.428468366694404(−1)	1.696700745266622(−1)
4	4.387642946878456(−1)	2.136246330297717(−1)
5	6.787965036904373(−1)	2.329324905722498(−1)
6	9.522620471509191(−1)	2.150021042138036(−1)
7	1.249165311141012(0)	1.596591146577856(−1)
8	1.561526358196975(0)	8.939650846589768(−2)
9	1.883496691223344(0)	3.512652914092340(−2)
10	2.213595570164661(0)	8.956321788320709(−3)
11	2.550023378308307(0)	1.353123731389520(−3)
12	2.895208615030500(0)	1.076566880888657(−4)
13	3.254368222416162(0)	3.781200408411502(−6)
14	3.639045691197643(0)	4.272835535767259(−8)
15	4.080805415015807(0)	7.218347932277564(−11)

3. Moment-related tests.

As already mentioned, the ability of the quadrature formula to reproduce the moments accurately is an unreliable test. This will now be documented by performing two tests, first a simple moment-reproducing test, then a more involved test based on Markov's remainder formula.

Test #1. Verify $R_n(f) = 0$ for $f(t) = t^k$, $\quad k = 0, 1, 2, \ldots, 2n-1.$

In other words, use the formulae in Tables 2.1 and 2.2 to check the identities (with $n = 15$)

$$\mu_k = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} [\tau_\nu^{(n)}]^k, \qquad k = 0, 1, 2, \ldots, 2n-1, \tag{3.1}$$

where μ_k are the moments $\mu_k = \int_0^\infty t^k \exp(-t^3/3)dt = 3^{(k-2)/3} \times \Gamma((k+1)/3)$, $k = 0, 1, 2, \ldots$.

Results of Test #1. Using double precision on the CDC 6500 (which corresponds to a precision of about 29 significant decimal digits) to carry out the computations indicated in (3.1), we obtain for the relative errors $\varepsilon_k = |(\mu_k - \sum_{\nu=1}^{n} \lambda_\nu^* [\tau_\nu^*]^k)/\mu_k|$ the results shown in Table 3.1. In the second and third columns are listed the errors ε_k resulting from the quadrature formula $(\tau_\nu^*, \lambda_\nu^*)$ of

Table 3.1. *Relative errors* ε_k *observed in reproducing the moments* μ_k *by the quadrature formulae of Tables* 2.1 *and* 2.2.

k	Table 2.1	Table 2.2
0	4.56(−16)	2.02(−17)
1	8.92(−16)	4.66(−17)
2	3.20(−15)	1.51(−16)
3	6.49(−15)	2.45(−16)
4	1.02(−14)	3.21(−16)
.	.	.
.	.	.
.	.	.
29	7.48(−14)	4.46(−16)

Table 2.1 and Table 2.2, respectively. The maximum error in each case is attained for $k = 29$.

Discussion. It is rather remarkable that both quadrature rules of Section 2, even though they differ already in the first or second decimal digit, manage to compute the moments to about 15 correct decimal digits. The reason for this is an extreme case of *correlation of errors.* If we represent the correct quadrature rule by a point $g_0 \in \mathbb{R}^{2n}$, and the vector of moments by $m_0 \in \mathbb{R}^{2n}$, then $g_0 = M_n m_0$ for some (nonlinear) map $M_n: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ defined in a neighborhood of m_0. For sufficiently small perturbations Δm of m_0, one has $\Delta g \approx J^0_{M_n} \Delta m$, where $J^0_{M_n}$ is the Jacobian matrix of M_n at m_0. Therefore, a small sphere $S(m_0; \varepsilon)$ of moment vectors, with center at m_0 and radius ε, is mapped under M_n, approximately, into an ellipsoid $E(g_0; \varepsilon)$ centered at g_0, whose half axes have lengths $\varepsilon \cdot \sigma_i(J^0_{M_n})$, with $\sigma_i(J^0_{M_n})$ the singular values of $J^0_{M_n}$, and directions given by the (orthonormal) eigenvectors of $J^0_{M_n}(J^0_{M_n})^T$. In our case, the ellipsoid $E(g_0; \varepsilon)$ happens to be extremely elongated and flat, the largest singular value being approx. 5.78×10^{11}, and the smallest 1.88×10^{-18}! It is reasonable to assume that the computed Gauss formula g^* is the exact Gauss formula belonging to some moment vector $m^* \in S(m_0; \varepsilon)$, where ε is of the order of magnitude of the machine precision, or a few orders larger (to account for rounding errors in the computational process). Conversely, then, to g^* there corresponds $m^* \in S(m_0; \varepsilon)$, hence $\|m^* - m_0\| \leqq \varepsilon$, explaining the relatively high accuracy of m^*. *The correlation of errors thus consists in the fact that the computed formula* g^* *lies, approximately, in the extremely elongated and flat ellipsoid* $E(g^0; \varepsilon)$. This correlation can be confirmed by subjecting either of the two quadrature rules of Section 2 to random errors of given magnitude ϱ, and letting ϱ vary through 10^{-1}, 10^{-2}, 10^{-3}, ... One will find that the resulting relative errors in the moments are no longer of the order of magnitude 10^{-15}, but rather of the order of magnitude ϱ, or significantly larger. The correlation of errors has been broken!

The discussion just given has merit only in a qualitative, not quantitative,

sense, the reason being that the moments μ_k vary in a wide range (from about 1.29 for $k = 0$ to about 7.14×10^9 for $k = 29$) and that one really ought to analyze the propagation of errors under M_n consistently in terms of *relative* errors. This can be done by computing a carefully defined condition number (cond M_n)(m_0) for the map M_n at m_0 (see [3, § 3.2, especially Eq. (3.11)]), with the result that (cond M_n)(m_0) $= 1.26 \times 10^{17}$ (for $n = 15$). This means that relative errors in the moments μ_k of magnitude ε must be expected to translate into relative errors in the Gauss formula having magnitude $\approx 10^{17} \cdot \varepsilon$. It would appear, therefore, that the formula in Table 2.1, given that it is accurate to only 1–2 decimal digits (cf. Section 4), was computed in a precision of about 20 decimal digits, assuming that the moments were computed correctly to machine precision.

Test # 2. Use the given quadrature nodes $\tau_\nu^{(n)}$ and weights $\lambda_\nu^{(n)}$ (for $n = 15$) to first generate the coefficients α_k, β_k, $k = 0, 1, 2, \ldots, n-1$, in the recursion formula

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \quad \pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \tag{3.2}$$

for the associated (monic) orthogonal polynomials $\{\pi_k(\cdot\,; d\lambda)\}$, where $\beta_0 = \int_0^\infty d\lambda(t)$. This is easily done (see, e.g., [3, Eq. (3.7)]) and yields the Jacobi matrix

$$J_n = J_n(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}. \tag{3.3}$$

Then, using the successive segments $J_1, J_2, \ldots, J_{n-1}$ of $J_n(d\lambda)$, generate (by methods already mentioned in Section 2) the nodes $\tau_\nu^{(k)}$ and weights $\lambda_\nu^{(k)}$ of the k-point Gaussian quadrature rule, $k = 1, 2, \ldots, n-1$, and check the identities

$$\mu_{2k} = \sum_{\nu=1}^{k} \lambda_\nu^{(k)} [\tau_\nu^{(k)}]^{2k} + \beta_0 \beta_1 \ldots \beta_k, \qquad k = 1, 2, \ldots, n-1. \tag{3.4}$$

(These follow readily from Markov's formula for the remainder term in Gaussian quadrature.)

Results of Test # 2. Using double precision as before, this test, too, disappointingly, is as unrevealing as Test # 1. Both quadrature rules of Section 2 confirm all identities in (3.4) to within a relative error of at most 7.24×10^{-14} and 4.36×10^{-16}, respectively.

4. Coefficient-based tests.

More effective are tests based on coefficients, either the coefficients in the three-term recurrence relation satisfied by the orthogonal polynomials, or coefficients of the orthogonal polynomials themselves. We propose two such tests.

Test # 3. Generate the coefficients α_k, β_k, $k = 0, 1, \ldots, n-1$, as in Test # 2; then check the relations

$$\left.\begin{aligned} \alpha_k &= D'_{k+1}/D_{k+1} - D'_k/D_k \\ \beta_k &= D_{k+1}D_{k-1}/D_k^2 \end{aligned}\right\} \quad k = 0(1)n-1 \text{ where} \tag{4.1}$$

$$D_0 = D_{-1} = 1,\ D_1 = \mu_0;\ D'_0 = 0,\ D'_1 = \mu_1; \tag{4.2}$$

$$D_k = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-1} \\ \mu_1 & \mu_2 & \cdots & \mu_k \\ \cdots & \cdots & \cdots & \cdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-2} \end{vmatrix}, \quad D'_k = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-2} & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k-1} & \mu_{k+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-3} & \mu_{2k-1} \end{vmatrix}, \quad k = 2, 3, \ldots.$$

Table 4.1. *Relative errors in the recursion coefficients α_k, β_k generated by the quadrature rules of Table 2.1 and Table 2.2.*

k	Table 2.1		Table 2.2	
	$\delta\alpha_k$	$\delta\beta_k$	$\delta\alpha_k$	$\delta\beta_k$
0	1.35(−15)	4.56(−16)	6.68(−17)	2.02(−17)
1	5.38(−15)	5.75(−15)	3.75(−17)	2.52(−16)
2	2.49(−15)	6.42(−15)	2.89(−17)	4.66(−19)
3	1.32(−13)	6.59(−14)	1.54(−16)	7.72(−17)
4	1.43(−12)	8.73(−13)	3.20(−16)	2.01(−16)
5	2.26(−11)	9.64(−12)	2.10(−16)	7.77(−16)
6	6.73(−10)	2.43(−10)	1.85(−16)	1.16(−15)
7	1.29(−8)	6.31(−9)	6.24(−16)	5.13(−16)
8	9.98(−8)	8.26(−8)	6.08(−16)	4.32(−16)
9	4.59(−7)	1.94(−7)	4.39(−16)	5.97(−16)
10	6.36(−6)	5.71(−6)	5.17(−16)	6.93(−16)
11	2.08(−4)	3.12(−5)	6.55(−16)	2.15(−15)
12	2.80(−3)	2.01(−3)	4.29(−14)	1.08(−14)
13	3.66(−2)	1.33(−3)	3.17(−13)	3.14(−13)
14	8.28(−2)	3.65(−1)	5.71(−12)	4.75(−13)

Results of Test # 3. Using the LINPACK double precision routine DGECO (see, e.g., [2, Ch. I]) to factor the Hankel matrices in (4.2), and computing the determinants $D_k, D'_k, k = 2, 3, \ldots$, as signed products of the diagonal elements of the upper triangular factors, one obtains the results shown in Table 4.1. Here,

$\delta\alpha_k$ and $\delta\beta_k$ are defined by $\delta\alpha_k = |(\alpha_k^* - \alpha_k)/\alpha_k|$, $\delta\beta_k = |(\beta_k^* - \beta_k)/\beta_k|$, where α_k^*, β_k^* are the recursion coefficients generated as in Test # 2 from the respective quadrature rule $(\tau_\nu^*, \lambda_\nu^*)$ in Table 2.1 and Table 2.2, while α_k, β_k are the recursion coefficients as computed from (4.1), (4.2).

Discussion. The map from the Gaussian quadrature formula $(\tau_\nu^{(n)}, \lambda_\nu^{(n)})_{\nu=1}^n$ to the recursion coefficients α_k, β_k, $k = 0, 1, \ldots, n-1$, is usually quite well-conditioned; see the discussion in [3, § 3.1]. In the present case, the appropriate condition number indeed computes to 28.0. This means that Test # 3 ought to be able not only to discriminate between a good and a bad quadrature formula, but also to determine, approximately, the accuracy of each. From the results in Table 4.1 it indeed becomes plausible that the quadrature rule of Table 2.1 is accurate to at most 1–2 decimal digits, while the one of Table 2.2 is accurate to at least 11 decimal digits.

Actually, our quadrature rule in Table 2.2 is probably accurate to all 16 digits shown. The reason why this is not evident from Table 4.1 is the fact that the Hankel matrices H_k and H_k' used in (4.2) also become ill-conditioned rather quickly, as k increases. Their triangular factorizations, therefore, suffer in accuracy accordingly. Fortunately, for the case at hand, double precision on the CDC 6500 is still sufficient to weather this progressive ill-conditioning. From the condition numbers furnished by the routine DGECO, and shown in Table 4.2, we can

Table 4.2. *Condition numbers of the Hankel matrices* H_k, H_k' *in* (4.2).

k	condH_k	condH_k'	k	condH_k	condH_k'
1	1.00(0)	1.00(0)	9	1.40(11)	2.90(11)
2	1.15(1)	7.18(0)	10	5.85(12)	1.29(13)
3	1.79(2)	1.48(2)	11	2.58(14)	6.02(14)
4	3.95(3)	4.17(3)	12	1.20(16)	2.93(16)
5	1.02(5)	1.33(5)	13	5.81(17)	1.48(18)
6	3.02(6)	4.61(6)	14	2.93(19)	7.76(19)
7	9.95(7)	1.72(8)	15	1.53(21)	4.20(21)
8	3.59(9)	6.85(9)			

see indeed that, in the worst case $k = 15$, at least 8–10 decimal digits are salvaged. However, it would be unreasonable to expect agreement in the recursion coefficients α_{14}, β_{14} to much more than 10 decimal digits. As it turned out (see Table 4.1), we observed agreement to about 11–12 decimal digits.

To make Test # 3 effective as a general test, one would normally have to consider the use of multiple-precision arithmetic. With the availability of precompilers, such as Augment [1], to convert single- or double-precision Fortran routines to multiple-precision routines, this would be quite feasible. However, we have not done so here.

For easy reference, we list in Table 4.3 what we believe are the correct values (to 16 decimals) of the coefficients α_k, β_k.

Table 4.3. *The recursion coefficients* α_k, β_k.

k	α_k	β_k
0	0.7290111329472270	1.2878993168540691
1	1.0422198256747441	0.2450009794174209
2	1.2537306422019648	0.3530735172799071
3	1.4061820889340039	0.4538065447547201
4	1.5304717088698266	0.5467091516329361
5	1.6371146876931010	0.6327914312656564
6	1.7313265280009314	0.7135915502415592
7	1.8162157284093990	0.7901716008181790
8	1.8938033162945061	0.8632766955003995
9	1.9654868263312374	0.9334529739837076
10	2.0322783394582394	1.0011143019264016
11	2.0949374105669606	1.0665830763064052
12	2.1540505128026898	1.1301163055170060
13	2.2100811161203424	1.1919228879829775
14	2.2634026387069418	1.2521754391488299

A simpler test, but one that checks only the nodes, is

Test #4. Compute the sum of the nodes, $s_n = \sum_{\nu=1}^{n} \tau_\nu^{(n)}$, and check against

$$s_n = D_n'/D_n, \tag{4.3}$$

where D_n, D_n' are the determinants defined in (4.2).

Results of Test #4. Using again the LINPACK routine DGECO, one finds

$$\begin{aligned} D_n'/D_n &= 25.7603125030, \\ s_n &= 25.4984452247 \quad \text{from Table 2.1,} \\ s_n &= 25.7603125030 \quad \text{from Table 2.2,} \end{aligned}$$

corroborating the conclusion reached earlier in Test # 3.

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20.4. [85] "ERROR BOUNDS FOR GAUSSIAN QUADRATURE OF ANALYTIC FUNCTIONS"

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[85] (with R. S. Varga) "Error Bounds for Gaussian Quadrature of Analytic Functions," *SIAM J. Numer. Anal*. **20**, 1170–1186 (1983).

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ERROR BOUNDS FOR GAUSSIAN QUADRATURE OF ANALYTIC FUNCTIONS*

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To Peter Henrici on his 60th birthday in friendship and admiration

Abstract. For Gaussian quadrature rules over a finite interval, applied to analytic or meromorphic functions, we develop error bounds from contour integral representations of the remainder term. As in previous work on the subject, we consider both circular and elliptic contours. In contrast with earlier work, however, we attempt to determine exactly where on the contour the kernel of the error functional attains its maximum modulus. We succeed in answering this question for a large class of weight distributions (including all Jacobi weights) when the contour is a circle. In the more difficult case of elliptic contours, we can settle the question for certain special Jacobi weight distributions with parameters $\pm\frac{1}{2}$, and we provide empirical results for more general Jacobi weights. We further point out that the kernel of the error functional, at any complex point outside the interval of integration, can be evaluated accurately and efficiently by a recursive procedure. The same procedure is useful also to evaluate certain correction terms that arise when poles are present in the integrand. The error bounds obtained are illustrated numerically for two examples—an integral representation for the Bessel function of order zero, and an integral related to the complex exponential integral.

1. Introduction. We consider Gaussian quadrature with respect to some positive measure $d\lambda(t)$ on a finite interval which we normalize to be $[-1, 1]$. Thus,

$$\int_{-1}^{1} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f), \tag{1.1}$$

where $\tau_\nu^{(n)}$ are the zeros of the nth degree orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ and $\lambda_\nu^{(n)}$ the corresponding Christoffel numbers. If f is single-valued holomorphic in a domain D which contains $[-1, 1]$ in its interior, and Γ is a contour in D surrounding $[-1, 1]$, the remainder term $R_n(\cdot)$ can be represented as a contour integral

$$R_n(f) = \frac{1}{2\pi i}\int_\Gamma K_n(z) f(z)\,dz, \tag{1.2}$$

where the kernel K_n is given by

$$K_n(z) = R_n\left(\frac{1}{z-\cdot}\right), \tag{1.3}$$

or, alternatively, by

$$K_n(z) = \frac{\rho_n(z)}{\pi_n(z)}. \tag{1.4}$$

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Here, $\pi_n(z)$ is the orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ evaluated at z, while $\rho_n(z)$ is defined by

$$\rho_n(z) = \int_{-1}^{1} \frac{\pi_n(t)}{z-t}\, d\lambda(t); \tag{1.5}$$

see, e.g., [4, § 1.4].

There is an extensive literature using (1.2) to estimate the error R_n in (1.1); see the references cited in [4, § 4.1.1] and more recent work in [1], [11], [12]. Basically, the estimates take the form

$$|R_n(f)| \leqq \frac{l(\Gamma)}{2\pi} \max_{z\in\Gamma} |K_n(z)| \cdot \max_{z\in\Gamma} |f(z)|, \tag{1.6}$$

where $l(\Gamma)$ denotes the length of Γ. The first maximum depends only on the quadrature rule (i.e., on $d\lambda$) and not on f, while the second depends only on f. Similar estimates hold for meromorphic functions, if the contributions from the poles are separated out. In all the literature on the subject, $\max_{z\in\Gamma} |K_n(z)|$ is either bounded from above, or estimated asymptotically for large n (or large z, or both). Our objective here is to point out that for a large class of measures $d\lambda$ (including the Jacobi measure $d\lambda(t) = (1-t)^\alpha(1+t)^\beta\, dt$ for arbitrary $\alpha > -1$, $\beta > -1$), and in the case where Γ is a circle $|z| = r$, $r > 1$, this maximum can be expressed exactly as either $K_n(r)$ or $|K_n(-r)|$ (Theorem 3.1) and can be evaluated accurately and efficiently by recursion (Section 4). For elliptic contours $\Gamma = \{z : z = \frac{1}{2}(\rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}),\ 0 \leqq \vartheta \leqq 2\pi\}$, $\rho > 1$, the problem is considerably more difficult. We are able, however, in the case of Jacobi measures with $\alpha = \beta = \pm\frac{1}{2}$ and $\alpha = -\frac{1}{2}$, $\beta = \frac{1}{2}$, to give explicit representations of the kernel K_n on Γ, and from these to determine the maximum points on the ellipse (Section 5). The latter turn out to be located on the real positive axis (Theorems 5.1 and 5.3), except when $\alpha = \beta = \frac{1}{2}$, in which case they are located on the imaginary axis, if n is odd (Theorem 5.2), or nearby, if n is even. For more general Jacobi measures we present empirical results. Section 6 contains numerical examples illustrating the quality of the error bounds obtained.

We begin by recalling a preliminary result from [7].

2. Inequalities for moment quadrature sums. Here and in the following we restrict ourselves to measures $d\lambda$ of the form

$$d\lambda(t) = w(t)\, dt, \qquad -1 < t < 1, \tag{2.1}$$

where the function w is nonnegative and integrable on $[-1, 1]$, with moments

$$\mu_k = \int_{-1}^{1} t^k\, d\lambda(t), \qquad k = 0, 1, 2, \cdots, \tag{2.2}$$

where $\mu_0 > 0$. The orthogonal polynomials associated with (2.1) are denoted by $\pi_n(\cdot) = \pi_n(\cdot\,; d\lambda)$, their zeros by $\tau_\nu^{(n)}$, and the corresponding Christoffel numbers by $\lambda_\nu^{(n)}$. The following theorem, proved in [7], shows that, for a large class of weight functions w, the Gaussian quadrature sums for approximating the moment μ_k approach this moment monotonically. (To suit our present purposes, we have slightly weakened both the assertions and the hypotheses of the theorem.)

THEOREM 2.1. *Let*

$$\mu_k^{(n)} = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} [\tau_\nu^{(n)}]^k, \qquad k = 1, 2, 3, \cdots, \quad n = 1, 2, 3, \cdots. \tag{2.3}$$

(a) *If $w(t)/w(-t)$ is nondecreasing on $(-1, 1)$, then*

$$0 \leqq \mu_k^{(1)} \leqq \mu_k^{(2)} \leqq \cdots \leqq \mu_k^{([k/2]+1)} = \mu_k^{([k/2]+2)} = \cdots = \mu_k. \tag{2.4}$$

(b) *If $w(t)/w(-t)$ is nonincreasing on $(-1, 1)$, then*

$$0 \leqq \mu_k^{(1)} \leqq \mu_k^{(2)} \leqq \cdots \leqq \mu_k^{([k/2]+1)} = \mu_k^{([k/2]+2)} = \cdots = \mu_k \tag{2.5}$$

if k is even and

$$\mu_k = \cdots = \mu_k^{([k/2]+2)} = \mu_k^{([k/2]+1)} \leqq \mu_k^{([k/2])} \leqq \cdots \leqq \mu_k^{(2)} \leqq \mu_k^{(1)} \leqq 0 \tag{2.6}$$

if k is odd.

We note, in particular, that for the Jacobi weight function $w(t) = (1-t)^\alpha (1+t)^\beta$, $\alpha > -1$, $\beta > -1$, one has

$$\frac{w(t)}{w(-t)} = \left(\frac{1+t}{1-t}\right)^{\beta-\alpha},$$

which is strictly increasing on $(-1, 1)$ if $\alpha < \beta$, equal to 1 if $\alpha = \beta$, and strictly decreasing on $(-1, 1)$ if $\alpha > \beta$. Accordingly, (2.4) holds if $\alpha \leqq \beta$, and (2.5), (2.6) if $\alpha > \beta$.

3. The maximum of the kernel K_n on a circle and corresponding error bounds. We assume a measure $d\lambda$ of the form (2.1) and propose to find the maximum of the kernel $K_n(z)$ in (1.3) on the circle $C_r = \{z : |z| = r\}$, where $r > 1$.

THEOREM 3.1. *There holds*

$$\max_{z \in C_r} |K_n(z)| = \begin{cases} K_n(r) & \text{if } w(t)/w(-t) \text{ is nondecreasing on } (-1, 1), \\ |K_n(-r)| & \text{if } w(t)/w(-t) \text{ is nonincreasing on } (-1, 1). \end{cases} \tag{3.1}$$

Remark. If $w(t) = w(-t)$ on $(-1, 1)$ then, by symmetry, $K_n(r) = |K_n(-r)|$, and either statement in (3.1) is valid.

Proof of Theorem 3.1. By expanding $(z-t)^{-1}$ in powers of t/z, one obtains from (1.3), when $|z| > 1$, that

$$K_n(z) = \sum_{k=2n}^{\infty} \frac{R_n(t^k)}{z^{k+1}}. \tag{3.2}$$

We have used the fact that $R_n(t^k) = 0$ for $0 \leqq k < 2n$. Therefore,

$$\max_{z \in C_r} |K_n(z)| \leqq \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}}. \tag{3.3}$$

If $w(t)/w(-t)$ is nondecreasing, then, by Theorem 2.1(a), since $[k/2] \geqq n$ for $k \geqq 2n$,

$$\mu_k = \mu_k^{([k/2]+1)} \geqq \mu_k^{(n+1)} \geqq \mu_k^{(n)}, \qquad k \geqq 2n,$$

hence, by (2.2) and (2.3),

$$R_n(t^k) \geqq 0 \quad \text{for all } k \geqq 2n.$$

Therefore,

$$K_n(r) = \sum_{k=2n}^{\infty} \frac{R_n(t^k)}{r^{k+1}} = \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}}.$$

Comparison with (3.3) shows that $\max_{z \in C_r} |K_n(z)| = K_n(r)$, proving (3.1) in case (a) of Theorem 2.1.

If $w(t)/w(-t)$ is nonincreasing, one obtains from (2.5), when k is even, as before that

$$R_n(t^k) \geqq 0 \quad \text{for all } k \text{ (even)} \geqq 2n,$$

while for $k \geqq 2n+1$ odd, $\mu_k = \mu_k^{([k/2]+1)} \leqq \mu_k^{(n+1)} \leqq \mu_k^{(n)}$ by (2.6), so that

$$R_n(t^k) \leqq 0 \quad \text{for all } k \text{ (odd)} \geqq 2n+1.$$

Consequently,

$$(-1)^k R_n(t^k) \geqq 0 \quad \text{for all } k \geqq 2n,$$

and

$$|K_n(-r)| = \left| -\sum_{k=2n}^{\infty} \frac{(-1)^k R_n(t^k)}{r^{k+1}} \right| = \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}},$$

yielding $\max_{z \in C_r} |K_n(z)| = |K_n(-r)|$. □

In the situations described in Theorem 3.1, the modulus of the kernel $K_n(z)$ thus attains its maximum on the circle C_r either at $z = r$ or at $z = -r$ on the real axis. For the Jacobi weight function $w(t) = (1-t)^\alpha (1+t)^\beta$, the remark after Theorem 2.1 implies that the maximum occurs at $z = r$ if $\alpha \leqq \beta$, and at $z = -r$ if $\alpha > \beta$.

We remark that the "bound" used in [12, Eqs. (5) and (6)] for $\max_{z \in C_r} |K_n(z)|$ in the case of Gegenbauer measures is actually $K_n(r)$, hence, by Theorem 3.1, *equal* to the maximum in question. The form given in [12] for $K_n(r)$ involves infinite series and the zeros of Gegenbauer polynomials. It requires considerably more effort to evaluate than the simple recursion (Eqs. (4.3)–(4.5)) to be described below in § 4. The approach via recursion, moreover, is not restricted to Gegenbauer measures, but is valid for essentially arbitrary measures.

The error bound (1.6), in combination with, say, the first case of Theorem 3.1, now yields the final error bound

$$|R_n(f)| \leqq r \cdot K_n(r) \cdot \max_{z \in C_r} |f(z)|. \tag{3.4}$$

Whether or not this represents a realistic estimation of the error depends largely on the behavior of f on the contour C_r. If f is highly oscillatory on C_r, then (3.4) is likely to be conservative. Some improvement, for specific functions f, may be achieved by optimizing the bound on the right of (3.4) as a function of r; see § 6 for examples.

If f is meromorphic, with poles close to the interval $[-1, 1]$, the quadrature rule (1.1) will converge only very slowly. Moreover, (3.4) ceases to be applicable, since f may no longer be analytic in C_r, $r > 1$. Valid error bounds can still be obtained by employing elliptic contours (see § 5), but they are of limited interest in cases of slow convergence.

It is well known, however, how the poles can be taken into account so as to restore the fast convergence one is accustomed to in the case of analytic functions. Assuming for simplicity that there are only a finite number of poles p_i in the finite complex plane, and that all are simple, then in fact (see, e.g., [10])

$$\int_{-1}^{1} f(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) - \sum_i K_n(p_i)(\operatorname{res} f)_{p_i} + R_n(f), \tag{3.5}$$

where $\tau_\nu^{(n)}$, $\lambda_\nu^{(n)}$ are as before, and $(\operatorname{res} f)_{p_i}$ denotes the residue of f at the pole p_i. For the remainder R_n we have the same representation as before,

$$R_n(f) = \frac{1}{2\pi i} \int_\Gamma K_n(z) f(z)\, dz, \tag{3.6}$$

where Γ is a contour enclosing the interval $[-1, 1]$ as well as the poles p_i; the error bound (3.4) continues to hold if the circle C_r, $r>1$, contains all poles p_i in its interior.

As a simple example, suppose that

$$f(t)=\frac{g(t)}{t^2+\omega^2}, \qquad \omega>0, \tag{3.7}$$

with g an entire function, real-valued on the real axis. Then (3.5), by an elementary calculation, reduces to

$$\int_{-1}^{1}\frac{g(t)}{t^2+\omega^2}\,d\lambda(t)=\sum_{\nu=1}^{n}\lambda_\nu^{(n)}\frac{g(\tau_\nu^{(n)})}{[\tau_\nu^{(n)}]^2+\omega^2}-\frac{1}{\omega}\operatorname{Im}[K_n(i\omega)g(i\omega)]+R_n(f), \tag{3.8}$$

the remainder being bounded by (3.4), where $r>\max(1,\omega)$ and f is given by (3.7).

4. Computation of $K_n(\pm r)$ and $K_n(z)$. For computational purposes, the second of the two expressions (1.3) and (1.4) for $K_n(z)$, that is,

$$K_n(z)=\frac{\rho_n(z)}{\pi_n(z)}, \tag{4.1}$$

is the more suitable one, as it is not subject to any loss of accuracy. (This is not sufficiently recognized in the literature; Lether [11], for example, refers to the form (4.1) as being "inconvenient".) Indeed, $\{\rho_k(z)\}$ and $\{\pi_k(z)\}$ both are solutions of the basic recurrence relation

$$y_{k+1}=(z-\alpha_k)y_k-\beta_k y_{k-1}, \qquad k=0,1,2,\cdots, \tag{4.2}$$

satisfied by the (monic) orthogonal polynomials $\pi_k(\cdot)=\pi_k(\cdot\,;d\lambda)$, whereby $y_{-1}=0$, $y_0=1$ for $\{\pi_k\}$, and $y_{-1}=1$ for $\{\rho_k\}$. (It is assumed that $\beta_0=\int_{-1}^{1}d\lambda(t)$.) If $z=\pm r$, $r>1$, so that $z\notin[-1,1]$, the solution $\{\rho_k(z)\}$ is the minimal solution of (4.2), hence uniquely determined by the single initial value $y_{-1}=1$; see [5]. It can be computed most effectively by backward recursion [5, § 5]: Let

$$r_\nu^{[\nu]}(z)=0, \qquad r_{k-1}^{[\nu]}(z)=\frac{\beta_k}{z-\alpha_k-r_k^{[\nu]}(z)}, \qquad k=\nu,\nu-1,\cdots,1,0. \tag{4.3}$$

Then, if $z\notin[-1,1]$, the limit $\lim_{\nu\to\infty}r_{k-1}^{[\nu]}(z)=r_{k-1}(z)$ exists, and

$$\rho_{-1}(z)=1, \qquad \rho_k(z)=r_{k-1}(z)\rho_{k-1}(z), \qquad k=0,1,2,\cdots,n. \tag{4.4}$$

Thus, to compute $\rho_n(z)$ to within a relative error of ε, one starts with some initial value $\nu_0>n$ of the index ν, and keeps increasing ν, say by 5, until $|r_{k-1}^{[\nu+5]}(z)-r_{k-1}^{[\nu]}(z)|\leqq\varepsilon|r_{k-1}^{[\nu+5]}(z)|$ for all $k=0,1,2,\cdots,n$. Thereafter, (4.4) is applied, with $r_{k-1}(z)$ approximated by $r_{k-1}^{[\nu+5]}(z)$ for the final index ν. The computation of $\pi_n(z)$ proceeds directly from (4.2), applied for $k=0,1,\cdots,n-1$, with $y_{-1}=0$, $y_0=1$.

In the important special case of the Jacobi weight function $w(t)=(1-t)^\alpha(1+t)^\beta$, $\alpha>-1$, $\beta>-1$, the iteration on the index ν in (4.3) can be dispensed with. An appropriate value for ν, when $z=\pm r$, $r>1$, is indeed known to be [5, Eq. (5.6′)], independently of α and β, the smallest integer ν satisfying

$$\nu\geqq n+\frac{\ln(1/\varepsilon)}{2\ln(r+\sqrt{r^2-1})}. \tag{4.5}$$

In this case, the computation of $\rho_n(z)$ by (4.3), (4.4) is particularly efficient, even for $z=\pm r$ relatively close to the interval $[-1,1]$. Some numerical values of ν/n in the case $\varepsilon=.5\times10^{-5}$ are shown in Table 4.1.

TABLE 4.1
Numerical values of ν/n for $\varepsilon = .5\times 10^{-5}$, where ν is the smallest integer satisfying (4.5).

r	$n=10$	$n=20$	$n=40$	$n=80$
1.01	5.4	3.20	2.100	1.5500
1.05	3.0	2.00	1.500	1.2500
1.10	2.4	1.70	1.350	1.1750
1.50	1.7	1.35	1.175	1.0875
2.00	1.5	1.25	1.125	1.0625
5.00	1.3	1.15	1.075	1.0375

Doubling the accuracy to $\varepsilon = .25\times 10^{-10}$ has the effect, essentially, of doubling $(\nu/n)-1$, as can be seen from (4.5). For the purpose of error estimation, however, five decimal digits are more than enough.

We stress the fact that the algorithm (4.3), (4.4) is valid for arbitrary complex $z \notin [-1, 1]$. The estimate for ν in (4.5), when $d\lambda$ is the Jacobi measure, however, becomes a bit more complicated. We now have to take the smallest integer satisfying [5, Eq. (5.6)]

$$\nu \geqq n + \frac{\ln(1/\varepsilon)}{2\ln\left|z+(z-1)^{1/2}(z+1)^{1/2}\right|}, \tag{4.6}$$

where the principal values of $\arg(z-1)$ and $\arg(z+1)$ are to be used in evaluating the square roots. If $z = iy$ is purely imaginary, (4.6) reduces to

$$\nu \geqq n + \frac{\ln(1/\varepsilon)}{2\ln\left(y+\sqrt{1+y^2}\right)}. \tag{4.7}$$

In particular, the algorithm (4.3), (4.4) may also be used to compute the numerators of $K_n(p_i) = \rho_n(p_i)/\pi_n(p_i)$ in (3.5) and of $K_n(i\omega) = \rho_n(i\omega)/\pi_n(i\omega)$ in (3.8). The denominators can be computed directly from the recursion (4.2).

5. The maximum of the kernel K_n on an ellipse and corresponding error bounds. Another frequent choice of the contour Γ is an ellipse $\mathscr{E}_\rho = \{z : z = \frac{1}{2}(u+u^{-1}),\ u = \rho e^{i\vartheta},\ 0 \leqq \vartheta \leqq 2\pi\}$ with foci at $z = \pm 1$ and sum of semiaxes equal to ρ, $\rho > 1$. As $\rho \downarrow 1$, the ellipse $\mathscr{E}_\rho$ shrinks to the interval $[-1, 1]$, while with increasing ρ it becomes more and more circle-like. Since

$$\frac{1}{z-t} = \frac{2}{u}\,\frac{1}{u^{-2}-2tu^{-1}+1} = 2\sum_{k=0}^{\infty}\frac{U_k(t)}{u^{k+1}},$$

where U_k denotes the Chebyshev polynomial of the second kind, the expansion analogous to (3.2) now reads

$$K_n(z) = 2\sum_{k=2n}^{\infty}\frac{R_n(U_k)}{u^{k+1}}, \qquad z = \frac{1}{2}\left(u+\frac{1}{u}\right). \tag{5.1}$$

One has symmetry with respect to the real axis, i.e., $|K_n(\bar{z})| = |K_n(z)|$, but the maximum of $|K_n(z)|$, $z \in \mathscr{E}_\rho$, is no longer always attained on the real axis.

The case of the Jacobi weight function $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha > -1$, $\beta > -1$, is of sufficient interest to be considered in some detail, although precise results are difficult to obtain for general parameter values. Note, however, that the known

identity for Jacobi polynomials, $\pi_n^{(\beta,\alpha)}(z)=(-1)^n\pi_n^{(\alpha,\beta)}(-z)$, implies $|K_n^{(\beta,\alpha)}(z)|=|K_n^{(\alpha,\beta)}(-z)|=|K_n^{(\alpha,\beta)}(-\bar{z})|$, so that an interchange of the parameters amounts to a reflection in the complex plane with respect to the imaginary axis. It suffices therefore to consider $\alpha \leqq \beta$.

5.1. Chebyshev measures of the first and second kind. Let first $\alpha=\beta=-\frac{1}{2}$, that is, $d\lambda(t)=(1-t^2)^{-1/2}\,dt$, the orthogonal polynomials thus being the Chebyshev polynomials T_k of the first kind. From the well-known formula

$$T_n(z)=\tfrac{1}{2}[(z+\sqrt{z^2-1})^n+(z-\sqrt{z^2-1})^n], \tag{5.2}$$

putting $z=\frac{1}{2}(u+u^{-1})$, one gets

$$T_n(z)=\tfrac{1}{2}(u^n+u^{-n}), \qquad z=\tfrac{1}{2}(u+u^{-1}).$$

Furthermore, using [9, Eq. 3.613.1], one finds

$$\int_{-1}^{1}\frac{T_n(t)}{z-t}(1-t^2)^{-1/2}\,dt=\int_0^{\pi}\frac{\cos n\vartheta}{z-\cos\vartheta}\,d\vartheta=\frac{\pi}{\sqrt{z^2-1}}(z-\sqrt{z^2-1})^n, \tag{5.3}$$

hence

$$\int_{-1}^{1}\frac{T_n(t)}{z-t}(1-t^2)^{-1/2}\,dt=\frac{2\pi}{(u-u^{-1})u^n}, \qquad z=\frac{1}{2}(u+u^{-1}).$$

It follows that

$$\frac{\rho_n(z)}{\pi_n(z)}=\frac{4\pi}{(u-u^{-1})u^n(u^n+u^{-n})}, \qquad z=\frac{1}{2}(u+u^{-1}),$$

from which, in particular,

$$\begin{aligned}&|K_n(z)|=\frac{2\pi}{\rho^n}\{[a_2(\rho)-\cos 2\vartheta][a_{2n}(\rho)+\cos 2n\vartheta]\}^{-1/2},\\ &z=\tfrac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta})\in\mathscr{E}_\rho,\end{aligned} \tag{5.4}$$

where

$$a_j(\rho)=\tfrac{1}{2}(\rho^j+\rho^{-j}), \qquad j=1,2,3,\cdots, \quad \rho>1. \tag{5.5}$$

LEMMA 5.1. *The functions in* (5.5) *satisfy*

$$\frac{a_{2n}(\rho)-1}{a_2(\rho)-1}\geqq n^2, \qquad n=1,2,3,\cdots, \quad \rho>1. \tag{5.6}$$

Proof. Multiplying numerator and denominator in (5.6) by $2\rho^{2n}$, and using (5.5), one gets

$$\frac{a_{2n}(\rho)-1}{a_2(\rho)-1}=\frac{\rho^{4n}+1-2\rho^{2n}}{\rho^{2(n-1)}(\rho^4+1-2\rho^2)}=\left\{\frac{\rho^{2n}-1}{\rho^{n-1}(\rho^2-1)}\right\}^2.$$

Observe that

$$\begin{aligned}\rho^{-(n-1)}\frac{\rho^{2n}-1}{\rho^2-1}&=\rho^{-(n-1)}[\rho^{2(n-1)}+\rho^{2(n-2)}+\cdots+1]\\ &=\rho^{n-1}+\rho^{n-3}+\cdots+\rho^{-(n-3)}+\rho^{-(n-1)}.\end{aligned}$$

Since $x+x^{-1}>2$ for any $x>1$, the sum on the right is larger than $2(n/2)=n$ if n is

even, and larger than $2[(n-1)/2]+1=n$ if $n\geqq 3$ is odd, hence $>n$ for any integer $n\geqq 2$, proving (5.6) with strict inequality for $n\geqq 2$. If $n=1$, (5.6) is an equality. □

THEOREM 5.1. *If* $d\lambda(t)=(1-t^2)^{-1/2}\,dt$ *on* $(-1,1)$, *then*

$$\max_{z\in\mathscr{E}_\rho}|K_n(z)|=K_n(\tfrac{1}{2}(\rho+\rho^{-1})), \tag{5.7}$$

i.e., the maximum of $|K_n(z)|$ *on* $\mathscr{E}_\rho$ *is attained on the real axis.*

Proof. By (5.4) it suffices to prove

$$(a_2-\cos 2\vartheta)(a_{2n}+\cos 2n\vartheta)\geqq(a_2-1)(a_{2n}+1),\qquad 0\leqq\vartheta\leqq\pi/2,$$

where $a_j=a_j(\rho)$ is given by (5.5). This is equivalent to

$$(1-\cos 2\vartheta)a_{2n}-(1-\cos 2n\vartheta)a_2+1-\cos 2\vartheta\cos 2n\vartheta\geqq 0,$$

or, introducing half angles, to

$$a_{2n}+1-(a_2-1)\frac{\sin^2 n\vartheta}{\sin^2\vartheta}-2\sin^2 n\vartheta\geqq 0, \tag{5.8}$$

if $\vartheta>0$. Since

$$\left|\frac{\sin n\vartheta}{\sin\vartheta}\right|=|U_{n-1}(\cos\vartheta)|\leqq n,$$

the left-hand side of (5.8) is larger than or equal to

$$a_{2n}+1-n^2(a_2-1)-2=(a_2-1)\left\{\frac{a_{2n}-1}{a_2-1}-n^2\right\},$$

which is nonnegative by Lemma 5.1. □

For the Chebyshev measure of the second kind, $d\lambda(t)=(1-t^2)^{1/2}\,dt$, the nth degree orthogonal polynomial is

$$U_n(z)=\frac{1}{2\sqrt{z^2-1}}[(z+\sqrt{z^2-1})^{n+1}-(z-\sqrt{z^2-1})^{n+1}],$$

which yields

$$U_n(z)=\frac{u^{n+1}-u^{-(n+1)}}{u-u^{-1}},\qquad z=\frac{1}{2}(u+u^{-1}),$$

while (cf. [9, Eq. 3.613.3])

$$\int_{-1}^{1}\frac{U_n(t)}{z-t}(1-t^2)^{1/2}\,dt=\int_0^\pi\frac{\sin(n+1)\vartheta\sin\vartheta}{z-\cos\vartheta}\,d\vartheta=\frac{\pi}{u^{n+1}},$$

$$z=\frac{1}{2}(u+u^{-1}).$$

Therefore,

$$|K_n(z)|=\frac{\pi}{\rho^{n+1}}\left\{\frac{a_2(\rho)-\cos 2\vartheta}{a_{2n+2}(\rho)-\cos 2(n+1)\vartheta}\right\}^{1/2},$$

$$z=\tfrac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta})\in\mathscr{E}_\rho. \tag{5.9}$$

THEOREM 5.2. *If* $d\lambda(t) = (1-t^2)^{1/2}\,dt$ *on* $(-1, 1)$, *and* n *is odd, then*

$$\max_{z\in\mathscr{E}_\rho} |K_n(z)| = \left|K_n\left(\frac{i}{2}(\rho-\rho^{-1})\right)\right|, \tag{5.10}$$

i.e., the maximum of $|K_n(z)|$ (n *odd*) *on* $\mathscr{E}_\rho$ *is attained on the imaginary axis.*

Proof. It is obvious that

$$\frac{a_2-\cos 2\vartheta}{a_{2n+2}-\cos 2(n+1)\vartheta} \leqq \frac{a_2+1}{a_{2n+2}-1}, \quad \text{for all } \vartheta, \text{ all } n,$$

with equality holding when $\vartheta = \pi/2$ and n is odd. With (5.9), this gives the desired result. □

If, in Theorem 5.2, n is even, computation shows that the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$ is attained slightly off the imaginary axis.

5.2. Jacobi measure with $\alpha = -\frac{1}{2}$ and $\beta = \frac{1}{2}$. The orthogonal polynomials in this case are those with respect to $d\lambda(t) = \sqrt{(1+t)/(1-t)}\,dt$, and are given by

$$p_n(z) = \frac{T_{2n+1}(\sqrt{\frac{1}{2}(z+1)})}{\sqrt{\frac{1}{2}(z+1)}},$$

where T_{2n+1} is the Chebyshev polynomial of degree $2n+1$. With $z = \frac{1}{2}(u+u^{-1})$, so that $\sqrt{\frac{1}{2}(z+1)} = (u+1)/(2\sqrt{u})$, we find by (5.2), after a little computation,

$$p_n(z) = \frac{u^{n+1}+u^{-n}}{u+1}, \qquad z = \frac{1}{2}(u+u^{-1}).$$

Furthermore,

$$\int_{-1}^{1} \frac{p_n(t)}{z-t}\sqrt{\frac{1+t}{1-t}}\,dt = \int_0^\pi \frac{2\cos(2n+1)\vartheta/2\cos\vartheta/2}{z-\cos\vartheta}\,d\vartheta$$

$$= \int_0^\pi \frac{\cos(n+1)\vartheta+\cos n\vartheta}{z-\cos\vartheta}\,d\vartheta,$$

hence, using (5.3),

$$\int_{-1}^{1} \frac{p_n(t)}{z-t}\sqrt{\frac{1+t}{1-t}}\,dt = \frac{2\pi(u+1)}{(u-u^{-1})u^{n+1}}, \qquad z = \frac{1}{2}(u+u^{-1}).$$

There follows

$$\frac{\rho_n(z)}{\pi_n(z)} = \frac{2\pi(u+1)^2}{(u-u^{-1})u^{n+1}(u^{n+1}+u^{-n})},$$

and, by an elementary computation,

$$|K_n(z)| = \frac{2\pi}{\rho^{n+1/2}} \frac{a_1(\rho)+\cos\vartheta}{\{[a_2(\rho)-\cos 2\vartheta][a_{2n+1}(\rho)+\cos(2n+1)\vartheta]\}^{1/2}}, \tag{5.11}$$

$$z = \frac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta}) \in \mathscr{E}_\rho,$$

where $a_j(\rho)$ is again given by (5.5).

LEMMA 5.2. *There holds*

$$\frac{a_1(\rho)a_{2n+1}(\rho)-1}{a_2(\rho)-1} > \left(n+\frac{1}{2}\right)^2, \qquad n = 1, 2, 3, \cdots, \quad \rho > 1. \tag{5.12}$$

Proof. A simple computation based on the definition (5.5) of $a_j(\rho)$ yields

$$\frac{a_1(\rho)a_{2n+1}(\rho)-1}{a_2(\rho)-1}=\frac{1}{2}\left\{\frac{\rho^{2n+2}-1}{\rho^n(\rho^2-1)}\right\}^2+\frac{1}{2}\left\{\frac{\rho^{2n}-1}{\rho^{n-1}(\rho^2-1)}\right\}^2.$$

Applying to each of the two squares on the right the reasoning used in the proof of Lemma 5.1 produces the lower bound $\frac{1}{2}[(n+1)^2+n^2]=n^2+n+\frac{1}{2}>n^2+n+\frac{1}{4}=(n+\frac{1}{2})^2$. □

THEOREM 5.3. *If* $d\lambda(t)=\sqrt{(1+t)/(1-t)}\,dt$ *on* $(-1, 1)$, *then*

$$\max_{z\in\mathscr{E}_\rho}|K_n(z)|=K_n(\tfrac{1}{2}(\rho+\rho^{-1})), \tag{5.13}$$

i.e., the maximum of $|K_n(z)|$ *on* $\mathscr{E}_\rho$ *is attained on the positive real axis.*

Proof. We shall show that the expression on the right of (5.11), considered as a function of ϑ on $[0, \pi]$, attains its maximum only at $\vartheta=0$. Using

$$a_2(\rho)=2[a_1(\rho)]^2-1,$$

we can write this assertion in the form

$$\frac{a_1+\cos\vartheta}{(a_1-\cos\vartheta)(a_{2n+1}+\cos(2n+1)\vartheta)}<\frac{a_1+1}{(a_1-1)(a_{2n+1}+1)},\qquad 0<\vartheta\leqq\pi,$$

where $a_j=a_j(\rho)$. Clearing the denominators, and multiplying out everything, produces an aggregate of terms that can be combined to suggest the introduction of half angles, and then yields the equivalent inequality

$$\frac{a_1(a_{2n+1}+1)}{a_1+1}-\frac{1}{2}(a_1-1)\frac{\sin^2((2n+1)\vartheta/2)}{\sin^2(\vartheta/2)}-\sin^2(2n+1)\frac{\vartheta}{2}>0.$$

Now the left-hand side is larger than or equal to

$$\frac{a_1(a_{2n+1}+1)}{a_1+1}-\frac{1}{2}(a_1-1)(2n+1)^2-1=2(a_1-1)\left\{\frac{a_1a_{2n+1}-1}{a_2-1}-\left(n+\frac{1}{2}\right)^2\right\},$$

which is strictly positive by Lemma 5.2. □

5.3. Gegenbauer measure. In the case $\alpha=\beta$ we have only empirical results based on computation. These seem to indicate the following. If $-1<\alpha\leqq-\frac{1}{2}$, we have the behavior exhibited by the Chebyshev polynomials of the first kind: The maximum of $|K_n^{(\alpha,\alpha)}(z)|$ on $\mathscr{E}_\rho$ is attained on the real axis, i.e., we have (5.7). If $-\frac{1}{2}<\alpha<0$, the maximum is attained on the imaginary axis if $n=1$; as n becomes larger, the maximum point moves along $\mathscr{E}_\rho$ to the real axis, more rapidly so, the larger ρ is. If $0\leqq\alpha$, the maximum is attained on the imaginary axis, except when n is even and ρ not too large, in which case it is assumed slightly off the imaginary axis. Thus, the Chebyshev polynomials of the second kind (cf. Theorem 5.2) are a prototype for the case $\alpha\geqq0$.

Another interesting empirical observation is the apparent monotonic decrease of $\max_{z\in\mathscr{E}_\rho}|K_n^{(\alpha,\alpha)}(z)|$ as a function of α, $\alpha>-1$, for fixed ρ and n.

5.4. General Jacobi measure. For arbitrary $-1<\alpha<\beta$ we again have only empirical information, the extent of computational experimentation being of necessity more limited. What appears to be happening, nevertheless, is the following: For all $-1<\alpha\leqq-\frac{1}{2}$, $\alpha<\beta$, we have (5.7), i.e., the maximum occurs on the positive real axis. For $-\frac{1}{2}<\alpha<\beta$, the maximum point for $|K_n^{(\alpha,\beta)}(z)|$ on $\mathscr{E}_\rho$ is located to the right of the imaginary axis and is moving toward the positive real axis as both ρ and n increase.

As a practical matter, it was determined that a generally good *estimate* of the maximum of $|K_n^{(\alpha,\beta)}(z)|$ on $\mathscr{E}_\rho$ can be found as follows, if $\alpha \leqq \beta$:

$$\max_{z\in\mathscr{E}_\rho} |K_n^{(\alpha,\beta)}(z)| \approx \begin{cases} K_n^{(\alpha,\beta)}(\tfrac{1}{2}(\rho+\rho^{-1})), & \text{if } -1<\alpha\leqq -\tfrac{1}{2}, \\ \max\left\{K_n^{(\alpha,\beta)}(\tfrac{1}{2}(\rho+\rho^{-1})), \left|K_n^{(\alpha,\beta)}\left(\frac{i}{2}(\rho-\rho^{-1})\right)\right|\right\}, & \text{otherwise.} \end{cases} \tag{5.14}$$

If $\alpha>\beta$, the estimate (5.14), by symmetry, continues to hold if $K_n^{(\alpha,\beta)}(\frac{1}{2}(\rho+\rho^{-1}))$ is replaced by $|K_n^{(\alpha,\beta)}(-\frac{1}{2}(\rho+\rho^{-1}))|$. The value of the kernel $K_n^{(\alpha,\beta)}(z)$ on the imaginary axis, $z=iy$, $y>0$, can be computed to a relative accuracy of ε as in (4.3), (4.4), where $z=iy$, and where ν may be taken to be the smallest integer satisfying (4.7).

5.5. Error bound. To obtain the error bound in final form, assume, for definiteness, that (5.7) holds. Since the ellipse $\mathscr{E}_\rho$ has length $l(\mathscr{E}_\rho)=4\varepsilon^{-1}E(\varepsilon)$, where

$$\varepsilon = \frac{2}{\rho+\rho^{-1}} \tag{5.15}$$

is the eccentricity of $\mathscr{E}_\rho$ and

$$E(\varepsilon)=\int_0^{\pi/2} \sqrt{1-\varepsilon^2\sin^2\vartheta}\,d\vartheta \tag{5.16}$$

the complete elliptic integral of the second kind, we obtain from (1.6)

$$|R_n(f)| \leqq \frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)\cdot K_n(\varepsilon^{-1})\cdot \max_{z\in\mathscr{E}_\rho}|f(z)|, \qquad \varepsilon=\frac{2}{\rho+\rho^{-1}}. \tag{5.17}$$

Again it is possible to optimize the bound on the right as a function of ρ. Also, the bound (5.17) can be used in connection with the modified quadrature rule (3.5) if $\mathscr{E}_\rho$ contains all the poles p_i.

6. Examples.

Example 6.1.

$$\int_{-1}^{1} \frac{\cos[\omega(t+1)]}{\sqrt{(3+t)(1-t)}}\,dt = \frac{\pi}{2}J_0(2\omega), \qquad \omega>0.$$

We take for $d\lambda$ the Jacobi measure $d\lambda(t)=(1-t)^{-1/2}\,dt$ with parameters $\alpha=-\frac{1}{2}$, $\beta=0$. Accordingly,

$$f(z)=\frac{\cos[\omega(z+1)]}{\sqrt{3+z}}, \tag{6.1}$$

the square root being understood in the sense of the principal value. We first illustrate the error bounds based on circular contours.

The singularity closest to the origin is the branch point at $z=-3$; hence all circles C_r with $1<r<3$ are admissible. To bound f on C_r, we note

$$|\cos[\omega(z+1)]| = \tfrac{1}{2}|e^{-\omega y}e^{i\omega(x+1)}+e^{\omega y}e^{-i\omega(x+1)}|$$

$$\leqq \tfrac{1}{2}(e^{-\omega y}+e^{\omega y}), \qquad z=x+iy,$$

and

$$|\sqrt{3+z}| = \sqrt{|3+z|} \geqq \sqrt{3-|z|},$$

so that

$$|f(z)| \leqq \frac{\cosh(\omega r)}{\sqrt{3-r}}, \qquad z \in C_r. \tag{6.2}$$

Since we are in the first case of Theorem 3.1, we obtain, according to (3.4),

$$|R_n(f)| \leqq r \cdot K_n(r) \cdot \frac{\cosh(\omega r)}{\sqrt{3-r}}, \qquad 1 < r < 3. \tag{6.3}$$

The bound on the right of (6.3) may be optimized as a function of r by using a simple dichotomous search procedure in combination with the recursive algorithm (4.3)–(4.5) for evaluating $K_n(r)$. A few optimal values r_{opt} of r thus computed, and corresponding optimal bounds, are shown in Table 6.1, together with the modulus of

TABLE 6.1
Optimal error bound (6.3) *and actual error.*

ω	n	r_{opt}	bound	error	ω	n	r_{opt}	bound	error
.5	5	2.853	1.19 (−6)	3.93 (−9)	8.0	5	1.628	3.29 (1)	1.05 (−1)
	10	2.928	3.83 (−14)	6.73 (−17)		10	2.481	4.90 (−5)	3.01 (−7)
	15	2.952	1.05 (−21)	1.25 (−24)		15	2.851	3.19 (−12)	3.50 (−15)
	20	2.964	2.68 (−29)	m.p.		20	2.925	1.03 (−19)	1.27 (−24)
1.0	5	2.828	4.69 (−6)	4.36 (−9)		25	2.951	2.83 (−27)	m.p.
	10	2.922	1.57 (−13)	6.33 (−17)	16.0	5	1.224	1.94 (6)	3.82 (−1)
	15	2.950	4.36 (−21)	1.10 (−24)		10	1.615	3.41 (2)	3.10 (−2)
	20	2.963	1.13 (−28)	m.p.		15	2.095	1.69 (−3)	9.38 (−7)
2.0	5	2.752	7.63 (−5)	3.88 (−7)		20	2.558	5.78 (−10)	5.22 (−13)
	10	2.908	2.89 (−12)	7.04 (−17)		25	2.832	3.70 (−17)	1.90 (−20)
	15	2.944	8.28 (−20)	1.38 (−24)		30	2.917	1.25 (−24)	3.64 (−27)
	20	2.960	2.17 (−27)	2.27 (−28)	32.0	5	1.074	1.33 (14)	5.21 (−1)
4.0	5	2.380	1.37 (−2)	7.69 (−5)		10	1.203	8.56 (11)	1.63 (−1)
	10	2.860	9.32 (−10)	5.98 (−14)		20	1.608	3.62 (4)	2.14 (−3)
	15	2.929	2.94 (−17)	4.92 (−25)		30	2.109	8.57 (−7)	3.05 (−12)
	20	2.952	8.02 (−25)	2.35 (−27)		40	2.612	7.48 (−20)	1.21 (−24)

the actual errors. (Numbers in parentheses indicate decimal exponents. Close to machine precision, the actual error may be larger than the bound; this is indicated by "m.p." for "machine precision".) The actual error was computed in double precision on the CDC 6500 computer (machine precision of approx. 29 decimal digits), using software for Gaussian quadrature rules currently under development and a well-known recursive procedure (see, e.g., [3]) for evaluating the Bessel function J_0.

Several interesting features are worth noting: The optimal radius r_{opt} increases with n, approaching the radius of convergence $r = 3$ rather quickly when ω is small or moderately large. This is so, presumably, because of the "weak" nature of the singularity. Increasing ω, on the other hand, has the effect of reducing r_{opt}. The bounds are seen to overestimate the error by several orders of magnitude, becoming ludicrously large when ω is large and n relatively small. The latter is caused by the highly oscillatory behavior of f on the circle C_r. The use of ellipses, snuggling closely around the interval $[-1, 1]$, improves the matter considerably; see Table 6.3. While it is true that the bounds are excessively conservative, it must also be noted that the actual errors decrease rapidly with increasing n. Using the bounds to estimate not the error, but the appropriate value of n to be used, yields an overestimation of n by only a few

units (1–2 in most cases, as was determined by additional computation). In this sense, therefore, the bounds obtained are not without practical interest.

For purposes of reference, we list the true values of the integral (to 27 decimals) in Table 6.2.

TABLE 6.2
True values of the integral in Example 6.1.

ω	$(\pi/2)J_0(2\omega)$
.5	1.20196 97153 17206 49913 66624 46
1.0	.35168 68134 78300 44589 24008 93
2.0	−.62384 14625 21423 05380 16654 91
4.0	.26962 84573 43048 89859 64559 11
8.0	−.27473 08229 73313 59029 11052 65
16.0	.21689 40013 17366 77422 90002 39
32.0	.14544 00510 86862 98391 53851 72

Using elliptic contours, we have in place of (6.2),

$$|f(z)| \leqq \frac{\cosh\left(\frac{1}{2}\omega(\rho-\rho^{-1})\right)}{\sqrt{3-\frac{1}{2}(\rho+\rho^{-1})}}, \qquad z \in \mathscr{E}_\rho. \tag{6.4}$$

The empirical information mentioned in § 5.4 suggests the use of (5.17), giving

$$|R_n(f)| \leqq \frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)\cdot K_n(\varepsilon^{-1})\cdot\frac{\cosh\left(\frac{1}{2}\omega(\rho-\rho^{-1})\right)}{\sqrt{3-\varepsilon^{-1}}}, \tag{6.5}$$
$$\varepsilon = 2/(\rho+\rho^{-1}), \quad 1<\rho<3+\sqrt{8}=5.828\cdots.$$

We have also optimized this bound as a function of ρ, using the polynomial approximations in [2] to evaluate $E(\varepsilon)$. The results are similar to those in Table 6.1, for relatively small ω, with the bounds being consistently somewhat smaller. The improvement becomes more pronounced with increasing ω, and is quite dramatic for $\omega = 16$ and $\omega = 32$, as is shown in Table 6.3.

TABLE 6.3
Optimal error bound (6.5) *and actual error.*

ω	n	ρ_{opt}	bound	error
16.0	5	1.138	2.64 (1)	3.82 (−1)
	10	2.116	5.15 (−1)	3.10 (−2)
	15	3.425	2.05 (−5)	9.38 (−7)
	20	4.589	1.91 (−11)	5.22 (−13)
	25	5.367	1.88 (−18)	1.90 (−20)
	30	5.625	7.11 (−26)	3.64 (−27)
32.0	5	1.046	7.65 (1)	5.21 (−1)
	10	1.068	5.28 (1)	1.63 (−1)
	20	2.063	8.09 (−2)	2.14 (−3)
	30	3.442	1.44 (−10)	3.05 (−12)
	40	4.678	9.87 (−23)	1.21 (−24)

Example 6.2.

$$I(\omega)=\int_{-1}^{1}\frac{e^{-t}}{t^2+\omega^2}\,dt, \qquad \omega>0.$$

The integral could be expressed in terms of the complex exponential integral $E_1(z)$ as

$$I(\omega)=\frac{1}{\omega}\{\mathrm{Im}\,[e^{i\omega}E_1(1+i\omega)]-\mathrm{Im}\,[e^{i\omega}E_1(-1+i\omega)]\}$$

(cf. [8, Eq. 5.1.43]). However, it is much simpler to evaluate it by the modified Gauss–Legendre quadrature rule (3.8) (where $g(t)=e^{-t}$).

We illustrate the use of ordinary Gaussian quadrature (i.e., without separating out the poles $\pm i\omega$), and compare error bounds based on circular and elliptic contours.

Circular contours C_r can be used only if $\omega>1$ and require $1<r<\omega$. If we take $d\lambda(t)=dt$, hence

$$f(z)=\frac{e^{-z}}{z^2+\omega^2},$$

we find

$$|f(z)|=\frac{e^{-r\cos\vartheta}}{\{(r^2\cos 2\vartheta+\omega^2)^2+r^4\sin^2 2\vartheta\}^{1/2}}, \qquad z=re^{i\vartheta}\in C_r.$$

An elementary calculation shows that the denominator attains its minimum at $\vartheta=\pi/2$, so that

$$|f(z)|\leqq\frac{e^{r}}{\omega^2-r^2}, \qquad z\in C_r, \quad 1<r<\omega, \quad d\lambda(t)=dt. \tag{6.6}$$

We will also consider $d\lambda(t)=e^{-t}\,dt$ on $[-1, 1]$, a measure for which part (b) of Theorem 2.1, hence the second statement in (3.1), is applicable. In this case

$$f(z)=\frac{1}{z^2+\omega^2},$$

and (6.6) is to be replaced by

$$|f(z)|\leqq\frac{1}{\omega^2-r^2}, \qquad z\in C_r, \quad 1<r<\omega, \quad d\lambda(t)=e^{-t}\,dt. \tag{6.7}$$

If ω and r are large, one expects the error bound based on (1.6) and (3.1) to be more realistic in the case $d\lambda(t)=e^{-t}\,dt$ than in the case $d\lambda(t)=dt$, on account of the absence of the exponential e^{r} in the bound of (6.7). Some selected numerical examples of error bounds that result from (1.6), (3.1) and (6.6), (6.7), after optimization in r, are shown in Table 6.4, together with the true errors. The true values of the integral were computed by the modified Gauss–Legendre formula (3.8), which converges quite rapidly, even for very small values of ω. We quote as typical the error bounds 1.59(−3), 5.45(−11), 3.11(−26) for $n=2$, 5 and 10, respectively, with associated optimal radii 6.066, 12.038, 22.022, which hold when $\omega=.1$. Some reference values for the integral $I(\omega)$ are given in Table 6.5.

Before turning to error bounds based on elliptic contours, we digress briefly to explain how the Gauss formulae with measure $d\lambda(t)=e^{-t}\,dt$ on $[-1, 1]$ were obtained.

TABLE 6.4
Optimal error bounds for Example 6.2, based on circular contours, and actual errors.

ω	n	$d\lambda(t)=dt$ r_{opt}	bound	$d\lambda(t)=e^{-t}dt$ r_{opt}	bound	error
1.6	5	1.414	3.20 (−3)	1.498	1.06 (−3)	1.19 (−7)
	10	1.540	1.86 (−7)	1.544	5.76 (−8)	4.57 (−13)
	15	1.559	7.99 (−12)	1.561	2.41 (−12)	1.73 (−18)
	20	1.569	3.04 (−16)	1.570	9.06 (−17)	6.54 (−24)
3.2	5	2.858	9.63 (−7)	2.941	6.32 (−8)	1.97 (−9)
	10	3.037	2.43 (−14)	3.060	1.37 (−15)	1.37 (−17)
	15	3.094	4.26 (−22)	3.104	2.26 (−23)	9.47 (−26)
6.4	5	5.379	2.87 (−9)	5.854	1.10 (−11)	4.45 (−12)
	10	5.995	7.54 (−20)	6.107	1.92 (−22)	4.70 (−24)

TABLE 6.5
True values of the integral in Example 6.2.

ω	$I(\omega)$
.1	30.30306 13396 82348 89801 1277
.2	14.48521 60752 92332 62573 9000
.4	6.49657 69543 56769 22643 33955
.8	2.53625 92876 02957 26987 44666
1.6	.80972 41454 64440 32089 68500 1
3.2	.22163 00516 42300 12649 17735 9
6.4	.05686 69117 77072 55597 11571 19

We found it expedient to employ the modified Chebyshev algorithm [6, § 2.4] to generate the recursion coefficients for the required orthogonal polynomials from "modified moments". For the latter we chose Legendre moments,

$$\int_{-1}^{1} P_n(t)\, e^{-t}\, dt = \sqrt{2\pi}\, i^{n-1/2} J_{n+1/2}(i), \qquad n = 0, 1, 2, \cdots \tag{6.8}$$

(cf. [9, Eq. 7.321]), where P_n is the Legendre polynomial. (Actually, they have to be normalized to correspond to the monic Legendre polynomials, which requires division by $k_n = (2n)!/(2^n n!^2)$.) Being expressible in terms of Bessel functions, these moments can be readily computed as minimal solution of the recurrence relation

$$y_{n+1} - (2n+1)y_n - y_{n-1} = 0, \qquad n = 1, 2, 3, \cdots, \tag{6.9}$$

especially since the initial value is simply

$$y_0 = e - e^{-1}. \tag{6.10}$$

Once the recursion coefficients for the orthogonal polynomials $\pi_n(\cdot\,; e^{-t}dt)$ are found, the corresponding Gauss formulae can be obtained from the associated Jacobi matrix by well-known procedures (cf., e.g., [4, § 5.1]).

Returning now to elliptic contours $\mathscr{E}_\rho$, where ρ is to be constrained by $1 < \rho < \omega + \sqrt{\omega^2+1}$, we have in place of (6.6),

$$|f(z)| \leqq \frac{\exp\left(-\frac{1}{2}(\rho+\rho^{-1})\cos\vartheta\right)}{\left\{\left[\frac{1}{4}(\rho^2+\rho^{-2})\cos 2\vartheta + \omega^2 + \frac{1}{2}\right]^2 + \frac{1}{16}(\rho^2-\rho^{-2})^2 \sin^2 2\vartheta\right\}^{1/2}}, \tag{6.11}$$

$$z = \tfrac{1}{2}(\rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}) \in \mathscr{E}_\rho, \qquad d\lambda(t) = dt.$$

The derivative with respect to ϑ of the radicand in the denominator of (6.11) computes to

$$-\sin 2\vartheta\{\cos 2\vartheta + (\rho^2+\rho^{-2})(\omega^2+\tfrac{1}{2})\},$$

and hence can only vanish at $\vartheta = 0$ and $\vartheta = \pi/2$ (modulo π). The value of the radicand at $\vartheta = \pi/2$ is clearly the smaller of the two, so that

$$(6.12)\qquad |f(z)| \leqq \frac{\exp\left(\frac{1}{2}(\rho+\rho^{-1})\right)}{\omega^2+\frac{1}{2}-\frac{1}{4}(\rho^2+\rho^{-2})}, \qquad z \in \mathscr{E}_\rho, \quad 1<\rho<\omega+\sqrt{\omega^2+1}, \quad d\lambda(t)=dt.$$

(The denominator in (6.12) is positive under the constraint imposed on ρ and ω.) A similar bound, without the exponential in the numerator, holds in the case $d\lambda(t) = e^{-t}\,dt$. Neither in the case $d\lambda(t) = dt$, nor in the case $d\lambda(t) = e^{-t}\,dt$ do we have any theoretical basis upon which to evaluate $\max_{z\in\mathscr{E}_\rho}|K_n(z)|$. Nevertheless, empirical work alluded to in § 5.3 suggests the use of the approximation $\max_{z\in\mathscr{E}_\rho}|K_n(z)| \approx |K_n((i/2)(\rho-\rho^{-1}))|$ in the case $d\lambda(t) = dt$. When $d\lambda(t) = e^{-t}\,dt$ on $[-1, 1]$, it was found

TABLE 6.6

Optimal error bounds for Example 6.2, based on elliptic contours, and actual errors.

		$d\lambda(t) = dt$		$d\lambda(t) = e^{-t}\,dt$		
ω	n	ρ_{opt}	bound	ρ_{opt}	bound	error
.1	5	1.066	1.81 (3)	1.052	6.23 (2)	3.11 (1)
	10	1.056	3.77 (2)	1.065	3.45 (2)	6.83 (0)
	15	1.078	2.74 (2)	1.074	1.83 (2)	2.96 (0)
	20	1.081	1.11 (2)	1.081	9.00 (1)	1.02 (0)
	40	1.092	3.98 (0)	1.092	3.39 (0)	1.94 (−2)
	80	1.098	2.61 (−3)	1.098	2.30 (−3)	6.54 (−6)
.2	5	1.148	1.52 (2)	1.136	7.87 (1)	3.86 (0)
	10	1.167	2.70 (1)	1.169	2.04 (1)	4.65 (−1)
	15	1.184	5.53 (0)	1.184	4.20 (0)	6.50 (−2)
	20	1.192	9.82 (−1)	1.192	7.68 (−1)	8.90 (−3)
	40	1.205	6.71 (−4)	1.205	5.38(−4)	3.15 (−6)
	80	1.212	1.65 (−10)	1.212	1.34 (−10)	3.94 (−13)
.4	5	1.359	7.27 (0)	1.360	4.45 (0)	1.98 (−1)
	10	1.410	2.66 (−1)	1.412	1.76 (−1)	3.97 (−3)
	15	1.431	7.93 (−3)	1.432	5.27 (−3)	8.07 (−5)
	20	1.442	2.12 (−4)	1.443	1.41 (−4)	1.63 (−6)
	40	1.459	6.99 (−11)	1.459	4.68 (−11)	2.75 (−13)
	80	1.468	3.90 (−24)	1.468	2.61 (−24)	3.51 (−26)
.8	5	1.892	1.02 (−1)	1.909	4.85 (−2)	1.68 (−3)
	10	1.981	1.32 (−4)	1.987	6.16 (−5)	1.12 (−6)
	15	2.013	1.30 (−7)	2.016	5.99 (−8)	7.41 (−10)
	20	2.030	1.14 (−10)	2.031	5.22 (−11)	4.89 (−13)
	40	2.055	4.26 (−23)	2.055	1.93 (−23)	9.46 (−26)
1.6	5	3.142	3.22 (−4)	3.191	7.62 (−5)	1.19 (−7)
	10	3.313	2.53 (−9)	3.327	5.54 (−10)	4.57 (−13)
	15	3.370	1.45 (−14)	3.377	3.09 (−15)	1.73 (−18)
	20	3.400	7.33 (−20)	3.403	1.54 (−20)	6.54 (−24)
3.2	5	5.796	5.96 (−7)	5.990	3.38 (−8)	1.97 (−9)
	10	6.198	9.34 (−15)	6.250	4.49 (−16)	1.37 (−17)
	15	6.322	1.00 (−22)	6.346	4.57 (−24)	9.47 (−26)
6.4	5	10.773	2.62 (−9)	11.764	9.38 (−12)	4.45 (−12)
	10	12.047	6.16 (−20)	12.281	1.46 (−22)	4.70 (−24)

by computation that the maximum is attained close to, or on the negative real axis, thus suggesting the approximation $\max_{z\in\mathcal{E}_\rho}|K_n(z)|\approx|K_n(-\frac{1}{2}(\rho+\rho^{-1}))|$ in the case $d\lambda(t)=e^{-t}dt$. With these approximations replacing $K_n(\varepsilon^{-1})$ in (5.17), the error estimate (5.17), when optimized as a function of ρ, yields the bounds shown in Table 6.6. It can be seen that the bounds in the case $d\lambda(t)=e^{-t}dt$ are consistently better than those for $d\lambda(t)=dt$, appreciably so, if ω is large.

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Gaussian Quadrature Involving Einstein and Fermi Functions With an Application to Summation of Series*

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Abstract. Polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\lambda)$, $k = 0,1,2,\ldots$, are constructed which are orthogonal with respect to the weight distributions $d\lambda(t) = (t/(e^t - 1))^r\,dt$ and $d\lambda(t) = (1/(e^t + 1))^r\,dt$, $r = 1,2$, on $(0,\infty)$. Moment-related methods being inadequate, a discretized Stieltjes procedure is used to generate the coefficients α_k, β_k in the recursion formula $\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t)$, $k = 0,1,2,\ldots$, $\pi_0(t) = 1$, $\pi_{-1}(t) = 0$. The discretization is effected by the Gauss-Laguerre and a composite Fejér quadrature rule, respectively. Numerical values of α_k, β_k, as well as associated error constants, are provided for $0 \leqslant k \leqslant 39$. These allow the construction of Gaussian quadrature formulae, including error terms, with up to 40 points. Examples of n-point formulae, $n = 5(5)40$, are provided in the supplements section at the end of this issue. Such quadrature formulae may prove useful in solid state physics calculations and can also be applied to sum slowly convergent series.

1. Introduction. We are interested in Gaussian quadrature on $[0,\infty]$ relative to the weight functions $\varepsilon_r(t) = (t/(e^t - 1))^r$ and $\varphi_r(t) = (1/(e^t + 1))^r$. These functions arise, for example, in solid state physics and are referred to, when $r = 1$, as *Einstein* and *Fermi functions*, respectively. Integrals with respect to the measure $d\lambda(t) = \varepsilon_r(t)\,dt$, $r = 1$ and 2, are widely used in phonon statistics and lattice specific heats [7, §10], [1, §2.4], and occur also in the study of radiative recombination processes [9, §9.2]. Specifically, the average energy of a quantum harmonic oscillator of frequency ω at temperature T (representing thermal vibrations of crystal lattice atoms) is given by

$$\bar{U} = \frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1}, \tag{1.1}$$

where $\hbar = h/2\pi$ (h is the Planck constant) and k is the Boltzmann constant. Therefore, $\bar{U} = kT\varepsilon_1(\hbar\omega/kT)$, where ε_1 is Einstein's function. Letting $g(\omega)$ denote the phonon density of states function, and integrating (1.1) over the entire frequency range, the total energy of thermal vibration of the crystal lattice becomes

$$U = \int_0^\infty \frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1} g(\omega)\,d\omega = \frac{k^2T^2}{\hbar}\int_0^\infty \varepsilon_1(t)\,g((kT/\hbar)t)\,dt. \tag{1.2}$$

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Furthermore, differentiating U with respect to temperature T, yields the crystal lattice heat capacity at constant volume,

$$C_v = \frac{\partial U}{\partial T} = \int_0^\infty \frac{(\hbar\omega/kT)^2}{(\exp(\hbar\omega/kT) - 1)^2} kg(\omega)\exp(\hbar\omega/kT)\, d\omega,$$

that is,

$$C_v = \frac{k^2 T}{\hbar}\int_0^\infty \varepsilon_2(t) f(t)\, dt \quad \text{where } f(t) = e^t g((kT/\hbar)t). \tag{1.3}$$

Similarly, integrals of the type $\int_0^\infty \varphi_1(t)f(t)\,dt$ (in fact, more generally $\int_0^\infty \varphi_1(t - t_0)f(t)\,dt$, for some parameter t_0) are encountered in the dynamics of electrons in metals, where they express the specific heat of the electron gas [8, §9.17]. For an application to heavy doped semiconductors, see also [10].

It will be shown in Section 4 that integration with respect to $d\lambda(t) = \varepsilon_1(t)\,dt$ and $d\lambda(t) = \varphi_1(t)\,dt$ is also useful in summing slowly convergent series whose general term is expressible in terms of a Laplace transform or its derivative.

Gaussian quadrature relative to the weight functions ε_r and φ_r will be particularly attractive in the case $r = 1$, since both weight functions then have poles with nonzero residues, the former at $2n\pi i$, $n = \pm 1, \pm 2, \ldots$, the latter at $(2n + 1)\pi i$, $n = 0, \pm 1, \pm 2, \ldots$. Classical integration, even based on Gauss-Laguerre quadrature, will often be too slow, but will be used to generate the desired quadrature rules, at least in the case of the weight function ε_r; see (2.3) below.

The problem, basically, amounts to generating the coefficients α_k, β_k in the recursion formula

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \qquad k = 0, 1, 2, \ldots,$$
$$\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1$$

for the (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\lambda)$, $k = 0, 1, 2, \ldots$. (β_0 is arbitrary, but will be defined as $\beta_0 = \int_0^\infty d\lambda(t)$.) Once the first n of these coefficients, α_k, β_k, $k = 0, 1, \ldots, n - 1$, and β_n, are known, the m-point Gaussian quadrature formula

$$\int_0^\infty f(t)\, d\lambda(t) = \sum_{\mu=1}^{m} \lambda_\mu f(\tau_\mu) + R_m(f),$$
$$R_m(f) = \gamma_m f^{(2m)}(\tau), \qquad 0 < \tau < \infty, \tag{1.4}$$

including the error constant γ_m, can easily be obtained for any m with $1 \leqslant m \leqslant n$. The nodes $\tau_\mu = \tau_\mu^{(m)}$, indeed, are the eigenvalues of the (symmetric tridiagonal) Jacobi matrix

$$J_m = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \ddots & \ddots & \ddots \sqrt{\beta_{m-1}} \\ 0 & & \sqrt{\beta_{m-1}} & \alpha_{m-1} \end{bmatrix},$$

while the weights $\lambda_\mu = \lambda_\mu^{(m)}$ are given by $\lambda_\mu = \beta_0 v_{\mu,1}^2$ in terms of the first components $v_{\mu,1}$ of the corresponding normalized eigenvectors; see, e.g., [3, §5.1]. Moreover,

$$\gamma_m = \frac{\beta_0 \beta_1 \cdots \beta_m}{(2m)!}, \qquad m = 1, 2, \ldots, n.$$

A number of methods are available, and have been analyzed in [4], for computing the recursion coefficients α_k, β_k. They are either based on the moments (or modified moments) of the weight distribution $d\lambda(t)$, or else use a suitable discretization of the inner product

$$(u, v) = \int_0^\infty u(t) v(t)\, d\lambda(t), \qquad u, v \in \mathbf{P},$$

where u, v are polynomials. In the next section we discuss the relative merits of these methods for constructing the particular orthogonal polynomials at hand.

2. Generation of the Recursion Coefficients. We consider first the weight function ε_r. The classical approach (for example, the Chebyshev algorithm; see [4, §2.3]) departs from the moments of the weight function, which, in the case at hand, can be expressed in terms of the Riemann zeta function $\zeta(z)$,

$$\mu_k = \int_0^\infty t^k \varepsilon_r(t)\, dt$$

$$= \begin{cases} (k+1)!\zeta(k+2), & r = 1, \\ (k+2)![\zeta(k+2) - \zeta(k+3)], & r = 2, \end{cases} \qquad k = 0, 1, 2, \ldots. \tag{2.1}$$

It is well-known, however, that the moments μ_k define the recursion coefficients α_k, β_k and the associated Gaussian quadrature formulae poorly in a numerical sense. The map G_n from the first $2n$ moments μ_k, $k = 0, 1, 2, \ldots, 2n-1$, to the weights $\lambda_\nu^{(n)}$ and nodes $\tau_\nu^{(n)}$ of the n-point Gaussian formula, in fact becomes progressively more ill-conditioned as n increases. This is illustrated in Table 2.1, where in the second and third column the condition number of this map (in the sense of [4, Eq. (3.11)f]) is shown as a function of n for $r = 1$ and $r = 2$, respectively. (Numbers in parentheses indicate decimal exponents.)

TABLE 2.1

The numerical condition of various maps relating to the construction of orthogonal polynomials $\pi_k(\cdot\,; \varepsilon_r\, dt)$, $r = 1, 2$.

n	cond G_n $r=1$	cond G_n $r=2$	cond $\tilde{G}_n$ $r=1$	n	cond H_n $r=1$	cond H_n $r=2$
3	1.686(2)	7.620(1)	1.415(1)	5	7.665(0)	7.980(0)
6	1.288(5)	7.171(4)	2.934(3)	10	2.163(1)	2.161(1)
9	9.092(7)	5.820(7)	9.795(5)	15	3.299(1)	3.356(1)
12	6.334(10)	4.471(10)	4.039(8)	20	4.256(1)	4.244(1)
15	4.409(13)	3.344(13)	1.878(11)	30	6.761(1)	6.783(1)
18	3.076(16)	2.465(16)	9.441(13)	40	8.531(1)	8.556(1)

Sometimes the condition can be improved by employing modified moments $\nu_k = \int_0^\infty p_k(t)\varepsilon_r(t)\,dt$, where $\{p_k\}$ is a system of (monic) polynomials suitably chosen. If the support interval is infinite, however, as in the case at hand, the improvement is often not sufficient to make this a viable alternative. The fourth column of Table 2.1 indeed confirms this. Here, $r = 1$, and $\varepsilon_1(t) \sim te^{-t}$ as $t \to \infty$, so that the monic Laguerre polynomials with parameter $\alpha = 1$,

$$p_k(t) = (-1)^k k! L_k^{(1)}(t), \qquad k = 0,1,2,\ldots,$$

appear to be the most natural choices for the polynomials p_k. The corresponding modified moments can be shown to be expressible in terms of the (forward) differences, with unit step, of the Riemann zeta function at $z = 2$,

$$\nu_k = \int_0^\infty p_k(t)\varepsilon_1(t)\,dt = (k+1)!\Delta^k\zeta(z)\big|_{z=2}, \qquad k = 0,1,2,\ldots. \tag{2.2}$$

The map $\tilde{G}_n$ in Table 2.1 is the map from the first $2n$ normalized modified moments $\tilde{\nu}_k = \nu_k[\int_0^\infty p_k^2(t)te^{-t}\,dt]^{-1/2}$, $k = 0,1,\ldots,2n-1$, to the weights $\lambda_\nu^{(n)}$ and nodes $\tau_\nu^{(n)}$ of the n-point Gaussian quadrature formula (1.4) (with $d\lambda(t) = \varepsilon_1(t)\,dt$). The entries in the fourth column exhibit the estimate derived in [4, Eq. (3.15)] for the condition of $\tilde{G}_n$. It can be seen that cond $\tilde{G}_n$, while somewhat smaller than cond G_n, is still growing unacceptably fast.

The modified Chebyshev algorithm (cf. [4, §2.4]), run in single precision on the CDC 6500 (machine precision: ca. 15 significant decimal digits), with the modified moments (2.2) computed in double precision, indeed loses accuracy very much in accordance with the growth of cond $\tilde{G}_n$; the number of correct decimal digits observed in α_k, β_k, $k = 3(3)18$, is 14, 11, 10, 6, 2, 0, respectively, not a single digit being correct for $k = 18$, not even the sign of β_{18}.

An additional complication arises in connection with the high-order differences in (2.2), which are subject to considerable cancellation errors. For $k = 40$, for example, one must expect a loss of approx. 12 decimal digits.

In contrast, methods based on discretization appear to be incomparably more effective, particularly if one uses the natural discretization based on the Gauss-Laguerre quadrature rule,

$$\begin{aligned}\int_0^\infty p(t)\left(\frac{t}{e^t-1}\right)^r dt &= \frac{1}{r}\int_0^\infty p(t/r)\left(\frac{t/r}{1-e^{-t/r}}\right)^r e^{-t}\,dt \\ &\approx \frac{1}{r}\sum_{k=1}^N \lambda_k^L p\left(\tau_k^L/r\right)\left(\frac{\tau_k^L/r}{1-e^{-\tau_k^L/r}}\right)^r, \qquad p \in \mathbf{P}.\end{aligned} \tag{2.3}$$

Here, τ_k^L are the zeros of the Laguerre polynomial of degree N, and λ_k^L the associated Christoffel numbers. The discretized Stieltjes procedure (cf. [4, §2.2]), based on (2.3), then converges fairly rapidly as $N \to \infty$. For example, to obtain the first 12 recursion coefficients ($n = 12$) to 12 correct decimals [25 correct decimals] requires $N = 49$ [$N = 127$], when $r = 1$, and $N = 41$ [$N = 85$], when $r = 2$. The first 40 coefficients ($n = 40$) can be obtained accurately to 25 decimal digits with $N = 281$ for $r = 1$ and $N = 201$ for $r = 2$. Also the numerical stability of the procedure,

which is roughly determined (cf. [4, §3.4]) by the condition of the map

$$H_n\colon (\lambda_1,\ldots,\lambda_n,\tau_1,\ldots,\tau_n) \to (\alpha_0,\ldots,\alpha_{n-1},\beta_0,\ldots,\beta_{n-1}),$$

is rather good. This can be seen from the last two columns of Table 2.1, which display the condition number of H_n in the sense of [4, Eq. (3.8)f].

One might expect that a discretization analogous to the one in (2.3) works well also for the weight function φ_r. This, however, is not the case, at least not if $r = 1$. Convergence turns out to be slow on account of the poles at $\pm i\pi$, which are twice as close to the real axis as in the case of ε_1. For example, to obtain 20 correct decimal digits (in the case $r = 1$ and for $n = 40$), requires $N = 361$. We used instead a discretization procedure based on the composite Fejér quadrature rule, decomposing the interval of integration into four subintervals, $[0,\infty] = [0,10] \cup [10,100] \cup [100,500] \cup [500,\infty]$. Using $N = 201$ for $r = 1$, and $N = 281$ for $r = 2$, on each subinterval, then yields the first $n = 40$ recursion coefficients accurately to 25 decimal digits. The same procedure (with $n = 50$ and $N = 251$) was also used to check the computation based on (2.3) for ε_r, $r = 1,2$. The maximum discrepancy observed was 1 unit in the 25th digit.

3. Numerical Results. Using the procedures outlined in the last two paragraphs of Section 2, we obtained the results shown in Tables 1–4 of the Appendix. The coefficients $\beta_0 = \zeta(2) = \pi^2/6$ in Table 1 and $\beta_0 = 2[\zeta(2) - \zeta(3)]$ in Table 2 (cf. Eq. (2.1)), agree to all 25 decimal digits with the values obtained from the 41S-table of the Riemann zeta function in [6]. Similarly, one checks the values $\beta_0 = \ln 2$ in Table 3 and $\beta_0 = \ln 2 - \frac{1}{2}$ in Table 4. Corresponding n-point Gaussian quadrature formulae, $n = 5(5)40$, for $r = 1$ and $r = 2$, can be found to 25 significant decimal digits in Tables 5–8 in the supplements section at the end of this issue.

We illustrate these formulae by computing the integrals

$$I_1 = \int_0^\infty e^{-t}\frac{t}{e^t - 1}\,dt = \zeta(2) - 1,$$

$$I_2 = \int_0^\infty e^{-t}\left(\frac{t}{e^t - 1}\right)^2 dt = 2[\zeta(2,2) - 2\zeta(3,2)],$$

$$I_3 = \int_0^\infty e^{-t}\frac{dt}{e^t + 1} = 1 - \ln 2,$$

$$I_4 = \int_0^\infty e^{-t}\frac{dt}{(e^t + 1)^2} = \frac{3}{2} - 2\ln 2,$$

where $\zeta(z, a)$ is the generalized zeta function. Table 3.1 shows the n-point approximations $I_i(n)$ to I_i, $i = 1,2$, together with the relative errors $r_i(n)$, for $n = 5(5)25$. Similarly, $I_i(n)$ and $r_i(n)$, $i = 3,4$, are shown in Table 3.2. In each entry the first digit in error is underlined. The error term in (1.4) yields the bounds γ_n/I_i, $i = 1,2,3,4$, for the relative error, which can be computed with the help of Tables 1–4 of the Appendix and the limit values in Tables 3.1, 3.2; they are summarized in Table 3.3 for $n = 5(5)25$. The bounds for I_2, I_4 are seen to be considerably sharper than those for I_1, I_3.

TABLE 3.1

Gaussian approximations of the integrals I_1 and I_2 and relative errors.

n	$I_1(n)$	$r_1(n)$	$I_2(n)$	$r_2(n)$
5	.644742	3.0(−4)	.4816385	4.1(−6)
10	.6449340594	1.1(−8)	.48164052105737	1.5(−12)
15	.644934066848017	3.2(−13)	.481640521058075731184	3.3(−19)
20	.64493406684822643131	8.0(−18)	.48164052105807573134587776	1.1(−25)
25	.6449340668482264364772	1.8(−22)		

TABLE 3.2

Gaussian approximations of the integrals I_3 and I_4 and relative errors.

n	$I_3(n)$	$r_3(n)$	$I_4(n)$	$r_4(n)$
5	.3068171	1.2(−4)	.113705528	9.7(−7)
10	.30685281854	2.9(−9)	.113705638880091	1.5(−13)
15	.3068528194400358	6.2(−14)	.11370563888010938116323	2.0(−20)
20	.306852819440054690208	1.2(−18)	.11370563888010938116553 58	6.1(−26)
25	.3068528194400546905827607	2.3(−23)		

TABLE 3.3

Relative error bounds for $I_i(n)$, $i = 1, 2, 3, 4$.

n	$\gamma_n/I_1(n)$	$\gamma_n/I_2(n)$	$\gamma_n/I_3(n)$	$\gamma_n/I_4(n)$
5	4.8(−2)	8.3(−5)	1.2(−2)	1.3(−5)
10	1.1(−4)	3.0(−10)	1.6(−5)	1.9(−11)
15	1.9(−7)	6.7(−16)	2.0(−8)	2.3(−17)
20	2.7(−10)	1.2(−21)	2.3(−11)	2.5(−23)
25	3.6(−13)	1.8(−27)	2.5(−14)	2.7(−29)

4. Summation of Series. As an application of Gaussian integration with weight functions ε_1 and φ_1, we consider the summation of series whose general term is expressible in terms of the derivative of a Laplace transform, or in terms of the Laplace transform itself. Suppose, for example, that $a_k = -F'(k)$, where

$$F(p) = \int_0^\infty e^{-pt} f(t)\, dt, \qquad \operatorname{Re} p \geqslant 1. \tag{4.1}$$

Then

$$\sum_{k=1}^{\infty} a_k = \sum_{k=1}^{\infty} \int_0^\infty te^{-kt} f(t)\, dt = \int_0^\infty \frac{t}{e^t - 1} f(t)\, dt,$$

that is,

$$-\sum_{k=1}^{\infty} F'(k) = \int_0^\infty f(t)\varepsilon_1(t)\, dt. \tag{4.2a}$$

Similarly, for "alternating" series, one obtains

$$-\sum_{k=1}^{\infty} (-1)^{k-1} F'(k) = \int_0^\infty f(t) t\varphi_1(t)\, dt \tag{4.2b}$$

and

$$\sum_{k=1}^{\infty} (-1)^{k-1} F(k) = \int_0^{\infty} f(t)\varphi_1(t)\, dt. \tag{4.2c}$$

If the series on the left are slowly convergent and the respective function f on the right is smooth, then low-order Gaussian quadrature applied to the integrals on the right provides one (among many other) possible summation procedure. If f exhibits singularities, then the weight function may have to be modified if the effectiveness of the procedure is to be preserved (cf. Example 4.4). In the following examples, "(a)", "(b)", "(c)" refers to a, b, c of Eq. (4.2).

Example 4.1. (a) $\Sigma_{k=1}^{\infty}(k+1)^{-2} = \pi^2/6 - 1$. Here, $-F'(p) = (p+1)^{-2}$, and $F(p) = (p+1)^{-1}$, the integration constant being zero on account of $F(p) \to 0$ as $p \to \infty$. Thus, $f(t) = e^{-t}$, and the second column of Table 3.1 shows the rapid convergence of Gaussian quadrature in this case. For example, 15-point quadrature already yields 12 correct decimal digits. In contrast, 10 000 terms of the series would give only 3-digit accuracy.

(b) $\Sigma_{k=1}^{\infty}(-1)^{k-1}(k+1)^{-2} = 1 - \pi^2/12$. Applying Gaussian quadrature to the integral in (4.2b) yields the results shown in Table 4.1. To guarantee, on the basis of Leibniz' convergence criterion, the same accuracy as the one achieved for $n = 15$ would require the summation of approximately 690 000 terms.

(c) $\Sigma_{k=1}^{\infty}(-1)^{k-1}(k+1)^{-1} = 1 - \ln 2$. The convergence behavior of Gaussian quadrature applied to the integral in (4.2c) is evident from the second column of Table 3.2.

TABLE 4.1

Gaussian approximations $K(n)$ of the integral

$$K = \int_0^{\infty} e^{-t}t(e^t+1)^{-1}\, dt \text{ and relative errors.}$$

n	$K(n)$	$r(n)$
5	.177753	1.2(−3)
10	.1775329780	6.5(−8)
15	.17753296657625	2.1(−12)
20	.1775329665758867915	5.5(−17)
25	.17753296657586781764027	1.3(−21)
30	.17753296657586781763792	1.4(−25)

Example 4.2. $F(p) = p^{-1}\exp(-1/p)$, $-F'(p) = (p-1)p^{-3}\exp(-1/p)$. The original function is here $f(t) = J_0(2\sqrt{t})$. This being an entire function, we expect Gaussian quadrature in (4.2) to converge rapidly. This is confirmed in Table 4.2, which shows the relative errors for the n-point formula, $n = 2(2)12$. The exact sums (to 24 significant digits), as determined by Gaussian quadrature, are, respectively,

$$\sum_{k=1}^{\infty} (k-1)k^{-3}\exp(-1/k) = .342918943844609780961838,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}(k-1)k^{-3}\exp(-1/k) = -.044155938134083605273692 8,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}k^{-1}\exp(-1/k) = .197107936397950656955672.$$

The first 10 000 terms of the series yield, respectively, 3, 7 and 4 correct decimal digits. The Bessel function J_0 was evaluated by means of the rational approximations in [5] indexed 5852, 6553 and 6953.

TABLE 4.2

Relative errors in Gaussian approximation of the integrals in (4.2, a–c), *where* $F(p) = p^{-1}\exp(-1/p)$.

n	(a)	(b)	(c)
2	4.48(–2)	8.95(–1)	1.77(–2)
4	3.80(–6)	2.39(–4)	9.65(–7)
6	3.35(–11)	3.71(–9)	6.32(–12)
8	7.01(–17)	1.13(–14)	1.05(–17)
10	6.86(–23)	1.08(–20)	1.27(–23)
12		1.93(–23)	

Example 4.3. $F(p) = (1 + p^2)^{-1/2}$, $-F'(p) = p(1 + p^2)^{-3/2}$. Here, $f(t) = J_0(t)$—again an entire function. Convergence of Gaussian quadrature in (4.2), while still satisfactory, is not quite as fast as in Example 4.2, presumably since the argument of J_0 is now essentially squared. The relative errors are shown in Table 4.3. For reference, we list the exact values of the respective sums:

$$\sum_{k=1}^{\infty} k(1 + k^2)^{-3/2} = .900524735348125924300853,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}k(1 + k^2)^{-3/2} = .234771442466894018686113,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}(1 + k^2)^{-1/2} = .440917473865185397183787.$$

The first 10 000 terms yield 3, 8 and 4 correct decimal digits, respectively.

TABLE 4.3

Relative errors in Gaussian approximation of the integrals in (4.2, a–c), *where* $F(p) = (1 + p^2)^{-1/2}$.

n	(a)	(b)	(c)
5	1.68(–3)	8.15(–3)	1.99(–4)
10	8.03(–7)	4.75(–6)	2.11(–7)
15	4.05(–10)	2.99(–9)	9.01(–12)
20	1.64(–13)	7.61(–13)	2.26(–14)
25	5.79(–17)	5.64(–16)	2.52(–19)
30	2.69(–20)	8.25(–20)	2.33(–21)
35	5.11(–24)	8.01(–23)	3.88(–25)

Example 4.4. $F(p) = 2p^{-1}(p+1)^{-1/2}$, $-F'(p) = (3p+2)p^{-2}(p+1)^{-3/2}$. Here we have an example in which the original function, $f(t) = 2\operatorname{erf}\sqrt{t}$, is no longer smooth, having a square root singularity at $t = 0$.

TABLE 4.4

Relative errors in Gaussian approximation of the integrals in (4.2, a–c), *where* $F(p) = 2p^{-1}(p+1)^{-1/2}$, *using weight functions* $t^{1/2}\varepsilon_1(t)$ *and* $t^{1/2}\varphi_1(t)$.

n	(a)	(b)	(c)
5	2.10(−5)	4.69(−5)	9.20(−6)
10	5.47(−10)	1.54(−9)	1.58(−10)
15	1.24(−14)	3.88(−14)	2.70(−15)
20	2.62(−19)	8.78(−19)	4.61(−20)
25	5.17(−24)	1.85(−23)	4.91(−25)

This severely retards convergence of Gaussian quadrature in (4.2). When $n = 40$, for example, the relative errors are still 4.29(−4), 7.19(−6) and 4.80(−4), respectively. Better results can be obtained by integrating with respect to the measures $t^{1/2}\varepsilon_1(t)\,dt$ and $t^{1/2}\varphi_1(t)\,dt$. The recursion coefficients for the corresponding orthogonal polynomials have been computed by a discretized Stieltjes procedure [4, §2.2] involving two different discretizations, one on the interval $[0, 10]$, where a Gauss-Jacobi quadrature with parameters $\alpha = 0$, $\beta = \frac{1}{2}$ (to account for the $t^{1/2}$-singularity at $t = 0$) was used, and one on the interval $[10, \infty]$, where we used Gauss-Laguerre quadrature as before. With the special Gaussian quadrature rules thus obtained, convergence of the summation process is very satisfactory; see Table 4.4. The exact values of the sums are:

$$\sum_{k=1}^{\infty} (3k+2)k^{-2}(k+1)^{-3/2} = 2.57194963231048057027 8028,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}(3k+2)k^{-2}(k+1)^{-3/2} = 1.48576152922341211086 9727,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}2k^{-1}(k+1)^{-1/2} = 1.03952653371156898297 1620.$$

The error function was evaluated by a double precison version of the incomplete gamma function routine in [2], observing that $\operatorname{erf}\sqrt{t} = g^*(\frac{1}{2}, t)$ in the notation of [2].

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Appendix A1: Recursion coefficients α_k, β_k and error constants γ_k for orthogonal polynomials $\pi_k(\cdot\,; \varepsilon_r\, dt)$, $r = 1, 2$.

TABLE 1

Recursion coefficients and error constants in the case $r = 1$

k	alpha(k)	beta(k)	gamma(k)
0	1.46152593880287699745207 3d+00	1.64493406684822643647241 5d+00	1.6449d+00
1	3.70419144432933951350226 2d+00	1.81178369064211248928965 4d+00	1.4901d+00
2	5.77099865692809179215988 2d+00	5.67628870626027778768085 6d+00	7.0487d-01
3	7.80608070072948527261140 7d+00	1.15674440865786914884453 0d+01	2.7178d-01
4	9.82866055395294278392255 1d+00	1.94738944501645174756653 1d+01	9.4512d-02
5	1.18447794112360364910901 3d+01	2.93905670892394954704987 7d+01	3.0864d-02
6	1.38570396078047165242914 6d+01	4.13146932970749604914140 2d+01	9.6602d-03
7	1.58667750919992474110350 2d+01	5.52445668086204093591887 9d+01	2.9323d-03
8	1.78747508374765567332058 9d+01	7.11790480008690859981968 0d+01	8.6965d-04
9	1.98814415970351793764488 0d+01	8.91173308654563427825961 5d+01	2.5327d-04
10	2.18871598802202487178386 7d+01	1.09058820379898012601492 5d+02	7.2688d-05
11	2.38921210166598538009194 2d+01	1.31003062393062578934732 3d+02	2.0611d-05
12	2.58964788978958002459438 7d+01	1.54949700904517282002534 0d+02	5.7857d-06
13	2.79003468474734671911419 7d+01	1.80898450690622217410000 4d+02	1.6102d-06
14	2.99038104249190019259580 2d+01	2.08849079031838126870065 2d+02	4.4482d-07
15	3.19069356092613806067493 4d+01	2.38801393094447527754953 5d+02	1.2210d-07
16	3.39097742128952054887448 6d+01	2.70755230964148621303754 6d+02	3.3325d-08
17	3.59123675702259148598959 8d+01	3.04710455116924196784213 1d+02	9.0503d-09
18	3.79147491157105707545482 5d+01	3.40666947563050247429533 4d+02	2.4469d-09
19	3.99169462262375166030906 3d+01	3.78624606168121484105390 2d+02	6.5894d-10
20	4.19189815638596184619646 5d+01	4.18583341820024215962743 2d+02	1.7681d-10
21	4.39208740715906045258995 8d+01	4.60543076215539730858729 9d+02	4.7287d-11
22	4.59226397235110282958586 1d+01	5.04503740108530105401869 3d+02	1.2609d-11
23	4.79242920977863110238750 6d+01	5.50465271907210214971632 3d+02	3.3531d-12
24	4.99258428199971300091478 4d+01	5.98427616539050604375254 0d+02	8.8944d-13
25	5.19273019101157167440789 5d+01	6.48390724523412965465671 3d+02	2.3539d-13
26	5.39286780569477520591043 1d+01	7.00354551207249600314949 4d+02	6.2163d-14
27	5.59299788373114209320288 3d+01	7.54319056130126639705665 3d+02	1.6384d-14
28	5.79312108926457599417934 9d+01	8.10284202492785112714942 1d+02	4.3103d-15
29	5.99323800724905675233741 1d+01	8.68249956709319633557093 2d+02	1.1320d-15
30	6.19334915519425398171056 0d+01	9.28216288027432189028916 9d+02	2.9682d-16
31	6.39345499284898091681009 7d+01	9.90183168204522163050825 8d+02	7.7711d-17
32	6.59355593023727572900844 0d+01	1.05415057122989259024757 1d+03	2.0317d-17
33	6.79365233436849130933913 0d+01	1.12011847308529153983354 0d+03	5.3049d-18
34	6.99374453487251859393047 7d+01	1.18808685153751335207714 4d+03	1.3834d-18
35	7.19383282875793028754561 6d+01	1.25805568595796367092245 2d+03	3.6032d-19
36	7.39391748444998262159668 3d+01	1.33002495716502287964304 3d+03	9.3747d-20
37	7.59399874523387115038691 6d+01	1.40399464728578241730416 7d+03	2.4365d-20
38	7.79407683220409365278645 2d+01	1.47996473963432069027809 1d+03	6.3263d-21
39	7.99415194680153713694991 7d+01	1.55793521860416242299349 2d+03	1.6410d-21

TABLE 2

Recursion coefficients and error constants in the case $r = 2$

k	alpha(k)	beta(k)	gamma(k)
0	8.11062384327196946205671 7d-01	8.85754327377264302145354 0d-01	8.8575d-01
1	2.08248956336093311367829 7d+00	5.72193233946137696459835 8d-01	2.5341d-01
2	3.18047273249234227604951 4d+00	1.75996219501089909295738 9d+00	3.7166d-02
3	4.23046468723256772889965 9d+00	3.45238491920311735455095 7d+00	4.2771d-03
4	5.26181418022251950724901 6d+00	5.64676938993690062369948 7d+00	4.3128d-04
5	6.28397033564142307i715338d+00	8.34435506217352358147149 6d+00	3.9986d-05
6	7.30077782673740213770257 d+00	1.15452306452023959104798 2d+01	3.4973d-06
7	8.31412489353619673288072 1d+00	1.52490492491051382696617 2d+01	2.9303d-07
8	9.32507041285987738682683 1d+00	1.94554143663828825957240 7d+01	2.3754d-08
9	1.03342645617961846458623 8d+01	2.41639787751439158430004 5d+01	1.8758d-09
10	1.13421332013309197007101 3d+01	2.93744559679276554937314 6d+01	1.4500d-10
11	1.23489691225713504962972 1d+01	3.50866118286110500889542 3d+01	1.1012d-11
12	1.33549814198743446366512 1d+01	4.13002540998990151813200 3d+01	8.2392d-13
13	1.43603240720341318464856 5d+01	4.80152234184732650543339 6d+01	6.0862d-14
14	1.53651133880888756128231 3d+01	5.52313863208469179594750 9d+01	4.4465d-15
15	1.63694391240620361225983 4d+01	6.29486299048838956600320 7d+01	3.2172d-16
16	1.73733718245461715733081 6d+01	7.11668577594125789868747 2d+01	2.3081d-17
17	1.83769678201780301442912 1d+01	7.98859868401421330837791 8d+01	1.6433d-18
18	1.93802727191250805156488 6d+01	8.91059450490226145431907 7d+01	1.1621d-19
19	2.03833239022289503509472 0d+01	9.88266693390557337946939 0d+01	8.1686d-21
20	2.13861523419118477650827 1d+01	1.09048104214932817651728 1d+02	5.7101d-22
21	2.23887839516662215500863 6d+01	1.19770200534808468381183 7d+02	3.9715d-23
22	2.33912406031241676691632 1d+01	1.30992914543529561182725 4d+02	2.7497d-24
23	2.43935409034834760288119 4d+01	1.42716207085573113291523 2d+02	1.8958d-25
24	2.53957007973782645206274 8d+01	1.54940042958884923285766 6d+02	1.3020d-26
25	2.63977340382619308238438 6d+01	1.67664390380223414041490 7d+02	8.9102d-28
26	2.73996525615114816959884 0d+01	1.80889220539524670602025 1d+02	6.0775d-29
27	2.84014667826138423917050 8d+01	1.94614507225928831222153 0d+02	4.1327d-30
28	2.94031858376067730762167 9d+01	2.08840226511943565234401 1d+02	2.8022d-31
29	3.04048177785551793413400 7d+01	2.23566356485118355732302 0d+02	1.8950d-32
30	3.14063697336839322217435 3d+01	2.38792877018812703366787 6d+02	1.2783d-33
31	3.24078480394864608643845 7d+01	2.54519769575340382749868 3d+02	8.6024d-35
32	3.34092583504319060838601 7d+01	2.70747017036089200488583 8d+02	5.7764d-36
33	3.44106057306297866726030 8d+01	2.87474603554245089309268 7d+02	3.8708d-37
34	3.54118947308601214554648 4d+01	3.04702514426559752346377 0d+02	2.5888d-38
35	3.64131294536546155943872 2d+01	3.22430735981243548214696 8d+02	1.7282d-39
36	3.74143136085610543891908 7d+01	3.40659255479578083537394 0d+02	1.1516d-40
37	3.84154505592954813577731 3d+01	3.59388061029254841786218 7d+02	7.6617d-42
38	3.94165433641538763882214 4d+01	3.78617141507778928663518 6d+02	5.0892d-43
39	4.04175948107940307908245 3d+01	3.98346486494547914140165 9d+02	3.3754d-44

Appendix A2: Recursion coefficients α_k, β_k and error constants γ_k for orthogonal polynomials $\pi_k(\cdot\,; \varphi_r\, dt)$, $r = 1, 2$.

TABLE 3

Recursion coefficients and error constants in the case $r = 1$

k	alpha(k)	beta(k)	gamma(k)
0	1.18656911041562545282172 3d+00	6.93147180559945309417232 1d-01	6.9315d-01
1	3.09635421539677738586809 7d+00	1.19335604578950865917894 6d+00	4.1359d-01
2	5.07222727953560374852628 0d+00	4.19180642454904245159008 3d+00	1.4447d-01
3	7.06012262790758023777336 2d+00	9.21536738543464197654493 2d+00	4.4379d-02
4	9.05256194010737706335959 6d+00	1.62391324482831839978390 6d+01	1.2869d-02
5	1.10472751063886195317398 0d+01	2.52614732168519574773802 4d+01	3.6122d-03
6	1.30433139659181852416813 8d+01	3.62823510512377164623103 8d+01	9.9286d-04
7	1.50402043436732842362534 3d+01	4.93019377192574730481120 8d+01	2.6896d-04
8	1.70376796404636421493986 8d+01	6.43204130607568426140696 4d+01	7.2081d-05
9	1.90355770435038157236964 1d+01	8.13379310689911466188374 9d+01	1.9160d-05
10	2.10337907995074268367692 9d+01	1.00354618123271473784436 3d+02	5.0599d-06
11	2.30322488535853145083692 2d+01	1.21370577337493043917911 3d+02	1.3293d-06
12	2.50309001997975271673052 4d+01	1.44385893306431224734119 9d+02	3.4770d-07
13	2.70297075867974358796298 3d+01	1.69400636069531256134342 2d+02	9.0616d-08
14	2.90286430913710667036819 2d+01	1.96414864201032565199563 6d+02	2.3543d-08
15	3.10276853164622371451901 8d+01	2.25428627173671221287900 7d+02	6.1002d-09
16	3.30268175533095659865082 2d+01	2.56441967164364867756573 3d+02	1.5770d-09
17	3.50260265387935546542077 2d+01	2.89454920441689966823885 1d+02	4.0683d-10
18	3.70253015928848239162740 9d+01	3.24467518441407602600283 2d+02	1.0476d-10
19	3.90246340060485777904308 8d+01	3.61479788608423642788150 9d+02	2.6935d-11
20	4.10240165952977073498458 3d+01	4.00491755062552531702251 1d+02	6.9148d-12
21	4.30234433766462720479551 2d+01	4.41503439130141974003133 2d+02	1.7729d-12
22	4.50229093195404220044823 8d+01	4.84514859772580840659335 9d+02	4.5401d-13
23	4.70224101600774382455944 5d+01	5.29526033934762937770853 4d+02	1.1614d-13
24	4.90219422570760149958097 0d+01	5.76536976830824897703862 1d+02	2.9681d-14
25	5.10215024798458544374120 0d+01	6.25547702180280594965603 0d+02	7.5782d-15
26	5.30210881197241926033936 6d+01	6.76558222404588840837687 4d+02	1.9333d-15
27	5.50206968196521413642196 0d+01	7.29568548791901332201781 5d+02	4.9283d-16
28	5.70203265175990584730205 3d+01	7.84578691636023064468649 7d+02	1.2554d-16
29	5.90199754007281462402868 5d+01	8.41588660354321659053084 6d+02	3.1958d-17
30	6.10196418679738281521690 1d+01	9.00598463588334318616046 4d+02	8.1303d-18
31	6.30193244992654996391106 6d+01	9.61608109290061820064451 6d+02	2.0672d-18
32	6.50190220300463598410363 0d+01	1.02461760479635053031723 8d+03	5.2532d-19
33	6.70187333300433976588944 3d+01	1.08962695689330390465559 1d+03	1.3343d-19
34	6.90184573854750730811182 4d+01	1.15663617187230342524069 7d+03	3.3873d-20
35	7.10181932840576901978026 7d+01	1.22564525557893255833299 0d+03	8.5956d-21
36	7.30179402023046923829291 6d+01	1.29665421345586893233232 7d+03	2.1803d-21
37	7.50176973947157137910848 1d+01	1.36966305058062666546426 6d+03	5.5280d-22
38	7.70174641845318573090801 2d+01	1.44467177169888280976332 4d+03	1.4011d-22
39	7.90172399557959358550040 5d+01	1.52168038125400174038206 3d+03	3.5498d-23

TABLE 4

Recursion coefficients and error constants in the case $r = 2$

k	alpha(k)	beta(k)	gamma(k)
0	6.69540463853843823238722 7d-01	1.93147180559945309417232 1d-01	1.9315d-01
1	1.66468613300982968001107 5d+00	3.70527871085168485680662 2d-01	3.5783d-02
2	2.61943184101575847660419 2d+00	1.15490785365260136536582 4d+00	3.4439d-03
3	3.59386536697407229975627 9d+00	2.41678287193756902772399 8d+00	2.7744d-04
4	4.57956061124442250923140 9d+00	4.17898336359848107116637 4d+00	2.0704d-05
5	5.57039324488908101318346 5d+00	6.44237334182313934233823 3d+00	1.4820d-06
6	6.56386385646327482128266 2d+00	9.20582454373696897223672 9d+00	1.0336d-07
7	7.55889043571058239101728 7d+00	1.24688599041073718623267 4d+01	7.0810d-09
8	8.55493150694510173535017 4d+00	1.62313604104084499222873 7d+01	4.7889d-10
9	9.55168042407351284402543 3d+00	2.04933282758509898983908 4d+01	3.2072d-11
10	1.05489474942684973675855 3d+01	2.52548003830860925222397 9d+01	2.1315d-12
11	1.15466077449982794940033 6d+01	3.05158205689630751679392 4d+01	1.4079d-13
12	1.25445748719504500792143 0d+01	3.62764310278857077257822 7d+01	9.2524d-15
13	1.35427870359185112255078 9d+01	4.25366698803941543418865 0d+01	6.0549d-16
14	1.45411985846388167319097 8d+01	4.92965707916051973434468 7d+01	3.9482d-17
15	1.55397749704140948072293 6d+01	5.65561632661262475600211 8d+01	2.5666d-18
16	1.65384894959772310588552 0d+01	6.43154731343523431708196 2d+01	1.6640d-19
17	1.75373211570112602326835 7d+01	7.25745230546481570736355 1d+01	1.0764d-20
18	1.85362531688566647125190 7d+01	8.13333297094291496385707 d+01	6.9479d-22
19	1.95352719345285255182456 1d+01	9.05919205095099410741957 2d+01	4.4767d-23
20	2.05343663056676925868460 6d+01	1.00350301315548550875474 0d+02	2.8797d-24
21	2.15335270428624100991377 3d+01	1.10608489336027848003307 8d+02	1.8497d-25
22	2.25327464146852066733228 3d+01	1.21366497056645412086556 7d+02	1.1865d-26
23	2.35320178951521043637384 4d+01	1.32624335700416860219787 3d+02	7.6022d-28
24	2.45313359322501878801390 6d+01	1.44382015394487871329833 4d+02	4.8653d-29
25	2.55306957685986648380941 9d+01	1.56639545310722693349002 4d+02	3.1106d-30
26	2.65300933009043351995364 3d+01	1.69396933784657406974867 3d+02	1.9869d-31
27	2.75295249686637149193193 7d+01	1.82654188416572333905593 2d+02	1.2681d-32
28	2.85289876651779462679205 7d+01	1.96411316157743525955812 3d+02	8.0864d-34
29	2.95284786577761073760216 d+01	2.10668323384365569164109 8d+02	5.1529d-35
30	3.05279955694559457791074 3d+01	2.25425215961178175356063 2d+02	3.2813d-36
31	3.15275362510464093015741 7d+01	2.40681999296458230478643 7d+02	2.0882d-37
32	3.25270988217642175770310 3d+01	2.56438678389740217480571 3d+02	1.3281d-38
33	3.35266815964358323594838 d+01	2.72695257873387010668878 4d+02	8.4422d-40
34	3.45262830661164662197572 0d+01	2.89451742048938337922900 0d+02	5.3635d-41
35	3.55259018750786819483264 4d+01	3.06708134919006400574662 9d+02	3.4059d-42
36	3.65255368013707082955744 9d+01	3.24464440215359801741690 8d+02	2.1617d-43
37	3.75251867403076768726280 1d+01	3.42720661423732173950861 0d+02	1.3715d-44
38	3.85248506903868371384699 6d+01	3.61476801805806053751981 9d+02	8.6975d-46
39	3.95245277412169598056539 8d+01	3.80732864418751931924518 0d+02	5.5135d-47

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Supplement to Gaussian Quadrature Involving Einstein and Fermi Functions with an Application to Summation of Series

By Walter Gautschi and Gradimir V. Milovanović

TABLE 5. Nodes and weights for n-point Gaussian quadrature with respect to the weight function $\varepsilon_1(t)=t/(e^t-1)$ on $(0,\infty)$, n=5(5)40.

n	zero(n)	weight(n)
1	3.47953513120353353588890 6d-01	7.41380189386494906464841 8d-01
2	1.78951927025139605907858 7d+00	7.11279396853423032472763 1d-01
3	4.31707303978456328656870 2d+00	1.81054421301512781269066 7d-01
4	8.12431643567460120570154 6d+00	1.11315658101999566093209 3d-02
5	1.39925950359118224547104 5d+01	8.84934965957596564226918 7d-05

n	zero(n)	weight(n)
1	1.71276458780017236297046 7d-01	4.01758198387197055076484 7d-01
2	8.91672856407162815596929 5d-01	6.17815150206859887652466 d-01
3	2.15469624199527692672815 0d+00	4.30923849167124315840373 6d-01
4	3.94096219443207530854601 4d+00	1.60183185347729222338213 6d-01
5	6.27305497812020058371775 6d+00	3.11160015683170754870668 8d-02
6	9.21983320840474898721393 6d+00	3.00295027990631405838509 9d-03
7	1.28961290242617706777009 2d+01	1.32440035631860816922064 6d-04
8	1.74926202022969845392108 9d+01	2.28073401532276726442836 5d-06
9	2.33750687668907578748948 0d+01	1.11147558728885265968394 6d-08
10	3.14809299087054779458130 4d+01	6.68950943393158581725695 4d-12

n	zero(n)	weight(n)
1	1.12268974288284042856013 4d-01	2.71767492267731795222131 8d-01
2	5.87294257083216930436910 0d-01	4.85220672722516409624547 7d-01
3	1.42713459417277950892293 5d+00	4.58158636136058741788124 9d-01
4	2.61623020439048607096017 9d+00	2.80605666023943532123822 4d-01
5	4.14850536768364111755672 7d+00	1.13514066897138807547123 6d-01
6	6.03351695166850480208509 2d+00	2.99830491853427659019226 5d-02
7	8.29429999093608652700738 6d+00	5.09866606521548674399018 0d-03
8	1.09638434361438614647795 8d+01	5.48204012808260357476353 2d-04
9	1.40858762892952760916770 3d+01	3.61856494244970902647720 6d-05
10	1.77199969115676923387147 7d+01	1.39822259523196334003746 0d-06
11	2.19512629780375894928657 7d+01	2.93660342005254183907506 2d-08
12	2.69084782159920048168814 3d+01	2.98212303575126914799924 0d-10
13	3.28045483537421831472054 2d+01	1.20307931027707265686040 1d-12
14	4.00464897407709594053175 1d+01	1.32454420689602526583047 8d-15
15	4.96764146416902790202546 7d+01	1.54641524512391028869307 6d-19

n	zero(n)	weight(n)
1	8.31029218594976671157530 8d-02	2.04288429181202180267975 3d-01
2	4.35728136584064778993156 4d-01	3.91883245125899283439544 2d-01
3	1.06229883691405284741428 0d+00	4.26639182793801662241121 0d-01
4	1.95301068878080904320771 74d+00	3.29214573867934538864974 3d-01
5	3.10028889980321810285271 4d+00	1.86350249823556742598582 3d-01
6	4.50298851669459863509035 5d+00	7.72593302003812206732065 6d-02
7	6.16722713886496362097725 9d+00	2.33088507382474243586868 2d-02
8	8.10449919862512183390060 1d+00	5.09189052084577575340272 8d-03
9	1.03298765387808544956907 4d+01	8.00960060842622663868908 6d-04
10	1.28617651360213205940917 8d+01	8.98726919329419296149400 5d-05
11	1.57228376318031334127832 5d+01	7.08416443596815758861596 5d-06
12	1.89416112774580831906485 5d+01	3.83537811178228593303754 4d-07
13	2.25547148446590365305031 0d+01	1.38196278781362563886173 5d-08
14	2.66103515788890708641027 6d+01	3.17304179024130819858569 5d-10
15	3.11739857532197339070956 6d+01	4.36963450614604022445570 2d-12
16	3.63384085302550150502920 7d+01	3.30847185656690038147140 9d-14
17	4.22433244509445413516050 3d+01	1.20739094520372320241283 9d-16
18	4.91188832472082961493640 5d+01	1.71000462743488713976706 9d-19
19	5.74046378807687764791353 0d+01	6.23202967060716076256261 d-23
20	6.82273924336591631468169 1d+01	2.07808092700654764130773 7d-27

n	zero(n)	weight(n)
1	6.58021124370695526971220 2d-02	1.63233861990601739232320 8d-01
2	3.45465259457614528868157 2d-01	3.26499579989291489567545 6d-01
3	8.43920391952837393017310 d-01	3.85715838114082893915224 8d-01
4	1.55480908018003402626055 2d+00	3.39303394455953083503508 4d-01
5	2.47200889823326217261226 5d+00	2.32225437396558059451486 2d-01
6	3.59218283329596870181928 9d+00	1.24261951914101941567812 4d-01
7	4.91608717167410439865323 0d+00	5.17857773464348075340898 4d-02
8	6.44817758961915052174599 9d+00	1.67541248307500520087797 0d-02
9	8.19537375803952736920524 5d+00	4.20150239952020976260747 5d-03
10	1.01661764764780284515676 4d+01	8.15322437143844557293439 6d-04
11	1.23705069498601025158321 1d+01	1.21992583161861510300595 3d-04
12	1.48199985560100353702862 9d+01	1.39839469979074401877363 8d-05
13	1.75284742873334463832915 1d+01	1.21629144219694143718963 d-06
14	2.05125471004008004244337 4d+01	7.92201470946587202280668 2d-08
15	2.37924020496707874749640 8d+01	3.79776523328978773087964 4d-09
16	2.73928749471819010185071 5d+01	1.31057989051702247500016 9d-10
17	3.13450052704785204465251 1d+01	3.16399491510559377271771 6d-12
18	3.56883619739012747901498 7d+01	5.14934672306995546987862 0d-14
19	4.04746855132508035639551 4d+01	5.37957637469731027628667 6d-16
20	4.57739110197266282359495 2d+01	3.37533645242342875946808 5d-18
21	5.16848516363488020834266 2d+01	1.15752008522318033383545 9d-20
22	5.83560087696983260231389 4d+01	1.88331366215468681778306 9d-23
23	6.60318712749873359499426 3d+01	1.15269699242510136735219 5d-26
24	7.51795842469932423696395 3d+01	1.70977885600094047095346 6d-30
25	8.69984767513285216405227 6d+01	2.02772492939636223776455 1d-35

n	zero(n)	weight(n)
1	5.43829882227842719690689 9d-02	1.35713845360344949146613 0d-01
2	2.85746753793168013431589 3d-01	2.78951667261605237240964 8d-01
3	6.98945140273044942037205 9d-01	3.47359688705968223550628 5d-01
4	1.28965159339642679311867 6d+00	3.32200209736645699999670 2d-01
5	2.05319735081154272934505 9d+00	2.56513168926610114692235 6d-01
6	2.98613396786968035765431 5d+00	1.61466346148783517727212 0d-01
7	4.08734526860999465409819 7d+00	8.27239676669614655379068 1d-02
8	5.35826017362937479048411 8d+00	3.43968823738542100546403 1d-02
9	6.80227614648590339949238 9d+00	1.15934902983194312234078 4d-02
10	8.42401118234867557670618 9d+00	3.16739663924958331249873 3d-03
11	1.02288717854658224389386 9d+01	7.01275752725745339889136 9d-04
12	1.22229858870023060916280 6d+01	1.25647958377295142822671 4d-04
13	1.44133324102032160362590 3d+01	1.81621234122732072162807 6d-05
14	1.68079383250029889184094 8d+01	2.10770851222812962559742 9d-06
15	1.94161060852138169743313 9d+01	1.95061246892081304269954 3d-07
16	2.22486826953848593310970 7d+01	1.42717243176447194945853 2d-08
17	2.53183965128376770628314 7d+01	8.16593532927494024241989 2d-10
18	2.86402952612540510667330 3d+01	3.60528508129825594545025 9d-11
19	3.22323310662971597437060 5d+01	1.20819895408565993910071 1d-12
20	3.61161610081239397761826 2d+01	3.01180851008543193814697 2d-14
21	4.03182714982872597661205 d+01	5.44676245008030353641033 2d-16
22	4.48716056473855766745581 1d+01	6.92534825934631929590710 8d-18
23	4.98180044591090222685170 1d+01	5.94750436422686477888407 8d-20
24	5.52120320889673686043965 4d+01	3.27385049439310523596220 4d-22
25	6.11273053261582591705811 2d+01	1.07616340160380972222353 3d-24
26	6.76677266128698911960279 1d+01	1.91181138405916700920959 9d-27
27	7.49893796084870698608513 2d+01	1.58053928907282743507436 3d-30
28	8.33492806305053823449948 2d+01	4.75893832879445629738665 1d-34
29	9.32388748264442145324861 8d+01	3.27886802771784575118322 5d-38
30	1.05921581387608865010462 5d+02	1.59713452723125731422675 3d-43

n	zero(n)	weight(n)
1	4.62963893905364803805065 1d-02	1.16020972162332619803241 5d-01
2	2.43390414716042161730978 4d-01	2.43074373086358786748373 4d-01
3	5.95874924296197627950847 9d-01	3.13971702802761157213635 3d-01
4	1.10067565053995437497665 9d+00	3.18079503807499942077740 9d-01
5	1.75423214496275505261557 7d+00	2.66796764436062236884354 8d-01
6	2.55349244893775814649419 5d+00	1.87743397581102047336021 5d-01
7	3.49674849222554231686125 7d+00	1.10897736354434059122021 4d-01
8	4.58401984872692939236104 9d+00	5.48573845435249480426382 6d-02
9	5.81688104466406297127484 3d+00	2.26906222393771795863500 4d-02
10	7.19797849003330683364481 0d+00	7.84757707524087508819466 4d-03
11	8.73059682162313023385630 6d+00	2.27079435345123553443555 0d-03
12	1.04184510263018156637512 6d+01	5.49959054371791506654282 7d-04
13	1.22656685375670854562471 5d+01	1.11423363860587336958996 5d-04
14	1.42768609704318680196690 3d+01	1.88549567711124704733319 8d-05
15	1.64572219749466324544991 4d+01	2.65764694074879614028771 6d-06
16	1.88126330519429161462027 7d+01	3.10829311714789449524137 1d-07
17	2.13497807706844121113844 3d+01	3.00147860889666129618190 0d-08
18	2.40762943815358523498992 6d+01	2.37822925894637163089701 9d-09
19	2.70009138422062702301410 7d+01	1.53472007453715562133484 4d-10
20	3.01336998772472742518067 4d+01	7.99427105095301631206041 8d-12
21	3.34863011891762941432974 5d+01	3.32573001824023232458338 6d-13
22	3.70722999101217867258585 2d+01	1.09111341225824955611553 4d-14
23	4.09076658962664699389671 4d+01	2.78094980572414631457269 0d-16
24	4.50113656496188309118193 4d+01	5.40781560496662052853313 9d-18
25	4.94061964834566469582353 2d+01	7.85010242772268626131802 5d-20
26	5.41199585833590115014096 6d+01	8.28207426413662777814428 5d-22
27	5.91871518076043137455737 6d+01	6.14267671487485442002980 5d-24
28	6.46515217060233584700268 9d+01	3.07023941375839423833370 0d-26
29	7.05700503571292609487003 0d+01	9.78720555067552495318360 5d-29
30	7.70195625207835851005311 d+01	1.84749004966455749318048 0d-31
31	8.41084553133244035337228 9d+01	1.86011082669201193065890 5d-34
32	9.19995744415592813254000 0d+01	8.54135706634936268153574 3d-38
33	1.00961180687956302294656 d+02	1.38380788149187843432743 d-41
34	1.11506608812949300315929 7d+02	4.85989358554629098558339 0d-46
35	1.24957078700955341387671 8d+02	1.07761738534855564194088 8d-51

n	zero(n)	weight(n)
1	4.02764262715531982161157 5d-02	1.01250605146515291665088 8d-01
2	2.11824602053612842400751 5d-01	2.15144413205638416685734 5d-01
3	5.18931044499821489377806 0d-01	2.85463083396965829731245 2d-01
4	9.59330967959662184062349 4d-01	3.01594666555367686162675 4d-01
5	1.53027042094464551122828 2d+00	2.68601456531691085406471 4d-01
6	2.22916692592364240026393 8d+00	2.04897621339353551034349 3d-01
7	3.05421813713650480101712 5d+00	1.34205640775911152282000 5d-01
8	4.00478888486796560817418 8d+00	7.53536616963982059454359 d-02
9	5.08144173331919467302116 5d+00	3.62081422636988930310071 0d-02
10	6.28567459057664777825182 3d+00	1.48826979186404494301892 6d-02
11	7.61957784039183021232627 8d+00	5.23583071503508483356130 1d-03
12	9.08559191344316354186877 2d+00	1.57800085545704542060256 1d-03
13	1.06864114091769567598776 d+01	4.07658245510871904620624 3d-04
14	1.24249886772919978220589 3d+01	9.02641746425837450276631 3d-05
15	1.43045787058009347473245 5d+01	1.71156205934654671852792 5d-05
16	1.63287937693041571266197 8d+01	2.77472434343792597767211 4d-06
17	1.85016595175064823853263 1d+01	3.83675021183451043771239 1d-07
18	2.08276742643709696576464 1d+01	4.51098045819409091004630 8d-08
19	2.33118755006205246663229 8d+01	4.49227779877859887300205 7d-09
20	2.59599176306382064948871 6d+01	3.77170868856665118323318 1d-10
21	2.87781649769548535124655 3d+01	2.65528558915741064597615 1d-11
22	3.17738047238196110060298 4d+01	1.55744508610359770363702 0d-12
23	3.49549857273195647055989 6d+01	7.55475525862432979083755 0d-14
24	3.83309910836149460962773 0d+01	3.00466788200425062471594 5d-15
25	4.19124552601189201350540 5d+01	9.70065774758568467201833 3d-17
26	4.57116409118963038768637 2d+01	2.51292704028705237755537 d-18
27	4.97427970044031347217078 6d+01	5.15246657090783487318934 9d-20
28	5.40226298679077521774241 6d+01	8.22869407781031769764502 2d-22
29	5.85709346299169438959462 2d+01	1.00421833916659618918785 9d-23
30	6.34114602868820778121430 4d+01	9.15214217687191218842339 8d-26
31	6.85731253527713211204220 6d+01	6.05669619490292349878402 3d-28
32	7.40917781103952984228510 9d+01	2.81096713023039357363746 4d-30
33	8.00128385260981092009921 4d+01	8.75453058716443858336657 8d-33
34	8.63954407144726152467963 6d+01	1.72762033772138246420979 0d-35
35	9.33192926013056053092449 7d+01	1.99965986553747005973978 0d-38
36	1.00896860752685756921813 0d+02	1.21765315276959889320090 3d-41
37	1.09297145167294471120737 4d+02	3.31439521142265512723055 1d-45
38	1.18798674457912870537357 0d+02	3.08725117727572216878610 5d-49
39	1.29934805532434200546178 6d+02	5.92393036058448437812820 8d-54
40	1.44079642887435866138543 0d+02	6.46305925437841199910479 8d-60

TABLE 6. Nodes and weights for n-point Gaussian quadrature with respect to the weight function $\varepsilon_2(t)=(t/(e^t-1))^2$ on $(0,\infty)$, n=5(5)40.

n	zero(n)	weight(n)
1	1.89807370266614777773441148d-01	4.00044332569487360445437 2d-01
2	9.85246352958302065844420 3d-01	3.78980799529545381765159 1d-01
3	2.38635153636072397563074 3d+00	9.98634537233989316707744 4d-02
4	4.45391292131601193759460 6d+00	6.80359185806610509041442 2d-03
5	7.55098536673390681527797 3d+00	6.21496967665231735688223 7d-05

n	zero(n)	weight(n)
1	9.21844491584762340884216 5d-02	2.15162634818383655382103 7d-01
2	4.81831122550832794490727 4d-01	3.27858216517749371389480 2d-01
3	1.16958193968495596692890 8d+00	2.30781538388429613519668 6d-01
4	2.14255028569661291495118 5d+00	9.03728974215952248931923 4d-02
5	3.39980372024179797993968 9d+00	1.93585312146937141269350 3d-02
6	4.96351810743301862371409 8d+00	2.11286565020677178459716 1d-03
7	6.88672252985468662018599 3d+00	1.05591931702471932203065 7d-04
8	9.26649448648182598230334 0d+00	2.04039028370036053687255 0d-06
9	1.22897170275799233008730 6d+01	1.10368845013701221534845 9d-08
10	1.64321079095245131296622 6d+01	7.33527738651483521329791 9d-12

n	zero(n)	weight(n)
1	5.99063588694919601265218 0d-02	1.44584766083352519595089 2d-01
2	3.14094413719093291981153 6d-01	2.56477548598910267531264 2d-01
3	7.65662563411407164577574 1d-01	2.42656188092763090013774 3d-01
4	1.40715015277607788053930 2d+00	1.52788870665435845438556 7d-01
5	2.23221608324839056223438 7d+00	6.59118847834677709505963 0d-02
6	3.23927306528461301415501 8d+00	1.91923451667195194817890 6d-02
7	4.43396126201060036911039 5d+00	3.66486773049207186902973 0d-03
8	5.82995009380859587431455 7d+00	4.43679179714267691832502 5d-04
9	7.44895117555175113297457 5d+00	3.27445411313471451853191 1d-05
10	9.32173548873663959892263 4d+00	1.39997519498915376173566 5d-06
11	1.14919448304024425274230 9d+01	3.22034022757389502589951 8d-08
12	1.40250260527871406037364 8d+01	3.55132609626066180693401 7d-10
13	1.70286242292636552297552 0d+01	1.54589827549126236718126 4d-12
14	2.07081596154848594398644 7d+01	1.82940420713290675086467 4d-15
15	2.55893773967515071903896 5d+01	2.29760117722024991677002 9d-19

n	zero(n)	weight(n)
1	4.40742922104099218999031 7d-02	1.08127236410254081282626 2d-01
2	2.31442306035826929046463 2d-01	2.06418095638150336976681 6d-01
3	5.55379023803058678821969 d-01	2.24644924749206397007868 0d-01
4	1.04[illegible]93873111501898609 61d+00	1.76126616127068918102325 7d-01
5	1.65650873353939230434030 1d+00	1.04055465827621597964453 2d-01
6	2.40539876510090053929463 1d+00	4.64172325063923218647881 3d-02
7	3.28794136463779213944134 4d+00	1.54421515560945209031959 3d-02
8	4.30663762138075896543439 7d+00	3.76861264289424951853558 7d-03
9	5.46737174950389204884068 3d+00	6.63471476539732297589160 1d-04
10	6.77906954986558428352795 8d+00	8.28677053478071362781577 3d-05
11	8.25346581955132611223106 4d+00	7.20879723160508300347959 9d-06
12	9.90536494928915823469325 3d+00	4.26840224842828935615939 6d-07
13	1.17535611091633220223562 1d+01	1.66816242107258233775015 6d-08
14	1.38225519447525385314137 7d+01	4.12483382100378306422237 0d-10
15	1.61454335549127858054687 9d+01	6.08105569165334124891240 2d-12
16	1.87690004569074501915722 1d+01	4.90523801572649738048100 7d-14
17	2.17636250734638676629044 6d+01	1.89996083916687106872874 7d-16
18	2.52451821787890838637183 8d+01	2.84867328489464006829455 3d-19
19	2.94349448150720116164641 4d+01	1.09808290266351366661407 4d-22
20	3.49002021123789773165076 5d+01	3.88334708031970108589796 6d-27

n	zero(n)	weight(n)
1	3.47387959960882275685078 5d-02	8.60475193795629923521013 4d-02
2	1.82581037847762750619048 6d-01	1.71463577770995226496395 2d-01
3	4.46787523396424889951835 2d-01	2.02318725291396082868217 3d-01
4	8.24722612762274446851702 8d-01	1.79719360757503386111612 5d-01
5	1.31324263910740003147042 8d+00	1.26693924987843834486233 9d-01
6	1.90946265743377000053964 9d+00	7.16194793596277443592699 6d-02
7	2.61150336060657985065944 1d+00	3.23199630334449099495846 3d-02
8	3.41906372819883460040800 6d+00	1.15294755805345706103952 1d-02
9	4.33367068194919906124523 3d+00	3.21637948228422575301840 9d-03
10	5.35859906121490375867961 0d+00	6.94759365251410710780736 1d-04
11	6.49861356166351907942931 4d+00	1.15163435694927203804893 9d-04
12	7.75974119152006281707778 7d+00	1.45185909828243256792731 5d-05
13	9.14921747988000809672399 0d+00	1.37793434140442015510990 2d-06
14	1.06756461871233523081237 7d+01	9.72043478619890588935216 3d-08
15	1.23493569670072958295219 4d+01	5.01354811599108982596003 7d-09
16	1.41829577379114370002473 6d+01	1.85066579628329206680673 d-10
17	1.61921343883010436181567 9d+01	4.75527653467454606766115 1d-12
18	1.83968346660954060863705 8d+01	8.20175895768586328929989 6d-14
19	2.08231078770276960210293 5d+01	9.04767694748344120500216 7d-16
20	2.35061376282678293145748 2d+01	5.97612286255517938930138 8d-18
21	2.64956152443985456494249 5d+01	2.15218789025874677452160 6d-20
22	2.98662036986725314047493 2d+01	3.67060780698732938151991 d-23
23	3.37408174401890060733081 4d+01	2.35267088931531607158825 2d-26
24	3.83543173889886680216250 2d+01	3.65550386194521246288191 4d-30
25	4.43097532142508731423138 7d+01	4.55663527583511811749827 2d-35

n	zero(n)	weight(n)
1	2.86064090145636262377991111d-02	7.13053998240821728617146 5d-02
2	1.50434172072815275533914 8d-01	1.46117974877420339698334 3d-01
3	3.68466304441300152774249 3d-01	1.81680281893456518437587 3d-01
4	6.80962316079757795220842 1d-01	1.74845008538748046469788 3d-01
5	1.08572338303511966568010 4d+00	1.37899891352862493649270 2d-01
6	1.58051633583206848661433 9d+00	9.05104469813504763013325 5d-02
7	2.16350840593902907015368 3d+00	4.94524221685388846628130 2d-02
8	2.83365722592966760113437 8d+00	2.23625215440045841606542 6d-02
9	3.59096486776575576864189 9d+00	8.30535838010289504947745 1d-03
10	4.43654334111457223615423 8d+00	2.51453763634283914724481 1d-03
11	5.37251432954832218686077 7d+00	6.16654782414153577559961 5d-04
12	6.40183045857110412409836 4d+00	1.21833202116538990804765 1d-04
13	7.52811807075303578010383 6d+00	1.92955021268281157178885 2d-05
14	8.75560450644221019497929 9d+00	2.43656494540372051429222 5d-06
15	1.00891432793700643800095 1d+01	2.43740543839766393321592 d-07
16	1.15343212813338266155895 5d+01	1.91597234852204827566248 2d-08
17	1.30976299508998092678443 4d+01	1.17147333328737766532659 4d-09
18	1.47866959992894870732745 3d+01	5.50067940032908820187084 1d-11
19	1.66105852004857744305767 8d+01	1.95232920182717705626389 7d-12
20	1.85802112757421480860210 2d+01	5.13557695406594719141100 5d-14
21	2.07089047146679670076793 3d+01	9.76907452813166983991558 8d-16
22	2.30132324973780385459593 0d+01	1.30284244973795418901443 1d-17
23	2.55142255944215605977214 8d+01	1.17075150057969791979888 8d-19
24	2.82393011280970268291797 9d+01	6.72925895087858626648965 8d-22
25	3.12254421401372193644302 5d+01	2.30578284919326983079090 8d-24
26	3.45248404397608521619996 0d+01	4.26419284117537291094332 3d-27
27	3.82158959104805701077513 8d+01	3.66663511820572646922569 8d-30
28	4.24277082292576747140747 1d+01	1.14799191032868238381828 9d-33
29	4.74071474133302894749919 9d+01	8.23175883744290537580975 0d-38
30	5.37889458716808878833679 d+01	4.18805758889348764108194 2d-43

n	zero(n)	weight(n)
1	2.42807420306990788518575 5d-02	6.07920965716334584220518 7d-02
2	1.27734796479714462664009 5d-01	1.27043396467467925232184 2d-01
3	3.13068780607323326287820 9d-01	1.63843094130104003050476 4d-01
4	5.79071239802448349074947 2d-01	1.66680206148679568548148 5d-01
5	9.24151990627652940476330 6d-01	1.42015934377888094668907 8d-01
6	1.34659859537002644900105 1d+00	1.03234138898142081153071 4d-01
7	1.84484268980130449101412 2d+00	6.42489218693435758653016 0d-02
8	2.41772190606238536358389 0d+00	3.41339054617608821168273 9d-02
9	3.06468687011693155621845 0d+00	1.53953425194008010207107 9d-02
10	3.78590901572997848377383 8d+00	5.85979812529157702792261 1d-03
11	4.58227562481112461553123 4d+00	1.87220730790860142297185 8d-03
12	5.45529876667476054152884 3d+00	4.99957607327120830537018 9d-04
13	6.40699132903185111499339 2d+00	1.11205221527485559156374 6d-04
14	7.43976221947603014732147 1d+00	2.05408246607751781379373 3d-05
15	8.55636040737119852290603 0d+00	3.14094163705513677670547 0d-06
16	9.75987194467801856014891 9d+00	3.96156243851291151498125 6d-07
17	1.10537592318027432195287 6d+01	4.10274260358645978888263 2d-08
18	1.24419297062251587749269 9d+01	3.46924724229260160182463 9d-09
19	1.39288264783810284263490 6d+01	2.37865785565459215239992 8d-10
20	1.55195404612703974488762 7d+01	1.31127068765193441462585 3d-11
21	1.72199495156115405487693 8d+01	5.75291222104127457087641 8d-13
22	1.90368951060264602996590 3d+01	1.98426520206317219854260 0d-14
23	2.09784123208168371234727 8d+01	5.30200458343649188491155 1d-16
24	2.30540367187040711614941 5d+01	1.07821324869152261232211 0d-17
25	2.52752237755977018182314 9d+01	1.63316801776339238966764 6d-19
26	2.76559376715230536789450 9d+01	1.79437449264176572351714 0d-21
27	3.02135033190856893798221 1d+01	1.38356018099286146034732 3d-23
28	3.29698845860810645712076 7d+01	7.17837789091846020302822 7d-26
29	3.59536877565904732866863 8d+01	2.37232409077166883283625 6d-28
30	3.92034778985012804577356 6d+01	4.63781576099778302437956 9d-31
31	4.27736674394894463781523 d+01	4.83242452461244065713084 8d-34
32	4.67460010468806417590511 4d+01	2.29554480728010922791259 6d-37
33	5.12551443726077436053102 0d+01	3.84804210822512329543578 9d-41
34	5.65588068383365118692002 0d+01	1.39988487734725680188704 9d-45
35	6.33203491912486349373670 5d+01	3.22708746669995523338260 7d-51

n	zero(n)	weight(n)
1	2.10712241587540543295026 0d-02	5.29300063477387294844224 4d-02
2	1.10880229559473791938119 9d-01	1.12228931978270120598722 8d-01
3	2.71885440098612946639426 8d-01	1.48682967807320163811657 6d-01
4	5.03208030549119376697228 5d-01	1.57530301367235861735206 5d-01
5	8.03661428356911454986847 1d-01	1.41978839905700869468247 3d-01
6	1.17191816192618314838547 0d+00	1.11125033628647604589406 4d-01
7	1.60668096468549460127927 7d+00	7.59684450178019471445889 0d-02
8	2.10686103301908390176570 5d+00	4.53231243977816377905920 9d-02
9	2.67173586404966140444393 d+00	2.35079791382209853856268 6d-02
10	3.30105642522603798575429 0d+00	1.05496900919542011291229 9d-02
11	3.99508442155248352795496 1d+00	4.07748706615404008332278 1d-03
12	4.75456163190541853940887 1d+00	1.35208320223628414867742 9d-03
13	5.58063449821947839099631 6d+00	3.83518478323537884019111 6d-04
14	6.47476718799018606269252 7d+00	9.28452647234826389134079 8d-05
15	7.43867146555339717860359 8d+00	1.91469246099603668110474 5d-05
16	8.47426763994645594469582 4d+00	3.35721071203962603397288 0d-06
17	9.58367699748916975867494 0d+00	4.99390486755684388522007 6d-07
18	1.07692384722428048893592 3d+01	6.28488691523454838499759 6d-08
19	1.20335412552526748693029 4d+01	6.66915427888599619534666 6d-09
20	1.33794677519451234156450 6d+01	5.94213303202646421042003 8d-10
21	1.48102448350113917569421 3d+01	4.42300860421492418121965 9d-11
22	1.63295041876241903107157 1d+01	2.73391529209210066957687 4d-12
23	1.79413544750740639458232 0d+01	1.39336496689978534392213 0d-13
24	1.96504695433705808064182 0d+01	5.80692491533856757661657 1d-15
25	2.14621983696978524963230 3d+01	1.95975553969916703648509 7d-16
26	2.33827045841059872889681 9d+01	5.29514897281956753508071 4d-18
27	2.54191465581591820237119 8d+01	1.13018293699142728211817 0d-19
28	2.75799140149433519420652 4d+01	1.87551476565115788557252 2d-21
29	2.98749450163242923373984 2d+01	2.37449468533258114754984 7d-23
30	3.23161601158612476636859 7d+01	2.24175812202491751554881 1d-25
31	3.49180723703610391835132 6d+01	1.53483987637553129908044 d-27
32	3.76986705790796016609776 1d+01	7.36122962689463277966699 7d-30
33	4.06807448915441221819694 2d+01	2.36684376528691965462331 1d-32
34	4.38939653483009684154309 0d+01	4.81809250508001353349831 4d-35
35	4.73783238931706743243905 7d+01	5.74914902360275550879304 7d-38
36	5.11902486217134454596211 8d+01	3.60763608881326849519822 5d-41
37	5.54145342434441594065181 1d+01	1.01186261329986235419464 0d-44
38	6.01909368509581567962914 7d+01	9.71586991261870857039421 7d-49
39	6.57870938537880080617493 4d+01	1.92429817798657448786877 7d-53
40	7.28925896736521439221536 1d+01	2.17477192651065076086938 1d-59

TABLE 7. Nodes and weights for n-point Gaussian quadrature with respect to the weight function $\varphi_1(t)=1/(e^t+1)$ on $(0,\infty)$, n=5(5)40.

n	zero(n)	weight(n)
1	3.00477100474524066903844 9d-01	3.23808346469071329648267 6d-01
2	1.52415287201707667862610 2d+00	3.00480823472689644177976 0d-01
3	3.71370450364614742034568 9d+00	6.55913957862621538074042 9d-02
4	7.18995752400301511089337 3d+00	3.24545172670557621753997 7d-03
5	1.27395431732222006115800 5d+01	2.11631052166055660442409 2d-05

n	zero(n)	weight(n)
1	1.52393576359858910498841 3d-01	1.79681859318660087476621 8d-01
2	7.86940359227187865071950 8d-01	2.73291654045550335189209 9d-01
3	1.89332081799802347342213 4d+00	1.75585971052299949604994 3d-01
4	3.48651605808340061343548 4d+00	5.51247018608678788690426 0d-02
5	5.63020130715004656285810 4d+00	8.73725343500577203541311 3d-03
6	8.40334445960585327803550 6d+00	6.99032308335997076633653 4d-04
7	1.19148458568235835408408 9d+01	2.63106541578784987702861 5d-05
8	1.63491709388165968710410 7d+01	3.96167710278401916542707 2d-07
9	2.20657769988164416980558 8d+01	1.71643177999686113420764 8d-09
10	2.99893749004295179578588 9d+01	9.25352267768802069256501 0d-13

n	zero(n)	weight(n)
1	1.01534494742408160438430 4d-01	1.23284793005194381414476 5d-01
2	5.28414733417862585883935 6d-01	2.19141969396062166863752 4d-01
3	1.27750060898574015593076 6d+00	1.97447381032153581315777 9d-01
4	2.34163136017582040835221 1d+00	1.07508492806625235184880 4d-01
5	3.73667783867356059466059 9d+00	3.65319603404886096042528 9d-02
6	5.48938437438776900847169 1d+00	7.98178367263880816723800 0d-03
7	7.62665217761886873402579 6d+00	1.13926326585504039011488 d-03
8	1.01791788471660544860381 6d+01	1.05227992840301541527237 7d-04
9	1.31882186992974500741042 1d+01	6.09481132527258684667980 7d-06
10	1.67116997011941540244258 7d+01	2.10206082446464250011566 3d-07
11	2.08333259270851600962103 5d+01	3.99347989827818202766479 2d-09
12	2.56804160618949002507224 5d+01	3.70617479062219456000149 1d-11
13	3.14637924722652671798434 2d+01	1.37676823292052302534649 6d-13
14	3.85867579870667032997678 4d+01	1.40212387062630020093786 1d-16
15	4.80819905203975628079985 1d+01	1.51354747627594870065896 3d-20

n	zero(n)	weight(n)
1	7.59688176609774301717 2034d-02	9.35807835793527710275 9111d-02
2	3.96895863442851782230 5818d-01	1.79158910770774495547 9337d-01
3	9.63385596145567591248 2977d-01	1.89423241806090363744 5891d-01
4	1.76728517413438742450 6506d+00	1.34572985968616349951 2049d-01
5	2.81137836075440025156 9433d+00	6.62341722376745531546 4508d-02
6	4.10784057499448705328 1519d+00	2.30907203114386216600 0433d-02
7	5.67043545803123933190 7316d+00	5.83833507844786194118 7718d-03
8	7.51184353108768576068 2423d+00	1.08444779437876066060 4086d-03
9	9.64579779870125774795 9729d+00	1.47858854110918344528 0375d-04
10	1.20893498925556501228 6601d+01	1.46383819196463747697 5172d-05
11	1.48642777399847442929 3775d+01	1.03335045557209622103 0406d-06
12	1.79984828954222597097 7647d+01	5.07174476516357466913 1819d-08
13	2.15280817636933074504 3338d+01	1.67331109101869130103 0526d-09
14	2.55007709685205040808 7777d+01	3.54694392261330571761 9910d-11
15	2.99814451092488368210 8873d+01	4.53989722472979703530 1348d-13
16	3.50621812012207397750 1572d+01	3.21229451919345572752 4076d-15
17	4.08816854763507580821 3746d+01	1.10017251704642451460 2555d-17
18	4.76685221895425966465 4355d+01	1.46657732613403143116 7121d-20
19	5.58592363672724628529 1701d+01	5.03642185715181813683 43071d-24
20	6.65727760331033273319 3395d+01	1.57824729200670908217 2119d-28

n	zero(n)	weight(n)
1	6.06236476949789013780 8309d-02	7.53164895261358532752 8696d-02
2	3.17427709410930415516 8326d-01	1.50513206517006932964 3495d-01
3	7.72616452267741704081 4321d-01	1.74353621130575661098 4920d-01
4	1.41959740420737788417 0178d+00	1.44449671207612334212 1589d-01
5	2.25707476921010502572 8954d+00	8.85006682187619761873 6240d-02
6	3.29050505507140251111 4510d+00	4.07154778442534262892 2120d-02
7	4.52825526925860916109 3324d+00	1.43445491320910604348 9963d-02
8	5.97810805954109275511 0909d+00	3.93802494233172581104 1528d-03
9	7.64710555588595551755 076d+00	8.49884270547141863848 5438d-04
10	9.54283609635043770939 9811d+00	1.44274667429621989349 1800d-04
11	1.16743905168314621325 6351d+01	1.91703273112474041063 6517d-05
12	1.40528500295877799041 9192d+01	1.97667906179775138131 9017d-06
13	1.66916686154947596531 5763d+01	1.56326826158607196928 4727d-07
14	1.96071779984819517755 0952d+01	9.34230743282458102682 4956d-09
15	2.28193174931833581327 5190d+01	4.14089379934666699466 4001d-10
16	2.63526850719602696458 5240d+01	1.32984782727752965890 1807d-11
17	3.02380716146306645960 7256d+01	3.00437588291355342722 9356d-13
18	3.45147688174542451973 1948d+01	4.59729038102168045325 8445d-15
19	3.92341884953743040550 8670d+01	4.53385261841303743720 3013d-17
20	4.44658511906657729732 6098d+01	2.69437167107815844424 8283d-19
21	5.03080097507014769102 6168d+01	8.77530954887263397418 6416d-22
22	5.69083432202074984440 5702d+01	1.35869712360370890146 7366d-24
23	6.45099943383722293859 8566d+01	7.92281227873279319444 7596d-28
24	7.35775105764932312800 7488d+01	1.11937118469023791096 9420d-31
25	8.53033847721682603336 7785d+01	1.26015680372366939782 0879d-36

n	zero(n)	weight(n)
1	5.04045071671897176600 1156d-02	6.29727388300600493920 7042d-02
2	2.64289352108690110770 8105d-01	1.29391182419270057104 8905d-01
3	6.44510259655841267848 5001d-01	1.58895947141334374044 5347d-01
4	1.18600314696325932070 6762d+00	1.45283581367794673598 9001d-01
5	1.88631367251467138799 6753d+00	1.02707442331599853196 8227d-01
6	2.74753564137406025688 0807d+00	5.68107862373996210936 4464d-02
7	3.77482892751903170033 3358d+00	2.49434085533364679376 5132d-02
8	4.97369743806014829066 4424d+00	8.83676219065582143060 7667d-03
9	6.34885055180635834811 4462d+00	2.55699576607844532365 6236d-03
10	7.90464901610431248796 8213d+00	6.07796392368713594352 9345d-04
11	9.64584686610347996027 1023d+00	1.18749124951985272729 3219d-04
12	1.15780303608293184586 2712d+01	1.90183223155247374515 5275d-05
13	1.37078161022203767487 6666d+01	2.48476382181250999452 4717d-06
14	1.60429879493460860010 7228d+01	2.63116489160775638759 8505d-07
15	1.85926679055613944063 6720d+01	2.23999142081260100220 0258d-08
16	2.13675531037374674317 4465d+01	1.51814762891785856848 9713d-09
17	2.43802360927628935145 0600d+01	8.09505612140086577355 995d-11
18	2.76456334402043559325 3567d+01	3.34813381165491340483 6031d-12
19	3.11815641288576395893 8504d+01	1.05592219481478434963 0319d-13
20	3.50095441682183570236 1876d+01	2.48704265348043661098 4178d-15
21	3.91559044591024512842 6502d+01	4.26453115538891742418 3103d-17
22	4.36534098780702919612 5651d+01	5.15670673185047356135 7608d-19
23	4.85436887736780169564 9898d+01	4.22287139994646446331 533d-21
24	5.38810403234957048975 4357d+01	2.22152678563276834612 2970d-23
25	5.97387345338396646064 016d+01	6.99201014740015699316 8816d-26
26	6.62201926688379035763 0170d+01	1.19106194415616293794 0958d-28
27	7.34807792325338925396 3821d+01	9.45114260908736222082 3362d-32
28	8.17763196244966616869 8358d+01	2.73220601373336915646 5250d-35
29	9.15959458474502059500 3182d+01	1.80588191202207605027 3723d-39
30	1.04196973885436261852 5074d+02	8.40765569530612261892 8261d-45

n	zero(n)	weight(n)
1	4.31162529815330921152685 7d-02	5.40812761836511449338848 5d-02
2	2.26288760940182725134516 6d-01	1.13298017904235050664930 0d-01
3	5.52598810890601120106915 3d-01	1.44847613963340682442772 5d-01
4	1.01815676705251623702920 1d+00	1.41740181301287773884129 6d-01
5	1.62035200328029158958184 1d+00	1.10716536462908098379216 0d-01
6	2.35958215234032404999448 5d+00	6.97911349448794134014845 5d-02
7	3.23893799911908461866682 6d+00	3.58690469873332511344834 1d-02
8	4.26242964765481383026562 3d+00	1.52373006774888213189524 0d-02
9	5.43364935904327830003018 6d+00	5.41830901134199902419334 7d-03
10	6.75563155553389355227630 7d+00	1.62618241954889556975243 9d-03
11	8.23130819307009790712971 1d+00	4.13430237406673217647903 0d-04
12	9.86392138162902160128714 8d+00	8.90650273429861655890131 7d-05
13	1.16572314712579560675704 2d+01	1.62308094256887528286854 9d-05
14	1.36156030964410089460994 1d+01	2.49450491914073560809023 2d-06
15	1.57440618489425784268444 6d+01	3.22021065771101640072781 0d-07
16	1.80483647897699317834147 8d+01	3.47441379383285224203622 3d-08
17	2.05350971729565187863900 6d+01	3.11460649258306815215618 1d-09
18	2.32117992692553965309989 3d+01	2.30368833860662821208248 3d-10
19	2.60871284315561679088799 3d+01	1.39446137284358584076030 0d-11
20	2.91710653961444020376312 9d+01	6.84263270671273141484275 3d-13
21	3.24751787006115872048314 0d+01	2.69182739787586207759435 2d-14
22	3.60129676852250624239572 5d+01	8.37937755854498617841771 1d-16
23	3.98003142940065708100528 4d+01	2.03245962501363846317226 6d-17
24	4.38560891370271338786126 4d+01	3.77138055877473686063667 9d-19
25	4.82029820683735298228055 4d+01	5.23646345801805159032355 0d-21
26	5.28686694321737146470120 7d+01	5.29545502421640963297277 6d-23
27	5.78875040369373339363719 1d+01	3.77164159140879809714405 7d-25
28	6.33030509997385543472471 1d+01	1.81323753220962406573297 1d-27
29	6.91720626082298728342535 3d+01	5.56730970653854037818735 1d-30
30	7.55710578551655546116821 9d+01	1.01333773217527017175657 2d-32
31	8.26080043955838994768767 8d+01	9.84572100056420908075601 7d-36
32	9.04451006269318825948002 5d+01	4.36473226686394028243130 7d-39
33	9.93495296071668628235209 4d+01	6.82606728080430659578477 6d-43
34	1.09832526780164825822739 6d+02	2.31147701687591679899830 9d-47
35	1.23209768383663463147622 8d+02	4.92360746158022862991821 d-53

n	zero(n)	weight(n)
1	3.76589835130351514997393 6d-02	4.73757657950525209421595 3d-02
2	1.97780911829622009106449 6d-01	1.00677233398879170695573 4d-01
3	4.83475052343421562982818 5d-01	1.32540035169157957870776 0d-01
4	8.91714881563821859710910 2d-01	1.36239116836890759003032 5d-01
5	1.42006907712302214953309 2d+00	1.14666792804864875846643 1d-01
6	2.06809492284144009649033 2d+00	7.94973940496404976747189 9d-02
7	2.83753931363912696172430 9d+00	4.59835697409760841211954 3d-02
8	3.73130282141519795486538 9d+00	2.23927413675631052922941 3d-02
9	4.75225536850671743598963 1d+00	9.28903246826232220056886 5d-03
10	5.90278295703793181800950 0d+00	3.31290128935510868083567 3d-03
11	7.18496503811123387931897 0d+00	1.02139565084314908732777 4d-03
12	8.60090502771868101127313 8d+00	2.72837561156936801556497 1d-04
13	1.01529534652375485964886 3d+01	6.31519129816737547178263 7d-05
14	1.18438073883801331410288 5d+01	1.26507961075170529567947 3d-05
15	1.36765486631723769390673 0d+01	2.18878106636569851388904 8d-06
16	1.56546696611924539881952 0d+01	3.26180793262692229913249 4d-07
17	1.77821065375187751111810 9d+01	4.17299181965588798583536 8d-08
18	2.00632851109615057563808 1d+01	4.56536117107615389611196 7d-09
19	2.25031801165434260879660 4d+01	4.25183822492466245146984 2d-10
20	2.51073888939016590188453 7d+01	3.35346803497600460468905 2d-11
21	2.78822191570351236447547 d+01	2.22660171213250925509 2974d-12
22	3.08348140291253721140943 0d+01	1.23613764847922711619872 1d-13
23	3.39732619440227184991527 7d+01	5.69359492248698720836042 2d-15
24	3.73067956432510464584542 0d+01	2.15637976733328100032325 2d-16
25	4.08459943798090662197455 8d+01	6.64692016981894857742081 8d-18
26	4.46030622711136660559167 8d+01	1.64781429408909389370210 0d-19
27	4.85921850001580906066954 5d+01	3.24020849341601489288486 2d-21
28	5.28299991156265540583982 9d+01	4.97220451668138394438417 7d-23
29	5.73362211958930402523673 5d+01	5.84056883034296425365909 0d-25
30	6.21345098695849330971882 7d+01	5.13133554383661757813748 3d-27
31	6.72536772079707194606745 0d+01	3.27810229376079769217330 0d-29
32	7.27294428161160645259431 8d+01	1.47044301511504172289179 7d-31
33	7.86070664653855452892467 6d+01	4.43083008159307886400237 7d-34
34	8.49454759044253057255027 5d+01	8.46715693912720916621888 8d-37
35	9.18241020428239730466871 6d+01	9.49671828369756214960915 0d-40
36	9.93550198518753602688221 3d+01	5.60603326700028658875738 d-43
37	1.07706636464257729580841 8d+02	1.47944047224283215669530 0d-46
38	1.17156490684870650354797 0d+02	1.33554469561202088220710 7d-50
39	1.28236008767219100653991 5d+02	2.48041824865681230354914 8d-55
40	1.42314196230481757867082 1d+02	2.60969335088797107954366 3d-61

TABLE 8. Nodes and weights for n-point Gaussian quadrature with respect to the weight function $\psi_2(t)=(1/(e^t+1))^2$ on $(0,\infty)$, n=5(5)40.

n	zero(n)	weight(n)
1	1.60452949179171005871872 2d-01	8.63180515113980361507013 4d-02
2	8.19082478537845820662453 9d-01	8.43219678341386226976142 1d-02
3	1.96520478615245983945830 4d+00	2.12761745430662212182868 1d-02
4	3.71044814625348560460455 3d+00	1.22241570858326620672172 4d-03
5	6.47189605597496451824449 4d+00	8.57096275916314390803784 2d-06

n	zero(n)	weight(n)
1	7.98346830245532970958292 8d-02	4.70317991168396223567934 0d-02
2	4.14297830986004655852686 5d-01	7.30907379185972419458026 3d-02
3	9.97207454137470109232396 4d-01	5.10021264993603538321139 5d-02
4	1.81962942457939935481227 3d+00	1.83960445642098834869230 0d-02
5	2.89950207529803084051210 2d+00	3.32643847329293276233772 9d-03
6	4.28168355190592841761151 7d+00	2.88592856250414107867706 7d-04
7	6.03104227594554055962984 1d+00	1.12682492619269151079139 5d-05
8	8.24389408038401992244296 9d+00	1.72131363286763148499302 8d-07
9	1.10997384302542724208139 2d+01	7.50363745187767562072466 8d-10
10	1.50600140776642600156971 6d+01	4.05902059369721720522831 5d-13

n	zero(n)	weight(n)
1	5.27309861533059966011526 6d-02	3.19995028365775777791055 61d-02
2	2.75329002532469803451508 4d-01	5.75330499190879242223814 0d-02
3	6.67276843443092766817388 6d-01	5.44515873542329347072685 9d-02
4	1.22030170218714632399571 9d+00	3.28316671746224500901151 5d-02
5	1.93292669416123314054290 6d+00	1.27000509599606821349646 5d-02
6	2.81399630587587786541262 2d+00	3.10589172607051194605586 9d-03
7	3.88024865780182787178838 5d+00	4.76882408608614462406276 0d-04
8	5.15214451976861610220925 7d+00	4.57559448776715778845111 5d-05
9	6.65303337160644082368476 1d+00	2.69669751837170198962372 2d-06
10	8.41237249041871469507148 1d+00	9.37340600950457028007584 9d-08
11	1.04716751022543949469899 8d+01	1.78763861269140326427310 0d-09
12	1.28942264844080851657406 5d+01	1.66279356809026140983055 4d-11
13	1.57852102945861989222862 2d+01	6.18642825449024628775120 4d-14
14	1.93461568809685973530213 2d+01	6.30757416906597403963049 3d-17
15	2.40933302797880327143082 2d+01	6.81516986221934686127314 8d-21

n	zero(n)	weight(n)
1	3.92495281104047429322002 0d-02	2.41670731274493708510569 6d-02
2	2.05535554960007626419084 8d-01	4.65941754047944222743085 2d-02
3	5.00130348992820627102325 9d-01	5.08620297667071825876609 6d-02
4	9.17605793669991637187948 3d-01	3.89007190105560185386430 6d-02
5	1.45447469103100190231296 0d+00	2.13776501007044942590461 3d-02
6	2.11178932946593526121554 7d+00	8.38153326035798032457060 2d-03
7	2.89541304910411068452794 7d+00	2.33106606615982001791618 6d-03
8	3.81417651191976627524649 4d+00	4.60838728715706437456151 3d-04
9	4.87788501146800629620947 7d+00	6.50516949502456452138737 8d-05
10	6.09673442915004658111809 7d+00	6.55314056773409248336274 8d-06
11	7.48207602187159834579607 1d+00	4.66489624438329265114435 4d-07
12	9.04774984688160328984445 4d+00	2.29925953989527924637102 0d-08
13	1.08115838420480420419075 4d+01	7.60410633980989492402996 8d-10
14	1.27972473540488678812889 5d+01	1.61435359898483920685361 6d-11
15	1.50370789630846995296626 2d+01	2.06857218791231878655628 2d-13
16	1.75770554077411003673039 8d+01	1.46489007595462238425843 6d-15
17	2.04864934942809249171335 8d+01	5.02041527897072381190139 0d-18
18	2.38796520291908910767916 7d+01	6.69608318777869768882276 4d-21
19	2.79747863317822072134831 4d+01	2.30059227735624335991638 1d-24
20	3.33313528039397845239703 0d+01	7.21232804093268640186175 2d-29

n	zero(n)	weight(n)
1	3.12108727955639275422641 06d-02	1.93831744692965915315238 5d-02
2	1.63707731829509564037590 1d-01	3.89207498680069900246461 2d-02
3	3.99327738243130471363646 5d-01	4.60982114808205403474309 0d-02
4	7.34469428777303507723095 5d-01	4.03360958822771902674805 5d-02
5	1.16601469101588565536809 9d+00	2.70458699022882388548963 8d-02
6	1.69295674013868135220381 4d+00	1.38841935850525058383433 6d-02
7	2.31716095303701636380470 2d+00	5.42537404646223366834821 1d-03
8	3.04288054250299686308393 3d+00	1.61300162146798421779924 9d-03
9	3.87554526215833125983446 1d+00	3.66720004903362294407900 4d-04
10	4.82078217951660307589762 4d+00	6.41523342272582923745075 1d-05
11	5.88417243807130219027982 5d+00	8.66102096121474272249792 8d-06
12	7.07158470247944187255971 6d+00	9.00354341602824822241150 5d-07
13	8.38970738950290159999562 1d+00	7.15095220288021785921085 5d-08
14	9.84656164056936370437379 6d+00	4.28389056345450059613483 4d-09
15	1.14519853834155055711443 8d+01	1.90172622508910976150909 4d-10
16	1.32181874329935288514667 8d+01	6.11400480113559864723492 5d-12
17	1.51605077903670165191031 9d+01	1.38239249297627509890100 9d-13
18	1.72985588025645341392551 3d+01	2.11668626562184281264418 5d-15
19	1.96580254002003868622408 1d+01	2.08855706401164951616375 1d-17
20	2.22736539579928116906077 2d+01	1.24171523227121230591881 2d-19
21	2.51945611495745942061065 5d+01	4.04560396401756169525269 5d-22
22	2.84945792477473729280092 6d+01	6.26581996659079557061800 0d-25
23	3.22952737910954369360872 0d+01	3.65470602600684723802723 6d-28
24	3.68289130274334091282270 5d+01	5.16480169991288951778987 5d-32
25	4.26917356393367841843218 9d+01	5.81575636846665832192833 6d-37

n	zero(n)	weight(n)
1	2.58822802615319535128016 5d-02	1.61650718251460592097048 8d-02
2	1.35897012809654851199003 2d-01	3.33294650883212869403543 7d-02
3	3.32021388734775488517225 3d-01	4.16015990343310625667579 8d-02
4	6.11766487230645420200505 3d-01	3.96550327179501860618760 1d-02
5	9.72642694252003546421136 5d-01	3.01699513882223331805702 7d-02
6	1.41317810925048642495047 2d+00	1.84005684401319432905569 7d-02
7	1.93361452983697676538845 4d+00	8.95499539701409203030517 0d-03
8	2.53595193958767871679819 4d+00	3.46887945726549354858378 4d-03
9	3.22337570986005126681500 0d+00	1.07228899134045675246477 3d-03
10	3.99950255060397780876235 7d+00	2.66076695253579604271265 9d-04
11	4.86789873686528567275262 8d+00	5.33197307677338355660092 0d-05
12	5.83200889972149737814654 6d+00	8.65963303914104779092225 8d-06
13	6.89535437025096095338343 6d+00	1.13988207518990604637906 3d-06
14	8.06180657433391016140359 6d+00	1.21195943075015947984732 6d-07
15	9.33582869876077755239063 1d+00	1.03420913444837995605478 3d-08
16	1.07226723619386051961474 5d+01	7.01981165085849065533007 2d-10
17	1.22285620032472531507581 6d+01	3.74700712531853850512056 9d-11
18	1.38609086914099051302684 8d+01	1.55097810210329473982710 8d-12
19	1.56285920880849127448593 6d+01	4.89441107262164215893665 8d-14
20	1.75423511499739486882139 9d+01	1.15336465096023891106338 4d-15
21	1.96153386979886425841027 2d+01	1.97848281006836127275994 4d-17
22	2.18639284139317656330250 8d+01	2.39322014271820583281116 5d-19
23	2.43089281488876125844446 5d+01	1.96040242011809239392327 5d-21
24	2.69774827643949940503155 9d+01	1.03156985747509687375576 7d-23
25	2.99062236144775797717247 8d+01	3.24746842112785216729662 3d-26
26	3.31468584115258551906539 1d+01	5.53301565941642541018842 6d-29
27	3.67770669480489353460272 9d+01	4.39124546479417188436072 4d-32
28	4.09247596495674274909451 1d+01	1.26965574423410955922115 6d-35
29	4.58344996016925934295552 d+01	8.39318222564375006703582 7d-40
30	5.21349414164747735220271 5d+01	3.90819833108670093130499 8d-45

n	zero(n)	weight(n)
1	2.20951735331255901839345 3d-02	1.38550978256702832883880 1d-02
2	1.16092353182799635664906 8d-01	2.91018608557695510833791 4d-02
3	2.83949711407800174692090 4d-01	3.76712566273750823818409 6d-02
4	5.23878048092414221969362 5d-01	3.80851192493926531525649 1d-02
5	8.33925569568502886138734 1d-01	3.15942351536975935747670 0d-02
6	1.21263530597870555632563 8d+00	2.16919239459257303432801 2d-02
7	1.65958596268979260236890 1d+00	1.22918292465216233253407 6d-02
8	2.17560179382021172289978 7d+00	5.72951977127393099519786 6d-03
9	2.76254118469927222590144 2d+00	2.19751136698948379184511 0d-03
10	3.42282143546613785887160 3d+00	6.96344862193064193040383 3d-04
11	4.15896841554986923613140 d+00	1.83376351458920200570948 6d-04
12	4.97338877879503716360589 5d+00	4.03462228036142771689799 6d-05
13	5.86837512367205173887761 4d+00	7.44100606481827429154243 7d-06
14	6.84624072447553893943973 3d+00	1.15121504265980164467768 5d-06
15	7.90947949131601604945125 4d+00	1.49167851702704306695276 8d-07
16	9.06089864892431732722192 3d+00	1.61298848764983345552280 4d-08
17	1.03037179030342147185219 6d+01	1.44799809200631988813476 1d-09
18	1.16416506758390332057493 0d+01	1.07205686381345782986088 8d-10
19	1.30789864888720424686886 4d+01	6.49414039864930398903416 8d-12
20	1.46206899538384633139308 9d+01	3.18853003446180293050921 9d-13
21	1.62725284544009099833803 9d+01	1.25492824491209867961973 7d-14
22	1.80412403194728877772225 6d+01	3.90798467877573331013442 8d-16
23	1.99347586235038537231010 5d+01	9.48212587572669153175586 6d-18
24	2.19625129686091937102608 6d+01	1.75997259575306656759433 7d-19
25	2.41358440329084461412713 1d+01	2.44426708835450509808106 4d-21
26	2.64685867401832477243568 0d+01	2.47232383752572278503790 1d-23
27	2.89779149562912380001166 7d+01	1.76121707552056809878091 4d-25
28	3.16856092154185780057825 2d+01	8.46853755413455002414615 5d-28
29	3.46200440123617156169370 7d+01	2.60053533291075448181335 3d-30
30	3.78194774650371047774801 9d+01	4.73400770251423201193002 3d-33
31	4.13378922050296757384049 6d+01	4.60017616805595687146864 d-36
32	4.52563863270673774508486 0d+01	2.03954166879719346431965 3d-39
33	4.97085502171998659863181 9d+01	3.18999832836126041727796 9d-43
34	5.49500001211371046132233 1d+01	1.08032044837011322958217 1d-47
35	6.16385712059240156202305 8d+01	2.30139089248380075462645 3d-53

n	zero(n)	weight(n)
1	1.92672519829316553908651 48-02	1.21178082780836937880133 3d-02
2	1.01283386041782977973573 2d-01	2.58042152339834795031140 1d-02
3	2.47927521221687191542970 d-01	3.43053128488967380112260 4d-02
4	4.57869233636184973669477 d-01	3.61970384242542044919000 8d-02
5	7.29570260935723154300680 73-01	3.19665085865257393429045 2d-02
6	1.06172422958227705960241 68+00	2.39118450629913796152928 4d-02
7	1.45366047253123397953063 03+00	1.51378380810463864276060 2d-02
8	1.90558013129430203959879 33+00	8.08388104026013314257379 9d-03
9	2.41852507436018785066573 1d+00	3.63722251800023904533092 8d-03
10	2.99411189887638329187814 5d+00	1.38185380568530014406818 2d-03
11	3.63418755758242198608912 4d+00	4.45370159380604217302658 1d-04
12	4.34057257064239302623690 2d+00	1.22428427762488838071630 7d-04
13	5.11496425562242857353763 1d+00	2.88343661321707987634559 5d-05
14	5.95897149681102234433417 5d+00	5.83476788984153404409690 9d-06
15	6.87421100905220627930720 3d+00	1.01533524729895555012088 0d-06
16	7.86240798979230875305535 5d+00	1.51814607088699970201736 3d-07
17	8.92547532866260117352114 6d+00	1.94617060006721905994366 2d-08
18	1.00655669679182635528985 32d+01	2.13196509028547463784624 8d-09
19	1.12851334571923101616397 7d+01	1.98739098700860459639088 4d-10
20	1.25869332021824357631312 6d+01	1.56856368138005420096625 1d-11
21	1.39741023063811952732440 8d+01	1.04204832723060706122991 2d-12
22	1.54501935003519656049943 2d+01	5.78769001721802624376197 0d-14
23	1.70192451043717780960852 6d+01	2.66677057588797970742030 3d-15
24	1.86858650563320875023591 4d+01	1.01032283286016433419168 4d-16
25	2.04553378620068563642717 d+01	3.11509761627283923422064 7d-18
26	2.23337617554478024065417 0d+01	7.72431598025899081406321 05d-20
27	2.43282266440133194439344 3d+01	1.51919133450402253300876 7d-21
28	2.64470485111170253144164 1d+01	2.33166243885737874346597 4d-23
29	2.87000838237938411722543 7d+01	2.73930377342987634739610 8d-25
30	3.10991604256174427212717 2d+01	2.40700177871601591496397 4d-27
31	3.36586831482343063951261 7d+01	1.53788259146453518937742 5d-29
32	3.63965107943294510126543 1d+01	6.89919212739192509977760 9d-32
33	3.93352724058536652091922 9d+01	2.07912196797451798132243 5d-34
34	4.25044311307010450610846 5d+01	3.97350220388638310463312 8d-37
35	4.59437017802616420068305 0d+01	4.45704605324906815745868 2d-40
36	4.97091212444506157875466 0d+01	2.63126292583014684501022 2d-43
37	5.38848924950567787119794 0d+01	6.94466688409045677007158 d-47
38	5.86097842577410784063914 8d+01	6.26947390405357922920107 8d-51
39	6.41495086882712996519876 4d+01	1.16446960991100357764966 4d-55
40	7.11885664236220273315669 3d+01	1.22524929887474809745991 2d-61

20.6. [119] "A NOTE ON THE CONTOUR INTEGRAL REPRESENTATION OF THE REMAINDER TERM FOR A GAUSS–CHEBYSHEV QUADRATURE RULE"

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[119] (with E. Tychopoulos and R. S. Varga) "A Note on the Contour Integral Representation of the Remainder Term for a Gauss–Chebyshev Quadrature Rule," *SIAM J. Numer. Anal.* **27**, 219–224 (1990).

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A NOTE ON THE CONTOUR INTEGRAL REPRESENTATION OF THE REMAINDER TERM FOR A GAUSS-CHEBYSHEV QUADRATURE RULE*

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Abstract. It is shown that the kernel $K_n(z)$, $n(\text{even}) \geqq 2$, in the contour integral representation of the remainder term of the n-point Gauss formula for the Chebyshev weight function of the second kind, as z varies on the ellipse $\mathscr{E}_\rho = \{z: z = \rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta},\ 0 \leqq \vartheta \leqq 2\pi\}$, $\rho > 1$, assumes its largest modulus on the imaginary axis if $\rho \geqq \rho_{n+1}$, where ρ_{n+1} is the root of a certain algebraic equation. If $1 < \rho < \rho_{n+1}$, the maximum is attained near the imaginary axis within an angular distance less than $\pi/(2n+2)$. The bounds $\{\rho_{n+1}\}$ decrease monotonically to 1.

Key words. Gauss-Chebyshev quadrature, remainder term for analytic functions, kernel of contour integral representation

AMS(MOS) subject classification. 65D32

1. We are dealing here with the remainder term $R_n(f)$ of the Gaussian quadrature rule for the Chebyshev weight function of the second kind,

$$\int_{-1}^{1} f(t)(1-t^2)^{1/2}\,dt = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f), \tag{1.1}$$

where $\tau_\nu^{(n)} = \cos(\nu\pi/(n+1))$, $\lambda_\nu^{(n)} = \pi \sin^2(\nu\pi/(n+1))/(n+1)$, $\nu = 1, 2, \cdots, n$. We assume that f is analytic inside of, and continuous on, an ellipse

$$\mathscr{E}_\rho = \{z: z = \tfrac{1}{2}(u + u^{-1}),\ u = \rho e^{i\vartheta},\ 0 \leqq \vartheta \leqq 2\pi\} \tag{1.2}$$

with foci at $z = \pm 1$ and with the sum of the semi-axes equal to ρ, $\rho > 1$. The remainder $R_n(f)$ of (1.1) has the form (cf. [1])

$$R_n(f) = \frac{1}{2\pi i} \int_{\mathscr{E}_\rho} K_n(z) f(z)\,dz, \tag{1.3}$$

so that

$$|R_n(f)| \leqq \frac{l(\mathscr{E}_\rho)}{2\pi} \max_{z \in \mathscr{E}_\rho} |f(z)| \cdot \max_{z \in \mathscr{E}_\rho} |K_n(z)|, \tag{1.3'}$$

where $l(\mathscr{E}_\rho)$ denotes the length of $\mathscr{E}_\rho$. Since $f(z)$ and $\mathscr{E}_\rho$ are assumed known, the first two terms on the right side of (1.3') can be calculated, and our interest then is in determining *where* on $\mathscr{E}_\rho$ the kernel $K_n(z)$ assumes its *maximum modulus*. In view of $K_n(\bar{z}) = \overline{K_n(z)}$ and $K_n(-\bar{z}) = -\overline{K_n(z)}$, the modulus of K_n is symmetric with respect to both coordinate axes:

$$|K_n(\bar{z})| = |K_n(z)|, \qquad |K_n(-\bar{z})| = |K_n(z)|. \tag{1.4}$$

Thus, consideration may be restricted to the first quarter of $\mathscr{E}_\rho$, i.e., to the interval $0 \leqq \vartheta \leqq \pi/2$ in (1.2).

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It is known that, when n is odd, the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$ is attained on the imaginary axis [1, Thm. 5.2]. It is remarked in [1] that when n is even, the maximum "... is attained slightly off the imaginary axis." The purpose of this note is to amplify this statement and make it more precise. Defining

$$a_j = a_j(\rho) = \tfrac{1}{2}(\rho^j + \rho^{-j}), \quad j = 1, 2, 3, \cdots, \quad \rho > 1, \tag{1.5}$$

we will prove, in fact, the following theorem.

THEOREM 1. *For each positive integer n with $n \geqq 2$, let $\rho_n > 1$ be the unique root of*

$$\frac{a_1(\rho)}{a_n(\rho)} = \frac{1}{n} \qquad (\rho > 1). \tag{1.6}$$

Then, if $n \geqq 2$ is even, we have

$$\max_{z \in \mathscr{E}_\rho} |K_n(z)| = \left| K_n\left(\frac{i}{2}(\rho - \rho^{-1})\right)\right| \quad \text{if } \rho \geqq \rho_{n+1}, \tag{1.7}$$

i.e., the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$, when $\rho \geqq \rho_{n+1}$, is attained on the imaginary axis. If $1 < \rho < \rho_{n+1}$, then the maximum in (1.7) is attained at some $z = z^* = \frac{1}{2}(\rho e^{i\vartheta^*} + \rho^{-1} e^{-i\vartheta^*}) \in \mathscr{E}_\rho$ with $(n/(n+1))\pi/2 < \vartheta^* < \pi/2$.

In Table 1 we display ρ_n for $n = 2(1)40$ to 10 decimal places. Since $\rho^{-(n-1)} < a_1(\rho)/a_n(\rho) < 2\rho/\rho^n = 2\rho^{-(n-1)}$ for $\rho > 1$, putting $\rho = \rho_n$ we obtain from (1.6) that

$$n^{1/(n-1)} < \rho_n < (2n)^{1/(n-1)}. \tag{1.8}$$

This shows, in particular, that $\rho_n \to 1$ as $n \to \infty$. The next theorem establishes monotonicity of the ρ_n and sharpens the bounds in (1.8).

THEOREM 2. *The roots $\rho_n > 1$ of (1.6) satisfy*

$$\rho_n > \rho_{n+1} \quad \text{for all } n \geqq 2. \tag{1.9}$$

Moreover, if $\lambda_n := (2n)^{1/n}$, and if μ_n, $n \geqq 2$, is the unique positive root (by Descartes' rule of signs) of

$$M_n(\mu) = 0, \qquad M_n(\mu) := \mu^{n+1} - n(\mu^2 + 1), \tag{1.10}$$

then

$$\lambda_n < \rho_n < \mu_n \quad \text{for all } n \geqq 2. \tag{1.11}$$

It is easily seen that the bounds in (1.11) are sharper than those in (1.8), except when $n = 2$, in which case the lower bounds are both equal to 2.

TABLE 1
The roots $\rho_n > 1$ of (1.6).

n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n
		11	1.3290434092	21	1.1956793660	31	1.1427199553
2	2.2966302629	12	1.3068931058	22	1.1884619640	32	1.1390810161
3	1.9318516526	13	1.2878200461	23	1.1818092074	33	1.1356405646
4	1.7390838834	14	1.2712053026	24	1.1756552136	34	1.1323822718
5	1.6180339887	15	1.2565878778	25	1.1699441267	35	1.1292915806
6	1.5341771340	16	1.2436169389	26	1.1646282627	36	1.1263554696
7	1.4722691130	17	1.2320204906	27	1.1596666536	37	1.1235622539
8	1.4244774799	18	1.2215842188	28	1.1550238943	38	1.1209014162
9	1.3863414780	19	1.2121368378	29	1.1506692205	39	1.1183634632
10	1.3551231521	20	1.2035397132	30	1.1465757653	40	1.1159398028

The proofs of Theorems 1 and 2 will be given in §§ 3 and 4, respectively. Section 2 contains some auxiliary results.

2.

LEMMA 1. *For each positive integer n, set*

$$\varphi_n(\sigma) := \frac{\sin \sigma\pi}{\sin((1-\sigma)\pi/(n+1))}, \qquad 0 \leqq \sigma \leqq 1, \tag{2.1}$$

where $\varphi_n(1) := \lim_{\sigma \uparrow 1} \varphi_n(\sigma)$. *Then* $\varphi_n(\sigma)$ *increases monotonically from* $\varphi_n(0) = 0$ *to* $\varphi_n(1) = n+1$ *as* σ *varies from zero to* 1.

Proof. Since $\sin \sigma\pi = \sin[(1-\sigma)\pi]$, we can write $\varphi_n(\sigma)$ as

$$\varphi_n(\sigma) = \frac{\sin[(n+1)u]}{\sin u} \quad \text{where} \quad \frac{(1-\sigma)\pi}{n+1} =: u,$$

so that $0 \leqq u \leqq \pi/(n+1)$. Furthermore,

$$\frac{\sin[(n+1)u]}{\sin u} = U_n(x) \qquad (\cos u =: x),$$

where $U_n(x)$ is the Chebyshev polynomial (of the second kind) of degree n. It is well known that $U_n(x)$ is increasing from $U_n(\cos(\pi/(n+1))) = 0$ to $U_n(1) = n+1$ as x increases from $\cos(\pi/(n+1))$ to 1 (hence σ increases from zero to 1), from which the assertions of Lemma 1 follow. □

LEMMA 2. *Let* φ_n *be as in Lemma* 1, *and set*

$$\psi_n(\sigma) := \cos \sigma\pi + (n+1)\varphi_n(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right), \qquad 0 \leqq \sigma \leqq 1. \tag{2.2}$$

Then $\psi_n(\sigma)$ *increases monotonically from* $\psi_n(0) = 1$ *to* $\psi_n(1) = (n+1)^2 - 1$ *as* σ *varies from zero to* 1.

Proof. The limit values follow directly from the limit values of φ_n in Lemma 1. Differentiating (2.2), we get

$$\begin{aligned}
\psi_n'(\sigma) &= -\pi \sin \sigma\pi + \pi\varphi_n(\sigma) \sin\left(\frac{1-\sigma}{n+1}\pi\right) + (n+1)\varphi_n'(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right) \\
&= -\pi \sin \sigma\pi + \pi \sin \sigma\pi + (n+1)\varphi_n'(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right) \\
&= (n+1)\varphi_n'(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right),
\end{aligned}$$

which is positive by Lemma 1. □

3.

Proof of Theorem 1. From [1, eq. (5.9)] we have

$$(\pi^{-1}\rho^{n+1}|K_n(z)|)^2 = \frac{a_2(\rho) - \cos 2\vartheta}{a_{2n+2}(\rho) - \cos 2(n+1)\vartheta}, \tag{3.1}$$

$$z = \tfrac{1}{2}(\rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}) \in \mathscr{E}_\rho.$$

By (1.4), it suffices to consider $0 \leqq \vartheta \leqq \pi/2$. Denote

$$\kappa_n(\vartheta) = \frac{a_2 - \cos 2\vartheta}{a_{2n+2} - \cos 2(n+1)\vartheta}, \tag{3.2}$$

where a_2, a_{2n+2} are as defined in (1.5). By symmetry,

$$\kappa_n'(0) = \kappa_n'\left(\frac{\pi}{2}\right) = 0. \tag{3.3}$$

Let

$$\vartheta_n := \frac{n}{n+1}\frac{\pi}{2}. \tag{3.4}$$

Since $\cos 2\vartheta \geqq \cos 2\vartheta_n$ for $0 \leqq \vartheta \leqq \vartheta_n$, we have

$$\kappa_n(\vartheta) \leqq \frac{a_2 - \cos 2\vartheta_n}{a_{2n+2}-1} = \kappa_n(\vartheta_n), \qquad 0 \leqq \vartheta \leqq \vartheta_n, \tag{3.5}$$

where the equality on the right follows from $\cos 2(n+1)\vartheta_n = \cos n\pi = 1$, since n is even. Differentiating (3.2) gives

$$[a_{2n+2} - \cos 2(n+1)\vartheta]\kappa_n'(\vartheta) + \kappa_n(\vartheta)\cdot 2(n+1)\sin 2(n+1)\vartheta = 2\sin 2\vartheta, \tag{3.6}$$

from which it follows that $(a_{2n+2}-1)\kappa_n'(\vartheta_n) = 2\sin 2\vartheta_n$, hence

$$\kappa_n'(\vartheta_n) > 0. \tag{3.7}$$

Letting $\max_{0\leqq\vartheta\leqq\pi/2}\kappa_n(\vartheta) = \kappa_n(\vartheta^*)$, we conclude from (3.5) and (3.7) that

$$\vartheta_n < \vartheta^* \leqq \frac{\pi}{2}. \tag{3.8}$$

Differentiating (3.6) once more, and then setting $\vartheta = \pi/2$, gives

$$\frac{1}{4}(a_{2n+2}+1)\kappa_n''\left(\frac{\pi}{2}\right) = (n+1)^2\frac{a_2+1}{a_{2n+2}+1} - 1 = \left[(n+1)\frac{a_1}{a_{n+1}}\right]^2 - 1, \tag{3.9}$$

since $a_2+1 = 2a_1^2$, $a_{2n+2}+1 = 2a_{n+1}^2$. From the definition of ρ_n (cf. (1.6)) and from the fact that $a_1(\rho)/a_{n+1}(\rho)$ for $\rho > 1$ decreases monotonically, we get from (3.9) that

$$\kappa_n''(\pi/2) \gtrless 0 \quad \text{iff } \rho \lessgtr \rho_{n+1}. \tag{3.10}$$

If $1 < \rho < \rho_{n+1}$, i.e., $\kappa_n''(\pi/2) > 0$, it is clear from the second relation in (3.3) that $\vartheta^* < \pi/2$ in (3.8), proving the second statement of the theorem.

If $\rho \geqq \rho_{n+1}$, i.e., $\kappa_n''(\pi/2) \leqq 0$, we now show that

$$\kappa_n'(\vartheta) > 0 \quad \text{for } \vartheta_n < \vartheta < \frac{\pi}{2} \qquad (\rho \geqq \rho_{n+1}). \tag{3.11}$$

We introduce the variable σ by

$$\vartheta = \frac{n+\sigma}{n+1}\frac{\pi}{2}, \qquad 0 < \sigma < 1. \tag{3.12}$$

Using $(n+\sigma)/(n+1) = 1-(1-\sigma)/(n+1)$, we can rewrite (3.6) in the form

$$\frac{[a_{2n+2}-\cos\sigma\pi]^2}{2\sin((1-\sigma)\pi/(n+1))}\kappa_n'(\vartheta) = a_{2n+2} - (n+1)a_2\varphi_n(\sigma) - \psi_n(\sigma), \tag{3.13}$$

with $\varphi_n(\sigma)$ and $\psi_n(\sigma)$ as defined in Lemmas 1 and 2, respectively. By the assumption $\rho \geqq \rho_{n+1}$, which implies $a_{n+1} \geqq (n+1)a_1$, hence

$$a_{2n+2} = 2a_{n+1}^2 - 1 \geqq 2(n+1)^2a_1^2 - 1 = (n+1)^2(a_2+1) - 1,$$

and using Lemmas 1 and 2, we find that the right-hand side of (3.13) is larger than or equal to

$$(n+1)^2(a_2+1)-1-(n+1)a_2\varphi_n(\sigma)-\psi_n(\sigma)$$
$$>(n+1)^2(a_2+1)-1-(n+1)^2a_2-[(n+1)^2-1]=0, \qquad 0<\sigma<1.$$

Therefore, $\kappa_n'(\vartheta)>0$ for $\vartheta_n<\vartheta<\pi/2$, showing that $\vartheta^*=\pi/2$ in (3.8). □

4. We precede the proof of Theorem 2 with the following lemma.

LEMMA 3. *With λ_n and μ_n as defined in Theorem 2, there holds*

$$\lambda_n>\mu_{n+1} \quad \textit{for all } n\geqq 2. \tag{4.1}$$

Proof. Since $M_n(\mu)$, $n\geqq 2$, in (1.10) has a unique positive zero μ_n, and since $M_n(+\infty)=+\infty$, it is evident that $M_{n+1}(\mu)>0$ implies $\mu>\mu_{n+1}$. It suffices, therefore, to show that

$$M_{n+1}(\lambda_n)>0 \quad \text{for } n\geqq 2. \tag{4.2}$$

This is clearly true when $n=2$, since $\lambda_2=2$ and $M_3(\lambda_2)=1$. We may thus assume that $n\geqq 3$.

We have

$$M_{n+1}(\lambda_n)=\lambda_n^2\cdot\lambda_n^n-(n+1)(\lambda_n^2+1)=\lambda_n^2\cdot 2n-(n+1)(\lambda_n^2+1)=-(n+1)+(n-1)\lambda_n^2.$$

When we write $\lambda_n=e^{l_n}$, $l_n=n^{-1}\log 2n$, there follows

$$M_{n+1}(\lambda_n)=-(n+1)+(n-1)\,e^{2l_n}=-(n+1)+(n-1)[1+2l_n+e^{2l_n}-(1+2l_n)]$$
$$=2[-1+(n-1)l_n]+(n-1)[e^{2l_n}-(1+2l_n)].$$

Here, the expression in the last bracket is clearly positive, and an elementary calculation shows that $-1+(n-1)l_n=-1+(1-n^{-1})\log 2n>0$ if $n\geqq 3$. □

Proof of Theorem 2. To establish (1.9), it suffices to prove the inequalities (1.11), since combining them with the inequality in Lemma 3 immediately gives $\rho_n>\lambda_n>\mu_{n+1}>\rho_{n+1}$ for all $n\geqq 2$.

Now (1.6) is equivalent to

$$L_n(\rho):=\rho^{2n}-n\rho^{n+1}-n\rho^{n-1}+1=0. \tag{4.3}$$

Clearly, L_n (by Descartes' rule of signs) has at most two positive zeros. Since $L_n(0)=1$, $L_n(1)=2-2n<0$, and $L_n(+\infty)=+\infty$, there are exactly two positive zeros, one in $(0,1)$ and the other in $(1,\infty)$. (Because ρ and ρ^{-1} occur symmetrically in (1.6), one zero is the reciprocal of the other.) The larger of the two, as in Theorem 1, is denoted by ρ_n.

We have

$$L_n(\rho)=\rho^{2n}+\rho^{2n-2}-\rho^{2n-2}-n\rho^{n-1}(\rho^2+1)+1$$
$$=\rho^{2n-2}(\rho^2+1)-\rho^{2n-2}-n\rho^{n-1}(\rho^2+1)+1,$$

so that the equation in (4.3), after division by $\rho^{n-1}(\rho^2+1)$, can be written in the form

$$\rho^{n-1}-\frac{\rho^{n-1}}{\rho^2+1}+\frac{1}{\rho^{n-1}(\rho^2+1)}=n. \tag{4.4}$$

Since $L_n(\rho_n)=0$, dropping the third term on the left of (4.4), we arrive at

$$\rho_n^{n-1}-\frac{\rho_n^{n-1}}{\rho_n^2+1}<n \quad \text{or} \quad \rho_n^{n+1}-n(\rho_n^2+1)<0.$$

In terms of the function M_n in (1.10), this says $M_n(\rho_n)<0$, and hence implies $\rho_n<\mu_n$, the right inequality in (1.11).

To prove the left inequality of (1.11), we will show that

$$L_n(\lambda_n)<0 \quad \text{for all } n\geqq 2. \tag{4.5}$$

We now express $L_n(\rho)$ from (4.3) as

$$\begin{aligned} L_n(\rho) &= \rho^{2n}-2n\rho^n+1+2n\rho^n-n\rho^n\left(\rho+\frac{1}{\rho}\right) \\ &= \rho^n(\rho^n-2n)+1+n\rho^n\left[2-\left(\rho+\frac{1}{\rho}\right)\right]. \end{aligned}$$

Since $\lambda_n=(2n)^{1/n}=e^{l_n}$, $l_n=n^{-1}\log 2n$, this gives

$$L_n(\lambda_n)=1+4n^2(1-\cosh l_n)=1-2n^2l_n^2-4n^2[\cosh l_n-1-\tfrac{1}{2}l_n^2].$$

The expression in brackets, when expanded in Taylor's series, involves only positive terms and hence is positive, while $1-2n^2l_n^2=1-2(\log 2n)^2<0$ for all $n\geqq 2$. This establishes (4.5) and completes the proof of Theorem 2. □

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The remainder term for analytic functions of Gauss–Radau and Gauss–Lobatto quadrature rules with multiple end points *

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Abstract: A study is undertaken of the kernels in the contour integral representations of the remainder terms for Gauss–Radau and Gauss–Lobatto quadrature rules over the interval $[-1, 1]$. It is assumed that the respective end points in these rules have multiplicity two, and that integration is with respect to one of the four Chebyshev weight functions. Of particular interest is the location on the contour where the modulus of the kernel attains its maximum value. Only elliptic contours are considered having foci at the points ± 1.

Keywords: Gauss–Radau and Gauss–Lobatto quadrature rules, multiple end points, remainder term for analytic functions, contour integral representation.

1. Introduction

We continue here the analysis of the remainder term of quadrature rules for analytic functions, initiated in [3,4] for Gaussian quadrature rules, to deal with Gauss–Radau and Gauss–Lobatto rules with multiple end points, in particular, end points of multiplicity two. The case of simple end points was treated in [2]. The object is to determine where precisely the kernel in the contour integral representation of the remainder attains its maximum modulus along the contour. Of special interest are elliptic contours. As in [2], we will concentrate on the four Chebyshev weight functions.

The Gauss–Radau rule with (positive) weight function w and end point -1 of multiplicity r is given by

$$\int_{-1}^{1} f(t)w(t)\,\mathrm{d}t = \sum_{\rho=0}^{r-1} \kappa_{\rho}^{\mathrm{R}} f^{(\rho)}(-1) + \sum_{\nu=1}^{n} \lambda_{\nu}^{\mathrm{R}} f\left(\tau_{\nu}^{\mathrm{R}}\right) + R_{n,r}^{\mathrm{R}}(f), \tag{1.1$_{\mathrm{R}}$}$$

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where the remainder $R_{n,r}^{\mathrm{R}}(f)$ is zero whenever f is a polynomial of degree $\leqslant 2n+r-1$,

$$R_{n,r}^{\mathrm{R}}(f)=0, \quad \text{all } f\in\mathbb{P}_{2n+r-1}. \tag{1.2$_{\mathrm{R}}$}$$

This in particular implies that τ_ν^{R} must be the zeros of the polynomial $\pi_n(\cdot;\, w^{\mathrm{R}})$ of degree n orthogonal on $[-1, 1]$ with respect to the weight function

$$w^{\mathrm{R}}(t)=(t+1)^r w(t). \tag{1.3$_{\mathrm{R}}$}$$

(The case where $+1$ is the given end point is easily reduced to (1.1$_{\mathrm{R}}$) by a change of variables.) Similarly, the Gauss–Lobatto rule (with end points of the same multiplicity, for simplicity) is

$$\int_{-1}^{1} f(t)w(t)\,\mathrm{d}t=\sum_{\rho=0}^{r-1}\kappa_\rho^{\mathrm{L}} f^{(\rho)}(-1)+\sum_{\nu=1}^{n}\lambda_\nu^{\mathrm{L}} f(\tau_\nu^{\mathrm{L}})+\sum_{\rho=0}^{r-1}(-1)^\rho\mu_\rho^{\mathrm{L}} f^{(\rho)}(1)+R_{n,r}^{\mathrm{L}}(f), \tag{1.1$_{\mathrm{L}}$}$$

where now

$$R_{n,r}^{\mathrm{L}}(f)=0, \quad \text{all } f\in\mathbb{P}_{2n+2r-1}, \tag{1.2$_{\mathrm{L}}$}$$

and τ_ν^{L} are the zeros of $\pi_n(\cdot;\, w^{\mathrm{L}})$, with

$$w^{\mathrm{L}}(t)=(t^2-1)^r w(t). \tag{1.3$_{\mathrm{L}}$}$$

Letting

$$\omega_{n,r}^{\mathrm{R}}(z;\, w)=(z+1)^r\pi_n(z;\, w^{\mathrm{R}}), \qquad \omega_{n,r}^{\mathrm{L}}(z;\, w)=(z^2-1)^r\pi_n(z;\, w^{\mathrm{L}}), \tag{1.4}$$

and defining

$$\rho_{n,r}^{\mathrm{R,L}}(z;\, w)=\int_{-1}^{1}\frac{\omega_{n,r}^{\mathrm{R,L}}(t;\, w)}{z-t}w(t)\,\mathrm{d}t, \quad z\in\mathbb{C}\setminus[-1, 1], \tag{1.5}$$

(where, to save space, we have combined two formulae into one), we have for the remainders in (1.1$_{\mathrm{R}}$) and (1.1$_{\mathrm{L}}$), when f is analytic in a domain $\mathscr{D}$ containing $[-1, 1]$,

$$R_{n,r}^{\mathrm{R,L}}(f)=\frac{1}{2\pi\mathrm{i}}\oint_\Gamma K_{n,r}^{\mathrm{R,L}}(z;\, w)f(z)\,\mathrm{d}z. \tag{1.6}$$

Here, Γ is any contour in $\mathscr{D}$ surrounding $[-1, 1]$, and the kernels $K_{n,r}^{\mathrm{R,L}}$ are given by

$$K_{n,r}^{\mathrm{R,L}}(z;\, w)=\frac{\rho_{n,r}^{\mathrm{R,L}}(z;\, w)}{\omega_{n,r}^{\mathrm{R,L}}(z;\, w)}, \quad z\in\Gamma. \tag{1.7}$$

This follows readily from Hermite's formula for the remainder term of interpolation (cf. [1, Theorem 3.6.1 and Corollary 3.6.3]) and subsequent integration over t. Clearly,

$$K_{n,r}^{\mathrm{R,L}}(\bar z;\, w)=\overline{K_{n,r}^{\mathrm{R,L}}(z;\, w)}. \tag{1.8}$$

It is useful to note that the normalization of the orthogonal polynomial π_n in (1.4) is unimportant, since any nonzero multiplicative factor will cancel out when the kernel is formed in (1.7). We shall frequently make use of this freedom later on, without special mention.

From (1.6) one obtains the estimate

$$|R_{n,r}^{\mathrm{R,L}}(f)|\leqslant\frac{1}{2\pi}l(\Gamma)\max_{z\in\Gamma}|K_{n,r}^{\mathrm{R,L}}(z;\, w)|\max_{z\in\Gamma}|f(z)|, \tag{1.9}$$

where $l(\Gamma)$ is the length of Γ. Our interest will focus on the first maximum in (1.9), where it is useful to know the location on Γ where the maximum is attained. For the actual computation of

$K_{n,r}^{R,L}(z; w)$, for fixed $z \in \Gamma$, we refer to the discussion in [4, §4]. In the following, we limit ourselves to elliptic contours,

$$\Gamma = \mathscr{E}_\rho = \{ z \in \mathbb{C} : z = \tfrac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta}), 0 \leqslant \theta \leqslant 2\pi \}, \quad \rho > 1, \tag{1.10}$$

which we consider to be more flexible than circular contours. Indeed, they can be chosen (by selecting ρ sufficiently close to 1) to snuggle tightly around the interval $[-1, 1]$, thereby avoiding possible singularities of f and preventing excessive growth of f along Γ. We shall furthermore assume throughout that $r = 2$ in $(1.1_{R,L})$, i.e., we are dealing only with end points of multiplicity 2.

We begin in Section 2 with collecting explicit expressions for the kernels $K_{n,2}^{R,L}(\cdot; w)$ in the cases where w is any one of the four Chebyshev weight functions. The study of their maxima on Γ is then carried out in Section 3 for Radau, and in Section 4 for Lobatto formulae. Precise theorems will be established whenever possible, numerical and asymptotic analyses given otherwise.

2. The remainder kernels for Chebyshev weight functions

In this section we are gathering explicit expressions for the kernels $K_{n,2}^{R,L}(z; w)$ in (1.7), in the case where w is any one of the four Chebyshev weight functions

$$\begin{aligned} w_1(t) &= (1-t^2)^{-1/2}, & w_2(t) &= (1-t^2)^{1/2}, \\ w_3(t) &= (1-t)^{-1/2}(1+t)^{1/2}, & w_4(t) &= (1-t)^{1/2}(1+t)^{-1/2}. \end{aligned} \tag{2.1}$$

The expressions will all be in terms of the variable u, which is connected with z through the familiar relation

$$z = \tfrac{1}{2}(u + u^{-1}), \quad |u| > 1. \tag{2.2}$$

Since the derivations are often very similar to those in [2], we will limit ourselves to brief indications. More details will be provided only when new considerations are required.

2.1. Gauss–Radau formulae

For $w = w_1$, we have from (1.3_R) that

$$w_1^R(t) = (t+1)^2 w_1(t) = (1-t)^{-1/2}(1+t)^{3/2},$$

so that by (1.4) and [2, Lemma 3.3]

$$\omega_{n,2}^R(z; w_1) = (1+z)\left\{ V_{n+1}(z) + \frac{2n+3}{2n+1} V_n(z) \right\}, \tag{2.3}$$

where V_n is the Chebyshev polynomial of the third kind. Therefore, by (1.5), since $(1+t)w_1(t) = w_3(t)$,

$$\rho_{n,2}^R(z; w_1) = \int_{-1}^{1} \frac{V_{n+1}(t) + \dfrac{2n+3}{2n+1} V_n(t)}{z-t} w_3(t)\, dt. \tag{2.4}$$

Now using in (2.3), (2.4) the known expressions for $V_n(z)$ and $\int_{-1}^{1} V_n(t)w_3(t)\,dt/(z-t)$ in terms of the variable u of (2.2) (cf. [2, Eq. (3.14)]), and applying (1.7), one obtains

$$K_{n,2}^{R}(z;\, w_1) = \frac{4\pi}{(u^2-1)u^n} \frac{u + \dfrac{2n+1}{2n+3}}{\dfrac{2n+1}{2n+3}\left[u^{n+2} + u^{-(n+1)}\right] + \left[u^{n+1} + u^{-n}\right]}. \tag{2.5}$$

In the case $w = w_2$, we have $w_2^{R}(t) = (1-t)^{1/2}(1+t)^{5/2}$, which requires two applications of [2, Lemma 3.2] to obtain

$$\omega_{n,2}^{R}(z;\, w_2) = U_{n+2}(z) + 4\frac{n+3}{2n+3}U_{n+1}(z) + \frac{(n+3)(2n+5)}{(n+1)(2n+3)}U_n(z), \tag{2.6}$$

with U_n denoting the Chebyshev polynomial of the second kind. In combination with (1.5) and [2, Eq. (3.6)], this then yields

$$K_{n,2}^{R}(z;\, w_2) = \frac{\pi(u^2-1)}{u^{n+4}} \times \frac{u^2 + \alpha_n u + \beta_n}{\beta_n\left[u^{n+3} - u^{-(n+3)}\right] + \alpha_n\left[u^{n+2} - u^{-(n+2)}\right] + \left[u^{n+1} - u^{-(n+1)}\right]},$$

$$\alpha_n = 4\frac{n+1}{2n+5}, \qquad \beta_n = \frac{(n+1)(2n+3)}{(n+3)(2n+5)}. \tag{2.7}$$

Similarly, when $w = w_3$, then $w_3^{R}(t) = (1-t)^{-1/2}(1+t)^{5/2}$, and two applications of [2, Lemma 3.3 and Eq. (3.14)] give

$$K_{n,2}^{R}(z;\, w_3) = \frac{2\pi(u+1)}{(u-1)u^{n+2}} \times \frac{u^2 + \alpha_n u + \beta_n}{\beta_n\left[u^{n+3} + u^{-(n+2)}\right] + \alpha_n\left[u^{n+2} + u^{-(n+1)}\right] + \left[u^{n+1} + u^{-n}\right]},$$

$$\alpha_n = \frac{2n+1}{n+2}, \qquad \beta_n = \frac{(n+1)(2n+1)}{(n+2)(2n+5)}. \tag{2.8}$$

Finally, for $w = w_4$, we have $w_4^{R}(t) = (1-t)^{1/2}(1+t)^{3/2}$, and [2, Lemma 3.2 and Eq. (3.6)] combine to produce

$$K_{n,2}^{R}(z;\, w_4) = \frac{2\pi(u-1)}{(u+1)u^{n+2}} \frac{u + \dfrac{n+1}{n+2}}{\dfrac{n+1}{n+2}\left[u^{n+2} - u^{-(n+2)}\right] + \left[u^{n+1} - u^{-(n+1)}\right]}. \tag{2.9}$$

2.2. *Gauss–Lobatto formulae*

For $w = w_1$ we have from (1.3_L) that

$$w_1^{L}(t) = (1-t^2)^2 w_1(t) = (1-t^2)^{3/2},$$

so that [2, Lemma 3.1] and the same argumentation as used in [2, §3.2] yields

$$\omega_{n,2}^{L}(z;\, w_1) = -\tfrac{1}{2}(n+1)(n+2)(1-z^2)\left\{U_{n+2}(z) - \frac{n+3}{n+1}U_n(z)\right\}. \tag{2.10}$$

Then (1.5) and $(1-t^2)w_1(t) = w_2(t)$, in conjunction with [2, Eq. (3.6)] and (1.7), gives

$$K_{n,2}^{L}(z;\, w_1) = \frac{4\pi}{(u^2-1)u^{n+2}} \frac{u^2 - \dfrac{n+1}{n+3}}{\dfrac{n+1}{n+3}\left[u^{n+3} - u^{-(n+3)}\right] - \left[u^{n+1} - u^{-(n+1)}\right]}. \tag{2.11}$$

In the case $w = w_2$, we have $w_2^{L}(t) = (1-t^2)^{5/2}$, thus by (1.4) and [2, Lemma 3.1], $\omega_{n,2}^{L}(z;\, w_2) = (1-z^2)^2\, T_{n+3}'''(z)$. Using repeatedly the differential equation for T_{n+3} and the expressions of T_{n+3} and T_{n+3}' in terms of the U's (cf. [2, §3.2]), we get

$$\begin{aligned}\omega_{n,2}^{L}(z;\, w_2) &= (n+3)\left\{\left((n+3)^2-1\right)(z^2-1) + 3z^2\right\}U_{n+2}(z) \\ &\quad -\tfrac{3}{2}(n+3)^2 z\left\{U_{n+3}(z) - U_{n+1}(z)\right\} \\ &= \tfrac{1}{4}(n+3)\left\{(n+1)(n+2)U_{n+4}(z) - 2(n+1)(n+5)U_{n+2}(z)\right. \\ &\quad \left. +(n+4)(n+5)U_n(z)\right\}.\end{aligned} \tag{2.12}$$

Inserted in (1.5), and using [2, Eq. (3.6)] and (1.7), this yields

$$\begin{aligned}K_{n,2}^{L}(z;\, w_2) &= \frac{\pi(u^2-1)}{u^{n+6}} \\ &\quad \times \frac{u^4 - \alpha_n u^2 + \beta_n}{\beta_n\left[u^{n+5} - u^{-(n+5)}\right] - \alpha_n\left[u^{n+3} - u^{-(n+3)}\right] + \left[u^{n+1} - u^{-(n+1)}\right]}, \\ \alpha_n &= 2\frac{n+1}{n+4}, \qquad \beta_n = \frac{(n+1)(n+2)}{(n+4)(n+5)}.\end{aligned} \tag{2.13}$$

Assume next $w = w_3$. Here, $w_3^{L}(t) = (1-t)^{3/2}(1+t)^{5/2}$, hence

$$\omega_{n,2}^{L}(z;\, w_3) = \text{const} \cdot (z^2-1)^2 P_n^{(3/2,5/2)}(z), \tag{2.14}$$

where $P_n^{(\alpha,\beta)}$ is the Jacobi polynomial with parameters α, β. The second formula in [5, Eq. (4.5.4)], with $\alpha = \beta = \frac{3}{2}$, yields

$$P_n^{(3/2,5/2)}(z) = \frac{1}{2n+5}\frac{(2n+5)P_n^{(3/2,3/2)}(z) + 2(n+1)P_{n+1}^{(3/2,3/2)}(z)}{z+1}. \tag{2.15}$$

On the other hand, from [5, Eq. (4.21.7)] one finds that

$$P_n^{(3/2,3/2)}(z) = \frac{4c_{n+2}}{(n+2)(n+3)}T_{n+2}''(z), \quad c_{n+2} = 4^{-(n+2)}\binom{2n+4}{n+2}.$$

Using this in (2.15), and disposing of the constant in (2.14) appropriately, gives

$$\omega_{n,2}^{L}(z;\, w_3) = (1-z)(1-z^2)\left\{T_{n+3}''(z) + \frac{(n+3)(n+4)}{(n+1)(n+2)}T_{n+2}''(z)\right\}.$$

Now the differential equation for Chebyshev polynomials, and an argument similar to the one that led to [2, Eq. (3.10)], finally yields

$$\omega_{n,2}^{\mathrm{L}}(z;\, w_3) = -\tfrac{1}{2}(n+2)(n+3)(1-z)\Big\{U_{n+3}(z) - \frac{n+4}{n+2}U_{n+1}(z) + \frac{n+4}{n+2}\Big[U_{n+2}(z) - \frac{n+3}{n+1}U_n(z)\Big]\Big\}. \tag{2.16}$$

Since $(1-t)w_3(t) = w_2(t)$, one readily obtains $\rho_{n,2}^{\mathrm{L}}(z;\, w_3)$ in terms of the integrals $\int_{-1}^{1} U_n(t)w_2(t)\,dt/(z-t)$, which then, together with (2.16), in the usual manner establishes

$$K_{n,2}^{\mathrm{L}}(z;\, w_3) = \frac{2\pi(u+1)}{(u-1)u^{n+4}} \times \frac{u^3 + \alpha_n(u^2-u) - \beta_n}{\beta_n\big[u^{n+4} - u^{-(n+4)}\big] + \alpha_n\big[u^{n+3} - u^{-(n+3)} - \big(u^{n+2} - u^{-(n+2)}\big)\big] - \big[u^{n+1} - u^{-(n+1)}\big]}, \tag{2.17}$$

$$\alpha_n = \frac{n+1}{n+3}, \qquad \beta_n = \frac{(n+1)(n+2)}{(n+3)(n+4)}.$$

Finally, the case $w = w_4$, by a change of variables, is easily reduced to the preceding case:

$$K_{n,2}^{\mathrm{L}}(z;\, w_4) = -K_{n,2}^{\mathrm{L}}(-z;\, w_3). \tag{2.18}$$

3. The maximum of the Radau kernels on elliptic contours

In this section we seek to determine the precise location of $\max_{z\in\mathscr{E}_\rho} |K_{n,2}^{\mathrm{R}}(z;\, w)|$ on the elliptic contour $\mathscr{E}_\rho$ (cf. (1.10)). Because of (1.8), it suffices to consider the upper half of the ellipse, i.e., $0 \leqslant \theta \leqslant \pi$ in (1.10). For $w = w_1$ and $w = w_4$ (cf. (2.1)), we shall prove that, for any fixed $\rho > 1$, the maximum occurs on the negative real axis, that is, for $\theta = \pi$ (Theorems 3.6 and 3.7). For the other two Chebyshev weights, the state of affairs is more complicated, and we limit ourselves, in Section 3.3, to stating conjectures based on numerical and asymptotic analyses. Section 3.1 contains a number of auxiliary results, some possibly of independent interest.

3.1. Preliminary lemmas

We begin with two elementary trigonometric inequalities.

Lemma 3.1. *We have, for* $n = 0, 1, 2, \ldots,$

$$\left|\frac{\sin n\theta}{\sin\theta}\right| \leqslant n, \qquad \left|\frac{\cos(2n+1)\theta}{\cos\theta}\right| \leqslant 2n+1. \tag{3.1}$$

Proof. The first inequality is well known. The second, being true for $n = 0$, follows by induction:

$$\left|\frac{\cos(2n+1)\theta}{\cos\theta}\right| = \left|\frac{2\cos\theta\cos 2n\theta - \cos(2n-1)\theta}{\cos\theta}\right| \leqslant 2|\cos 2n\theta| + \left|\frac{\cos(2n-1)\theta}{\cos\theta}\right| \leqslant 2 + (2n-1) = 2n+1. \quad \square$$

For the remaining results, we define

$$a_j = a_j(\rho) = \tfrac{1}{2}(\rho^j + \rho^{-j}), \quad j = 1, 2, 3, \ldots, \quad \rho > 1. \tag{3.2}$$

Lemma 3.2. *For any* $\rho > 1$, *there holds*

$$\frac{a_{2n}(\rho) - 1}{a_2(\rho) - 1} \geqslant n^2, \quad \frac{a_{2n+1}(\rho) - 1}{a_1(\rho) - 1} > (2n+1)^2, \qquad n = 1, 2, 3, \ldots . \tag{3.3}$$

Proof. The first inequality is known [4, Lemma 5.1]. The second is proved similarly:

$$\frac{a_{2n+1} - 1}{a_1 - 1} = \left\{ \frac{\rho^{2n+1} - 1}{\rho^n(\rho - 1)} \right\}^2$$

$$= \{\rho^n + \rho^{n-1} + \cdots + \rho^{-(n-1)} + \rho^{-n}\}^2 > (2n+1)^2. \qquad \square$$

Lemma 3.3. *For any* $\rho > 1$, *there holds*

$$\frac{1}{2n+3}\frac{a_{2n+3}(\rho) - 1}{a_1(\rho) - 1} - \frac{1}{2n+1}\frac{a_{2n+1}(\rho) - 1}{a_1(\rho) - 1} > 2. \tag{3.4}$$

Proof. We first note that

$$\frac{1}{2n+3}\left(\rho^{(2n+3)/2} - \rho^{-(2n+3)/2}\right) - \frac{1}{2n+1}\left(\rho^{(2n+1)/2} - \rho^{-(2n+1)/2}\right) > 0. \tag{3.5}$$

Indeed, for $\rho = 1$, the left-hand side vanishes, while its derivative is

$$\tfrac{1}{2}\left(\rho^{n+1/2} + \rho^{-n-5/2} - \rho^{n-1/2} - \rho^{-n-3/2}\right) = \tfrac{1}{2}\left(\rho^{1/2} - \rho^{-1/2}\right)\left(\rho^n - \rho^{-n-2}\right) > 0.$$

Now the left-hand side of (3.4) can be written as

$$\frac{1}{2n+3}\left(\frac{\rho^{(2n+3)/2} - \rho^{-(2n+3)/2}}{\rho^{1/2} - \rho^{-1/2}}\right)^2 - \frac{1}{2n+1}\left(\frac{\rho^{(2n+1)/2} - \rho^{-(2n+1)/2}}{\rho^{1/2} - \rho^{-1/2}}\right)^2,$$

which by (3.5) and subsequent application of the second inequality in Lemma 3.2 is seen to be larger than

$$\left[\frac{1}{2n+3}\left(\frac{2n+3}{2n+1}\right)^2 - \frac{1}{2n+1}\right]\left(\frac{\rho^{(2n+1)/2} - \rho^{-(2n+1)/2}}{\rho^{1/2} - \rho^{-1/2}}\right)^2$$

$$> \left[\frac{2n+3}{(2n+1)^2} - \frac{1}{2n+1}\right](2n+1)^2 = 2n + 3 - (2n+1) = 2. \qquad \square$$

Lemma 3.4. *For any* $\rho > 1$, *and* $\theta \in [0, \pi]$, *there holds*

$$\left[a_{2n+2}(\rho) - 1\right]\sin^2\theta - \left[a_2(\rho) - 1\right]\sin^2(n+1)\theta \geqslant 0.$$

Proof. By the first inequality in (3.3), the left-hand side is larger than, or equal to

$$\left[(n+1)^2\sin^2\theta - \sin^2(n+1)\theta\right]\left[a_2(\rho) - 1\right],$$

which is nonnegative by virtue of the first inequality in (3.1). $\square$

Lemma 3.5. *For any $\rho > 1$, and $\theta \in [0, \pi]$, we have*

$$\left(\frac{1}{2n+3}[a_{2n+3}(\rho)-1] - \frac{1}{2n+1}[a_{2n+1}(\rho)-1]\right)\cos^2\tfrac{1}{2}\theta$$
$$+ [a_1(\rho)-1]\left(\frac{1}{2n+1}\cos^2\tfrac{1}{2}(2n+1)\theta - \frac{1}{2n+3}\cos^2\tfrac{1}{2}(2n+3)\theta\right) \geqslant 0.$$

Proof. By Lemma 3.3, the left-hand side, after division by $a_1 - 1$, is larger than

$$2\cos^2\tfrac{1}{2}\theta + \frac{1}{2n+1}\cos^2\tfrac{1}{2}(2n+1)\theta - \frac{1}{2n+3}\cos^2\tfrac{1}{2}(2n+3)\theta$$
$$= 1 + \cos\theta + \frac{1}{2(2n+1)}[1+\cos(2n+1)\theta] - \frac{1}{2(2n+3)}[1+\cos(2n+3)\theta]$$
$$=: s(\theta).$$

Now, $s(\pi) = 0$, and

$$s'(\theta) = -\sin\theta - \tfrac{1}{2}\sin(2n+1)\theta + \tfrac{1}{2}\sin(2n+3)\theta = -\sin\theta + \cos(2n+2)\theta\sin\theta$$
$$= -\sin\theta[1-\cos(2n+2)\theta] \leqslant 0 \quad \text{for } 0 \leqslant \theta \leqslant \pi.$$

Therefore, $s(\theta) \geqslant 0$ on $[0, \pi]$. □

3.2. Main results

We are now ready to establish the desired results for the weight functions w_1 and w_4.

Theorem 3.6. *We have, for any $\rho > 1$,*

$$\max_{z\in\mathscr{E}_\rho}\left|K_{n,2}^{\mathrm{R}}(z; w_1)\right|$$
$$= \left|K_{n,2}^{\mathrm{R}}\left(-\tfrac{1}{2}(\rho+\rho^{-1}); w_1\right)\right|$$
$$= \frac{4\pi}{(\rho-1)\rho^{n+1}} \frac{\rho - \dfrac{2n+1}{2n+3}}{\dfrac{2n+1}{2n+3}\left[\rho^{n+2}-\rho^{-(n+2)}\right] - \dfrac{2}{2n+3}\left[\rho^{n+1}-\rho^{-(n+1)}\right] - \left[\rho^n - \rho^{-n}\right]}. \tag{3.6}$$

Remark. The denominator in the last expression of (3.6) is positive, since it vanishes for $\rho = 1$ and its derivative computes to

$$(\rho-1)\left[\frac{(n+2)(2n+1)}{2n+3}\left(\rho^n - \rho^{-(n+3)}\right) + n\left(\rho^{n-1} - \rho^{-(n+2)}\right)\right],$$

which is clearly positive for $\rho > 1$.

Proof of Theorem 3.6. By virtue of (2.2) and (1.10), we have $z \in \mathscr{E}_\rho$ if and only if $u = \rho e^{i\theta}$. It suffices, therefore, to study the modulus of the kernel $K_{n,2}^{\mathrm{R}}$ in (2.5) for $u = \rho e^{i\theta}$, $0 \leqslant \theta \leqslant \pi$.

Straightforward calculus shows that

$$\left\{\left|\frac{u + \dfrac{2n+1}{2n+3}}{u+1}\right| : u = \rho e^{i\theta},\ 0 \leqslant \theta \leqslant \pi\right\}$$

attains its maximum at $\theta = \pi$. We must show, therefore, that

$$(u-1)\left(\frac{2n+1}{2n+3}\left[u^{n+2}+u^{-(n+1)}\right]+\left[u^{n+1}+u^{-n}\right]\right)$$
$$=u\left\{\frac{2n+1}{2n+3}\left[u^{n+2}-u^{-(n+2)}\right]+\frac{2}{2n+3}\left[u^{n+1}-u^{-(n+1)}\right]-\left[u^{n}-u^{-n}\right]\right\}$$

has minimum modulus at $\theta = \pi$. Since $|u| = \rho$, it suffices to study the modulus of the expression in braces, the square of which, considered as a function of θ for fixed $\rho > 1$, we denote by $f(\theta)$. An elementary (though tedious) computation gives

$$\frac{1}{4}\frac{2n+3}{2n+1}[f(\theta)-f(\pi)] = \frac{2n+1}{2n+3}\sin^2(n+2)\theta + \frac{4}{(2n+1)(2n+3)}\sin^2(n+1)\theta$$
$$+\frac{2n+3}{2n+1}\sin^2 n\theta + 2\left[a_{2n+2}\sin^2\theta - a_2\sin^2(n+1)\theta\right]$$
$$-\frac{4}{2n+1}\left[a_{2n+1}\cos^2\tfrac{1}{2}\theta - a_1\cos^2\tfrac{1}{2}(2n+1)\theta\right]$$
$$+\frac{4}{2n+3}\left[a_{2n+3}\cos^2\tfrac{1}{2}\theta - a_1\cos^2\tfrac{1}{2}(2n+3)\theta\right],$$

where $a_j = a_j(\rho)$ is as defined in (3.2). Subtracting 1 from each a_j appearing in this expression and adding back the respective trigonometric terms, results in a purely trigonometric expression and an expression involving terms containing $a_j - 1$. Using elementary trigonometric identities, the former expression can be shown to be

$$\frac{2n+1}{2n+3}\left(\sin(n+2)\theta+\frac{2}{2n+1}\sin(n+1)\theta-\frac{2n+3}{2n+1}\sin n\theta\right)^2 \geqslant 0.$$

To the latter, we apply Lemmas 3.4 and 3.5 to obtain

$$2\left[(a_{2n+2}-1)\sin^2\theta-(a_2-1)\sin^2(n+1)\theta\right]$$
$$+4\left\{\left[\frac{1}{2n+3}(a_{2n+3}-1)-\frac{1}{2n+1}(a_{2n+1}-1)\right]\cos^2\tfrac{1}{2}\theta\right.$$
$$\left.+(a_1-1)\left[\frac{1}{2n+1}\cos^2\tfrac{1}{2}(2n+1)\theta-\frac{1}{2n+3}\cos^2\tfrac{1}{2}(2n+3)\theta\right]\right\}\geqslant 0. \qquad \square$$

Theorem 3.7. *We have, for any* $\rho > 1$,

$$\max_{z\in\mathscr{E}_\rho}\left|K_{n,2}^{\mathrm{R}}(z;\,w_4)\right| = \left|K_{n,2}^{\mathrm{R}}\left(-\tfrac{1}{2}(\rho+\rho^{-1});\,w_4\right)\right|$$
$$= 2\pi\frac{\rho+1}{(\rho-1)\rho^{n+2}}\,\frac{\rho-\dfrac{n+1}{n+2}}{\dfrac{n+1}{n+2}\left[\rho^{n+2}-\rho^{-(n+2)}\right]-\left[\rho^{n+1}-\rho^{-(n+1)}\right]}. \tag{3.7}$$

Remark. The positivity of the last denominator in (3.7) is shown similarly as in the remark following Theorem 3.6.

Proof of Theorem 3.7. We now must analyze the modulus of the kernel $K_{n,2}^{\mathrm{R}}$ in (2.9) with $u = \rho e^{i\theta}$, $0 \leqslant \theta \leqslant \pi$. As in the proof of Theorem 3.6, it is elementary to show that

$$\left\{ \left| \frac{u + \dfrac{n+1}{n+2}}{u+1} \right| : u = \rho e^{i\theta},\ 0 \leqslant \theta \leqslant \pi \right\}$$

takes on its maximum at $\theta = \pi$, and the same is true for $|u-1|$. It suffices, therefore, to show that

$$g(\theta) := \left| \frac{n+1}{n+2} \left[u^{n+2} - u^{-(n+2)} \right] + \left[u^{n+1} - u^{-(n+1)} \right] \right|^2$$

has a minimum at $\theta = \pi$. We have

$$\frac{1}{4} \frac{n+2}{n+1} [g(\theta) - g(\pi)] = \frac{n+1}{n+2} \sin^2(n+2)\theta + \frac{n+2}{n+1} \sin^2(n+1)\theta + 2\left[a_{2n+3} \cos^2 \tfrac{1}{2}\theta - a_1 \cos^2 \tfrac{1}{2}(2n+3)\theta \right].$$

Proceeding as in the proof of Theorem 3.6, we decompose this into a purely trigonometric expression, and one involving terms with $a_j - 1$. The former turns out to be

$$\frac{n+1}{n+2} \left(\sin(n+2)\theta + \frac{n+2}{n+1} \sin(n+1)\theta \right)^2 \geqslant 0,$$

while the latter becomes

$$2\left[(a_{2n+3} - 1) \cos^2 \tfrac{1}{2}\theta - (a_1 - 1) \cos^2 \tfrac{1}{2}(2n+3)\theta \right]$$
$$\geqslant 2(a_1 - 1)\left[(2n+3)^2 \cos^2 \tfrac{1}{2}\theta - \cos^2 \tfrac{1}{2}(2n+3)\theta \right] \geqslant 0,$$

on account of the second inequalities in (3.3) and (3.1). □

3.3. Numerical and asymptotic results

Numerical experimentation revealed that the behavior of $|K_{n,2}^{\mathrm{R}}(z; w)|$ for $z \in \mathscr{E}_\rho$, in the cases $w = w_2$ and $w = w_3$, is considerably more complicated than in the cases of the other Chebyshev weights treated in Section 3.2. The location of the maximum not only depends on n, but for some n also on the value of ρ.

More specifically, for $w = w_2$, numerical evidence suggests that when $1 \leqslant n \leqslant 11$, then

$$\max_{z \in \mathscr{E}_\rho} \left| K_{n,2}^{\mathrm{R}}(z; w_2) \right| = \left| K_{n,2}^{\mathrm{R}}\left(-\tfrac{1}{2}(\rho + \rho^{-1}); w_2 \right) \right|, \tag{3.8}$$

while for $n \geqslant 12$ there exist numbers $1 < \rho_n' < \rho_n$ such that (3.8) holds if either $1 < \rho \leqslant \rho_n'$ or $\rho \geqslant \rho_n$. Inbetween, the maximum point on $\mathscr{E}_\rho$ moves from close (and to the left of) the imaginary axis towards the negative real axis as ρ increases from ρ_n' to ρ_n. Numerical values of ρ_n' and ρ_n for $12 \leqslant n \leqslant 20$ are given in Table 3.1.

Table 3.1
The bounds ρ_n', ρ_n, $n = 12, \ldots, 20$, for Radau formulae with Chebyshev weight w_2

n	ρ_n'	ρ_n
12	1.6304	2.3454
13	1.4073	3.4034
14	1.3160	4.7165
15	1.2602	5.8433
16	1.2214	6.7472
17	1.1928	7.5730
18	1.1701	8.3574
19	1.1523	9.1161
20	1.1373	9.8574

Table 3.2
The bounds ρ_n, $n = 2, \ldots, 20$, for Radau formulae with Chebyshev weight w_3

n	ρ_n
2	2.1789
3	1.4045
4	1.2308
5	1.1549
6	1.1131
7	1.0871
8	1.0697
9	1.0573
10	1.0481
11	1.0411
12	1.0356
13	1.0312
14	1.0276
15	1.0246
16	1.0221
17	1.0200
18	1.0182
19	1.0166
20	1.0153

An asymptotic analysis for $\rho \downarrow 1$ and $\rho \to \infty$ yields results consistent with the findings above. Indeed, as $\rho \downarrow 1$, one obtains by a lengthy computation that

$$\left| K_{n,2}^{\mathrm{R}}(z;\, w_2) \right|_{z \in \mathscr{E}_\rho} \sim \begin{cases} \dfrac{(2n+3)(2n+5)\pi}{4(n+1)(n+2)(n+3)} & \text{if } \theta = 0, \\ \dfrac{180\pi}{(n+1)(n+2)(n+3)(2n+3)(2n+5)} (\rho - 1)^{-4} & \text{if } \theta = \pi, \end{cases} \tag{3.9}$$

whereas for $0 < \theta < \pi$, the behavior is O(1) or $O((\rho - 1)^{-1})$, the latter only for isolated values of $\theta \in (0, \pi)$ satisfying

$$(n+1)(2n+3)\sin(n+3)\theta + 4(n+1)(n+3)\sin(n+2)\theta + (n+3)(2n+5)\sin(n+1)\theta = 0.$$

Likewise, as $\rho \to \infty$, one finds

$$\left| K_{n,2}^{\mathrm{R}}(z;\, w_2) \right|_{z \in \mathscr{E}_\rho} \sim \frac{(n+3)(2n+5)}{(n+1)(2n+3)} \rho^{-(2n+3)} \times \left\{ 1 - \frac{48(n+2)}{(2n+3)(2n+5)} \rho^{-1} \cos\theta \right\}^{1/2}. \tag{3.10}$$

For $w = w_3$, numerical results suggest the existence of numbers $\rho_n > 1$ such that for $n \geqslant 2$

$$\max_{z\in\mathscr{E}_\rho} \left| K_{n,2}^{\mathrm{R}}(z;\, w_3) \right| = \begin{cases} \left| K_{n,2}^{\mathrm{R}}\left(-\tfrac{1}{2}(\rho+\rho^{-1});\, w_3\right) \right| & \text{if } 1 < \rho \leqslant \rho_n, \\ K_{n,2}^{\mathrm{R}}\left(\tfrac{1}{2}(\rho+\rho^{-1});\, w_3\right) & \text{if } \rho \geqslant \rho_n, \end{cases} \tag{3.11}$$

while for $n = 1$, the first relation holds for all $\rho > 1$. Table 3.2 lists the quantities ρ_n for $2 \leqslant n \leqslant 20$, which evidently are the roots of the equation

$$\left| K_{n,2}^{\mathrm{R}}\left(-\tfrac{1}{2}(\rho+\rho^{-1});\, w_3\right) \right| = K_{n,2}^{\mathrm{R}}\left(\tfrac{1}{2}(\rho+\rho^{-1});\, w_3\right).$$

An asymptotic analysis for $\rho \downarrow 1$ and $\rho \to \infty$ again corroborates these results. In the former limit, we find

$$\left| K_{n,2}^{\mathrm{R}}(z;\, w_3) \right|_{z\in\mathscr{E}_\rho} \sim \begin{cases} 2\pi(\rho-1)^{-1} & \text{if } \theta = 0, \\ \dfrac{180\pi}{(n+1)(2n+1)(2n+3)(2n+5)}(\rho-1)^{-4} & \text{if } \theta = \pi, \end{cases} \tag{3.12}$$

with values of $O(1)$ or $O((\rho-1)^{-1})$ for $\theta \in (0, \pi)$, while in the latter limit we have

$$\left| K_{n,2}^{\mathrm{R}}(z;\, w_3) \right|_{z\in\mathscr{E}_\rho} \sim \frac{2(n+2)(2n+5)\pi}{(n+1)(2n+1)}\rho^{-(2n+3)} \times \left(1 + \frac{2(2n^2-5)}{(n+1)(n+2)}\rho^{-1}\cos\theta\right)^{1/2}. \tag{3.13}$$

4. The maximum of the Lobatto kernels on elliptic contours

As in the previous section, it suffices to study $|K_{n,2}^{\mathrm{L}}|$ on the upper half, $0 \leqslant \theta \leqslant \pi$, of the ellipse $\mathscr{E}_\rho$ (cf. (1.10)). For $w = w_1$ and $w = w_2$, since $|K_{n,2}^{\mathrm{L}}(-\bar{z};\, w_i)| = |K_{n,2}^{\mathrm{L}}(z;\, w_i)|$, $i = 1, 2$, we can even restrict ourselves to the interval $0 \leqslant \theta \leqslant \frac{1}{2}\pi$. We have a rigorous result only for $w = w_1$, stating that $|K_{n,2}^{\mathrm{L}}|$ attains its maximum on the real axis. For the other Chebyshev weight functions, we present numerical and asymptotic results in Section 4.2.

4.1. Main result

For the Chebyshev weight function of the first kind, $w = w_1$, we prove the following theorem.

Theorem 4.1. *For any $\rho > 1$, we have*

$$\max_{z\in\mathscr{E}_\rho} \left| K_{n,2}^{\mathrm{L}}(z;\, w_1) \right| = K_{n,2}^{\mathrm{L}}\left(\tfrac{1}{2}(\rho+\rho^{-1});\, w_1\right) = \frac{4\pi}{(\rho^2-1)\rho^{n+2}} \frac{\rho^2 - \dfrac{n+1}{n+3}}{\dfrac{n+1}{n+3}\left[\rho^{n+3} - \rho^{-(n+3)}\right] - \left[\rho^{n+1} - \rho^{-(n+1)}\right]}. \tag{4.1}$$

Remark. The last denominator in (4.1) is positive, which can be seen similarly as in the remark to Theorem 3.7.

Proof of Theorem 4.1. Referring to the expression (2.11) for $K_{n,2}^{\mathrm{L}}$, we first note that

$$\left|\frac{u^2-\frac{n+1}{n+3}}{u^2-1}\right| = \left|1+\frac{2}{n+3}\frac{1}{u^2-1}\right| \leqslant 1+\frac{2}{n+3}\frac{1}{\rho^2-1} = \frac{\rho^2-\frac{n+1}{n+3}}{\rho^2-1},$$

i.e., the modulus on the left attains its maximum for $u=\rho e^{i\theta}$ at $\theta=0$. It remains, therefore, to determine the minimum of

$$h(\theta) := \left|\frac{n+1}{n+3}\left[u^{n+3}-u^{-(n+3)}\right]-\left[u^{n+1}-u^{-(n+1)}\right]\right|^2, \quad u=\rho e^{i\theta}.$$

An elementary calculation shows that

$$\frac{1}{4}\frac{n+3}{n+1}[h(\theta)-h(0)] = \frac{n+1}{n+3}\sin^2(n+3)\theta+\frac{n+3}{n+1}\sin^2(n+1)\theta + 2\left[a_{2n+4}\sin^2\theta - a_2\sin^2(n+2)\theta\right],$$

where $a_j=a_j(\rho)$ is as defined in (3.2). Subtracting 1 from the a_j and readjusting the first two terms produces an aggregate of purely trigonometric terms and of terms involving a_j-1. The former becomes

$$\frac{n+1}{n+3}\left(\sin(n+3)\theta+\frac{n+3}{n+1}\sin(n+1)\theta\right)^2 \geqslant 0,$$

whereas the latter, by the first inequalities in (3.3) and (3.1), is larger than, or equal to

$$2(n+2)^2[a_2-1]\sin^2\theta - 2[a_2-1]\sin^2(n+2)\theta$$
$$\geqslant 2[a_2-1]\sin^2(n+2)\theta - 2[a_2-1]\sin^2(n+2)\theta = 0.$$

This establishes $h(\theta)-h(0)\geqslant 0$ and completes the proof of Theorem 4.1. □

4.2. Numerical and asymptotic results

For $w=w_2$, it is found numerically that $|K_{n,2}^{\mathrm{L}}(\cdot;w_2)|$ attains its maximum on $\mathscr{E}_\rho$ on the real axis if $1\leqslant n\leqslant 9$. The same holds for $n\geqslant 10$, if $1<\rho\leqslant\rho_n$ for some $\rho_n>1$, while for $\rho\geqslant\rho_n$ the maximum occurs on the imaginary axis. Clearly, ρ_n must be such that

$$K_{n,2}^{\mathrm{L}}\left(\tfrac{1}{2}(\rho+\rho^{-1});w_2\right) = \left|K_{n,2}^{\mathrm{L}}\left(\tfrac{1}{2}i(\rho-\rho^{-1});w_2\right)\right|, \quad \rho=\rho_n. \tag{4.2}$$

The root ρ_n of (4.2) was determined for $10\leqslant n\leqslant 20$ by means of a bisection procedure, using

Table 4.1
The roots ρ_n of (4.2)

n	ρ_n
10	1.7531
11	1.4925
12	1.3730
13	1.3012
14	1.2525
15	1.2169
16	1.1898
17	1.1683
18	1.1509
19	1.1365
20	1.1244

(2.13) (with $u = \rho$ and $u = \mathrm{i}\rho$, respectively) to evaluate the left- and right-hand sides of (4.2). The results are shown in Table 4.1.

Asymptotically, as $\rho \downarrow 1$, we find by a lengthy computation that at $\theta = 0$,

$$K_{n,2}^{\mathrm{L}}\left(\tfrac{1}{2}(\rho+\rho^{-1});\, w_2\right) \sim \frac{45\pi}{(n+1)(n+2)(n+3)(n+4)(n+5)}(\rho-1)^{-4},$$

while at $\theta = \frac{1}{2}\pi$,

$$K_{n,2}^{\mathrm{L}}\left(\tfrac{1}{2}\mathrm{i}(\rho-\rho^{-1});\, w_2\right) = \begin{cases} \mathrm{O}(1), & \text{when } n \text{ is even,} \\ \mathrm{O}\big((\rho-1)^{-1}\big), & \text{otherwise.} \end{cases}$$

For $\theta \in (0, \frac{1}{2}\pi)$, the kernel is O(1) in general, except when θ satisfies

$$(n+1)(n+2)\sin(n+5)\theta - 2(n+1)(n+5)\sin(n+3)\theta + (n+4)(n+5)\sin(n+4)\theta = 0,$$

in which case it has a peak of $\mathrm{O}((\rho-1)^{-1})$. Likewise, as $\rho \to \infty$,

$$\left|K_{n,2}^{\mathrm{L}}(z;\, w_2)\right|_{z\in\mathscr{E}_\rho} \sim \frac{(n+4)(n+5)\pi}{(n+1)(n+2)\rho^{2n+5}} \times\left[1-2\left(1-\frac{12(n+3)}{(n+2)(n+4)}\right)\cos 2\theta\right]^{1/2},$$

which shows that the maximum is indeed attained on the real axis when $1 - 12(n+3)/(n+2)(n+4) < 0$, i.e., $n < 10$, and on the imaginary axis, otherwise.

Finally, for $w = w_3$, numerical as well as asymptotic computations indicate that $|K_{n,2}^{\mathrm{L}}(z;\, w_3)|_{z\in\mathscr{E}_\rho}$ always takes on its maximum on the positive real axis (i.e., for $\theta = 0$), but it seems difficult to prove this rigorously.

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ON THE REMAINDER TERM FOR ANALYTIC FUNCTIONS OF GAUSS-LOBATTO AND GAUSS-RADAU QUADRATURES

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Dedicated to Wolfgang Thron on his 70th birthday

ABSTRACT. We study the kernels in the contour integral representation of the remainder term of Gauss-Lobatto and Gauss-Radau quadratures, in particular the location of their maxima on circular and elliptic contours. Quadrature rules with Chebyshev weight functions of all four kinds receive special attention, but more general weights are also considered.

1. Introduction. Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1,1]$ and $\mathcal{D}$ be its interior. Let f be analytic in $\mathcal{D}$ and continuous on $\overline{\mathcal{D}}$. We consider an interpolatory quadrature rule

$$\int_{-1}^{1} f(t)w(t)\,dt = \sum_{\nu=1}^{N} \lambda_\nu f(\tau_\nu) + R_N(f) \tag{1.1}$$

with

$$-1 \le \tau_N < \tau_{N-1} < \cdots < \tau_1 \le 1 \tag{1.2}$$

30.

$$\omega_N(z) = \omega_N(z;w) = \prod_{\nu=1}^{N}(z-\tau_\nu), \quad z \in \mathbf{C}, \tag{1.3}$$

denote its node polynomial (which in general depends on w), and define

$$\rho_N(z;w) = \int_{-1}^{1} \frac{\omega_N(t;w)}{z-t} w(t)\,dt, \quad z \in \mathbf{C}\backslash[-1,1], \tag{1.4}$$

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then, as is well known, the remainder term R_N in (1.1) admits the contour integral representation

$$R_N(f) = \frac{1}{2\pi i} \oint_\Gamma K_N(z;w) f(z)\, dz, \tag{1.5}$$

where the "kernel" K_N can be expressed, e.g., in the form

$$K_N(z;w) = \frac{\rho_N(z;w)}{\omega_N(z;w)}, \quad z \in \Gamma. \tag{1.6}$$

This is easily verified by applying the residue theorem to the integral $(2\pi i)^{-1} \oint_\Gamma [f(z)\omega_N(t)/((z-t)\omega_N(z))]\, dz$ and subsequent integration in t, recalling that the weights λ_ν in (1.1) are given by $\lambda_\nu = \int_{-1}^{1} [\omega_N(t)/((t-\tau_\nu)\omega_N'(\tau_\nu))] w(t)\, dt$, since (1.1) is interpolatory. Note that ω_N in (1.3) and (1.4) may be multiplied by any constant $c \neq 0$ without affecting the validity of (1.6). It is also evident from (1.6) that

$$K_N(\bar{z};w) = \overline{K_N(z;w)}. \tag{1.7}$$

In order to estimate the error in (1.1) by means of

$$|R_N(f)| \leq (2\pi)^{-1} \ell(\Gamma) \max_{z\in\Gamma} |K_N(z;w)| \cdot \max_{z\in\Gamma} |f(z)|, \tag{1.8}$$

where $\ell(\Gamma)$ is the length of the contour Γ, it becomes necessary to study the magnitude of $|K_N|$ on Γ. This has been done in a number of papers (see [1, §4.1.1] for references) for Gauss = type and other quadrature formulae, and for contours Γ that are either concentric circles centered at the origin or confocal ellipses with focal points at ± 1. The thrust of this work has been directed towards upper bounds, or asymptotic estimates, for the maximum of $|K_N|$ in (1.8). In an attempt to remove uncertainties inherent in such estimates, we determined in [2] (see also [3]), for Gauss formulae, the precise location on Γ where $|K_N|$ attains its maximum, and we suggested simple recursive techniques to evaluate $K_N(z;w)$ for any $z \in \mathbf{C}\backslash[-1,1]$. Here we investigate, in the same spirit, quadrature rules of Gauss-Lobatto and Gauss-Radau type, especially for any of the four Chebyshev weight functions

$$\begin{aligned} w_1(t) &= (1-t^2)^{-\frac{1}{2}}, & w_2(t) &= (1-t^2)^{\frac{1}{2}}, \\ w_3(t) &= (1-t)^{-\frac{1}{2}}(1+t)^{\frac{1}{2}}, & w_4(t) &= (1-t)^{\frac{1}{2}}(1+t)^{-\frac{1}{2}}. \end{aligned} \tag{1.9}$$

In Section 2 we consider circular contours and general weight functions. In Section 3 explicit formulae are derived for the Lobatto and Radau kernels $K_N(\cdot;w)$ with $w = w_i$, $i = 1,2,3,4$. Their maximum moduli are analyzed in Section 4, both on circular and elliptic contours.

2. Some general results for circular contours. In this section, $\Gamma = C_r$, $C_r = \{z \in \mathbf{C} : |z| = r\}$, where $r > 1$. For positive weight functions w and quadrature rules of Gaussian type, with $N = n$, it is known from [2] that

$$\max_{z\in C_r} |K_n(z;w)| = \begin{cases} K_n(r;w) & \text{if } w(t)/w(-t) \text{ is nondecreasing on } (-1,1), \\ |K_n(-r;w)| & \text{if } w(t)/w(-t) \text{ is nonincreasing on } (-1,1). \end{cases} \tag{2.1}$$

We now explore the implications of this result to Gauss-Lobatto (Subsection 2.1) and Gauss-Radau formulae (Subsection 2.2).

2.1. *Gauss-Lobatto formulae.* These are the quadrature rules (1.1) with $N = n+2$, $\tau_N = -1$, $\tau_1 = 1$ and $R_N(f) = 0$ whenever $f \in \mathbf{P}_{2n+1}$ (the class of polynomials of degree $\leq 2n+1$). They are clearly interpolatory. We denote $w^L(t) = (1-t^2)w(t)$ and write $\pi_n(\cdot;w^L)$ for the polynomial of degree n (suitably normalized) orthogonal with respect to the weight function w^L. It is well known that

$$\omega_{n+2}(z;w) = (1-z^2)\pi_n(z;w^L), \tag{2.2}$$

from which there follows

$$\begin{aligned} \rho_{n+2}(z;w) &= \int_{-1}^{1} \frac{(1-t^2)\pi_n(t;w^L)}{z-t} w(t)\,dt \\ &= \int_{-1}^{1} \frac{\pi_n(t;w^L)}{z-t} w^L(t)\,dt = \rho_n(z;w^L) \end{aligned}$$

and, therefore, by (1.6),

$$K_{n+2}(z;w) = \frac{K_n(z;w^L)}{1-z^2}. \tag{2.3}$$

Here, $K_n(\cdot;w^L)$ is the kernel for the n-point Gauss formula relative to the weight function w^L. Since $|1-z^2|$ attains its minima on C_r at

$z = r$ and $z = -r$, and since $w^L(t)/w^L(-t) = w(t)/w(-t)$, we have as an immediate consequence of (2.1) that

$$\max_{z\in C_r} |K_{n+2}(z;w)| = \begin{cases} \frac{1}{r^2-1} K_n(r;w^L), \\ \frac{1}{r^2-1} |K_n(-r;w^L)|, \end{cases} \tag{2.4}$$

depending on whether $w(t)/w(-t)$ is nondecreasing or nonincreasing, respectively. In particular (cf. [2, p. 1172]), for the Jacobi weight function $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha > -1$, $\beta > -1$, the first relation in (2.4) holds if $\alpha \le \beta$ and the second if $\alpha > \beta$.

2.2. *Gauss-Radau formulae.* There are pairs of such formulae, namely, (1.1) with $N = n+1$, $\tau_N = -1$, and (1.1) with $N = n+1$, $\tau_1 = 1$, both having $R_n(f) = 0$ for $f \in \mathbf{P}_{2n}$. It suffices to consider one of them, say the former, since the kernels of the two formulae are simply related. If we denote $w(-t) = w^*(t)$ and write $K_N^{(\mp 1)}(\cdot;w)$ for the kernel of the Radau formula with $\tau_N = -1$ and $\tau_1 = 1$, respectively, a simple computation indeed will show that $K_N^{(+1)}(z;w) = -\overline{K_N^{(-1)}(-\bar{z};w^*)}$, where bars indicate complex conjugation. Therefore,

$$|K_N^{(+1)}(z;w)| = |K_N^{(-1)}(-\bar{z};w^*)|, \tag{2.5}$$

i.e., the modulus of $K_N^{(+1)}$ for the weight function w at the point z has the same value as the modulus of $K_N^{(-1)}$ for the weight function w^* at the point $-\bar{z}$, the mirror image of z with respect to the imaginary axis.

For the Radau formula with $\tau_N = -1$, we write $w^R(t) = (1+t)w(t)$ and have, as is well known,

$$\omega_{n+1}(z;w) = (1+z)\pi_n(z;w^R). \tag{2.6}$$

There follows, similar to the case of Lobatto formulae,

$$K_{n+1}(z;w) = \frac{K_n(z;w^R)}{1+z}, \tag{2.7}$$

where $K_n(\cdot;w^R)$ is the kernel for the n-point Gauss formula relative to the weight function w^R. Since $|1+z|$ on C_r attains its minimum at $z = -r$, we can now apply the second result in (2.1), giving

$$\max_{z\in C_r} |K_{n+1}(z;w)| = \frac{|K_n(-r;w^R)|}{r-1}, \tag{2.8}$$

provided $w^R(t)/w^R(-t)$ is nonincreasing on $(-1,1)$. Unfortunately, this condition is not satisfied for the Chebyshev weights w_1, w_2, w_3 (cf. (1.9)). We conjecture, in fact, that the maximum in (2.8) is attained at $z = r$, rather than $z = -r$, when $w = w_3$ (cf. Subsection 4.2).

3. Remainder kernels for Chebyshev weight functions. In this section, after some preliminaries on orthogonal polynomials, we provide explicit formulae, for Lobatto = and Radau = type rules, of $K_N(\cdot; w)$ when $w = w_i$, $i = 1, 2, 3, 4$ (cf. (1.9)).

3.1. *Preliminaries.* We shall need some facts about Jacobi polynomials with half-integer parameters. They are given here in a form general enough to be applicable (if need be) to Lobatto and Radau formulae with multiple fixed points.

Lemma 3.1. *The polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t^2)^{-1/2+k}$, $k \geq 0$ an integer, is given by $T_{n+k}^{(k)}(t)$, where T_m denotes the m^{th} = degree Chebyshev polynomial of the first kind.*

Proof. See Equation (4.21.7) in [4] and the paragraph following this equation. □

The following two lemmas are also known, but are stated here in a form more suitable for our purposes. We recall that Chebyshev polynomials U_n, V_n of the second and third kind (orthogonal relative to the weight functions $(1-t^2)^{1/2}$ and $(1-t)^{-1/2}(1+t)^{1/2}$, respectively) are given by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad V_n(\cos\theta) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}. \tag{3.1}$$

Lemma 3.2. *Let $U_{n,k}$ be the polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t)^{1/2}(1+t)^{1/2+k}$, $k \geq 0$*

an integer. Then

$$(3.2_0) \qquad U_{n,0}(t) = U_n(t),$$

(3.2_k)

$$U_{n,k}(t) = \frac{1}{1+t}\left\{U_{n+1,k-1}(t) + \frac{(n+k+\frac{1}{2})(n+k+1)}{(n+\frac{1}{2}k+\frac{1}{2})(n+\frac{1}{2}k+1)}U_{n,k-1}(t)\right\},$$

$$k = 1, 2, 3, \ldots.$$

Proof. Define $U_{n,k}(t) = [(n!(n+k+1)!\sqrt{\pi})/(2\Gamma(n+k/2+1)\Gamma(n+k/2+3/2))]P_n^{(1/2,1/2+k)}(t)$, and use the second relation in [**4**, Equation (4.5.4)] with $\alpha = 1/2$, $\beta = -1/2 + k$. □

Lemma 3.3. *Let $V_{n,k}$ be the polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t)^{-1/2}(1+t)^{1/2+k}$, $k \geq 0$ an integer. Then*

$$(3.3_0) \qquad V_{n,0}(t) = V_n(t),$$

(3.3_k)

$$V_{n,k}(t) = \frac{1}{1+t}\left\{V_{n+1,k-1}(t) + \frac{(n+k)(n+k+\frac{1}{2})}{(n+\frac{1}{2}k)(n+\frac{1}{2}k+\frac{1}{2})}V_{n,k-1}(t)\right\},$$

$$k = 1, 2, 3, \ldots.$$

Proof. Define $V_{n,k}(t) = [(n!(n+k)!\sqrt{\pi})/(\Gamma(n+k/2+1/2)\Gamma(n+k/2+1))]P_n^{(-1/2,1/2+k)}(t)$, and use the second relation in [**4**, Equation (4.5.4)] with $\alpha = -1/2$, $\beta = -1/2 + k$. □

3.2. *Chebyshev-Lobatto formulae.* We begin with the weight function w_1 and consider (1.1) with $w = w_1$, $N = n+2$, $\tau_N = -1$, $\tau_1 = 1$, $R_N(f) = 0$ for $f \in \mathbf{P}_{2n+1}$. Since the nodes τ_ν, $2 \leq \nu \leq N-1$, are the zeros of $\pi_n(\cdot; (1-t^2)w_1) = \pi_n(\cdot; w_2)$, we may take

$$(3.4) \qquad \omega_{n+2}(z; w_1) = (1-z^2)U_n(z),$$

giving

$$(3.5)\quad \rho_{n+2}(z;w_1)=\int_{-1}^{1}\frac{(1-t^2)U_n(t)}{z-t}w_1(t)\,dt=\int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt.$$

Now it is well known (cf. [2, p. 1177]) that

$$(3.6)\qquad U_n(z)=\frac{u^{n+1}-u^{-(n+1)}}{u-u^{-1}},\quad \int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt=\frac{\pi}{u^{n+1}},$$

where z and u are related by the familiar conformal map

$$(3.7)\qquad z=\frac{1}{2}(u+u^{-1}),\quad |u|>1,$$

which transforms the exterior of the unit circle, $\{u\in\mathbf{C}:|u|>1\}$, into the whole z-plane cut along $[-1,1]$. Concentric circles $|u|=\rho$, $\rho>1$, thereby are mapped into confocal ellipses

$$(3.8)\qquad \mathcal{E}_\rho=\{z\in\mathbf{C}:z=\frac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta}),\ 0\le\vartheta\le 2\pi\}$$

with foci at ±1 and sum of semiaxes equal to ρ.

Substituting (3.6) in (3.4) and (3.5), and noting that $z^2-1=(u-u^{-1})^2/4$, one obtains

$$(3.9)\qquad K_{n+2}(z;w_1)=-\frac{4\pi}{u^{n+1}(u-u^{-1})(u^{n+1}-u^{-(n+1)})}.$$

Proceeding to the weight function w_2, we recall that the nodes τ_ν, $2\le\nu\le N-1$, are now the zeros of $\pi_n(\cdot;(1-t^2)w_2)=\pi_n(\cdot;(1-t^2)^{3/2})$, hence, by Lemma 3.1 (with $k=2$), the zeros of T''_{n+2}. Therefore,

$$\omega_{n+2}(z;w_2)=(1-z^2)T''_{n+2}(z),$$

which, by the differential equation satisfied by T_{n+2}, becomes

$$\omega_{n+2}(z;w_2)=zT'_{n+2}(z)-(n+2)^2T_{n+2}(z).$$

With the help of

$$T_{n+2}(z) = \frac{1}{2}[U_{n+2}(z) - U_n(z)], \quad T'_{n+2}(z) = (n+2)U_{n+1}(z)$$

one then gets

$$\omega_{n+2}(z; w_2) = \frac{n+2}{2}\{-(n+2)[U_{n+2}(z) - U_n(z)] + 2zU_{n+1}(z)\},$$

which can be simplified, using the recurrence relation $2zU_{n+1} = U_{n+2} + U_n$, to

$$\omega_{n+2}(z; w_2) = -\frac{(n+1)(n+2)}{2}\left\{U_{n+2}(z) - \frac{n+3}{n+1}U_n(z)\right\}. \tag{3.10}$$

In terms of the variable u, cf. (3.7), using the first relation in (3.6), this can be written as

$$\omega_{n+2}(z; w_2) = -\frac{(n+1)(n+2)}{2(u-u^{-1})}\Big\{u^{n+3} - u^{-(n+3)} - \frac{n+3}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\Big\}.$$

From (3.10) and the second relation in (3.6), we find

$$\begin{aligned}\rho_{n+2}(z; w_2) &= -\frac{(n+1)(n+2)}{2}\Big\{\int_{-1}^{1}\frac{U_{n+2}(t)}{z-t}w_2(t)\,dt \\ &\qquad - \frac{n+3}{n+1}\int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt\Big\} \\ &= -\frac{(n+1)(n+2)\pi}{2u^{n+1}}\left\{u^{-2} - \frac{n+3}{n+1}\right\}.\end{aligned}$$

Therefore, finally,

$$K_{n+2}(z; w_2) = \frac{\pi}{u^{n+1}}\frac{u^{-1} - u^{-3} - \frac{n+3}{n+1}(u-u^{-1})}{u^{n+3} - u^{-(n+3)} - \frac{n+3}{n+1}(u^{n+1} - u^{-(n+1)})}. \tag{3.11}$$

In the case $w = w_3$ we have $\omega_{n+2}(t; w_3) = (1-t^2)\pi_n(t; (1-t)^{1/2}(1+t)^{3/2})$; hence, by Lemma 3.2 (with $k=1$) and (3.2_1),

$$\omega_{n+2}(z; w_3) = (1-z^2)U_{n,1}(z) = (1-z)\left\{U_{n+1}(z) + \frac{n+2}{n+1}U_n(z)\right\}.$$

Using (3.6) together with $1 - z = -(u-1)^2/2u$ yields

$$\omega_{n+2}(z; w_3) = -\frac{1}{2}\frac{u-1}{u+1}\left\{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\right\}.$$

Furthermore,

$$\begin{aligned}\rho_{n+2}(z; w_3) &= \int_{-1}^{1} \frac{\omega_{n+2}(t; w_3)}{z-t} w_3(t)\, dt \\ &= \int_{-1}^{1} \frac{U_{n+1}(t) + \frac{n+2}{n+1} U_n(t)}{z-t} w_2(t)\, dt \\ &= \frac{\pi}{u^{n+1}}\left(u^{-1} + \frac{n+2}{n+1}\right),\end{aligned}$$

giving

(3.12)

$$K_{n+2}(z; w_3) = -\frac{2\pi}{u^{n+1}}\frac{u+1}{u-1}\frac{u^{-1} + \frac{n+2}{n+1}}{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}(u^{n+1} - u^{-(n+1)})}.$$

The case $w = w_4$ is easily transformed to the previous case, since $w_4(t) = w_3(-t)$ implies $\omega_{n+2}(z; w_4) = (-1)^n \omega_{n+2}(-z; w_3)$ and $\rho_{n+2}(z; w_4) = (-1)^{n+1}\rho_{n+2}(-z; w_3)$. Therefore, $K_{n+2}(z; w_4) = -K_{n+2}(-z; w_3)$ or, equivalently,

$$K_{n+2}(z; w_4) = -\overline{K_{n+2}(-\bar{z}; w_3)}. \tag{3.13}$$

The kernel for $w = w_4$ is thus obtained from that for $w = w_3$ essentially by reflection on the imaginary axis.

3.3. *Chebyshev-Radau formulae.* In analogy to (3.6) one has

$$V_n(z) = \frac{u^{n+1} + u^{-n}}{u+1}, \quad \int_{-1}^{1} \frac{V_n(t)}{z-t} w_3(t)\, dt = \frac{2\pi}{(u-1)u^n}. \tag{3.14}$$

The first relation follows from the second relation in (3.1) by writing all cosines in exponential form, using Euler's formula, and then putting $u = e^{i\theta}$. To prove the second relation, substitute $t = \cos\theta$ to obtain

$$\begin{aligned}\int_{-1}^{1} \frac{V_n(t)}{z-t} w_3(t)\, dt &= 2\int_0^{\pi} \frac{\cos(n+\frac{1}{2})\theta \cos\frac{1}{2}\theta}{z - \cos\theta}\, d\theta \\ &= \int_0^{\pi} \frac{\cos(n+1)\theta + \cos n\theta}{z - \cos\theta}\, d\theta,\end{aligned}$$

and then use Equation (5.3) in [2] and the equation immediately following it to evaluate the last integral.

For reasons indicated in Subsection 2.2, we consider only Radau formulae with the fixed point at -1. Thus, $N = n+1$, $\tau_N = -1$ in (1.1), and $R_N(f) = 0$ for $f \in \mathbf{P}_{2n}$. We treat in turn the four weight functions w_i, $i = 1,2,3,4$ (cf. (1.9)).

For $w = w_1$, in view of $\pi_n(\cdot;(1+t)w_1) = \pi_n(\cdot;w_3)$, we can take $\omega_{n+1}(z;w_1) = (1+z)V_n(z)$, which, by the first relation in (3.14) and $1+z = (u+1)^2/2u$, gives

$$\omega_{n+1}(z;w_1) = \frac{1}{2}(u+1)(u^n + u^{-(n+1)})$$

and, by the second relation in (3.14),

$$\rho_{n+1}(z;w_1) = \frac{2\pi}{(u-1)u^n},$$

hence

$$K_{n+1}(z;w_1) = \frac{4\pi u}{(u^2-1)(u^{2n+1}+1)}. \tag{3.15}$$

In the case $w = w_2$, we are led to $\pi_n(\cdot;(1+t)w_2) = \pi_n(\cdot;(1-t)^{1/2}(1+t)^{3/2})$ and may apply Lemma 3.2 and (3.2_1) to obtain

$$\omega_{n+1}(z;w_2) = (1+z)U_{n,1}(z) = U_{n+1}(z) + \frac{n+2}{n+1}U_n(z).$$

Using (3.6), we find

$$\omega_{n+1}(z;w_2) = \frac{1}{u-u^{-1}}\left\{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\right\}$$

and

$$\rho_{n+1}(z;w_2) = \frac{\pi}{u^{n+1}}\left(u^{-1} + \frac{n+2}{n+1}\right),$$

giving

$$K_{n+1}(z;w_2) = \frac{\pi}{u^{n+1}}\frac{1 - u^{-2} + \frac{n+2}{n+1}\left(u - u^{-1}\right)}{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)}. \tag{3.16}$$

For $w = w_3$, since $\pi_n(\cdot; (1+t)w_3) = \pi_n(\cdot; (1-t)^{-1/2}(1+t)^{3/2})$, we can appeal to Lemma 3.3 (with $k = 1$) and (3.3_1) and obtain, similarly as above, using (3.14), that

(3.17)

$$K_{n+1}(z; w_3) = \frac{2\pi}{u^n}\frac{u+1}{u-1}\frac{u^{-1} + \frac{2n+3}{2n+1}}{u^{n+2} + u^{-(n+1)} + \frac{2n+3}{2n+1}(u^{n+1} + u^{-n})}.$$

Finally, when $w = w_4$, we have $(1+t)w_4 = w_2$, so that $\omega_{n+1}(z; w_4) = (1+z)U_n(z)$, and we find, using (3.6), that

$$K_{n+1}(z; w_4) = \frac{2\pi}{u^{n+1}}\frac{u-1}{(u+1)(u^{n+1} - u^{-(n+1)})}. \tag{3.18}$$

4. The maximum of the kernel for Chebyshev weight functions. In this section we present results, in part theoretical, in part empirical, concerning the location of the maximum of $|K_N(z; w)|$ as z varies on the circle C_r or the ellipse $\mathcal{E}_\rho$, both for Lobatto and Radau type formulae, and for the Chebyshev weight functions $w = w_i$, $i = 1, 2, 3, 4$ (cf. (1.9)).

4.1. *Lobatto formulae.* For circular contours, the question of interest is already settled by the discussion in Subsection 2.1, for any of the four Chebyshev weight functions (in fact, for arbitrary Jacobi weights). For elliptic contours $\mathcal{E}_\rho$ (cf. (3.8)) we must insert $u = \rho e^{i\vartheta}$ in the respective formulae for $K_{n+2}(\cdot; w_i)$ and study the behavior of $|K_{n+2}(\cdot; w_i)|$ as a function of ϑ. Because of (1.7), it suffices to consider $0 \le \vartheta \le \pi$, and for the weight functions w_1 and w_2 to consider $0 \le \vartheta \le \pi/2$, because of the additional symmetry $|K_{n+2}(-\bar{z}; w_i)| = |K_{n+2}(z; w_i)|$, $i = 1, 2$.

The analysis is simplest in the case of $w = w_1$. We have

$$|u^m - u^{-m}|^2 = \rho^{2m} + \rho^{-2m} - 2\cos 2m\vartheta, \quad u = \rho e^{i\vartheta},$$

which, for any natural number m, attains its minimum $(\rho^m - \rho^{-m})^2$ at $\vartheta = 0$. Therefore, from (3.9), one immediately obtains

$$\begin{aligned} \max_{z \in \mathcal{E}_\rho} |K_{n+2}(z; w_1)| &= K_{n+2}\left(\frac{1}{2}(\rho + \rho^{-1}); w_1\right) \\ &= \frac{4\pi}{(\rho - \rho^{-1})(\rho^{2n+2} - 1)}. \end{aligned} \tag{4.1}$$

Thus, we have

Theorem 4.1. *The kernel of the $(n+2)$-point Lobatto formula for the Chebyshev weight function w_1 attains its maximum on the ellipse $\mathcal{E}_\rho$ on the real axis; the value of the maximum is given by* (4.1).

For $w = w_2$ and $w = w_3$ we have only empirical and asymptotic results. In the case $w = w_2$, computation shows that $|K_{n+2}(z; w_2)|$, $z \in \mathcal{E}_\rho$, attains its maximum on the real axis if $n = 1$ or $n = 2$. If n is odd and ≥ 3, the maximum is attained on the real axis if $1 < \rho < \rho_n$, and on the imaginary axis if $\rho_n < \rho$ (at either place if $\rho = \rho_n$). If $n \geq 4$ is even, the behavior is more complicated: we have a maximum on the real axis if $1 < \rho < \rho_n'$, on the imaginary axis if $\rho_n < \rho$, and in between if $\rho_n' < \rho < \rho_n$, where ρ_n', ρ_n are certain numbers satisfying $1 < \rho_n' < \rho_n$. Numerical values for $n = 3(1)20$ have been determined by a bisection procedure and are shown in Table 4.1.

TABLE 4.1. The bounds ρ_n', ρ_n, $n = 3(1)20$, for Lobatto formulae with Chebyshev weight w_2.

n	ρ_n'	ρ_n	n	ρ_n'	ρ_n	n	ρ_n'	ρ_n
3		1.4142	9		1.0350	15		1.0127
4	1.2093	1.5955	10	1.0287	1.3138	16	1.0113	1.2237
5		1.1170	11		1.0235	17		1.0099
6	1.0822	1.4483	12	1.0199	1.2756	18	1.0089	1.2051
7		1.0580	13		1.0169	19		1.0080
8	1.0451	1.3671	14	1.0147	1.2466	20	1.0073	1.1896

The empirical observations above can be verified asymptotically as $\rho \downarrow 1$, or as $\rho \to \infty$, for any fixed n. In the first case, a lengthy calculation reveals that when $\vartheta = 0$ (i.e., $z = (\rho + \rho^{-1})/2$),

(4.2)
$$\left| K_{n+2}\left(\frac{1}{2}(\rho + \rho^{-1}; w_2\right)\right| \sim \frac{3\pi}{(n+1)(n+2)(n+3)}(\rho - 1)^{-2}, \quad \rho \downarrow 1,$$

whereas, for other values of ϑ, including $\vartheta = \pi/2$, K_{n+2} is either $O(1)$ or $O((\rho - 1)^{-1})$ as $\rho \downarrow 1$. Interestingly, for example, there

are local peaks of $O((\rho-1)^{-1})$ for values $\vartheta \in (0,\pi/2)$ satisfying $(n+1)\sin(n+3)\vartheta - (n+3)\sin(n+1)\vartheta = 0$. When $\rho \to \infty$, one finds

(4.3)
$$|K_{n+2}(z;w_2)| \sim \frac{(n+3)\pi}{(n+1)\rho^{2n+3}}\left\{1-2\frac{n^2-5}{(n+1)(n+3)}\rho^{-2}\cos 2\vartheta\right\}^{1/2}, \quad \rho\to\infty.$$

For $n=1$ and 2, the coefficient multiplying $\cos 2\vartheta$ in (4.3) is positive, while for $n \geq 3$ it is negative, which explains the behavior observed, at least when ρ is large.

In the case $w = w_3$, there is numerical evidence that the maximum of $|K_{n+2}(\cdot;w_3)|$ on $\mathcal{E}_\rho$ is attained consistently on the positive real axis. This can be verified asymptotically, both for $\rho \downarrow 1$ and $\rho \to \infty$. In the first case,

$$\left|K_{n+2}\left(\frac{1}{2}(\rho+\rho^{-1});w_3\right)\right| \sim \frac{(2n+3)\pi}{(n+1)(n+2)}(\rho-1)^{-2}, \quad \rho\downarrow 1, \tag{4.4}$$

the value at $z = -(\rho+\rho^{-1})/2$ being of the same order, but with smaller coefficient $3\pi/((n+1)(n+2)(2n+3))$. Again, there are sharp peaks of $O((\rho-1)^{-1})$ at values of $\vartheta \in (0,\pi)$ satisfying, this time, $(n+1)\sin(n+2)\vartheta + (n+2)\sin(n+1)\vartheta = 0$. In the second case,

(4.5)
$$|K_{n+2}(z;w_3)| \sim \frac{2(n+2)\pi}{(n+1)\rho^{2n+3}}\left\{1+2\frac{2n^2+4n+1}{(n+1)(n+2)}\rho^{-1}\cos\vartheta\right\}^{1/2}, \quad \rho\to\infty.$$

The same behavior, modulo reflection at the imaginary axis, holds for $w = w_4$, by virtue of (3.13).

4.2. *Radau formulae; circular contours.* The case w_1, again, is amenable to analytic treatment. We now have $z = re^{i\theta}$, $r > 1$, and, by (3.7),

$$u = z + \sqrt{z^2-1} = e^{i\theta}\left(r + \sqrt{r^2 - e^{-2i\theta}}\right), \tag{4.6}$$

where the branch of the square root is taken that assigns positive values to positive arguments. There follows

$$\frac{u}{u^2-1} = \frac{1}{u-u^{-1}} = \left(2e^{i\theta}\sqrt{r^2-e^{-2i\theta}}\right)^{-1},$$

hence

$$\left|\frac{u}{u^2-1}\right| \leq \frac{1}{2\sqrt{r^2-1}},$$

the bound being attained for $\theta = 0$ and $\theta = \pi$. Furthermore,

$$\begin{aligned}|u^{2n+1}+1| &= \left|\left(r+\sqrt{r^2-e^{-2i\theta}}\right)^{2n+1}+e^{-(2n+1)i\theta}\right| \\ &\geq \left|r+\sqrt{r^2-e^{-2i\theta}}\right|^{2n+1}-1 \geq \left(r+\sqrt{r^2-1}\right)^{2n+1}-1,\end{aligned}$$

with equality holding for $\theta = \pi$. Consequently, by (3.15),

$$\max_{z\in C_r}|K_{n+1}(z;w_1)| = |K_{n+1}(-r;w_1)| = \frac{4\pi}{R-R^{-1}}\frac{1}{R^{2n+1}-1}, \tag{4.7}$$

where

$$R = r+\sqrt{r^2-1}. \tag{4.8}$$

We have shown

Theorem 4.2. *The kernel of the $(n+1)$-point Radau formula (with fixed node at -1) for the Chebyshev weight function w_1 attains its maximum modulus on C_r on the negative real axis; the maximum is given by* (4.7), (4.8).

For $w = w_2$, we conjecture

$$\begin{aligned}\max_{z\in C_r}|K_{n+1}(z;w_2)| &= |K_{n+1}(-r;w_2)| \\ &= \frac{\pi}{R^{n+2}}\frac{\left(R-R^{-1}\right)\left(R-\frac{n+1}{n+2}\right)}{\frac{n+1}{n+2}\left(R^{n+2}-R^{-(n+2)}\right)-\left(R^{n+1}-R^{-(n+1)}\right)}\end{aligned}$$

(where the denominator is easily shown to be positive for $R > 1$), and, for $w = w_3$,

$$\begin{aligned}\max_{z\in C_r}|K_{n+1}(z;w_3)| &= K_{n+1}(r;w_3) \\ &= \frac{2\pi}{R^{n+1}}\frac{R+1}{R-1}\frac{R+\frac{2n+1}{2n+3}}{\frac{2n+1}{2n+3}\left(R^{n+2}+R^{-(n+1)}\right)+\left(R^{n+1}+R^{-n}\right)},\end{aligned}$$

where R is given by (4.8). When $w = w_4$, the kernel (3.18) is

sufficiently simple to be treated analytically. Note, first of all, that by (4.6) we have $|u| \geq R$ (with equality for $\theta = \pi$), hence

$$|u^{n+1} - u^{-(n+1)}| \geq |u|^{n+1} - \frac{1}{|u|^{n+1}} \geq R^{n+1} - \frac{1}{R^{n+1}},$$

again with equality holding for $\theta = \pi$. Next, from the relation (3.7) between z and u, there follows $(z-1)/(z+1) = [(u-1)/(u+1)]^2$, so that

$$\left|\frac{u-1}{u+1}\right|^4 = \left|\frac{z-1}{z+1}\right|^2 = \frac{r^2 - 2r\cos\theta + 1}{r^2 + 2r\cos\theta + 1} \leq \left(\frac{r+1}{r-1}\right)^2 = \left(\frac{R+1}{R-1}\right)^4.$$

Here again, the bound is attained for $\theta = \pi$. Consequently, by (3.18),

$$\max_{z \in C_r} |K_{n+1}(z; w_4)| = |K_{n+1}(-r; w_4)| = 2\pi \frac{R+1}{R-1} \frac{1}{R^{2n+2} - 1}. \tag{4.9}$$

This proves

Theorem 4.3. *The kernel of the $(n+1)$-point Radau formula (with fixed node at -1) for the Chebyshev weight function w_4 attains its maximum modulus on C_r on the negative real axis; the maximum is given by* (4.9), (4.8).

4.3. *Radau formulae; elliptic contours.* Putting $u = \rho e^{i\vartheta}$ in (3.15), one obtains, for $w = w_1$,

$$|K_{n+1}(z; w_1)| = \frac{4\pi\rho}{[(\rho^4 - 2\rho^2\cos 2\vartheta + 1)(\rho^{4n+2} + 2\rho^{2n+1}\cos(2n+1)\vartheta + 1)]^{1/2}},$$

which clearly takes on its maximum at $\vartheta = \pi$. Thus,

$$\max_{z \in \mathcal{E}_\rho} |K_{n+1}(z; w_1)| = \left|K_{n+1}\left(-\frac{1}{2}(\rho + \rho^{-1})\right)\right| = \frac{4\pi\rho}{(\rho^2 - 1)(\rho^{2n+1} - 1)}, \tag{4.10}$$

and we have

Theorem 4.4. *The kernel of the $(n+1)$-point Radau formula (with fixed node at -1) for the Chebyshev weight function w_1 attains its*

maximum modulus on $\mathcal{E}_\rho$ on the negative real axis; the maximum is given by (4.10).

For $w = w_2$ and $w = w_3$, the kernel is found by computation to behave more curiously. In the former case, we have a situation similar to the Lobatto formula for the same weight function, namely, the maximum is attained on the negative real axis, when $n = 1, 2, 3$, and also when $n \geq 4$, but then only if $1 < \rho < \rho_n'$ or $\rho_n < \rho$, where ρ_n', ρ_n are shown in Table 4.2; otherwise, the maximum point moves on the ellipse $\mathcal{E}_\rho$ from somewhere close to the imaginary axis to the negative real axis as ρ increases.

TABLE 4.2. The bounds $\rho_n', \rho_n, n = 4(1)10$, for Radau formulae with Chebyshev weight w_2.

n	ρ_n'	ρ_n	n	ρ_n'	ρ_n
			7	1.0681	12.267
4	1.2845	4.7385	8	1.0506	14.385
5	1.1518	7.7651	9	1.0394	16.470
6	1.0965	10.087	10	1.0317	18.533

Asymptotically one finds, consistent with the above, that

(4.11)
$$|K_{n+1}(z; w_2)| \sim \frac{(n+2)\pi}{(n+1)\rho^{2n+2}} \left\{1 - 2\frac{2n+3}{(n+1)(n+2)}\rho^{-1}\cos\vartheta\right\}^{\frac{1}{2}}, \quad \rho \to \infty,$$

and

(4.12)
$$\left|K_{n+1}\left(-\frac{1}{2}(\rho+\rho^{-1}); w_2\right)\right| \sim \frac{6\pi}{(n+1)(n+2)(2n+3)}(\rho-1)^{-2}, \quad \rho \downarrow 1,$$

the value at the other end approaching the finite limit $(2n+3)\pi/(2(n+1)(n+2))$ when $\rho \downarrow 1$, and there being the familiar peaks of $O((\rho-1)^{-1})$ when $(n+1)\sin(n+2)\vartheta + (n+2)\sin(n+1)\vartheta = 0$, $0 < \vartheta < \pi$.

For $w = w_3$, there is numerical evidence to suggest that the maximum is attained on the negative real axis for $1 < \rho < \rho_n$ and on the positive real axis for $\rho > \rho_n$, where ρ_n is as shown in Table 4.3.

TABLE 4.3. The values ρ_n, $n = 1(1)10$, for Radau formulae with Chebyshev weight w_3.

n	ρ_n	n	ρ_n
1	1.1339	6	1.0022
2	1.0318	7	1.0015
3	1.0126	8	1.0010
4	1.0063	9	1.0008
5	1.0036	10	1.0006

There is, again, asymptotic corroboration:

(4.13)
$$|K_{n+1}(z; w_3)| \sim \frac{2(2n+3)\pi}{(2n+1)\rho^{2n+2}} \left\{1 + 4\frac{4n^2+4n-1}{(2n+1)(2n+3)}\rho^{-1}\cos\vartheta\right\}, \quad \rho \to \infty,$$

and

(4.14)
$$\left|K_{n+1}\left(-\frac{1}{2}(\rho+\rho^{-1}); w_3\right)\right| \sim \frac{6\pi}{(n+1)(2n+1)(2n+3)}(\rho-1)^{-2}, \quad \rho \downarrow 1.$$

There are secondary peaks, as $\rho \downarrow 1$, of order $O((\rho-1)^{-1})$ at $\vartheta = 0$ and at values of $\vartheta \in (0, \pi)$ satisfying $(2n+1)\cos(n+3/2)\vartheta + (2n+3)\cos(n+1/2)\vartheta = 0$.

The values ρ_n in Table 4.3 are conjectured to be solutions of the equation

(4.15)
$$\frac{\rho^{2n+3} + 1 + \frac{2n+3}{2n+1}\rho\left(\rho^{2n+1}+1\right)}{\rho^{2n+3} - 1 - \frac{2n+3}{2n+1}\rho\left(\rho^{2n+1}-1\right)} = \left(\frac{\rho+1}{\rho-1}\right)^2 \frac{\rho + \frac{2n+1}{2n+3}}{\rho - \frac{2n+1}{2n+3}}$$

expressing equality of the values of $|K_{n+1}(\cdot; w_3)|$ at both real vertices of the ellipse $\mathcal{E}_\rho$.

Finally, when $w = w_4$, Equation (3.18) for $u = \rho e^{i\vartheta}$ implies

$$|K_{n+1}(z; w_4)| = \frac{2\pi}{\rho^{n+1}} \left\{\frac{\rho^2 - 2\rho\cos\vartheta + 1}{(\rho^2+2\rho\cos\vartheta+1)(\rho^{2n+2}+\rho^{-(2n+2)} - 2\cos(2n+2)\vartheta)}\right\}^{\frac{1}{2}},$$

which is largest when $\vartheta = \pi$, giving

$$\max_{z\in\mathcal{E}_\rho} |K_{n+1}(z; w_4)| = \left|K_{n+1}\left(-\frac{1}{2}\left(\rho+\rho^{-1}\right); w_4\right)\right|$$

$$= 2\pi \frac{\rho+1}{\rho-1}\frac{1}{\rho^{2n+2}-1}. \tag{4.16}$$

Thus, we have

Theorem 4.5. *The kernel of the $(n+1)$-point Radau formula (with fixed node at -1) for the Chebyshev weight function w_4 attains its maximum modulus on $\mathcal{E}_\rho$ on the negative real axis; the maximum is given by* (4.16).

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20.9. [126] "Gauss–Radau and Gauss–Lobatto quadratures with double end points"

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Gauss–Radau and Gauss–Lobatto quadratures with double end points *

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Abstract

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We develop explicit formulae for generalized Gauss–Radau and Gauss–Lobatto quadrature rules having end points of multiplicity 2 and containing Chebyshev weight functions of any of the four kinds.

Keywords: Generalized Gauss–Radau and Gauss–Lobatto rules, Chebyshev weight functions.

1. Introduction

Gaussian quadrature formulae for special weight functions, especially of Chebyshev type, have been known for a long time. Already in 1864, Mehler [11] studied the general case of Jacobi weights and noted the remarkable simplifications afforded by the Chebyshev weight function of the first kind. Chebyshev weights of the other kinds were later considered independently by Posse [12] and Stieltjes [13]. Markov [10] soon thereafter obtained the Radau and Lobatto versions of the (1st-kind) Gauss–Chebyshev formula (in which one or both of the end points are included among the nodes). The more general case of Jacobi weights, in particular all four Chebyshev weights, had to wait until 1952 when Bouzitat [1] developed the corresponding Gauss–Radau and Gauss–Lobatto formulae in detail. Explicit (as opposed to numerical) generalizations of these formulae to end points having multiplicity > 1 do not appear to have received much attention, except for the generalized Gauss–Lobatto formula with Legendre weight, which was studied by Gatteschi [2]. In the present paper, we develop for all four Chebyshev weight functions both Gauss–Radau and Gauss–Lobatto formulae having end points of multiplicity 2. This supplements earlier work of ours [7] devoted solely to a study of their remainder terms (for analytic functions). We expect these new quadrature rules to be potentially

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useful in applications, most likely in the solution of boundary value problems by spectral methods, where Lobatto-type formulae have been in use for some time.

Section 2 is devoted to Radau-type formulae. We begin in Section 2.1 with positivity results for general weight functions and then develop the desired multiple end point formulae in detail for the Chebyshev weight function of the first kind in Section 2.2, and for the other Chebyshev weights more summarily in Section 2.3. The same program is carried out in Section 3 for Lobatto-type formulae. Section 4 concludes with numerical examples.

2. Gauss–Radau formulae

In this section we develop the Gauss–Radau formula on the interval $[-1, 1]$, with a double node at the end point -1, both for general weight functions and weight functions of Chebyshev type. In the latter case we give detailed derivations only for the Chebyshev weight function of the first kind. For the other three Chebyshev weights the derivation is similar and will only be briefly summarized.

2.1. General weight function

Given any positive integrable weight function w on $[-1, 1]$, the associated Gauss–Radau quadrature rule to be studied has the form

$$\int_{-1}^{1} f(t)w(t)\,dt = \kappa_0^R f(-1) + \kappa_1^R f'(-1) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + E_n^R(f), \tag{2.1}$$

and is characterized by the requirement of having maximal degree of exactness $2n+1$,

$$E_n^R(f) = 0 \quad \text{if } f \in \mathbb{P}_{2n+1}. \tag{2.2}$$

It is well known that the nodes $\tau_\nu = \tau_\nu^R$ must be the zeros of $\pi_n(\cdot) = \pi_n(\cdot; w^R)$, the nth-degree orthogonal polynomial relative to the weight function

$$w^R(t) = (1+t)^2 w(t). \tag{2.3}$$

The weights in (2.1) admit various representations, the ones obtained via interpolation having the form

$$\kappa_0^R = \frac{1}{\pi_n(-1)} \int_{-1}^{1} \left[1 - \frac{\pi_n'(-1)}{\pi_n(-1)}(1+t)\right] \pi_n(t)w(t)\,dt, \tag{2.4$_0$}$$

$$\kappa_1^R = \frac{1}{\pi_n(-1)} \int_{-1}^{1} (1+t)\pi_n(t)w(t)\,dt, \tag{2.4$_1$}$$

$$\lambda_\nu^R = \int_{-1}^{1} \frac{(1+t)^2 \pi_n(t)}{(1+\tau_\nu)^2 \pi_n'(\tau_\nu)(t-\tau_\nu)} w(t)\,dt, \quad \nu = 1, 2, \ldots, n. \tag{2.4$_\nu$}$$

The weights λ_ν^R for the interior nodes can be re-expressed by a standard application of the Christoffel–Darboux formula as follows:

$$\lambda_\nu^R = -\frac{\|\pi_n\|_R^2}{(1+\tau_\nu)^2 \pi_{n+1}(\tau_\nu)\pi_n'(\tau_\nu)} = \frac{\lambda_\nu}{(1+\tau_\nu)^2}. \tag{2.5$_\nu$}$$

Here, $\|\cdot\|_R$ is the L_2-norm weighted by w^R, the polynomials π_n, π_{n+1} are assumed monic, and λ_ν are the weights of the Gaussian quadrature rule relative to the weight function w^R.

Theorem 2.1. *All weights in* (2.1) *are positive.*

Proof. The positivity of λ_ν^R follows immediately from the second equality in (2.5$_\nu$). For the weights in the boundary terms we easily obtain from (2.1), (2.2) that

$$\kappa_0^R = \frac{1}{\pi_n^2(-1)} \int_{-1}^{1} \left[1 - \frac{2\pi_n'(-1)}{\pi_n(-1)}(1+t)\right] \pi_n^2(t) w(t)\, dt, \tag{2.6}$$

$$\kappa_1^R = \frac{1}{\pi_n^2(-1)} \int_{-1}^{1} (1+t)\pi_n^2(t) w(t)\, dt, \tag{2.7}$$

from which their positivity follows at once, since $\pi_n'(-1)/\pi_n(-1) < 0$. □

The λ_ν and τ_ν in (2.5$_\nu$), being the Gauss weights and nodes for the weight function w^R (cf. (2.3)), are best computed in terms of eigenvalues and eigenvectors of the symmetric, tridiagonal Jacobi matrix $J_n(w^R)$ of order n. The latter, in turn, can be obtained from the Jacobi matrix $J_{n+1}(w)$ of order $n+1$ (assumed known or computable) by applying one step of the QR algorithm with shift -1 and then discarding the last row and column; cf. [5, §5.1] or [9].

2.2. Chebyshev weight of the first kind

In this subsection we let $w(t) = (1-t^2)^{-1/2}$ on $[-1, 1]$, so that by (2.3),

$$w^R(t) = (1-t)^{-1/2}(1+t)^{3/2} \tag{2.8}$$

is the Jacobi weight with parameters $\alpha = -\frac{1}{2}$, $\beta = \frac{3}{2}$. The corresponding (monic) orthogonal polynomial of degree n, by [7, Eq. (2.3)], is given by

$$\pi_n(t; w^R) = \frac{1}{2^{n+1}} \frac{1}{1+t} \left\{ V_{n+1}(t) + \frac{2n+3}{2n+1} V_n(t) \right\}, \tag{2.9}$$

where V_n is the Chebyshev polynomial of the third kind,

$$V_n(\cos\theta) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}. \tag{2.10}$$

As is well known, and easily derived from (2.10), V_n satisfies the differential equation

$$(1-t^2)V_n''(t) + (1-2t)V_n'(t) + n(n+1)V_n(t) = 0. \tag{2.11}$$

For convenience we let

$$\tilde{\pi}_n(t) = 2^{n+1}\pi_n(t; w^R). \tag{2.12}$$

Lemma 2.2. *The polynomial* $\tilde{\pi}_n$ *in* (2.12), *with* w^R *given by* (2.8), *satisfies for any* $n \geqslant 1$

$$\tilde{\pi}_n(-1) = \tfrac{2}{3}(-1)^n(n+1)(2n+3), \tag{2.13}$$

$$\tilde{\pi}_n'(-1) = \tfrac{2}{15}(-1)^{n+1} n(n+1)(n+2)(2n+3). \tag{2.14}$$

Proof. Letting $\theta \to \pi$ in (2.10), and using the rule of Bernoulli–L'Hospital, gives

$$V_n(-1) = (-1)^n(2n+1). \tag{2.15}$$

Putting $t = -1$ in (2.11) then yields

$$V_n'(-1) = \tfrac{1}{3}(-1)^{n+1}n(n+1)(2n+1). \tag{2.16}$$

Another application of Bernoulli–L'Hospital's rule, this time to the right-hand side of (2.9), gives

$$\tilde{\pi}_n(-1) = V_{n+1}'(-1) + \frac{2n+3}{2n+1}V_n'(-1),$$

which together with (2.16) yields (2.13).

To prove (2.14), first multiply (2.9) by $1+t$, differentiate the resulting equation twice, and then set $t = -1$, to get

$$\tilde{\pi}_n'(-1) = \tfrac{1}{2}\left\{V_{n+1}''(-1) + \frac{2n+3}{2n+1}V_n''(-1)\right\}. \tag{2.17}$$

Differentiating (2.11) once, and then letting $t = -1$ and using (2.16), on the other hand, gives

$$V_n''(-1) = \tfrac{1}{15}(-1)^n(n-1)n(n+1)(n+2)(2n+1),$$

which, inserted in (2.17), yields the desired result. □

Theorem 2.3. *The weights* κ_0^R *and* κ_1^R *in* (2.1), *where* $w(t) = (1-t^2)^{-1/2}$, *are given by*

$$\kappa_0^R = \tfrac{3}{5}\pi\frac{6n^2+12n+5}{(n+1)(2n+1)(2n+3)}, \tag{2.18}$$

$$\kappa_1^R = \frac{3\pi}{(n+1)(2n+1)(2n+3)}. \tag{2.19}$$

Proof. In the following we need the integral relation

$$\int_{-1}^{1} V_n(t)(1-t^2)^{-1/2}\,dt = (-1)^n\pi, \quad n \geqslant 0, \tag{2.20}$$

which is easily derived from (2.10) by the change of variable $t = \cos\theta$.

The formula (2.19) is a direct consequence of (2.4_1) together with (2.9), (2.20), (2.12) and (2.13).

To prove (2.18), we first note from (2.4_0) that

$$\kappa_0^R = \frac{1}{\tilde{\pi}_n(-1)}\int_{-1}^{1}\tilde{\pi}_n(t)w(t)\,dt - \frac{\tilde{\pi}_n'(-1)}{\tilde{\pi}_n(-1)}\kappa_1^R. \tag{2.21}$$

We now show, for w as given in the theorem, that

$$\int_{-1}^{1}\tilde{\pi}_n(t)w(t)\,dt = 2\pi(-1)^n\frac{(n+1)^2}{2n+1}. \tag{2.22}$$

To do this, we expand $\tilde{\pi}_n$ in Chebyshev polynomials of the third kind,

$$\tilde{\pi}_n(t) = \sum_{k=0}^{n} c_k V_k(t), \tag{2.23}$$

so that, by (2.9), (2.12),

$$(1+t)\sum_{k=0}^{n} c_k V_k(t) = V_{n+1}(t) + \frac{2n+3}{2n+1} V_n(t).$$

Using $tV_0 = \frac{1}{2}(V_0 + V_1)$ and $tV_k = \frac{1}{2}(V_{k+1} + V_{k-1})$ for $k = 1, 2, \ldots$, this can be written as

$$\left(\tfrac{3}{2}c_0 + \tfrac{1}{2}c_1\right)V_0 + \sum_{k=1}^{n-1}\left(\tfrac{1}{2}c_{k-1} + c_k + \tfrac{1}{2}c_{k+1}\right)V_k + \left(\tfrac{1}{2}c_{n-1} + c_n\right)V_n + \tfrac{1}{2}c_n V_{n+1}$$
$$= V_{n+1} + \frac{2n+3}{2n+1} V_n.$$

Equating coefficients on both sides yields

$$\begin{aligned} &3c_0 + c_1 = 0, \qquad c_{k-1} + 2c_k + c_{k+1} = 0; \quad k = 1, 2, \ldots, n-1, \\ &c_{n-1} + 2c_n = 2\frac{2n+3}{2n+1}, \qquad c_n = 2. \end{aligned} \tag{2.24}$$

The last two equations determine $c_n = 2$ and $c_{n-1} = -2(2n-1)/(2n+1)$. The second equation in the first line is a linear difference equation with constant coefficients and has the general solution

$$c_k = (a + bk)(-1)^k.$$

There are two boundary conditions for determining a and b: the first relation in (2.24) and the value of c_{n-1} found above. These give

$$a = \frac{2(-1)^n}{2n+1}, \qquad b = \frac{4(-1)^n}{2n+1},$$

hence

$$c_k = \frac{2(-1)^{n+k}}{2n+1}(1+2k), \quad 0 \leqslant k \leqslant n. \tag{2.25}$$

(It is easily verified that (2.25) is also valid in the case $n = 1$.) Now using (2.20), we get from (2.23)

$$\int_{-1}^{1} \tilde{\pi}_n(t) w(t)\, dt = \sum_{k=0}^{n} c_k \int_{-1}^{1} V_k(t) w(t)\, dt = \pi \sum_{k=0}^{n} (-1)^k c_k,$$

which, upon inserting (2.25) in the sum on the far right, yields (2.22).

The formula (2.18) now follows from (2.21), (2.22), (2.19) and (2.13), (2.14). □

While expressions for the weights λ_ν^R have already been given in (2.4_ν), (2.5_ν) for general weight functions w, alternative, more explicit, formulae can be obtained for Chebyshev weight functions. Those for the Chebyshev weight of the first kind, given in the next theorem, are particularly simple.

Theorem 2.4. *The weights* λ_ν^R *in* (2.1), *where* $w(t) = (1-t^2)^{-1/2}$, *are expressible in the form*

$$\lambda_\nu^R = \frac{\pi}{(n+1)(2n+1)(2n+3)} \frac{4(n+1)^2 + 1 + \left(4(n+1)^2 - 1\right)\tau_\nu}{1+\tau_\nu}, \quad \nu = 1, 2, \ldots, n, \tag{2.26}$$

where τ_ν *are the zeros of the polynomial* $\pi_n(\cdot; w^R)$ *in* (2.9).

Proof. The point of departure is the first equation in (2.5$_\nu$), where $\pi_n(\cdot) = \pi_n(\cdot\,; w^R)$ is the monic Jacobi polynomial with parameters $\alpha = -\frac{1}{2}$, $\beta = \frac{3}{2}$ (cf. (2.8)). From well-known formulae for the norm and leading coefficient of Jacobi polynomials one finds

$$\|\pi_n\|_R^2 = \frac{\pi}{2^{2n+1}} \frac{2n+3}{2n+1}.$$

A simple computation based on [14, Eq. (4.5.7)], transcribed to monic polynomials, yields

$$\pi_n'(\tau_\nu) = -2(n+1)\frac{\pi_{n+1}(\tau_\nu)}{1-\tau_\nu^2}.$$

Therefore, by (2.5$_\nu$),

$$\lambda_\nu^R = \frac{\pi}{2^{2n+2}} \frac{2n+3}{(n+1)(2n+1)} \frac{1-\tau_\nu}{(1+\tau_\nu)\pi_{n+1}^2(\tau_\nu)}. \tag{2.27}$$

To complete the proof, we show that

$$\pi_{n+1}(\tau_\nu) = \frac{2n+3}{2^{n+1}} T_{n+1}(\tau_\nu), \tag{2.28}$$

where T_{n+1} is the Chebyshev polynomial of the first kind, of degree $n+1$, and that

$$T_{n+1}^2(\tau_\nu) = \frac{1-\tau_\nu}{4(n+1)^2 + 1 + \big(4(n+1)^2 - 1\big)\tau_\nu}. \tag{2.29}$$

Letting $t = \tau_\nu = \cos\theta_\nu$ in (2.9) and using (2.10), we find

$$\cos(n+\tfrac{3}{2})\theta_\nu + \frac{2n+3}{2n+1}\cos(n+\tfrac{1}{2})\theta_\nu = 0,$$

from which, by the addition formula for the cosine,

$$\tan(n+1)\theta_\nu \tan\tfrac{1}{2}\theta_\nu = -2(n+1). \tag{2.30}$$

Squaring both sides and using $\tan^2\alpha = \cos^{-2}\alpha - 1$ gives

$$\left(\frac{1}{T_{n+1}^2(\tau_\nu)} - 1\right)\frac{1-\tau_\nu}{1+\tau_\nu} = 4(n+1)^2,$$

which implies (2.29).

To prove (2.28), we use again (2.9) [with n replaced by $n+1$] together with (2.10) to obtain

$$\pi_{n+1}(\tau_\nu) = \frac{1}{2^{n+3}} \frac{1}{(2n+3)\cos^3\frac{1}{2}\theta_\nu}\big\{(2n+3)\cos(n+\tfrac{5}{2})\theta_\nu + (2n+5)\cos(n+\tfrac{3}{2})\theta_\nu\big\}. \tag{2.31}$$

The expression in braces is now written as

$$(2n+3)\big[\cos(n+\tfrac{5}{2})\theta_\nu + \cos(n+\tfrac{3}{2})\theta_\nu\big] + 2\cos(n+\tfrac{3}{2})\theta_\nu,$$

and reduced by means of elementary trigonometric identities to

$$4\cos(n+1)\theta_\nu \cos\tfrac{1}{2}\theta_\nu\big[(2n+3)\cos^2\tfrac{1}{2}\theta_\nu - (n+1)\big]$$
$$-2\sin(n+1)\theta_\nu \sin\tfrac{1}{2}\theta_\nu\big[2(2n+3)\cos^2\tfrac{1}{2}\theta_\nu + 1\big].$$

Applying (2.30) to the last term simplifies the expression to

$$4(2n+3)^2 \cos(n+1)\theta_\nu \cos^3\tfrac{1}{2}\theta_\nu,$$

which, inserted in (2.31), yields (2.28). □

2.3. Other Chebyshev weight functions

(a) We begin with the Chebyshev weight of the second kind, $w(t) = (1-t^2)^{1/2}$, for which in place of (2.8) we now have

$$w^{\mathrm{R}}(t) = (1-t)^{1/2}(1+t)^{5/2}. \tag{2.32}$$

The corresponding (monic) orthogonal polynomial, by [7, Eq. (2.6)], is

$$\begin{aligned} \pi_n(t;\, w^{\mathrm{R}}) &= \frac{1}{2^{n+2}}\tilde{\pi}_n(t), \\ \tilde{\pi}_n(t) &= \frac{1}{(1+t)^2}\left\{U_{n+2}(t) + 4\frac{n+3}{2n+3}U_{n+1}(t) + \frac{(n+3)(2n+5)}{(n+1)(2n+3)}U_n(t)\right\}. \end{aligned} \tag{2.33}$$

Here,

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}$$

is the Chebyshev polynomial of the second kind, which satisfies the differential equation

$$(1-t^2)U_n''(t) - 3tU_n'(t) + n(n+2)U_n(t) = 0. \tag{2.34}$$

To derive the analogue of Lemma 2.2, one now has to apply the rule of Bernoulli–L'Hospital twice to $\tilde{\pi}_n$, and use two differentiations of the differential equation (2.34), to obtain the values of $\tilde{\pi}_n$ and $\tilde{\pi}_n'$ at -1. Other than that, the derivation proceeds along the same lines as before. We state the results as Lemma 2.5.

Lemma 2.5. *For the polynomial $\tilde{\pi}_n$ defined in* (2.33) *we have, for any $n \geqslant 1$,*

$$\tilde{\pi}_n(-1) = \tfrac{2}{15}(-1)^n(n+2)(n+3)(2n+5), \tag{2.35}$$

$$\tilde{\pi}_n'(-1) = \tfrac{2}{105}(-1)^{n+1}n(n+2)(n+3)(n+4)(2n+5). \tag{2.36}$$

The proof of the next theorem is similar to the proof of Theorem 2.3, using

$$\int_{-1}^{1} \frac{1}{1+t}U_n(t)(1-t^2)^{1/2}\,dt = (-1)^n\pi, \quad n \geqslant 0, \tag{2.37}$$

in place of (2.20) and Lemma 2.5 in place of Lemma 2.2. We omit the details.

Theorem 2.6. *The weights κ_0^{R} and κ_1^{R} in* (2.1), *where $w(t) = (1-t^2)^{1/2}$, are given by*

$$\kappa_0^{\mathrm{R}} = \tfrac{15}{7}\pi\frac{10n^2+40n+21}{(n+1)(n+2)(n+3)(2n+3)(2n+5)}, \tag{2.38}$$

$$\kappa_1^{\mathrm{R}} = \frac{45\pi}{(n+1)(n+2)(n+3)(2n+3)(2n+5)}. \tag{2.39}$$

The weights λ_ν^R corresponding to interior nodes could again be expressed in terms of n and τ_ν alone, as was done in Theorem 2.4 for the Chebyshev weight of the first kind, but the expressions are now rather more complicated and do not seem to offer any advantage over the general formula (2.5$_\nu$). We therefore do not state them here.

(b) For the Chebyshev weight of the third kind, $w(t) = (1-t)^{-1/2}(1+t)^{1/2}$, we have $w^R(t) = (1-t)^{-1/2}(1+t)^{5/2}$, and two applications of [6, Lemma 3.3] give

$$\begin{aligned} \pi_n(t; w^R) &= \frac{1}{2^{n+2}}\tilde{\pi}_n(t), \\ \tilde{\pi}_n(t) &= \frac{1}{(1+t)^2}\left\{V_{n+2}(t) + \frac{2n+5}{n+1}V_{n+1}(t) + \frac{(n+2)(2n+5)}{(n+1)(2n+1)}V_n(t)\right\}, \end{aligned} \tag{2.40}$$

with V_n defined as in (2.10). Since

$$\int_{-1}^{1} \tilde{\pi}_n(t)w(t)\,dt = \int_{-1}^{1} (1+t)\tilde{\pi}_n(t)(1-t^2)^{-1/2}\,dt,$$

the techniques used in the proof of Theorem 2.3, in particular (2.20), become applicable and yield the following theorem.

Theorem 2.7. *The weights κ_0^R and κ_1^R in (2.1), where $w(t) = (1-t)^{-1/2}(1+t)^{1/2}$, are given by*

$$\kappa_0^R = \tfrac{30}{7}\pi\frac{5n^2+15n+7}{(n+1)(n+2)(2n+1)(2n+3)(2n+5)}, \tag{2.41}$$

$$\kappa_1^R = \frac{45\pi}{(n+1)(n+2)(2n+1)(2n+3)(2n+5)}. \tag{2.42}$$

(c) Finally, the Chebyshev weight of the fourth kind, $w(t) = (1-t)^{1/2}(1+t)^{-1/2}$, has $w^R(t) = (1-t)^{1/2}(1+t)^{3/2}$, so that [6, Lemma 3.2] yields

$$\begin{aligned} \pi_n(t; w^R) &= \frac{1}{2^{n+1}}\tilde{\pi}_n(t), \\ \tilde{\pi}_n(t) &= \frac{1}{1+t}\left\{U_{n+1}(t) + \frac{n+2}{n+1}U_n(t)\right\}. \end{aligned} \tag{2.43}$$

The relation

$$\int_{-1}^{1} \tilde{\pi}_n(t)w(t)\,dt = \int_{-1}^{1} \frac{1}{1+t}\tilde{\pi}_n(t)(1-t^2)^{1/2}\,dt$$

allows us to proceed as in the proof of Theorem 2.6, to obtain the following theorem.

Theorem 2.8. *The weights κ_0^R and κ_1^R in (2.1), where $w(t) = (1-t)^{1/2}(1+t)^{-1/2}$, are given by*

$$\kappa_0^R = \tfrac{6}{5}\pi\frac{3n^2+9n+5}{(n+1)(n+2)(2n+3)}, \tag{2.44}$$

$$\kappa_1^R = \frac{3\pi}{(n+1)(n+2)(2n+3)}. \tag{2.45}$$

Although the zeros of the polynomial $\pi_n(\cdot; w^R)$ for any of the four Chebyshev weights could be computed as roots of certain trigonometric equations, it is more convenient, and probably faster, to use the general procedure described at the end of Section 2.1 to compute not only the zeros, but also the respective Christoffel numbers λ_ν.

3. Gauss–Lobatto formulae

Here we briefly report on the results obtained by carrying out the program of Section 2 for Gauss–Lobatto quadrature rules on $[-1, 1]$ having double nodes at each end point.

3.1. General weight function

Let w be again a positive integrable weight function on $[-1, 1]$. Our concern is with the quadrature rule

$$\int_{-1}^{1} f(t)w(t)\,dt = \kappa_0^L f(-1) + \kappa_1^L f'(-1) + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + \mu_0^L f(1) - \mu_1^L f'(1) + E_n^L(f) \tag{3.1}$$

of maximum degree of exactness $2n + 3$,

$$E_n^L(f) = 0 \quad \text{if } f \in \mathbb{P}_{2n+3}. \tag{3.2}$$

The nodes $\tau_\nu = \tau_\nu^L$ are then the zeros of the orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; w^L)$, where

$$w^L(t) = (1-t^2)^2 w(t). \tag{3.3}$$

The formula (3.1) enjoys perfect symmetry whenever w is an even function; indeed,

$$\begin{aligned} &\mu_0^L = \kappa_0^L, \qquad \mu_1^L = \kappa_1^L, \\ &\tau_{n+1-\nu}^L + \tau_\nu^L = 0, \quad \lambda_{n+1-\nu}^L = \lambda_\nu^L, \qquad \nu = 1, 2, \ldots, n, \end{aligned} \qquad (w \text{ even}). \tag{3.4}$$

Interpolation theory provides explicit formulae for the weights in (3.1), viz.,

$$\kappa_0^L = \frac{1}{4\pi_n(-1)} \int_{-1}^{1} \left[1 + \left(1 - \frac{\pi_n'(-1)}{\pi_n(-1)}\right)(1+t)\right](1-t)^2 \pi_n(t) w(t)\,dt, \tag{3.5$_0$}$$

$$\kappa_1^L = \frac{1}{4\pi_n(-1)} \int_{-1}^{1} (1+t)(1-t)^2 \pi_n(t) w(t)\,dt, \tag{3.5$_1$}$$

and similar formulae for μ_0^L, μ_1^L (with the point -1 replaced by $+1$, the sign of π_n' reversed, and $1+t$, $1-t$ replaced by $1-t$ and $1+t$, respectively). Likewise,

$$\lambda_\nu^L = \int_{-1}^{1} \frac{(1-t^2)^2 \pi_n(t)}{(1-\tau_\nu^2)^2 \pi_n'(\tau_\nu)(t-\tau_\nu)} w(t)\,dt, \quad \nu = 1, 2, \ldots, n. \tag{3.5$_\nu$}$$

This can be transformed by the Christoffel–Darboux formula to

$$\lambda_\nu^L = -\frac{\|\pi_n\|_L^2}{(1-\tau_\nu^2)^2 \pi_{n+1}(\tau_\nu)\pi_n'(\tau_\nu)} = \frac{\lambda_\nu}{(1-\tau_\nu^2)^2}, \tag{3.6$_\nu$}$$

with notations analogous to those in (2.5$_\nu$). The last equation, containing the Gauss nodes τ_ν and weights λ_ν relative to the weight function w^L in (3.3), is again the one most convenient for computation. The required Jacobi matrix $J_n(w^L)$ is now obtained from $J_{n+2}(w)$ by applying two QR steps in succession, one with shift 1, the other with shift -1, the last row and column being discarded each time.

Theorem 3.1. *The values of* κ_0^L, κ_1^L, μ_0^L, μ_1^L *and* λ_ν^L, $\nu = 1, 2, \ldots, n$, *are all positive.*

Proof. The positivity of λ_ν^L is immediate from (3.6$_\nu$). The one for κ_0^L and κ_1^L follows by respectively inserting

$$f(t) = \frac{1}{4\pi_n^2(-1)}\left[1 + \left(1 - \frac{2\pi_n'(-1)}{\pi_n(-1)}\right)(1+t)\right](1-t)^2\pi_n^2(t)$$

and

$$f(t) = \frac{1}{4\pi_n^2(-1)}(1+t)(1-t)^2\pi_n^2(t)$$

in (3.1), and noting (3.2) and the fact that $\pi_n'(-1)/\pi_n(-1)$ is negative. A similar argument (with the changes indicated after (3.5$_1$)) works for μ_0^L, μ_1^L. □

3.2. Chebyshev weight of the first kind

The lemmas and theorems contained in this and the following subsection look deceptively simple, but are the result of rather lengthy computations. The lemmas are included here to facilitate verification by the interested reader.

For the Chebyshev weight of the first kind, $w(t) = (1-t^2)^{-1/2}$, we have $w^L = (1-t^2)^{3/2}$, and [7, Eq. (2.10)] yields

$$\begin{aligned} \pi_n(t;\, w^L) &= \frac{1}{2^{n+2}}\tilde{\pi}_n(t), \\ \tilde{\pi}_n(t) &= \frac{1}{t^2-1}\left\{U_{n+2}(t) - \frac{n+3}{n+1}U_n(t)\right\}. \end{aligned} \tag{3.7}$$

Lemma 3.2. *The polynomial* $\tilde{\pi}_n$ *in* (3.7) *satisfies, for all* $n \geqslant 1$,

$$\tilde{\pi}_n(-1) = \tfrac{2}{3}(-1)^n(n+2)(n+3), \tag{3.8}$$

$$\tilde{\pi}_n'(-1) = \tfrac{2}{15}(-1)^{n+1}n(n+2)(n+3)(n+4). \tag{3.9}$$

Proof. Bernoulli–L'Hospital's rule applied to (3.7) and subsequent use of the differential equation (2.34) at $t = -1$ yield the first relation. The second is obtained by differentiating $(t^2-1)\tilde{\pi}_n(t)$ twice to express $\tilde{\pi}_n'(-1)$ in terms of $U_n''(-1)$, $U_{n+2}''(-1)$ and $\tilde{\pi}_n(-1)$, and then using (3.8) and the differential equation (2.34), differentiated once and evaluated at $t = -1$, to complete the computation. □

Theorem 3.3. *The weights of the boundary terms in* (3.1), *where* $w(t) = (1-t^2)^{-1/2}$, *are given by*

$$\kappa_0^L = \mu_0^L = \tfrac{3}{10}\pi \frac{3n^2+12n+10}{(n+1)(n+2)(n+3)}, \tag{3.10}$$

$$\kappa_1^L = \mu_1^L = \frac{3\pi}{4(n+1)(n+2)(n+3)}. \tag{3.11}$$

Proof. Equality between the κ's and μ's is a consequence of symmetry. Equation (3.11) follows directly from (3.5_1), (2.37) and (3.8). To prove (3.10), we first note from (3.5_0) that

$$\kappa_0^L = \frac{1}{4\tilde{\pi}_n(-1)} \int_{-1}^{1} (1-t)^2 \tilde{\pi}_n(t) w(t)\, dt + \left(1 - \frac{\tilde{\pi}_n'(-1)}{\tilde{\pi}_n(-1)}\right) \kappa_1^L, \tag{3.12}$$

and then use

$$\int_{-1}^{1} (1-t)^2 \tilde{\pi}_n(t) w(t)\, dt = \int_{-1}^{1} \frac{1}{(1+t)} (1-t) \tilde{\pi}_n(t) (1-t^2)^{1/2}\, dt$$

and expansion of $(1-t)\tilde{\pi}_n(t)$ in Chebyshev polynomials of the second kind, together with (2.37), to proceed as in the proof of Theorem 2.6. □

3.3. Other Chebyshev weight functions

(a) For the Chebyshev weight of the second kind, $w(t) = (1-t^2)^{1/2}$, we have $w^L(t) = (1-t^2)^{5/2}$, so that [7, Eq. (2.12)] gives

$$\begin{aligned} \pi_n(t) &= \frac{1}{2^{n+4}} \tilde{\pi}_n(t), \\ \tilde{\pi}_n(t) &= \frac{1}{(1-t^2)^2} \left\{ U_{n+4}(t) - 2\frac{n+5}{n+2} U_{n+2}(t) + \frac{(n+4)(n+5)}{(n+1)(n+2)} U_n(t) \right\}. \end{aligned} \tag{3.13}$$

Lemma 3.4. *For the polynomial* $\tilde{\pi}_n$ *in* (3.13), *we have for all* $n \geqslant 1$

$$\tilde{\pi}_n(-1) = \tfrac{4}{15}(-1)^n (n+3)(n+4)(n+5), \tag{3.14}$$

$$\tilde{\pi}_n'(-1) = \tfrac{4}{105}(-1)^{n+1} n(n+3)(n+4)(n+5)(n+6). \tag{3.15}$$

Proof. The first equation follows from (3.13) by two applications of Bernoulli–L'Hospital's rule, and the second by differentiating $(1-t^2)^2\tilde{\pi}_n(t)$ three times at $t=-1$. □

Theorem 3.5. *The weights of the boundary terms in* (3.1), *where* $w(t) = (1-t^2)^{1/2}$, *are given by*

$$\kappa_0^L = \mu_0^L = \tfrac{15}{14}\pi \frac{5n^2+30n+28}{(n+1)(n+2)(n+3)(n+4)(n+5)}, \tag{3.16}$$

$$\kappa_1^L = \mu_1^L = \frac{45\pi}{4(n+1)(n+2)(n+3)(n+4)(n+5)}. \tag{3.17}$$

Proof. As in the proof of Theorem 3.3, the formula for κ_1^L follows from (3.5_1), (2.37) and (3.14). For κ_0^L we use (3.12) in conjunction with (3.14), (3.15), (3.17) and

$$\int_{-1}^{1}(1-t)^2\tilde{\pi}_n(t)w(t)\,dt=\int_{-1}^{1}\frac{1}{1+t}(1+t)(1-t)^2\tilde{\pi}_n(t)w(t)\,dt.$$

The last integral is evaluated by expanding $(1+t)(1-t)^2\tilde{\pi}_n(t)$ in Chebyshev polynomials of the second kind and using once more (2.37). □

(b) Continuing with the third-kind Chebyshev weight $w(t)=(1-t)^{-1/2}(1+t)^{1/2}$, for which $w^L(t)=(1-t)^{3/2}(1+t)^{5/2}$, we get from [7, Eq. (2.16)]

$$\pi_n(t;\,w^L)=\frac{1}{2^{n+3}}\tilde{\pi}_n(t),$$
$$\tilde{\pi}_n(t)=\frac{1}{(t-1)(t+1)^2}\left\{U_{n+3}(t)-\frac{n+4}{n+2}U_{n+1}(t)+\frac{n+4}{n+2}\left[U_{n+2}(t)-\frac{n+3}{n+1}U_n(t)\right]\right\}. \tag{3.18}$$

Techniques similar to those used in Section 3.2 yield the following lemma.

Lemma 3.6. *The polynomial* $\tilde{\pi}_n$ *in* (3.18) *satisfies, for* $n\geqslant 1$,

$$\tilde{\pi}_n(-1)=\tfrac{2}{15}(-1)^n(n+3)(n+4)(2n+5), \tag{3.19}$$
$$\tilde{\pi}_n'(-1)=\tfrac{2}{105}(-1)^{n+1}n(n+3)(n+4)(n+5)(2n+5), \tag{3.20}$$
$$\tilde{\pi}_n(1)=\tfrac{2}{3}(n+3)(n+4), \tag{3.21}$$
$$\tilde{\pi}_n'(1)=\tfrac{2}{15}n(n+3)(n+4)(n+5). \tag{3.22}$$

Theorem 3.7. *The weights of the boundary terms in* (3.1), *where* $w(t)=(1-t)^{-1/2}(1+t)^{1/2}$, *are given by*

$$\kappa_0^L=\tfrac{15}{28}\pi\frac{10n^2+50n+49}{(n+1)(n+2)(n+3)(n+4)(2n+5)}, \tag{3.23}$$
$$\kappa_1^L=\frac{45\pi}{4(n+1)(n+2)(n+3)(n+4)(2n+5)}, \tag{3.24}$$
$$\mu_0^L=\tfrac{3}{20}\pi\frac{(2n+5)(6n^2+30n+25)}{(n+1)(n+2)(n+3)(n+4)}, \tag{3.25}$$
$$\mu_1^L=\tfrac{3}{4}\pi\frac{2n+5}{(n+1)(n+2)(n+3)(n+4)}. \tag{3.26}$$

(c) Finally, the Gauss–Lobatto formula for the Chebyshev weight of the fourth kind, $w(t)=(1-t)^{1/2}(1+t)^{-1/2}$, is readily obtained from the one for the third kind by the change of variable $t\leftrightarrow -t$. As a result, the weights κ_0, κ_1 formerly associated with the node -1 become those at the node 1, and vice versa, whereas the interior weights become associated in reverse order with the new nodes $-\tau_{n+1-\nu}$, $\nu=1,2,\ldots,n$.

4. Examples

It seems to be a widely-held belief, already expressed by Christoffel (cf. [4, p.86]), that the use of preassigned nodes in Gauss-type quadrature formulae, chosen judiciously at locations where the integrand function is predominant, should be advantageous. Our first example is intended to question, if not dispel, this belief. We experiment with integrands on $[-1, 1]$ that peak at the left end point -1 with a severity that can be controlled by a parameter. If we choose, according to the expectation expressed above, a Gauss–Radau formula with preassigned node at -1, we should see advantages over straight Gaussian integration, presumably even more so if both the function value and its derivative at -1 are preassigned. Somewhat disappointingly to us, Example 1 will show that this need not be the case. On the other hand, Example 3, in another context, will demonstrate that the use of preassigned nodes can indeed be helpful. Since the example involves computing Bessel–Fourier coefficients, hence the use of Bessel functions, we precede it by Example 2—an integral identity involving Bessel functions—which allows us to test our computer program for Bessel functions (a FORTRAN transcription of the algorithm in [3]).

All computations reported in this section were carried out in double precision on the Cyber 205 (machine precision ca. 29 decimal places).

Example 1(a).

$$I = \frac{\omega}{\pi}\int_{-1}^{1} \frac{(1-t^2)^{1/2}}{(1+t)^2+\omega^2}\,dt, \quad \omega > 0.$$

Here we treat $(1-t^2)^{1/2} = w(t)$ as a weight function (Chebyshev second kind), so that

$$f(t) = \frac{\omega}{\pi}\frac{1}{(1+t)^2+\omega^2}. \tag{4.1}$$

Clearly, this function exhibits a peak at $t = -1$, with increasing steepness as $\omega \downarrow 0$, and indeed approximates the Dirac delta function centered at $t = -1$. It seems reasonable, therefore, to employ the Gauss–Radau rule (2.1), (2.38), (2.39), using

$$f(-1) = \omega_0, \qquad f'(-1) = 0, \tag{4.2}$$

where $\omega_0 = 1/(\pi\omega)$. We are comparing this rule with the ordinary Gaussian rule having the same weight function w and the same number n of interior nodes. For each of these two rules, we determine the smallest value of n such that the two consecutive quadrature approximations for n and $n+1$, as well as those for $n+1$ and $n+2$, agree with each other to within a relative error of $\frac{1}{2}\cdot 10^{-20}$. The results are shown in Table 4.1 for $\omega_0 = 16^{-1}, 8^{-1}, \ldots, 1, \ldots, 32, 64$. It can be seen that for "flat" functions (ω_0 small), both formulae converge rapidly, with Gauss–Radau (R)

Table 4.1
Comparison of Gauss–Radau and Gauss quadrature for Example 1(a)

ω_0	16^{-1}	8^{-1}	4^{-1}	2^{-1}	1	2	4	8	16	32	64
R	11	15	21	30	43	60	84	118	167	234	320
G	12	16	22	30	43	61	85	118	166	233	321

Table 4.2
Comparison of Gauss–Radau and Gauss quadrature for Example 1(b)

ω_0	16^{-1}	8^{-1}	4^{-1}	2^{-1}	1	2	4	8	16	32	64
R	8	10	12	15	21	31	46	68	108	158	298
G	9	10	13	16	22	32	47	69	108	158	298

having a slight edge on Gauss (G). With increasing ω_0, convergence slows down as expected, and neither formula has any significant advantage over the other. The same experiment was repeated with an asymmetric (with respect to $t=-1$) function obtained by multiplying f in (4.1) by $\frac{1}{2}(1-t)$. This yields values ω_0 and $-\frac{1}{2}\omega_0$ in place of (4.2), but produces results which are almost identical with those of Table. 4.1.

To convince ourselves that this behavior is not tied to the special nature of the function (4.1), we selected another approximation to the Dirac delta function, namely the one in the following example.

Example 1(b).

$$I=\sqrt{\frac{\omega}{\pi}}\int_{-1}^{1} e^{-\omega(1+t)^2}(1-t^2)^{1/2}\,dt, \quad \omega>0.$$

We carried out the same experiment as in Example 1(a), with $\omega=\pi\omega_0^2$, $\omega_0=16^{-1}, 8^{-1},\ldots,1,\ldots,32, 64$. Here, the function f is given by

$$f(t)=\omega_0\, e^{-\pi\omega_0^2(1+t)^2}, \tag{4.3}$$

and its value and derivative at $t=-1$ are the same as in (4.2). The results obtained are shown in Table 4.2. They clearly exhibit a behavior similar to the one in Table 4.1. Again, multiplication in (4.3) by $\frac{1}{2}(1-t)$ does not affect the results appreciably.

What can be learned from this example is that the addition of a quadrature point to a Gauss formula, even if strategically placed and of multiplicity >1, and the consequent modest increase in polynomial degree of exactness, is simply not enough to cope with severely ill-behaved integrands such as those in Examples 1(a), 1(b).

Example 2.

$$\int_0^1 J_0(\omega t)\frac{dt}{\sqrt{1-t^2}}=\tfrac{1}{2}\pi\left[J_0\left(\tfrac{1}{2}\omega\right)\right]^2, \quad \omega>0.$$

This is a well-known relation involving the Bessel function of order zero (cf. [8, Eq. 6.552.4]). Since the weight function as well as the integrand $f(t)=J_0(\omega t)$ are even functions, the Gauss–Lobatto formula (3.1) applied to the integral from -1 to 1 (which is twice the integral of Example 2) yields, when again halved,

$$\int_0^1 f(t)(1-t^2)^{-1/2}\,dt \approx \mu_0^{\mathrm{L}} f(1)-\mu_1^{\mathrm{L}} f'(1)+\sum_{\nu=1+\lfloor n/2\rfloor}^{n}{}' \lambda_\nu^{\mathrm{L}} f\left(\tau_\nu^{\mathrm{L}}\right), \tag{4.4}$$

Table 4.3
Relative errors of (4.4) for Example 2

n	$\omega = 0.5$	$\omega = 1.0$	$\omega = 2.0$	$\omega = 4.0$	$\omega = 8.0$	$\omega = 16.0$
2	$3.5\cdot10^{-10}$	$9.8\cdot10^{-8}$	$3.5\cdot10^{-5}$	$7.4\cdot10^{-2}$	$1.4\cdot10^{0}$	$2.4\cdot10^{0}$
5	$2.5\cdot10^{-20}$	$4.4\cdot10^{-16}$	$1.0\cdot10^{-11}$	$1.6\cdot10^{-6}$	$3.7\cdot10^{-3}$	$7.5\cdot10^{0}$
8		$2.3\cdot10^{-25}$	$2.9\cdot10^{-19}$	$3.1\cdot10^{-12}$	$5.8\cdot10^{-7}$	$2.9\cdot10^{-1}$
11			$4.2\cdot10^{-26}$	$1.0\cdot10^{-18}$	$1.4\cdot10^{-11}$	$8.3\cdot10^{-4}$
14				$1.8\cdot10^{-26}$	$8.7\cdot10^{-17}$	$4.6\cdot10^{-7}$
17					$1.7\cdot10^{-22}$	$7.5\cdot10^{-11}$
20						$4.4\cdot10^{-15}$
23						$1.1\cdot10^{-19}$
26						$1.1\cdot10^{-24}$

where the prime in the summation is to indicate that the weight λ_ν^{L} in the first term must be halved if n is odd. Here,

$$f(1) = J_0(\omega), \qquad f'(1) = -\omega J_1(\omega), \tag{4.5}$$

and, if n is odd, $\tau_{1+\lfloor n/2\rfloor}^{\mathrm{L}} = 0$, so that

$$f\left(\tau_{1+\lfloor n/2\rfloor}^{\mathrm{L}}\right) = 1, \quad n \text{ odd}. \tag{4.6}$$

It should be noted that the computation of $J_0(\omega)$ by the familiar backward recurrence scheme yields also $J_1(\omega)$ at essentially no cost. The relative error of (4.4) (which is readily computable, since the exact answer is known) is shown in Table 4.3 for selected values of n and ω. Tabulation is halted in each column once the vicinity of machine precision is reached.

For reference, we list in Table 4.4 the true values of the integral to 25 significant digits.

If we count (4.5) as one function evaluation and disregard the cost of evaluating (4.6), we find that (4.4) requires exactly $\lfloor \frac{1}{2}(n+2)\rfloor$ nontrivial function evaluations. The same effort is required by the $(n+2)$-point Gauss–Chebyshev formula, which, having the same degree of exactness $2n+3$ as (4.4), indeed produces comparable results.

Example 3.

$$I_k = \int_0^1 \sqrt{\frac{t}{1-t}}\, \mathrm{e}^{-t} J_0(j_{0,k}t)\, \mathrm{d}t, \quad j_{0,k} = k\text{th zero of } J_0, \quad k = 1, 2, 3, \ldots .$$

The integrals here, except for normalization, are Fourier coefficients of the function $[t(1-t)]^{-1/2}\exp(-t)$ in the orthogonal system $\{J_0(j_{0,k}t)\}_{k=1}^{\infty}$. Their exact values are probably not

Table 4.4
Exact values of the integral in Example 2

ω	$\frac{1}{2}\pi[J_0(\frac{1}{2}\omega)]^2$
0.5	1.52228086677934197176650 4
1.0	1.38344050456868563898800 6
2.0	0.91974444547346406612607 56
4.0	0.07873943468335510847352319
8.0	0.24775851822556763234808 32
16.0	0.04628194233018786678533456

Table 4.5
Relative errors—and their ratios (r)—of the Gauss–Lobatto (L) and Gauss (G) formulae applied to the integrals of Example 3

n	$k=1$			$k=4$			$k=7$			$k=10$		
	L	G	r	L	G	r	L	G	r	L	G	r
2	$3.1\cdot10^{-7}$	$8.1\cdot10^{-3}$	$3.8\cdot10^{-5}$	$1.6\cdot10^{0}$	$1.0\cdot10^{1}$	$1.6\cdot10^{-1}$	$1.5\cdot10^{0}$	$6.2\cdot10^{0}$	$2.5\cdot10^{-1}$	$3.0\cdot10^{0}$	$8.2\cdot10^{0}$	$3.6\cdot10^{-1}$
5	$2.5\cdot10^{-14}$	$1.7\cdot10^{-9}$	$1.5\cdot10^{-5}$	$2.9\cdot10^{-4}$	$6.2\cdot10^{-2}$	$4.6\cdot10^{-3}$	$8.9\cdot10^{-2}$	$1.3\cdot10^{0}$	$7.1\cdot10^{-2}$	$9.9\cdot10^{0}$	$1.1\cdot10^{0}$	$8.8\cdot10^{0}$
8	$6.2\cdot10^{-23}$	$3.9\cdot10^{-18}$	$1.6\cdot10^{-5}$	$1.8\cdot10^{-9}$	$4.3\cdot10^{-6}$	$4.3\cdot10^{-4}$	$2.0\cdot10^{-4}$	$1.6\cdot10^{-2}$	$1.3\cdot10^{-2}$	$2.6\cdot10^{-1}$	$3.3\cdot10^{0}$	$7.8\cdot10^{-2}$
11				$9.4\cdot10^{-15}$	$1.0\cdot10^{-12}$	$9.5\cdot10^{-3}$	$4.2\cdot10^{-8}$	$1.2\cdot10^{-5}$	$3.6\cdot10^{-3}$	$4.8\cdot10^{-4}$	$2.9\cdot10^{-2}$	$1.7\cdot10^{-2}$
14				$2.1\cdot10^{-20}$	$1.3\cdot10^{-16}$	$1.7\cdot10^{-4}$	$1.8\cdot10^{-12}$	$1.4\cdot10^{-9}$	$1.3\cdot10^{-3}$	$1.7\cdot10^{-7}$	$3.0\cdot10^{-5}$	$5.7\cdot10^{-3}$
17				$1.3\cdot10^{-25}$	$1.5\cdot10^{-22}$	$8.7\cdot10^{-4}$	$2.2\cdot10^{-17}$	$3.8\cdot10^{-14}$	$5.8\cdot10^{-4}$	$1.7\cdot10^{-11}$	$6.9\cdot10^{-9}$	$2.4\cdot10^{-3}$
20							$9.5\cdot10^{-23}$	$3.3\cdot10^{-19}$	$2.9\cdot10^{-4}$	$5.3\cdot10^{-16}$	$4.7\cdot10^{-13}$	$1.1\cdot10^{-3}$
23										$6.0\cdot10^{-21}$	$1.1\cdot10^{-17}$	$5.6\cdot10^{-4}$
26										$7.0\cdot10^{-26}$	$7.9\cdot10^{-23}$	$8.8\cdot10^{-4}$

Table 4.6
Exact values of the integrals in Example 3

k	I_k
1	0.31114536231578812574318 08
2	−0.03189867185858781126668228
3	0.06441715855367780488160133
4	−0.02011734319990536683786198
5	0.03396279031350273365741716
6	−0.01449294488742138939879033
7	0.02274181563294370855827056
8	−0.01134211831713856256822432
9	0.01699275052361748571975268
10	−0.00933113406670990841481 3902

known analytically, but we have confidence in their determination by two independent methods: the Gauss–Lobatto formula (3.1), (3.23)–(3.26) on the one hand, and the ordinary Gauss formula on the other, both relative to the Chebyshev weight function of the third kind,

$$w(t) = (1-t)^{-1/2}(1+t)^{1/2}. \tag{4.7}$$

A change of variable brings the integral into the canonical form (3.1), with w as in (4.7), and

$$f(t) = \tfrac{1}{2}e^{-(1/2)(1+t)}J_0\left(\tfrac{1}{2}j_{0,k}(1+t)\right), \quad -1 \leqslant t \leqslant 1. \tag{4.8}$$

Thus,

$$f(-1) = \tfrac{1}{2}, \qquad f'(-1) = -\tfrac{1}{4}, \qquad f(1) = 0, \qquad f'(1) = -\tfrac{1}{4}\,e^{-1}j_{0,k}J_1(j_{0,k}). \tag{4.9}$$

Since these boundary values are easily precomputable, we will not count them here in the cost of evaluating the quadrature sum of (3.1). We therefore compare the results of (3.1) with those obtained, at the same cost, by the n-point Gauss formula for the weight function (4.7). We did our computations for $k = 1,\ldots,10$ and $n = 1,\ldots,30$, but in Table 4.5 show only selected results. The three entries headed by L, G and r represent respectively the relative error of the generalized Gauss–Lobatto formula (3.1), the relative error of the Gauss formula, and the ratio of the two errors. It can be seen that the Gauss-Lobatto formula produces results which are several orders of magnitude more accurate than those furnished (at comparable cost) by the Gauss formula. This is entirely due to the higher degree of exactness, $2n+3$, of the Gauss–Lobatto formula; indeed, repeating the computations with G the $(n+2)$-point Gauss formula (which has also degree of exactness $2n+3$) gives results which are even slightly more accurate than those produced by L.

The (presumed) true values of the integrals, for $k = 1,\ldots,10$, are given to 25 significant decimal places in Table 4.6.

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20.10. [137] “Gauss-type Quadrature Rules for Rational Functions”

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Gauss-type Quadrature Rules for Rational Functions*

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Abstract. When integrating functions that have poles outside the interval of integration, but are regular otherwise, it is suggested that the quadrature rule in question ought to integrate exactly not only polynomials (if any), but also suitable rational functions. The latter are to be chosen so as to match the most important poles of the integrand. We describe two methods for generating such quadrature rules numerically and report on computational experience with them.

Introduction

Traditionally, Gauss quadrature rules are designed to integrate exactly polynomials of maximum possible degree. This is meaningful for integrand functions that are "polynomial-like". For integrands having poles (outside the interval of integration) it would be more natural to include also rational functions among the functions to be exactly integrated. In this paper we consider n-point quadrature rules that exactly integrate m rational functions (with prescribed location and multiplicity of the poles) as well as polynomials of degree $2n-m-1$, where $0 \leq m \leq 2n$. The limit case $m = 2n$, in which only rational functions are being integrated exactly, is a rational counterpart of the classical Gauss formula; the latter corresponds to the other limit case $m = 0$.

In §1 we characterize these new quadrature rules in terms of classical (polynomial) Gauss formulae with modified weight functions. We also identify special choices of poles that are of interest in applications. The computation of the quadrature rules is discussed in §2, and numerical examples are given in §3.

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1. Gauss quadrature for rational functions

Let $d\lambda$ be a measure on the real line having finite moments of all orders. Let $\zeta_\mu \in \mathbb{C}$, $\mu = 1, 2, \ldots, M$, be distinct real or complex numbers such that

$$\zeta_\mu \neq 0 \quad \text{and} \quad 1 + \zeta_\mu t \neq 0 \quad \text{for} \quad t \in \overline{\text{supp}(d\lambda)}, \qquad \mu = 1, 2, \ldots, M \,. \tag{1.1}$$

For given integers m, n with $1 \leq m \leq 2n$, we wish to find an n-point quadrature rule that integrates exactly (against the measure $d\lambda$) polynomials of degree $2n - m - 1$ as well as the m rational functions

$$(1 + \zeta_\mu t)^{-s}, \qquad \mu = 1, 2, \ldots, M, \qquad s = 1, 2, \ldots, s_\mu, \tag{1.2}$$

where $s_\mu \geq 1$ and

$$\sum_{\mu=1}^{M} s_\mu = m. \tag{1.3}$$

In the extreme case $m = 2n$ (where polynomials of degree -1 are understood to be identically zero) the formula integrates exactly $2n$ rational functions (with poles of multiplicities s_μ at $-1/\zeta_\mu$), but no nontrivial polynomials. The formula, therefore, can be thought of as the rational analogue of the classical Gauss formula; the latter corresponds to the other limit case $m = M = 0$.

The solution of our problem is given by the following theorem.

THEOREM 1.1. *Define*

$$\omega_m(t) = \prod_{\mu=1}^{M} (1 + \zeta_\mu t)^{s_\mu}, \tag{1.4}$$

a polynomial of degree m. Assume that the measure $d\lambda/\omega_m$ admits a (polynomial) *n-point Gaussian quadrature formula*

$$\int_{\mathbb{R}} f(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu^G f(t_\nu^G) + R_n^G(f), \qquad R_n^G(\mathbb{P}_{2n-1}) = 0, \tag{1.5}$$

with nodes t_ν^G contained in the support of $d\lambda$,

$$t_\nu^G \in \text{supp}(d\lambda). \tag{1.6}$$

Define

$$t_\nu = t_\nu^G, \qquad \lambda_\nu = w_\nu^G \omega_m(t_\nu^G), \qquad \nu = 1, 2, \ldots, n. \tag{1.7}$$

Then

$$\int_{\mathbb{R}} g(t) d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu g(t_\nu) + R_n(g), \tag{1.8}$$

where

$$R_n(g) = 0 \quad \text{if} \quad \begin{cases} g(t) = (1+\zeta_\mu t)^{-s}, & \mu = 1,2,\dots,M;\ s = 1,2,\dots,s_\mu, \\ g \in \mathbb{P}_{2n-m-1}\ . \end{cases} \tag{1.9}$$

Conversely, (1.8) *with* $t_\nu \in \operatorname{supp}(d\lambda)$ *and* (1.9) *imply* (1.5), (1.6) *with* t_ν^G, w_ν^G *as defined in* (1.7).

Remark. Theorem 1.1, for real ζ_μ and either all $s_\mu = 1$ and $m = 2n$, or all but one $s_\mu = 2$ and $m = 2n-1$, is due to Van Assche and Vanherwegen [13]. The quadrature rule (1.5), especially its convergence properties for analytic functions f, has previously been studied by López and Illán [9, 10].

Proof of Theorem 1.1. Assume first (1.5), (1.6). For $\mu = 1,2,\dots,M; s = 1,2,\dots,s_\mu$, define

$$q_{\mu,s}(t) = \frac{\omega_m(t)}{(1+\zeta_\mu t)^s}\ . \tag{1.10}$$

Since $m \le 2n$ and $s \ge 1$, we have $q_{\mu,s} \in \mathbb{P}_{m-s} \subset \mathbb{P}_{2n-1}$, and therefore, by (1.5),

$$\begin{aligned} \int_{\mathbb{R}} \frac{d\lambda(t)}{(1+\zeta_\mu t)^s} &= \int_{\mathbb{R}} q_{\mu,s}(t)\frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu^G q_{\mu,s}(t_\nu^G) \\ &= \sum_{\nu=1}^{n} w_\nu^G \frac{\omega_m(t_\nu^G)}{(1+\zeta_\mu t_\nu^G)^s} = \sum_{\nu=1}^{n} \frac{\lambda_\nu}{(1+\zeta_\mu t_\nu)^s}\ , \end{aligned}$$

where (1.7) has been used in the last step and none of the denominators on the far right vanishes by (1.6) and (1.1). This proves the assertion in the top line of (1.9). The bottom part of (1.9) follows similarly: Let p be an arbitrary polynomial in $\mathbb{P}_{2n-m-1}$. Then, since $p\omega_m \in \mathbb{P}_{2n-1}$, again by (1.5) and (1.7),

$$\begin{aligned} \int_{\mathbb{R}} p(t)\,d\lambda(t) &= \int_{\mathbb{R}} p(t)\omega_m(t)\frac{d\lambda(t)}{\omega_m(t)} \\ &= \sum_{\nu=1}^{n} w_\nu^G p(t_\nu^G)\omega_m(t_\nu^G) = \sum_{\nu=1}^{n} \lambda_\nu p(t_\nu). \end{aligned}$$

To prove the converse, we first note that w_ν^G is well defined by (1.7), since $\omega_m(t_\nu) \neq 0$ by the assumption on t_ν and (1.1). One then easily verifies that (1.5) holds for all polynomials (1.10) (of degree $< m$) and all polynomials of the form $p\omega_m$ where $p \in \mathbb{P}_{2n-1-m}$. The collection of these polynomials, however, spans $\mathbb{P}_{2n-1}$. □

We will concentrate on six special choices of the parameters ζ_μ that are of interest in applications.

Case 1 (Simple real poles). All $s_\mu = 1$ in (1.2) (hence $M = m$), and all ζ_μ are real, distinct, and nonzero,

$$\zeta_\nu = \xi_\nu \in \mathbb{R}, \quad \xi_\nu \neq 0, \quad \nu = 1, 2, \ldots, m. \tag{1.11a}$$

In this case the polynomial ω_m has the form

$$\omega_m(t) = \prod_{\nu=1}^{m} (1 + \xi_\nu t), \quad \xi_\nu \in \mathbb{R}. \tag{1.11b}$$

If the support of $d\lambda$ is an interval, ω_m does not change sign on it because of (1.1).

Case 2 (Simple conjugate complex poles). All $s_\mu = 1$ (hence $M = m$), m even, and the ζ_μ occur in $m/2$ (distinct) pairs of conjugate complex numbers (cf. [9]),

$$\zeta_\nu = \xi_\nu + i\eta_\nu, \quad \zeta_{\nu+m/2} = \xi_\nu - i\eta_\nu, \quad \nu = 1, 2, \ldots, m/2, \tag{1.12a}$$

where $\xi_\nu \in \mathbb{R}$ and $\eta_\nu > 0$. Here,

$$\omega_m(t) = \prod_{\nu=1}^{m/2} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2], \tag{1.12b}$$

which is strictly positive for real t.

Case 2′ (Simple conjugate complex poles plus a simple real pole). All $s_\mu = 1$ (hence $M = m$), m (odd) ≥ 3, and, slightly changing the indexing of the ζ's,

$$\zeta_0 \in \mathbb{R}, \quad \zeta_\nu = \xi_\nu + i\eta_\nu, \quad \zeta_{\nu+(m-1)/2} = \xi_\nu - i\eta_\nu, \quad \nu = 1, 2, \ldots, (m-1)/2, \tag{1.13a}$$

where $\zeta_0 = \xi_0 \neq 0$ and $\xi_\nu \in \mathbb{R}$, $\eta_\nu > 0$ for $1 \leq \nu \leq (m-1)/2$. Then

$$\omega_m(t) = (1 + \xi_0 t) \prod_{\nu=1}^{(m-1)/2} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2]. \tag{1.13b}$$

Case 3 (Real poles of order 2). All $s_\mu = 2$ in (1.2) (hence $2M = m$), and all ζ_μ are nonzero, real and distinct,

$$\zeta_\nu = \xi_\nu \in \mathbb{R}, \quad \xi_\nu \neq 0, \quad s_\nu = 2, \quad \nu = 1, 2, \ldots, m/2. \tag{1.14a}$$

The polynomial ω_m now has the form

$$\omega_m(t) = \prod_{\nu=1}^{m/2} (1 + \xi_\nu t)^2 \tag{1.14b}$$

and is nonnegative for real t, and positive on the support of $d\lambda$.

Case 3′ (Real poles of order 2 plus a simple real pole). Here, all $\zeta_\mu = \xi_\mu$ are nonzero, real and distinct, $s_\nu = 2$ for $\nu = 1, 2, \ldots, M-1$ and $s_M = 1$. Thus, $m = 2M - 1$, and

$$\omega_m(t) = (1 + \xi_M t) \prod_{\nu=1}^{M-1} (1 + \xi_\nu t)^2, \quad M = \frac{m+1}{2}, \quad m(\text{odd}) \geq 3. \tag{1.15}$$

If $M = n$, i.e., $m = 2n - 1$, the quadrature rule (1.5) is then identical with the "orthogonal quadrature rule" of [13], having as nodes the zeros of the rational function $(1 + \zeta_n t)^{-1} + \sum_{\nu=1}^{n-1} a_\nu (1 + \zeta_\nu t)^{-1}$ which is orthogonal (relative to the measure $d\lambda$) to 1 and to $(1 + \zeta_\mu t)^{-1}$, $\mu = 1, 2, \ldots, n-1$. As in Case 1, the polynomial ω_m preserves its sign on the interval on which $d\lambda$ is supported.

Case 4 (Conjugate complex poles of order 2). All $s_\mu = 2$ (hence $2M = m$), $m = 0 \pmod 4$, and the ζ_μ, $\mu = 1, 2, \ldots, m/2$, occur in $m/4$ conjugate complex pairs, similarly as in Case 2. Thus,

$$\omega_m(t) = \prod_{\nu=1}^{m/4} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2]^2. \tag{1.16}$$

In all six cases, the measure $d\lambda/\omega_m$ admits a Gaussian n-point formula for each $n = 1, 2, 3, \ldots$, so that the assumption of Theorem 1.1 is fulfilled for each n.

Putting $f(t) = \omega_m(t) g(t)$ in (1.5) and using (1.7), we get

$$\int_{\mathbb{R}} g(t) d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu g(t_\nu) + R_n^G(\omega_m g), \tag{1.17}$$

where from the well-known expression for the remainder term of Gaussian quadrature rules, one has

$$R_n^G(\omega_m g) = \gamma_n (\omega_m g)^{(2n)}(\tau), \quad \gamma_n = \frac{\hat{\beta}_0 \hat{\beta}_1 \cdots \hat{\beta}_n}{(2n)!}. \tag{1.18}$$

Here, τ is some number in the smallest interval containing the support of $d\lambda$, and $\hat{\beta}_k = \beta_k(d\lambda/\omega_m)$ are the β-recursion coefficients for the measure $d\lambda/\omega_m$ (cf. (2.1) below). The latter are computed as part of the algorithms to be described in the next section.

2. Computation of the quadrature rule (1.5)

We propose essentially two methods for generating the basic quadrature rule (1.5), the first being most appropriate if the support of $d\lambda$ is a finite interval, the other more effective, though possibly slower, when the support interval of $d\lambda$ is unbounded.

2.1. Method based on partial fraction decomposition and modification algorithms. To compute the n-point formula (1.5), it suffices to compute the nth-degree orthogonal polynomial $\hat{\pi}_n(\,\cdot\,) = \pi_n(\,\cdot\,; d\hat{\lambda})$ relative to the measure $d\hat{\lambda} = d\lambda/\omega_m$, or, more precisely, the recursion coefficients $\hat{\alpha}_k = \alpha_k(d\hat{\lambda})$, $\hat{\beta}_k = \beta_k(d\hat{\lambda})$, $k = 0, 1, \ldots, n-1$, in the three-term recurrence relation satisfied by these (monic) polynomials:

$$\begin{aligned} \hat{\pi}_{k+1}(t) &= (t - \hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k\hat{\pi}_{k-1}(t), \\ & \qquad k = 0, 1, \ldots, n-1, \\ \hat{\pi}_0(t) &= 1, \qquad \hat{\pi}_{-1}(t) = 0. \end{aligned} \tag{2.1}$$

The nodes t_ν^G and weights w_ν^G in (1.5) can then be obtained by standard techniques via an eigensystem problem for the (symmetric, tridiagonal) Jacobi matrix of order n having the $\hat{\alpha}_k$, $k = 0, 1, \ldots, n-1$, on the diagonal, and $\sqrt{\hat{\beta}_k}$, $k = 1, 2, \ldots, n-1$, on the side diagonals (see, e.g., [7], [4, §6]). The coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ in turn are expressible in terms of the orthogonal polynomials $\hat{\pi}_k$ as

$$\begin{aligned} \hat{\alpha}_k &= \frac{(t\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_k, \hat{\pi}_k)}, \quad 0 \le k \le n-1, \\ \hat{\beta}_0 = (\hat{\pi}_0, \hat{\pi}_0), \quad \hat{\beta}_k &= \frac{(\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_{k-1}, \hat{\pi}_{k-1})}, \quad 1 \le k \le n-1, \end{aligned} \tag{2.2}$$

where $(\,\cdot\,,\,\cdot\,)$ denotes the inner product

$$(u, v) = \int_{\mathbb{R}} u(t)v(t)d\hat{\lambda}(t). \tag{2.3}$$

(If the error constant γ_n in (1.18) is desired, one needs to compute, in addition, $\hat{\beta}_n$.)

The basic idea of computing the coefficients in (2.2) is as follows. Suppose we can construct an N-point quadrature rule for $d\hat{\lambda} = d\lambda/\omega_m$, where $N > n$, which is exact for polynomials of degree $\le 2n-1$:

$$\int_{\mathbb{R}} p(t)d\hat{\lambda}(t) = \sum_{k=1}^{N} W_k p(T_k), \qquad p \in \mathbb{P}_{2n-1}. \tag{2.4}$$

Here the weights W_k are not necessarily all positive. Denote the discrete measure implied by the sum on the right by $d\Lambda_N$:

$$\int_{\mathbb{R}} p(t)d\Lambda_N(t) = \sum_{k=1}^{N} W_k p(T_k). \tag{2.5}$$

Then from the formulae in (2.2) one easily sees by induction that

$$\begin{aligned} \alpha_k(d\hat{\lambda}) &= \alpha_k(d\Lambda_N), \\ \beta_k(d\hat{\lambda}) &= \beta_k(d\Lambda_N), \end{aligned} \qquad k = 0, 1, \ldots, n-1. \tag{2.6}$$

Thus, the desired recursion coefficients are the first n of the α- and β-coefficients belonging to the discrete measure $d\Lambda_N$. These can be generated by Stieltjes's procedure, which is implemented in the routine `sti` of [4]. (The faster routine `lancz` of [4], implementing the Lanczos method, would also be applicable here, even though $d\Lambda_N$ is not necessarily a positive measure.)

We next show how a quadrature rule of type (2.4), with $N = O(mn)$, can be constructed by means of partial fraction decomposition and suitable modification algorithms. For this, we consider separately Cases 1–3′ identified in §1. The analysis of Case 4 becomes so tedious that we will not pursue it any further in this context; see, however, §2.2.

2.1.1. *Simple real poles.* We set up the partial fraction decomposition of $1/\omega_m$ in the form

$$\frac{1}{\omega_m(t)} = \frac{1}{\prod_{\nu=1}^{m}(1+\xi_\nu t)} = \sum_{\nu=1}^{m} \frac{c_\nu}{t + (1/\xi_\nu)}, \tag{2.7}$$

where

$$c_\nu = \frac{\xi_\nu^{m-2}}{\prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m}(\xi_\nu - \xi_\mu)}, \quad \nu = 1, 2, \ldots, m, \tag{2.8}$$

and an empty product in (2.8) (when $m = 1$) is to be taken as 1. Then, with $d\hat{\lambda} = d\lambda/\omega_m$,

$$\int_{\mathbb{R}} p(t)d\hat{\lambda}(t) = \sum_{\nu=1}^{m} \int_{\mathbb{R}} p(t) \frac{c_\nu d\lambda(t)}{t + (1/\xi_\nu)}.$$

The integrals on the right involve measures $c_\nu d\lambda$ modified by linear divisors. For such measures, the associated recursion coefficients can be obtained from those of $c_\nu d\lambda$ (assumed known) by a suitable modification algorithm (cf. [4, §5]). Unless $x_\nu = -1/\xi_\nu$ is very close to the support interval of $d\lambda$, the most appropriate algorithm is the one embodied in the routine `gchri` of [4] with `iopt` = 1. Otherwise, the routine `chri` of [4] (again with `iopt` = 1) is preferable. A basic ingredient of the routine `gchri` is the modified Chebyshev algorithm (cf. [2, §2.4]) using modified moments $\int_{\mathbb{R}} \pi_k(t; d\lambda)c_\nu d\lambda(t)/(t - x_\nu)$, $k = 0, 1, 2, \ldots, 2n-1$. These in turn are generated by backward recurrence as minimal solution of the three-term recurrence relation for the measure $d\lambda$; cf. [1, §5].

Having obtained, in whichever way, the first n of the α- and β-coefficients for the modified measure $c_\nu d\lambda(t)/(t-x_\nu)$, and hence the Gaussian quadrature formula[1]

$$\int_{\mathbb{R}} p(t)\,\frac{c_\nu d\lambda(t)}{t+(1/\xi_\nu)} = \sum_{\tau=1}^{n} w_\tau^{(\nu)} p(t_\tau^{(\nu)}), \qquad p \in \mathbb{P}_{2n-1}, \tag{2.9}$$

via eigensystem techniques, we then get

$$\begin{aligned}\int_{\mathbb{R}} p(t)\,\frac{d\lambda(t)}{\omega_m(t)} &= \sum_{\nu=1}^{m} \int_{\mathbb{R}} p(t)\,\frac{c_\nu d\lambda(t)}{t+(1/\xi_\nu)} \\ &= \sum_{\nu=1}^{m}\sum_{\tau=1}^{n} w_\tau^{(\nu)} p(t_\tau^{(\nu)}), \qquad p \in \mathbb{P}_{2n-1},\end{aligned}$$

hence the desired quadrature rule (2.4), with $N = mn$ and

$$\begin{aligned} T_{(\nu-1)n+\tau} &= t_\tau^{(\nu)}, \\ W_{(\nu-1)n+\tau} &= w_\tau^{(\nu)}, \end{aligned} \qquad \nu = 1,2,\dots,m; \quad \tau = 1,2,\dots,n. \tag{2.10}$$

The procedure described works best if the support of $d\lambda$ is a finite interval. Otherwise, the modified Chebyshev algorithm underlying the procedure is likely to suffer from ill-conditioning; cf. Example 3.4. Another difficulty that may adversely affect the accuracy of the results, in particular if $m = 2n$, is the possibility that the constants $c_\nu \operatorname{sgn}_{t\in\operatorname{supp}(d\lambda)}(t + 1/\xi_\nu)$ become very large and alternate in sign; cf. Example 3.2. This will cause serious cancellation errors in evaluating inner products relative to the measure $d\Lambda_N$ (there being blocks of weights W_k which are very large positive alternating with blocks of weights which are very large negative). In such cases, either m has to be lowered, perhaps down to $m = 1$, or else the method discussed in §2.2 invoked, which will be more effective (but possibly more expensive).

2.1.2. *Simple conjugate complex poles.* We now consider Case 2 of §1, i.e., conjugate complex parameters $\zeta_\nu = \xi_\nu + i\eta_\nu$, $\zeta_{\nu+m/2} = \bar{\zeta}_\nu$, where $\xi_\nu \in \mathbb{R}$, $\eta_\nu > 0$ and m is even. In this case, an elementary computation yields the partial fraction decomposition

$$\frac{1}{\omega_m(t)} = \sum_{\nu=1}^{m/2} \frac{c_\nu + d_\nu t}{\left(t + \frac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2 + \left(\frac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2}, \qquad t \in \mathbb{R}, \tag{2.11}$$

[1] In order to produce positive β-coefficients, as required in the routine for Gauss quadrature formulae, one inputs the measure $|c_\nu/(t-x_\nu)|d\lambda(t)$ and, if this entails a change of sign, reverses the sign of all Gauss weights after exiting from the Gauss quadrature routine.

where

$$\begin{aligned} c_\nu &= \tfrac{1}{\eta_\nu}\left(\tfrac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\ \mathrm{Im}\ p_\nu + \tfrac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\ \mathrm{Re}\ p_\nu\right), \\ d_\nu &= \tfrac{1}{\eta_\nu}\mathrm{Im}\ p_\nu \end{aligned} \tag{2.12}$$

and

$$p_\nu = \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} \frac{(\xi_\nu + i\eta_\nu)^2}{(\xi_\nu - \xi_\mu)^2 - (\eta_\nu^2 - \eta_\mu^2) + 2i\eta_\nu(\xi_\nu - \xi_\mu)} \tag{2.13}$$

with $p_1 = 1$ if $m = 2$. One can then proceed as in §2.1.1, except that the modification of the measure $d\lambda$ now involves multiplication by a nonconstant linear function (if $d_\nu \neq 0$) in addition to division by a quadratic. The former modification is handled by the routine `chri` of [4] with `iopt` = 1, the latter by the routine `gchri` with `iopt` = 2 (or, if more appropriate, by `chri` with `iopt` = 5). The quadrature rule (2.4) so obtained has $N = mn/2$.

If the poles $-1/\zeta_\mu$ are located in conjugate pairs on a line parallel to the imaginary axis, then by an elementary calculation one can show that all p_ν are real, hence $d_\nu = 0$, and there is no need to call `chri`.

2.1.2′. *Simple conjugate complex poles plus a simple real pole.* We are now in Case 2′ of §1, with m odd, $\zeta_0 = \xi_0 \in \mathbb{R}$ and the remaining ζ_μ conjugate complex as in Case 2. This yields

$$\frac{1}{\omega_m(t)} = \frac{c_0'}{t + (1/\xi_0)} + \sum_{\nu=1}^{(m-1)/2} \frac{c_\nu' + d_\nu' t}{\left(t + \frac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2 + \left(\frac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\right)^2}, \quad t \in \mathbb{R}, \tag{2.14}$$

where

$$\begin{aligned} c_0' &= \frac{\xi_0^{m-2}}{\prod_{\nu=1}^{(m-1)/2}[(\xi_0 - \xi_\nu)^2 + \eta_\nu^2]}, \\ c_\nu' &= \frac{1}{\eta_\nu}\left(\frac{\xi_\nu}{\xi_\nu^2+\eta_\nu^2}\ \mathrm{Im}\ p_\nu' + \frac{\eta_\nu}{\xi_\nu^2+\eta_\nu^2}\ \mathrm{Re}\ p_\nu'\right), \\ d_\nu' &= \frac{1}{\eta_\nu}\ \mathrm{Im}\ p_\nu' \end{aligned} \tag{2.15}$$

and

$$p_\nu' = \frac{\xi_\nu + i\eta_\nu}{\xi_\nu - \xi_0 + i\eta_\nu}\, p_\nu, \tag{2.16}$$

with p_ν the same as in (2.13) with m replaced by $m - 1$. The technique called for is a combination of the one in §2.1.1, to deal with the first term in (2.14), and the one in §2.1.2, to deal with the remaining terms, and yields a quadrature rule (2.4) with $N = (m + 1)n/2$.

2.1.3. *Real poles of order 2.* This is Case 3 of §1, and leads to the partial fraction decomposition

$$\frac{1}{\omega_m(t)} = \sum_{\nu=1}^{m/2} \left(\frac{c_\nu}{t+1/\xi_\nu} + \frac{d_\nu}{(t+1/\xi_\nu)^2} \right), \tag{2.17}$$

$$c_\nu = -\frac{2\xi_\nu^{m-3} \sum_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} \frac{\xi_\mu}{\xi_\nu - \xi_\mu}}{\prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} (\xi_\nu - \xi_\mu)^2}, \tag{2.18}$$

$$d_\nu = \frac{\xi_\nu^{m-4}}{\prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} (\xi_\nu - \xi_\mu)^2}, \tag{2.19}$$

where $c_1 = 0$, $d_1 = \xi_1^{-2}$ when $m = 2$. Here, $N = mn$ in (2.4).

2.1.3′. *Real poles of order 2 plus a simple real pole.* Similarly as in §2.1.3, the partial fraction decomposition has now the form

$$\frac{1}{\omega_m(t)} = \frac{c'_M}{t+1/\xi_M} + \sum_{\nu=1}^{M-1} \left(\frac{c'_\nu}{t+1/\xi_\nu} + \frac{d'_\nu}{(t+1/\xi_\nu)^2} \right), \quad M = (m+1)/2, \quad m \text{ odd}, \tag{2.20}$$

$$c'_M = \frac{\xi_M^{m-2}}{\prod_{\nu=1}^{M-1} (\xi_M - \xi_\nu)^2},$$

$$c'_\nu = -\frac{\xi_\nu^{m-3} \left(\xi_M + 2(\xi_\nu - \xi_M) \sum_{\substack{\mu=1 \\ \mu\neq\nu}}^{M-1} \frac{\xi_\mu}{\xi_\nu - \xi_\mu} \right)}{(\xi_\nu - \xi_M)^2 \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{M-1} (\xi_\nu - \xi_\mu)^2},$$

$$d'_\nu = \frac{\xi_\nu^{m-4}}{(\xi_\nu - \xi_M) \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{M-1} (\xi_\nu - \xi_\mu)^2}.$$

Empty sums and products (when $M = 2$) have their conventional values 0 and 1, respectively. Again, $N = mn$ in (2.4).

The presence of two terms in the summations of (2.17) and (2.20) complicates matters considerably, as they call for two applications of the routine `gchri`: First, we must generate sufficiently many of the recursion coefficients for the measure $d\lambda(t)/(t - x_\nu)$, $x_\nu = -1/\xi_\nu$, in order next to generate the desired recursion coefficients for $d\lambda(t)/(t - x_\nu)^2$ by backward recursion – a recursion based on the recurrence relation generated in the first application of `gchri` (which in turn requires backward recursion!). The procedure nevertheless works well if the x_ν are not too close to the support interval of $d\lambda$; see Example 3.3.

2.2. Discretization method. In this method, the inner product (2.3) is approximated by a discrete (positive) inner product,

$$(u,v) = \int_{\mathbb{R}} u(t)v(t)\,\frac{d\lambda(t)}{\omega_m(t)} \approx \sum_{k=1}^{N} \omega_k^{(N)} u(\tau_k^{(N)})v(\tau_k^{(N)}) =: (u,v)_N, \quad N > n, \tag{2.21}$$

whereupon the formulae (2.2) are applied with the inner product $(\,\cdot\,,\cdot\,)$ replaced by $(\,\cdot\,,\cdot\,)_N$ throughout. This yields approximations

$$\hat{\alpha}_{k,N} \approx \hat{\alpha}_k, \quad \hat{\beta}_{k,N} \approx \hat{\beta}_k, \quad k = 0,1,\ldots,n-1. \tag{2.22}$$

In effect we are generating the polynomials orthogonal with respect to the discrete inner product $(\,\cdot\,,\cdot\,)_N$ in order to approximate the desired orthogonal polynomials.

The computation of the approximate coefficients (2.22) can be done by either Stieltjes's procedure or Lanczos's algorithm (cf., e.g., [3, §§6–7]). Both are implemented in the routine `mcdis` of [4].

With any reasonable choice of the discretization (2.21), it will be true that the procedure converges as $N \to \infty$,

$$\lim_{N\to\infty} \hat{\alpha}_{k,N} = \hat{\alpha}_k, \quad \lim_{N\to\infty} \hat{\beta}_{k,N} = \hat{\beta}_k, \quad 0 \le k \le n-1. \tag{2.23}$$

A natural choice, indeed, is given by

$$\tau_k^{(N)} = t_k^{(N)}(d\lambda), \quad \omega_k^{(N)} = \frac{w_k^{(N)}(d\lambda)}{\omega_m(\tau_k^{(N)})}, \quad k = 1,2,\ldots,N, \tag{2.24}$$

where $t_k^{(N)}(d\lambda)$ are the zeros of the orthogonal polynomial $\pi_N(\,\cdot\,;d\lambda)$, and $w_k^{(N)}(d\lambda)$ the respective Christoffel numbers.

The discretization method is conceptually simpler, and sometimes more stable, than the methods of §2.1, but may become significantly more expensive, regardless of the choice of m, if poles are close to the interval of integration, or if high accuracy is desired; cf. Examples 3.1 and 3.5. Note also that Case 4 that was skipped in §2.1 can easily be handled by the present method; see Example 3.6.

3. Numerical Examples

All examples in this section were computed on the Cyber 205 in both single and double precision. The respective machine precisions are 7.11×10^{-15} and 5.05×10^{-29}

Example 3.1. $I_1(\omega) = \int_{-1}^{1} \frac{\pi t/\omega}{\sin(\pi t/\omega)}\,dt, \quad \omega > 1.$

Here, $d\lambda(t) = dt$, and the poles of the integrand are located at the integer multiples of ω. It is natural, then, to make our quadrature rule (1.8) exact for m elementary rational functions matching the m poles closest to the origin, say those at

$-(m/2)\omega, \ldots, -\omega, \omega, \ldots, (m/2)\omega$ when m is even. This suggests to identify $-1/\zeta_\mu$ in (1.2) with these poles, i.e., in (1.11a) to set

$$\xi_\nu = (-1)^\nu/(\omega\lfloor(\nu+1)/2\rfloor), \quad \nu = 1, 2, \ldots, m. \tag{3.1}$$

Best accuracy is expected when $m = 2n$, in which case the method described in §2.1.1 was found to work rather well, the only difficulty being the relatively slow convergence of the backward recurrence algorithm for computing the $2n$ modified (Legendre) moments associated with the measure $dt/(t \pm \omega)$ when ω is very close to 1. For single-precision accuracy $\epsilon = \frac{1}{2} \times 10^{-10}$ and double-precision accuracy $\epsilon^d = \frac{1}{2} \times 10^{-25}$, and $n = 20$, the respective starting indices k_0 and k_0^d in the backward recursion yielding the desired accuracy are shown in Table 3.1 for selected values of ω.

ω	k_0	k_0^d
2.0	50	63
1.5	53	71
1.1	67	106
1.01	124	247

TABLE 3.1. *Starting indices for backward recurrence when* $n = 20$

Other than that, the method appears to be very stable and produces quadrature rules that are rapidly converging. In Table 3.2, the results of the n-point rule (1.17)

ω	n	n-point rational Gauss	γ_n	err. Gauss
2.0	1	2.1	3.94(-1)	1.43(-1)
	4	2.33248722	3.50(-7)	7.18(-5)
	7	2.332487232246550235	2.61(-15)	2.73(-8)
	10	2.33248723224655024110 7076	1.48(-24)	1.02(-11)
1.1	2	4.43	1.73(-2)	2.60(-1)
	5	4.467773637	2.00(-9)	2.09(-2)
	8	4.46777364638776571	5.61(-18)	1.53(-3)
	11	4.46777364638776578923 6123	1.66(-27)	1.09(-4)
1.01	3	8.429	2.53(-4)	4.20(-1)
	6	8.4301845803	6.27(-12)	1.85(-1)
	9	8.43018458047084205 82	7.52(-21)	8.37(-2)
	12	8.43018458047084205897 1264	1.23(-30)	3.75(-2)

TABLE 3.2. *Numerical results for* $I_1(\omega)$, *error constants, and comparison with Gauss quadrature*

applied to $g(t) = (\pi t/\omega)/\sin(\pi t/\omega)$ in double precision are shown for $\omega = 2$, 1.1 and 1.01, along with the error constants γ_n of (1.18). Also shown in the last column are the relative errors of the n-point Gauss-Legendre rule. For $\omega = 2$, the exact answer is known to be $8C/\pi$, where C is Catalan's constant (cf. [8, Eq. 3.747(2)]). The value shown in Table 3.2 for $n = 10$ agrees with it to all 25 decimal digits given. Ordinary Gauss-Legendre quadrature is seen to converge rather slowly, as ω approaches 1. In contrast, convergence of the rational Gauss quadrature rule is fast even for ω very close to 1. The extra effort required in this case is expended, as illustrated in Table 3.1, at the time when the rule is generated.

		method of §2.1		method of §2.2	
ω	n	SP	DP	SP	DP
2.0	1	.001	.004	.007	.178
	4	.008	.036	.010	.224
	7	.027	.125	.028	.220
	10	.065	.296	.016	.423
1.1	2	.002	.014	.060	1.554
	5	.013	.063	.068	1.649
	8	.036	.177	.098	1.274
	11	.080	.376	.104	1.461
1.01	3	.005	.037	.460	20.10
	6	.020	.104	.446	41.51
	9	.050	.244	.458	10.44
	12	.102	.487	.525	12.65

TABLE 3.3. *Timings* (in seconds) *of the methods in* §§2.1 *and* 2.2 *applied to Example* 3.1

Identical results were obtained by the discretization method of §2.2, but with substantially greater effort, particularly for higher accuracies and for ω close to 1. Respective timings are shown in Table 3.3, both for single-precision (SP) and double-precision (DP) accuracy requirements of $\frac{1}{2} \times 10^{-10}$ and $\frac{1}{2} \times 10^{-25}$, respectively.

While the choice $m = 2n$ indeed gives best accuracy, other choices of m may be preferable if the effort and time to generate the quadrature rule is of any importance. It turns out that with the method of partial fractions, $m = 2\lfloor (n+1)/2 \rfloor$ gives almost the same accuracy at about half the effort, whereas $m = 2$ gives considerably less accuracy but requires only about one-tenth the effort. The discretization method of §2.2, on the other hand, requires essentially the same effort regardless of the choice of m. Some timings required to generate the quadrature rules for various m and n, and the relative errors achieved, are shown in Table 3.4

			method of §2.1		method of §2.2		
ω	n	m	SP	DP	SP	DP	err
2.0	10	2	.008	.037	.014	.399	1.10(-17)
		10	.033	.153	.015	.409	1.47(-25)
		20	.065	.296	.016	.423	1.58(-25)
1.1	11	2	.009	.047	.095	1.402	2.20(-13)
		12	.045	.213	.100	1.426	2.80(-23)
		22	.080	.376	.104	1.461	6.68(-26)
1.01	12	2	.011	.065	.526	12.65	1.15(-13)
		12	.052	.258	.511	12.46	9.10(-25)
		24	.102	.487	.526	12.65	3.55(-27)

TABLE 3.4. *Timings and errors for selected* $m \leq 2n$

If $m = 2$, the values of n for which full accuracy of about 10^{-25} is attained are 15, 21 and 22 for $\omega = 2.0$, 1.1 and 1.01, respectively. Interestingly, the timings involved are only about half those for $m = 2\lfloor (n+1)/2 \rfloor$ shown in Table 3.4.

Example 3.2. $I_2(\omega) = \int_0^1 \frac{t^{-1/2}\Gamma(1+t)}{t+\omega}\, dt, \quad 0 < \omega < 1.$

Here we take $d\lambda(t) = t^{-1/2}\, dt$ on [0,1]. If we wish to match the first $2n-1$ poles of the gamma function at the negative integers as well as the pole at $-\omega$, we set $m = 2n$ in

$$\begin{aligned} \xi_1 &= \tfrac{1}{\omega}\,, \\ \xi_\nu &= \tfrac{1}{\nu-1}, \qquad \nu = 2,3,\ldots,m. \end{aligned} \tag{3.2}$$

The rational n-point Gauss rule (1.7), (1.17), generated by the method of §2.1.1, then produces (in double precision) results as shown in Table 3.5, where $\omega = \frac{1}{2}$. In the last column we list the absolute value of the difference between double-precision and single-precision results. In contrast to Example 3.1, we now see a case in which the accuracy reaches a limit (at about $n = 10$) and deteriorates, rather than improves, as n is further increased. (When $n = 20$, the calculation even breaks down in single precision!). The last column in Table 3.5 provides a clear hint as to what is happening: a steady growth in numerical instability. Closer examination reveals the true cause of this instability. The constants c_ν in the partial fraction decomposition (2.7) become very large and alternate in sign. Thus, for example, $c_{18} = -2.3375\ldots \times 10^9$ and $c_{19} = 2.3336\ldots \times 10^9$ when $n = 18$. This produces blocks of large coefficients W_k in (2.10) that alternate in sign from block to block, causing severe cancellation errors in summations such as

(2.5) (which are abundant in Stieltjes's algorithm). The phenomenon evidently is a manifestation of the asymmetric distribution of the poles of the gamma function.

n	n-point rational Gauss	$\lvert DP - SP\rvert$
2	1.746	2.24(−13)
6	1.75012059121	7.05(−11)
10	1.7501205912613354153 86	3.36(−8)
14	1.75012059126133541 59	1.52(−5)
18	1.7501205912613356	4.31(−3)

TABLE 3.5. *Numerical results for* $I_2(\omega)$, $\omega = .5$

The method of §2.2, in contrast, does not suffer from any numerical instability and produces for $n = 12$, with comparable effort, the value

$$I_2(.5) = 1.75012059126133541539461 0, \tag{3.3}$$

believed to be correct to all 25 digits shown.

Matching only n poles, and thus taking $m = n$ in (3.2), stabilizes the procedure of §2.1.1 considerably, and as a consequence produces the correct result (3.3) (except for a discrepancy of 1 unit in the last decimal place) for $n = 11$. An even more stable procedure results from taking $m = 2$ and, amazingly, yields the correct answer (to all digits shown!) already for $n = 13$.

Example 3.3. $I_3(\omega) = \int_{-1}^{1} \left(\frac{\pi t/\omega}{\sin(\pi t/\omega)}\right)^2 dt, \quad \omega > 1.$

Similarly as in Example 3.1, we take

$$\xi_\nu = (-1)^\nu/(\omega\lfloor(\nu+1)/2\rfloor), \qquad \nu = 1, 2, \ldots, m/2. \tag{3.4}$$

We applied the procedure described in §2.1.3 for $\omega = 2$, 1.5, 1.1 and 1.01, both in single and double precision, requesting accuracies of $\epsilon = \frac{1}{2} \times 10^{-10}$ and $\epsilon^d = \frac{1}{2} \times 10^{-25}$,

ω	k_1	k_1^d	k_2	k_2^d
2.0	130	163	50	63
1.5	133	191	53	71
1.1	177	306	67	106
1.01	384	727	124	247

TABLE 3.6. *Starting indices for two backward recurrences when* $n = 20$

respectively. When $m = 2n$ and $n = 20$, starting indices k_1, k_1^d in the first application of the backward recursion that were found to meet the accuracy requirements for the poles closest to [-1,1], and the analogous starting indices k_2, k_2^d in the second application, are shown in Table 3.6 for the four values of ω. As expected, the procedure becomes laborious as ω approaches 1. Selected double-precision results produced by the n-point rational Gauss rule, along with error constants, are shown in Table 3.7. The last column shows the relative error of results generated by the n-point Gauss-Legendre rule. For $\omega = 2$, the exact answer is known to be $I_3(2) = 4 \ln 2$ ([8, Eq. 3.837(2)]) and is correctly reproduced to 25 digits when $n = 11$. Note again the fast convergence of the rational Gauss quadrature rule, even for ω very close to 1, in contrast to the relatively slow convergence of the ordinary Gauss rule, especially for ω close to 1.

ω	n	n-point rational Gauss	γ_n	err. Gauss
2.0	2	2.75	9.90(-3)	4.36(-2)
	5	2.77258868	1.16(-9)	4.70(-5)
	8	2.7725887222397811	3.28(-18)	2.92(-8)
	11	2.77258872223978123766892	9.72(-28)	1.52(-11)
1.1	2	15.5	3.00(-2)	6.69(-1)
	6	16.5328175	8.54(-12)	6.79(-2)
	10	16.5328177384604181	7.21(-24)	3.42(-3)
	14	16.532817738460418301558898	2.35(-37)	1.40(-4)
1.01	2	184.	6.34(-2)	9.64(-1)
	6	188.674782	2.20(-11)	7.06(-1)
	10	188.674784224994172	1.88(-23)	4.00(-1)
	14	188.67478422499417427083 25	6.15(-37)	1.92(-1)

TABLE 3.7. *Numerical results for $I_3(\omega)$, error constants, and comparison with Gauss quadrature*

While the choice $m = 2\lfloor (n+1)/2 \rfloor$ produced similar advantages as in Example 3.1 — an increase of speed by a factor of about 2 at only a slight loss of accuracy — the choice $m = 2$ offered no significant gains in accuracy over the Gauss-Legendre rule, unlike $m = 4$, which did (since a symmetric *pair* of double poles is now accounted for).

We also applied the discretization method of §2.2 and obtained identical results with somewhat less effort in the case $\omega = 2$, and about the same effort in the case $\omega = 1.1$. For $\omega = 1.01$, however, we were unable to attain the requested double-precision accuracy with a discretization parameter $N \leq 800$ (in (2.21)).

Example 3.4. $I_4 = \int_0^\infty \frac{t}{e^t - 1} e^{-t} dt$.

The appropriate measure here is $d\lambda(t) = e^{-t}dt$ on [0,∞]. Since the integrand has poles at the integer multiples of $2\pi i$, we let $\zeta_\nu = -1/(2\nu\pi i) = i/(2\nu\pi)$, and thus in

(1.12) take

$$\xi_\nu = 0, \quad \eta_\nu = \frac{1}{2\nu\pi}, \quad \nu = 1, 2, \ldots, m/2. \tag{3.5}$$

The quantity p_ν in (2.13) being real, and thus $d_\nu = 0$ in (2.12), there is no nonconstant linear factor in the numerators of (2.11). This simplifies somewhat the procedure in §2.1.2, as it obviates the need to apply the routine `chri`.

In Table 3.8 we compare the performance (in double precision and for $m = 2n$) of our rational quadrature routine with Gauss-Laguerre quadrature (applied to $f(t) = t/(e^t - 1)$) and the Gaussian quadrature rule (applied to $f(t) = e^{-t}$) associated with "Einstein's weight function" $t/(e^t - 1)$; for the latter see [6]. The respective relative errors are shown in the last two columns. It can be seen that the Gauss-Laguerre and Gauss-Einstein quadratures are comparable in accuracy, the former being somewhat more accurate for small values of n, the latter for larger values of n. Both quadrature rules, however, are incomparably inferior to the rational Gauss formula, which for $n = 15$ produces the true value of the integral, $\zeta(2) - 1 = (\pi^2/6) - 1$, to 25 correct decimal digits. (Actually, the last digit is off by one unit.) The results become even slightly more accurate when we choose $m = 2\lfloor (n+1)/2 \rfloor$, and are still better, by several orders of magnitude, than those for Gauss-Laguerre and Gauss-Einstein quadrature when $m = 2$.

n	n-point rational Gauss	err GL	err GE
1	.59	9.76(−2)	4.09(−1)
5	.644934055	1.50(−5)	2.97(−4)
10	.6449340668482264 28	2.22(−8)	1.15(−8)
15	.644934066848226436472415 1	1.59(−11)	3.25(−13)

TABLE 3.8. *Numerical results for I_4 and comparison with Gauss-Laguerre and Gauss-Einstein quadrature*

The high accuracy of our rational quadrature rules in this example is all the more remarkable as the routine `gchri`, used in their construction (by the methods of §2.1.2), is subject to ill-conditioning, causing the recursion coefficients for the relevant orthogonal polynomials to gradually lose accuracy (by as much as 10 decimals, when $n = 15$ and $m = 2n$).

This weakness is accentuated when one tries to deal with more difficult integrals, for example,

$$I(\theta) = \int_0^\infty \frac{t}{e^t - 1} \sqrt{1 + \tfrac{1}{2}\theta t}\, dt = \int_0^\infty \frac{t}{1 - e^{-t}} \sqrt{1 + \tfrac{1}{2}\theta t} \cdot e^{-t} dt, \quad \theta > 0, \tag{3.6}$$

which has an additional branch point singularity at $t = -2/\theta$. Here, when $\theta = .75$, the n-point rational Gauss formula (in double precision and for $m = 2n$) gives only about

13 correct decimal places for $n = 15$, and 18 for $n = 30$. By the time n reaches 33, the ill-conditioning in the routine gchri has built up to such a level that the method fails (by producing a negative β-recursion coefficient). To get higher accuracy, one needs to apply the discretization method of §2.2, which is more stable, but becomes fairly expensive if pushed much beyond $n = 30$. Using $d\lambda(t) = e^{-t}dt$, and hence the N-point Gauss-Laguerre formula, to effect the discretization in (2.21), and requesting an accuracy of $\frac{1}{2} \times 10^{-25}$ for the desired recursion coefficients, we have observed timings of the order 12–16 seconds, and discretization parameters N as large as $N = 370$, for $33 \leq n \leq 40$. The rational Gauss formula so produced then yields relative errors of 4.26×10^{-21} for $n = 35$, and 9.65×10^{-23} for $n = 40$. This is still better, by about 4 decimal orders of accuracy, than Gauss-Laguerre quadrature applied to the second form of the integral in (3.6), and Gauss-Einstein quadrature applied to the first form.

Generalized Fermi-Dirac integrals (cf. [12]) are similar to $I(\theta)$ except that $t/(e^t - 1)$ is replaced by $t^k/(e^{-\eta+t} + 1)$, where η is a real parameter and $k = 1/2$, $3/2$ or $5/2$. The poles are now located at $\eta \pm (2\nu - 1)i\pi$, $\nu = 1, 2, 3, \ldots$. The use of rational Gauss quadrature to compute such integrals is dealt with elsewhere [5].

Example 3.5. $I_5(\eta) = \int_0^\infty \frac{t}{e^{-\eta+t}-1} e^{-t}dt, \quad \eta < 0.$

Again, we take $d\lambda(t) = e^{-t}dt$ and note that the poles are now at $\eta \pm 2\nu\pi i$, $\nu = 0, 1, 2, \ldots$. Accordingly, in (1.13) we take

$$\xi_0 = -\frac{1}{\eta}, \quad \xi_\nu = -\frac{\eta}{\eta^2 + 4\nu^2\pi^2}, \quad \eta_\nu = \frac{2\nu\pi}{\eta^2 + 4\nu^2\pi^2}, \quad \nu = 1, 2, \ldots, (m-1)/2, \tag{3.7}$$

and use the procedure of §2.1.2′. Selected results (for $m = 2n - 1$), comparing rational Gauss formulae with Gauss-Laguerre formulae, are shown in Table 3.9. In the case

η	n	n-point rational Gauss	err GL
−.1	3	.4503	1.16(−1)
	6	.4501936153	5.13(−2)
	9	.450193614441350	2.70(−2)
	12	.45019361444134784096	1.55(−2)
−1.0	2	.113	2.14(−1)
	6	.1111093520	5.07(−3)
	11	.1111093516052317322	1.81(−4)
	16	.11110935160523173201050 65	1.26(−5)
−10.0	2	.122(−4)	1.79(−1)
	6	.113502121(−4)	1.57(−4)
	11	.11350211463539057 8(−4)	7.31(−9)
	16	.1135021146353905701870968(−4)	1.20(−12)

TABLE 3.9. *Numerical results for I_5 and comparison with Gauss-Laguerre quadrature*

$\eta = -.1$, we were able to go only up to $n = 13$; when $n = 14$, our procedure failed by producing a negative β-coefficient in (2.2). The difficulty is caused by the ill-conditioning (mentioned after (2.10)) affecting the modified Chebyshev procedure. Even though our procedure was successful for $n = 13$, it had to work hard to take care of the pole at $\eta = -.1$: Backward recursion to compute modified moments had to start at $\nu = 584$ to get single-precision accuracy $\frac{1}{2} \times 10^{-10}$, and at $\nu = 2650$ to get double-precision accuracy $\frac{1}{2} \times 10^{-25}$.

Replacing the numerator te^{-t} in the integrand by t^k, where $k = 1/2, 3/2$ or $5/2$, and adding a factor $\sqrt{1 + \frac{1}{2}\theta t}$ as in (3.6), produces the Bose-Einstein integral whose computation by rational Gauss quadrature is discussed in [5].

Example 3.6. $I_6 = \int_0^\infty \left(\frac{t}{e^t - 1}\right)^2 e^{-t} dt$.

Here, as in Example 3.4, we take $d\lambda(t) = e^{-t}dt$ and parameters ξ_ν, η_ν as in (3.5), except that there are only $m/4$ of them, m being divisible by 4. In Table 3.10 we give

n	n-point rational Gauss	err GL	err GE
2	.47	3.71(−2)	1.61(−2)
8	.4816405209	1.16(−6)	5.99(−10)
14	.4816405210580757311	4.36(−9)	7.26(−18)
20	.4816405210580757313458777	2.80(−11)	1.09(−25)

TABLE 3.10. *Numerical results for I_5 and comparison with Gauss-Laguerre and Gauss-Einstein quadrature*

the results for $m = 2n$ (n even) obtained by the discretization method of §2.2, analogous to those of Table 3.8 but using the square of the Einstein function as weight function in GE. (The method of §2.1, as mentioned earlier, was not implemented.) What is remarkable in this example is the competitiveness of the Gauss-Einstein quadrature rule vis-à-vis the rational Gauss rule.

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S-orthogonality and construction of Gauss–Turán-type quadrature formulae[1]

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Dedicated to William B. Gragg on his 60th birthday

Abstract

Using the theory of s-orthogonality and reinterpreting it in terms of the standard orthogonal polynomials on the real line, we develop a method for constructing Gauss–Turán-type quadrature formulae. The determination of nodes and weights is very stable. For finding all weights, our method uses an upper triangular system of linear equations for the weights associated with each node. Numerical examples are included.

Keywords: Gauss–Turán-type quadratures; s-orthogonal polynomials; Nonnegative measure; Extremal polynomial; Weights; Nodes; Degree of precision; Stieltjes procedure

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1. Introduction

Let $\mathcal{P}_m$ be the set of all algebraic polynomials of degree at most m. In 1950, Turán [21] studied numerical quadratures of the form

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \sum_{i=0}^{k-1}\sum_{\nu=1}^{n} A_{i,\nu} f^{(i)}(\tau_\nu) + R_{n,k}(f), \tag{1.1}$$

where

$$A_{i,\nu} = \int_{-1}^{1} l_{\nu,i}(t)\,\mathrm{d}t \quad (\nu = 1,\ldots,n;\ i = 0,1,\ldots,k-1)$$

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and $l_{v,i}(t)$ are the fundamental polynomials of Hermite interpolation. The coefficients $A_{i,v}$ are Cotes numbers of higher order. Evidently, the formula (1.1) is exact if $f \in \mathscr{P}_{kn-1}$ and the points $-1 \leqslant \tau_1 < \cdots < \tau_n \leqslant 1$ are arbitrary.

For $k=1$ the formula (1.1), i.e.,

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \sum_{v=1}^{n} A_{0,v} f(\tau_v) + R_{n,1}(f),$$

can be exact for all polynomials of degree at most $2n-1$ if the nodes τ_v are the zeros of the Legendre polynomial P_n, and it is the well-known Gauss–Legendre quadrature rule.

Because of Gauss's result it is natural to ask whether knots τ_v can be chosen so that the quadrature formula (1.1) will be exact for algebraic polynomials of degree not exceeding $(k+1)n-1$. Turán [21] showed that the answer is negative for $k=2$, and for $k=3$ it is positive. He proved that the knots τ_v should be chosen as the zeros of the monic polynomial $\pi_n^*(t) = t^n + \cdots$ which minimizes the integral

$$\int_{-1}^{1} [\pi_n(t)]^4\,\mathrm{d}t,$$

where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \cdots + a_1 t + a_0$.

More generally, the answer is negative for even, and positive for odd k, and then τ_v are the zeros of the polynomial minimizing

$$\int_{-1}^{1} [\pi_n(t)]^{k+1}\,\mathrm{d}t.$$

When $k=1$, then π_n^* is the monic Legendre polynomial $\hat{P}_n$.

Because of the above, we put $k=2s+1$. It is also interesting to consider, instead of (1.1), more general *Gauss–Turán-type* quadrature formulae

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{i=0}^{2s} \sum_{v=1}^{n} A_{i,v} f^{(i)}(\tau_v) + R_{n,2s}(f), \tag{1.2}$$

where $\mathrm{d}\lambda(t)$ is a nonnegative measure on the real line $\mathbb{R}$, with compact or infinite support, for which all moments

$$\mu_k = \int_{\mathbb{R}} t^k\,\mathrm{d}\lambda(t), \quad k=0,1,\ldots,$$

exist and are finite, and $\mu_0 > 0$. It is known that formula (1.2) is exact for all polynomials of degree at most $2(s+1)n-1$, i.e.,

$$R_{n,2s}(f) = 0 \quad \text{for } f \in \mathscr{P}_{2(s+1)n-1}.$$

The knots τ_v $(v=1,\ldots,n)$ in (1.2) are the zeros of the monic polynomial $\pi_n^s(t)$, which minimizes the integral

$$F(a_0, a_1, \ldots, a_{n-1}) = \int_{\mathbb{R}} [\pi_n(t)]^{2s+2}\,\mathrm{d}\lambda(t),$$

where $\pi_n(t)=t^n+a_{n-1}t^{n-1}+\cdots+a_1t+a_0$. This minimization leads to the conditions

$$\int_{\mathbb{R}}[\pi_n(t)]^{2s+1}t^k\,d\lambda(t)=0 \quad (k=0,1,\ldots,n-1). \tag{1.3}$$

Usually, instead of $\pi_n^s(t)$ we write $P_{s,n}(t)$.

The case $d\lambda(t)=w(t)\,dt$ on $[a,b]$ has been investigated by the Italian mathematicians Ossicini [15], Ghizzetti and Ossicini [7] and Guerra [9, 10]. It is known that there exists a unique $P_{s,n}(t)=\prod_{\nu=1}^{n}(t-\tau_\nu)$, whose zeros τ_ν are real, distinct and located in the interior of the interval $[a,b]$. These polynomials are known as *s-orthogonal* (or *s*-self associated) *polynomials* in the interval $[a,b]$ with respect to the weight function w (for more details see [4, 15–17]). For $s=0$ we have the standard case of orthogonal polynomials, and (1.2) then becomes the well-known Gauss–Christoffel formula.

An iterative process for computing the coefficients of *s*-orthogonal polynomials in a special case, when the interval $[a,b]$ is symmetric with respect to the origin and the weight function w is an even function, was proposed by Vincenti [24]. He applied his process to the Legendre case. When n and s increase, the process becomes numerically unstable.

At the Third Conference on Numerical Methods and Approximation Theory (Niš, 18–21 August, 1987) (see [13]) we presented a stable method for numerically constructing *s*-orthogonal polynomials and their zeros. It uses an iterative method with quadratic convergence based on a discretized Stieltjes procedure and the Newton–Kantorovič method. Since the proceedings of this conference may not be widely available, we recall this method in Section 2. In Section 3, we develop a numerical procedure for calculating the coefficients $A_{i,\nu}$ in (1.2). Some alternative methods were proposed by Stroud and Stancu [20] (see also [19]) and Milovanović and Spalević [14]. Remarks on the Chebyshev measure are made in Section 4. Finally, a few numerical examples are presented in Section 5.

2. Construction of *s*-orthogonal polynomials

The basic idea for our method to numerically construct *s*-orthogonal polynomials with respect to the measure $d\lambda(t)$ on the real line $\mathbb{R}$ is a reinterpretation of the "*orthogonality conditions*" (1.3). For given n and s, we put $d\mu(t)=d\mu^{s,n}(t)=(\pi_n(t))^{2s}\,d\lambda(t)$. The conditions can then be written as

$$\int_{\mathbb{R}}\pi_k^{s,n}(t)t^\nu\,d\mu(t)=0 \quad (\nu=0,1,\ldots,k-1),$$

where $\{\pi_k^{s,n}\}$ is a sequence of monic orthogonal polynomials with respect to the new measure $d\mu(t)$. Of course, $P_{s,n}(\cdot)=\pi_n^{s,n}(\cdot)$. As we can see, the polynomials $\pi_k^{s,n}$ $(k=0,1,\ldots)$ are implicitly defined, because the measure $d\mu(t)$ depends on $\pi_n^{s,n}(t)$. A general class of such polynomials was introduced and studied by Engels (cf. [2, pp. 214–226]).

We will write simply $\pi_k(\cdot)$ instead of $\pi_k^{s,n}(\cdot)$. These polynomials satisfy a three-term recurrence relation

$$\begin{aligned}&\pi_{\nu+1}(t)=(t-\alpha_\nu)\pi_\nu(t)-\beta_\nu\pi_{\nu-1}(t), \quad \nu=0,1,\ldots,\\ &\pi_{-1}(t)=0, \qquad \pi_0(t)=1,\end{aligned} \tag{2.1}$$

Table 1

n	$d\mu^{s,n}(t)$	Orthogonal polynomials			
0	$(\pi_0^{s,0}(t))^{2s}\,d\lambda(t)$	$\boxed{\pi_0^{s,0}}$			
1	$(\pi_1^{s,1}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,1}$	$\boxed{\pi_1^{s,1}}$		
2	$(\pi_2^{s,2}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,2}$	$\pi_1^{s,2}$	$\boxed{\pi_2^{s,2}}$	
3	$(\pi_3^{s,3}(t))^{2s}\,d\lambda(t)$	$\pi_0^{s,3}$	$\pi_1^{s,3}$	$\pi_2^{s,3}$	$\boxed{\pi_3^{s,3}}$
⋮					

where, because of orthogonality,

$$\alpha_v = \alpha_v(s,n) = \frac{(t\pi_v, \pi_v)}{(\pi_v, \pi_v)} = \frac{\int_{\mathbb{R}} t\pi_v^2(t)\,d\mu(t)}{\int_{\mathbb{R}} \pi_v^2(t)\,d\mu(t)},$$
$$\beta_v = \beta_v(s,n) = \frac{(\pi_v, \pi_v)}{(\pi_{v-1}, \pi_{v-1})} = \frac{\int_{\mathbb{R}} \pi_v^2(t)\,d\mu(t)}{\int_{\mathbb{R}} \pi_{v-1}^2(t)\,d\mu(t)}, \tag{2.2}$$

and, by convention, $\beta_0 = \int_{\mathbb{R}} d\mu(t)$.

The coefficients α_v and β_v are the fundamental quantities in the constructive theory of orthogonal polynomials. They provide a compact way of representing orthogonal polynomials, requiring only a linear array of parameters. The coefficients of orthogonal polynomials, or their zeros, in contrast, need two-dimensional arrays.

Knowing the coefficients α_v and β_v $(v=0,1,\ldots,n-1)$ gives us access to the first $n+1$ orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_n$. Of course, for a given n, we are interested only in the last of them, i.e., $\pi_n \equiv \pi_n^{s,n}$. Thus, for $n=0,1,\ldots$, the diagonal (boxed) elements in Table 1 are our s-orthogonal polynomials $\pi_n^{s,n}$.

A stable procedure for finding the coefficients α_v and β_v is the discretized Stieltjes procedure, especially for infinite intervals of orthogonality (see [3–6]). Unfortunately, in our case this procedure cannot be applied directly, because the measure $d\mu(t)$ involves an unknown polynomial $\pi_n^{s,n}$. Consequently, we consider the system of nonlinear equations

$$f_0 \equiv \beta_0 - \int_{\mathbb{R}} \pi_n^{2s}(t)\,d\lambda(t) = 0,$$
$$f_{2v+1} \equiv \int_{\mathbb{R}} (\alpha_v - t)\pi_v^2(t)\pi_n^{2s}(t)\,d\lambda(t) = 0 \quad (v=0,1,\ldots,n-1), \tag{2.3}$$
$$f_{2v} \equiv \int_{\mathbb{R}} (\beta_v\pi_{v-1}^2(t) - \pi_v^2(t))\pi_n^{2s}(t)\,d\lambda(t) = 0 \quad (v=1,\ldots,n-1),$$

which follows from (2.2).

Let $\boldsymbol{x}$ be a $(2n)$-dimensional column vector with components $\alpha_0, \beta_0, \ldots, \alpha_{n-1}, \beta_{n-1}$ and $\boldsymbol{f}(\boldsymbol{x})$ a $(2n)$-dimensional vector with components $f_0, f_1, \ldots, f_{2n-1}$, given by (2.3), in which $\pi_0, \pi_1, \ldots, \pi_n$ are

thought of as being expressed in terms of the α's and β's via (2.1). If $W = W(\boldsymbol{x})$ is the corresponding Jacobian of $\boldsymbol{f}(\boldsymbol{x})$, then we can apply Newton–Kantorovič's method

$$\boldsymbol{x}^{[k+1]} = \boldsymbol{x}^{[k]} - W^{-1}(\boldsymbol{x}^{[k]})\boldsymbol{f}(\boldsymbol{x}^{[k]}) \quad (k = 0, 1, \ldots) \tag{2.4}$$

for determining the coefficients of the recurrence relation (2.1). If a sufficiently good approximation $\boldsymbol{x}^{[0]}$ is chosen, the convergence of the method (2.4) is quadratic.

Notice that the elements of the Jacobian can be easily computed in the following manner.

First, we have to determine the partial derivatives $a_{v,i} = \partial\pi_v/\partial\alpha_i$ and $b_{v,i} = \partial\pi_v/\partial\beta_i$. Differentiating the recurrence relation (2.1) with respect to α_i and β_i, we obtain

$$a_{v+1,i} = (t - \alpha_v)a_{v,i} - \beta_v a_{v-1,i}, \qquad b_{v+1,i} = (t - \alpha_v)b_{v,i} - \beta_v b_{v-1,i},$$

where

$$a_{v,i} = 0, \quad b_{v,i} = 0 \quad (v \leqslant i),$$

$$a_{i+1,i} = -\pi_i(t), \quad b_{i+1,i} = -\pi_{i-1}(t).$$

These relations are the same as those for π_v, but with other (delayed) initial values. The elements of the Jacobian are

$$\begin{aligned}
\frac{\partial f_{2v+1}}{\partial \alpha_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)[(\alpha_v - t)p_{v,i}(t) + \tfrac{1}{2}\delta_{v,i}\pi_v^2(t)\pi_n(t)]\,\mathrm{d}\lambda(t),\\
\frac{\partial f_{2v+1}}{\partial \beta_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)(\alpha_v - t)q_{v,i}(t)\,\mathrm{d}\lambda(t),\\
\frac{\partial f_{2v}}{\partial \alpha_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)(\beta_v p_{v-1,i}(t) - p_{v,i}(t))\,\mathrm{d}\lambda(t),\\
\frac{\partial f_{2v}}{\partial \beta_i} &= 2\int_{\mathbb{R}} \pi_n^{2s-1}(t)[(\beta_v q_{v-1,i}(t) - q_{v,i}(t)) + \tfrac{1}{2}\delta_{v,i}\pi_{v-1}^2(t)\pi_n(t)]\,\mathrm{d}\lambda(t),
\end{aligned} \tag{2.5}$$

where

$$p_{v,i}(t) = \pi_v(t)(a_{v,i}\pi_n(t) + sa_{n,i}\pi_v(t)), \qquad q_{v,i}(t) = \pi_v(t)(b_{v,i}\pi_n(t) + sb_{n,i}\pi_v(t)),$$

and $\delta_{v,i}$ is the Kronecker delta.

All of the above integrals in (2.3) and (2.5) can be computed exactly, except for rounding errors, by using a Gauss–Christoffel quadrature formula with respect to the measure $\mathrm{d}\lambda(t)$,

$$\int_{\mathbb{R}} g(t)\,\mathrm{d}\lambda(t) = \sum_{v=1}^{N} A_v^{(N)} g(\tau_v^{(N)}) + R_N(g), \tag{2.6}$$

taking $N = (s+1)n$ knots. This formula is exact for all polynomials of degree at most $2N - 1 = 2(s+1)\cdot n - 1 = 2(n-1) + 2ns + 1$.

Thus, for all calculations we use only the fundamental three-term recurrence relation (2.1) for the orthogonal polynomials $\pi_k(\cdot\,; \mathrm{d}\lambda)$ and the Gauss–Christoffel quadrature (2.6). As intial values $\alpha_v^{[0]} = \alpha_v^{[0]}(s,n)$ and $\beta_v^{[0]} = \beta_v^{[0]}(s,n)$ we take the values obtained for $n-1$, i.e., $\alpha_v^{[0]} = \alpha_v(s, n-1)$, $\beta_v^{[0]} = \beta_v(s, n-1)$, $v \leqslant n-2$. For $\alpha_{n-1}^{[0]}$ and $\beta_{n-1}^{[0]}$ we use corresponding extrapolated values.

In the case $n=1$ we solve the equation

$$\phi(\alpha_0)=\phi(\alpha_0(s,1))=\int_{\mathbb{R}}(t-\alpha_0)^{2s+1}\,\mathrm{d}\lambda(t)=0,$$

and then determine

$$\beta_0=\beta_0(s,1)=\int_{\mathbb{R}}(t-\alpha_0)^{2s}\,\mathrm{d}\lambda(t).$$

The zeros $\tau_\nu=\tau_\nu(s,n)$ $(\nu=1,\dots,n)$ of $\pi_n^{s,n}$, i.e., the nodes of the Gauss–Turán-type quadrature formula (1.2), we obtain very easily as eigenvalues of a (symmetric tridiagonal) Jacobi matrix J_n using the QR algorithm, namely,

$$J_n=\begin{bmatrix}\alpha_0 & \sqrt{\beta_1} & & & \mathrm{O}\\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}}\\ \mathrm{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1}\end{bmatrix},$$

where $\alpha_\nu=\alpha_\nu(s,n)$, $\beta_\nu=\beta_\nu(s,n)$ $(\nu=0,1,\dots,n-1)$.

3. Calculation of coefficients

Let $\tau_\nu=\tau_\nu(s,n)$, $\nu=1,\dots,n$, be the zeros of the s-orthogonal (monic) polynomial $\pi_n(t)\,(\equiv\pi_n^{s,n}(t))$. In order to find the coefficients $A_{i,\nu}$ in the Gauss–Turán-type quadrature formula

$$\int_{\mathbb{R}}f(t)\,\mathrm{d}\lambda(t)=\sum_{i=0}^{2s}\sum_{\nu=1}^{n}A_{i,\nu}f^{(i)}(\tau_\nu)+R(f), \tag{3.1}$$

we define

$$\Omega_\nu(t)=\left(\frac{\pi_n(t)}{t-\tau_\nu}\right)^{2s+1}=\prod_{i\neq\nu}(t-\tau_i)^{2s+1}\quad(\nu=1,\dots,n). \tag{3.2}$$

Then the coefficients $A_{i,\nu}$ can be expressed in the form (see [19])

$$A_{i,\nu}=\frac{1}{i!(2s-i)!}\left[D^{2s-i}\frac{1}{\Omega_\nu(t)}\int_{\mathbb{R}}\frac{\pi_n(x)^{2s+1}-\pi_n(t)^{2s+1}}{x-t}\,\mathrm{d}\lambda(x)\right]_{t=\tau_\nu},$$

where D is the differentiation operator. In particular, for $i=2s$, we have

$$A_{2s,\nu}=\frac{1}{(2s)!(\pi_n'(\tau_\nu))^{2s+1}}\int_{\mathbb{R}}\frac{\pi_n(x)^{2s+1}}{x-\tau_\nu}\,\mathrm{d}\lambda(x),$$

i.e.,

$$A_{2s,\nu}=\frac{B_\nu^{(s)}}{(2s)!(\pi_n'(\tau_\nu))^{2s}} \quad (\nu=1,\dots,n),$$

where $B_\nu^{(s)}$ are the Christoffel numbers of the following Gaussian quadrature (with respect to the measure $\mathrm{d}\mu(t)=\pi_n^{2s}(t)\,\mathrm{d}\lambda(t)$):

$$\int_{\mathbb{R}} g(t)\,\mathrm{d}\mu(t)=\sum_{\nu=1}^{n} B_\nu^{(s)} g(\tau_\nu)+R_n(g), \quad R_n(\mathscr{P}_{2n-1})=0. \tag{3.3}$$

Since $B_\nu^{(s)}>0$, we conclude that $A_{2s,\nu}>0$. The expressions for the other coefficients ($i<2s$) become very complicated. For numerical calculation we could use a triangular system of linear equations obtained from the formula (3.1) by replacing f with the Newton polynomials: $1, t-\tau_1,\dots,(t-\tau_1)^{2s+1}$, $(t-\tau_1)^{2s+1}(t-\tau_2),\dots,(t-\tau_1)^{2s+1}(t-\tau_2)^{2s+1}\cdots(t-\tau_n)^{2s}$ (cf. [4, Section 2.2.4]).

In this paper we take instead the polynomials

$$f_{k,\nu}(t)=(t-\tau_\nu)^k\Omega_\nu(t)=(t-\tau_\nu)^k\prod_{i\neq\nu}(t-\tau_i)^{2s+1}, \tag{3.4}$$

where $0\leqslant k\leqslant 2s$, $1\leqslant\nu\leqslant n$.

Since the quadrature (3.1) is exact for all polynomials of degree at most $2(s+1)n-1$ and

$$\deg f_{k,\nu}=(n-1)(2s+1)+k\leqslant(2s+1)n-1,$$

we see that (3.1) is exact for the polynomials (3.4), i.e.,

$$R(f_{k,\nu})=0 \quad (0\leqslant k\leqslant 2s,\ 1\leqslant\nu\leqslant n).$$

Thus, we have

$$\sum_{i=0}^{2s}\sum_{j=1}^{n} A_{i,j} f_{k,\nu}^{(i)}(\tau_j)=\int_{\mathbb{R}} f_{k,\nu}(t)\,\mathrm{d}\lambda(t),$$

i.e.,

$$\sum_{i=0}^{2s} A_{i,\nu} f_{k,\nu}^{(i)}(\tau_\nu)=\mu_{k,\nu}, \tag{3.5}$$

because for every $j\neq\nu$ we have $f_{k,\nu}^{(i)}(\tau_j)=0$ when $0\leqslant i\leqslant 2s$. Here, we have put

$$\mu_{k,\nu}=\int_{\mathbb{R}} f_{k,\nu}(t)\,\mathrm{d}\lambda(t)=\int_{\mathbb{R}}(t-\tau_\nu)^k\prod_{i\neq\nu}(t-\tau_i)^{2s+1}\mathrm{d}\lambda(t).$$

For each ν, we have in (3.5) a system of $2s+1$ linear equations in the same number of unknowns, $A_{i,\nu}$, $i=0,1,\dots,2s$.

Using Leibniz's formula of differentiation, one easily proves the following auxiliary result.

Lemma 3.1. *For the polynomials $f_{k,v}$ given by* (3.4), *we have*

$$f_{k,v}^{(i)}(\tau_v)=\begin{cases}0, & i<k,\\ i^{(k)}\Omega_v^{(i-k)}(\tau_v), & i\geqslant k,\end{cases}$$

where $i^{(k)}=i(i-1)\cdots(i-k+1)$ [with $0^{(0)}=1$] and Ω_v is defined in (3.2).

Lemma 3.1 shows that each system of linear equations (3.5) is upper triangular. Thus, once all zeros of the s-orthogonal polynomial π_n, i.e., the nodes of the quadrature formula (3.1), are known, the determination of its weights $A_{i,v}$ is reduced to solving the n linear systems of $(2s+1)$ equations

$$\begin{bmatrix} f_{0,v}(\tau_v) & f'_{0,v}(\tau_v) & \cdots & f_{0,v}^{(2s)}(\tau_v)\\ & f'_{1,v}(\tau_v) & \cdots & f_{1,v}^{(2s)}(\tau_v)\\ & & \ddots & \\ & & & f_{2s,v}^{(2s)}(\tau_v)\end{bmatrix}\begin{bmatrix}A_{0,v}\\ A_{1,v}\\ \vdots\\ A_{2s,v}\end{bmatrix}=\begin{bmatrix}\mu_{0,v}\\ \mu_{1,v}\\ \vdots\\ \mu_{2s,v}\end{bmatrix}.$$

Put $a_{k,k+j}=f_{k-1,v}^{(k-1+j)}(\tau_v)$, so that the matrix of the system has elements $a_{l,j}$ $(1\leqslant l,j\leqslant 2s+1)$, with $a_{l,j}=0$ for $j<l$. Then, by Lemma 3.1,

$$a_{l,j}=(j-1)^{(l-1)}\Omega_v^{(j-l)}(\tau_v)\quad (j\geqslant l;\ 1\leqslant l,j\leqslant 2s+1). \tag{3.6}$$

Lemma 3.2. *Let $\tau_1,\ldots,\tau_n$ be the zeros of the s-orthogonal polynomial π_n. For the elements $a_{l,j}$, defined by* (3.6), *the following relations hold*:

$$a_{k,k}=(k-1)!a_{1,1}\quad (1\leqslant k\leqslant 2s+1),$$

$$a_{k,k+j}=-(2s+1)(k+j-1)^{(k-1)}\sum_{l=1}^{j}u_l a_{l,j}\quad \begin{pmatrix}1\leqslant k\leqslant 2s-j+1\\ j=1,\ldots,2s\end{pmatrix},$$

where

$$a_{1,1}=\Omega_v(\tau_v)=[\pi_n'(\tau_v)]^{2s+1},$$

$$u_l=\sum_{i\neq v}(\tau_i-\tau_v)^{-l}\quad (l=1,\ldots,2s). \tag{3.7}$$

Proof. The first relation is an immediate consequence of the definition of $a_{k,k}$ and Lemma 3.1. To prove the second, define $v(t)=\sum_{i\neq v}(t-\tau_i)^{-1}$. Since $\Omega_v(t)=\prod_{i\neq v}(t-\tau_i)^{2s+1}$ we have that

$$\Omega_v'(t)=(2s+1)v(t)\Omega_v(t)$$

and

$$\Omega_v^{(j)}(t)=\frac{d^{j-1}}{dt^{j-1}}(\Omega_v'(t))=(2s+1)\frac{d^{j-1}}{dt^{j-1}}(v(t)\Omega_v(t))$$

$$=(2s+1)\sum_{l=0}^{j-1}\binom{j-1}{l}\Omega_v^{(j-1-l)}(t)v^{(l)}(t).$$

Then, (3.6) becomes

$$a_{k,k+j}=(k+j-1)^{(k-1)}(2s+1)\sum_{l=1}^{j}\binom{j-1}{l-1}v^{(l-1)}(\tau_v)\Omega_v^{(j-l)}(\tau_v).$$

Since

$$v^{(l-1)}(\tau_v)=(-1)^{l-1}(l-1)!\sum_{i\neq v}(\tau_v-\tau_i)^{-l}=-(l-1)!u_l$$

and

$$\Omega_v^{(j-l)}(\tau_v)=\frac{a_{l,j}}{(j-1)^{(l-1)}}=\frac{(j-l)!}{(j-1)!}a_{l,j},$$

we get

$$a_{k,k+j}=-(2s+1)(k+j-1)^{(k-1)}\sum_{l=1}^{j}u_l a_{l,j}. \qquad \square$$

Using the normalization

$$\hat{a}_{k,j}=\frac{a_{k,j}}{(j-1)!a_{1,1}} \quad (1\leqslant k,\ j\leqslant 2s+1), \tag{3.8}$$

and putting

$$b_k=(k-1)A_{k-1,v} \quad (1\leqslant k\leqslant 2s+1),$$

$$\hat{\mu}_{k,v}=\frac{\mu_{k,v}}{(\pi_n'(\tau_v))^{2s+1}}=\int_{\mathbb{R}}(t-\tau_v)^k\left(\prod_{i\neq v}\frac{t-\tau_i}{\tau_v-\tau_i}\right)^{2s+1}\mathrm{d}\lambda(t), \tag{3.9}$$

we have the following result:

Theorem 3.3. *For fixed v $(1\leqslant v\leqslant n)$, the coefficients $A_{i,v}$ in the Gauss–Turán-type quadrature formula* (3.1) *are given by*

$$\begin{aligned} b_{2s+1} &= (2s)!A_{2s,v}=\hat{\mu}_{2s,v},\\ b_k &= (k-1)!A_{k-1,v}=\hat{\mu}_{k-1,v}-\sum_{j=k+1}^{2s+1}\hat{a}_{k,j}b_j \quad (k=2s,\ldots,1), \end{aligned} \tag{3.10}$$

where $\hat{\mu}_{k,v}$ are given by (3.9), *and*

$$\hat{a}_{k,k}=1, \qquad \hat{a}_{k,k+j}=-\frac{2s+1}{j}\sum_{l=1}^{j}u_l\hat{a}_{l,j} \quad (k=1,\ldots,2s;\ j=1,\ldots,2s-k+1), \tag{3.11}$$

the u_l being defined by (3.7).

Proof. The relations (3.11) follow directly from Lemma 3.2 and the normalization (3.8).

The coefficients b_k $(1 \leqslant k \leqslant 2s+1)$ are obtained from the corresponding upper triangular system of equations $\hat{A}\boldsymbol{b} = \boldsymbol{c}$, where

$$\hat{A} = [\hat{a}_{ij}], \quad \boldsymbol{b} = [b_1, \ldots, b_{2s+1}]^{\mathrm{T}}, \quad \boldsymbol{c} = [\hat{\mu}_{0,v}, \ldots, \hat{\mu}_{2s,v}]^{\mathrm{T}}. \qquad \square$$

The normalized moments $\hat{\mu}_{k,v}$ can be computed exactly, except for rounding errors, by using the same Gauss–Christoffel formula as in the construction of s-orthogonal polynomials, i.e., (2.6) with $N = (s+1)n$ knots.

4. Some remarks on the Chebyshev measure

In this section we discuss the particulary interesting case of the Chebyshev measure $\mathrm{d}\lambda(t) = (1-t^2)^{-1/2}\,\mathrm{d}t$. In 1930, Bernstein [1] showed that the monic Chebyshev polynomial $\hat{T}_n(t) = T_n(t)/2^{n-1}$ minimizes all integrals of the form

$$\int_{-1}^{1} \frac{|\pi_n(t)|^{k+1}}{\sqrt{1-t^2}}\,\mathrm{d}t \quad (k \geqslant 0).$$

Thus, the Chebyshev–Turán formula

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \sum_{i=0}^{2s} \sum_{v=1}^{n} A_{i,v} f^{(i)}(\tau_v) + R_n(f), \tag{4.1}$$

with $\tau_v = \cos((2v-1)\pi/2n)$ $(v = 1, \ldots, n)$, is exact for all polynomials of degree at most $2(s+1)n - 1$. Turán stated the problem of explicit determination of $A_{i,v}$ and its behavior as $n \to +\infty$ (see [22, Problem XXVI]). Some characterizations and solution for $s = 2$ were obtained by Micchelli and Rivlin [12], Riess [18], and Varma [23]. One simple answer to Turán's question was given by Kis [11]. His result can be stated in the following form: If g *is an even trigonometric polynomial of degree at most* $2(s+1)n - 1$, *then*

$$\int_0^{\pi} g(\theta)\,\mathrm{d}\theta = \frac{\pi}{n(s!)^2} \sum_{j=0}^{s} \frac{S_j}{4^j n^{2j}} \sum_{v=1}^{n} g^{(2j)}\left(\frac{2v-1}{2n}\pi\right),$$

where S_{s-j} $(j = 0, 1, \ldots, s)$ *denote the elementary symmetric polynomials with respect to the numbers* $1^2, 2^2, \ldots, s^2$, *i.e.*,

$$S_s = 1, \qquad S_{s-1} = 1^2 + 2^2 + \cdots + s^2, \ldots, \qquad S_0 = 1^2 \cdot 2^2 \cdots s^2.$$

Consequently,

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \frac{\pi}{n(s!)^2} \sum_{j=0}^{s} \frac{S_j}{4^j n^{2j}} \sum_{v=1}^{n} [D^{2j} f(\cos\theta)]_{\theta=(2v-1/2n)\pi}.$$

Using the expansion

$$D^{2k} f(\cos\theta) = \sum_{i=1}^{2k} d_{k,i}(t) f^{(i)}(t), \quad t = \cos\theta, \quad k > 0,$$

where the functions $d_{k,j} \equiv d_{k,j}(t)$ are given recursively by

$$d_{k+1,1} = (1-t^2)d''_{k,1} - td'_{k,1},$$

$$d_{k+1,2} = (1-t^2)d''_{k,2} - td'_{k,2} + 2(1-t^2)d'_{k,1} - td_{k,1},$$

$$d_{k+1,i} = (1-t^2)d''_{k,i} - td'_{k,i} + 2(1-t^2)d'_{k,i-1} - td_{k,i-1} + (1-t^2)d_{k,i-2}, \quad (i = 3,\ldots,2k),$$

$$d_{k+1,2k+1} = 2(1-t^2)d'_{k,2k} - td_{k,2k} + (1-t^2)d_{k,2k-1},$$

$$d_{k+1,2k+2} = (1-t^2)d_{k,2k},$$

with $d_{1,1} = -t$ and $d_{1,2} = 1 - t^2$, we obtain (4.1). For example, when $s = 3$, we have

$$A_{0,v} = \frac{\pi}{n}, \qquad A_{1,v} = \frac{\pi\tau_v}{2304n^7}(784n^4 + 56n^2 - 1),$$

$$A_{2,v} = \frac{\pi}{2304n^7}[(784n^4 - 392n^2 + 31)(1-\tau_v^2) + 168n^2 - 15],$$

$$A_{3,v} = -\frac{\pi\tau_v}{2304n^7}[(336n^2 - 89)(1-\tau_v^2) + 15],$$

$$A_{4,v} = \frac{\pi}{2304n^7}[(56n^2 - 65)(1-\tau_v^2)^2 + 45(1-\tau_v^2)],$$

$$A_{5,v} = \frac{\pi\tau_v}{2304n^7}[674(1-\tau_v^2)^2 - 240(1-\tau_v^2)], \qquad A_{6,v} = \frac{\pi}{2304n^7}(1-\tau_v^2)^3.$$

To conclude, we mention the corresponding formula (3.3) for the Chebyshev weight,

$$\int_{\mathbb{R}} g(t)\frac{\hat{T}_n^{2s}(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \frac{\pi}{4^{sn}n}\binom{2s}{s}\sum_{v=1}^{n} g(\tau_v) + R_n(g), \tag{4.2}$$

where $\tau_v = \cos(2v-1)(\pi/2n)$ $(v = 1,\ldots,n)$. Note that all weights are equal, i.e., the formula (4.2) is one of Chebyshev type.

5. Numerical examples

Using the procedures outlined in Sections 2 and 3 for constructing s-orthogonal polynomials and calculating the coefficients in Gauss–Turán-type quadrature formulae, we prepared corresponding software with the following types of polynomials $\pi_n(\cdot;\mathrm{d}\lambda)$ (identified by the integer `ipoly`):

```
c ipoly - integer identifying the kind of polynomials:
c
c  0 = nonclassical polynomials with given coefficients
c      in the three-term recurrence relation
c  1 = Legendre polynomials on [-1,1]
c  2 = Legendre polynomials on [0,1]
```

```
c  3 = Chebyshev polynomials of the first kind
c  4 = Chebyshev polynomials of the second kind
c  5 = Jacobi polynomials with parameters al=.5, be=-.5
c  6 = Jacobi polynomials with parameters al,be
c  7 = generalized Laguerre polynomials with parameter al
c  8 = Hermite polynomials
c  9 = generalized Gegenbauer polynomials with parameters al,be
c 10 = polynomials for the logistic weight
c       w(t)=e^{-t}/(1+e^{-t})^2 on the real line
c
c al,be - parameters for Jacobi, generalized Laguerre
c         and generalized Gegenbauer polynomials
c For ipoly=9, the weight function is given by
c w(x)=|x|^mu(1-x^2)^al, where be=(mu-1)/2.
```

All computations were done on the MICROVAX 3400 computer using VAX FORTRAN Ver. 5.3 in D- and Q-arithmetic, with machine precision $\approx 2.76\times 10^{-17}$ and $\approx 1.93\times 10^{-34}$, respectively. For example, taking $d\lambda(t)=e^{-t}\,dt$ on $(0,+\infty)$, for $s=2$ and $n=5$ we obtain the results in D-arithmetic shown in Table 2.

Finally, we give an example where it is preferable to use a formula of Turán type rather than the standard Gaussian formula,

$$\int_{\mathbb{R}} f(t)\,d\lambda(t)=\sum_{v=1}^{n} A_v f(t_v)+R_n(f) \tag{5.1}$$

for which $R_n(\mathscr{P}_{2n-1})=0$. The example is

$$I=\int_{-1}^{1} e^t\sqrt{1-t^2}\,dt=1.77549968921218094687857653 72\ldots .$$

Here we have $f(t)=e^t$ and $d\lambda(t)=\sqrt{1-t^2}\,dt$ on $[-1,1]$ (the Chebyshev measure of the second kind). Notice that $f^{(i)}(t)=f(t)$ for every $i\geqslant 0$.

The Gaussian formula (5.1) and the corresponding Gauss–Turán formula (3.1) give

$$I\approx I_n^{\mathrm{G}}=\sum_{v=1}^{n} A_v e^{t_v} \tag{5.2}$$

and

$$I\approx I_{n,s}^{\mathrm{T}}=\sum_{v=1}^{n} C_v^{(s)} e^{\tau_v}, \tag{5.3}$$

respectively, where $C_v^{(s)}=\sum_{i=0}^{2s} A_{i,v}$.

Table 3 shows the relative errors $|(I_{n,s}^{\mathrm{T}}-I)/I_{n,s}^{\mathrm{T}}|$ for $n=1(1)5$ and $s=0(1)5$. (Numbers in parentheses indicate decimal exponents and m.p. stands for machine precision.)

For $s=0$ the quadrature formula (5.3) reduces to (5.2), i.e., $I_{n,0}^{\mathrm{T}}\equiv I_n^{\mathrm{G}}$. Notice that Turán's formula (5.3) with n nodes has the same degree of exactness as the Gaussian formula with $(s+1)n$ nodes, which explains its superior behavior in Table 3.

Table 2
Example. Laguerre case ($s=2$, $n=5$)

k	alpha (k)	beta (k)
0	0.206241261660323E+01	0.111900724691563E+17
1	0.817357215072019E+01	0.627220780166491E+01
2	0.143542025111386E+02	0.314187808183856E+02
3	0.206411614818251E+02	0.761775799352482E+02
4	0.268361238086797E+02	0.141467716850165E+03
zero(1) = 0.511080817827157E+00		zero(2) = 0.365040485156886E+01
$A(0,1)$ = 0.831408096794173E+00		$A(0,2)$ = 0.167454288564437E+00
$A(1,1)$ = 0.878844153076445E−01		$A(1,2)$ = −0.133418640886195E+00
$A(2,1)$ = 0.777008304959738E−01		$A(2,2)$ = 0.101695158354974E+00
$A(3,1)$ = 0.776770118733145E−02		$A(3,2)$ = −0.233384486558624E−01
$A(4,1)$ = 0.124333607217694E−02		$A(4,2)$ = 0.920099700677729E−02
zero(3) = 0.100115534444780E+02		zero(4) = 0.204527761237753E+02
$A(0,3)$ = 0.113746188754331E−02		$A(0,4)$ = 0.152753792492066E−06
$A(1,3)$ = −0.204892563320579E−02		$A(1,4)$ = −0.410956732811768E−06
$A(2,3)$ = 0.191860247042219E−02		$A(2,4)$ = 0.484507006038965E−06
$A(3,3)$ = −0.903002129075339E−03		$A(3,4)$ = −0.288211914479617E−06
$A(4,3)$ = 0.265091858385108E−03		$A(4,4)$ = 0.791425834311650E−07
zero(5) = 0.374416573313175E+02		
$A(0,5)$ = 0.546801190168267E−13		
$A(1,5)$ = −0.192133308928889E−12		
$A(2,5)$ = 0.271424024484902E−12		
$A(3,5)$ = −0.181974618995712E−12		
$A(4,5)$ = 0.492724906167396E−13		

Table 3
Relative errors in quadrature sums $I_{n,s}^{\mathrm{T}}$

n	$s=0$	$s=1$	$s=2$	$s=3$	$s=4$	$s=5$
1	1.15(−1)	4.71(−3)	9.72(−5)	1.21(−6)	1.01(−8)	5.98(−11)
2	2.38(−3)	2.05(−7)	3.06(−12)	1.36(−17)	2.40(−23)	1.88(−29)
3	1.97(−5)	1.15(−12)	4.02(−21)	9.26(−31)	m.p.	m.p.
4	8.76(−8)	1.71(−18)	4.68(−31)	m.p.	m.p.	m.p.
5	2.43(−10)	9.40(−25)	m.p.	m.p.	m.p.	m.p.

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Gauss Quadrature for Refinable Weight Functions

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A two-parameter class of refinable functions is considered and Gaussian quadrature rules having these functions as weight functions. A discretization method is described for generating the recursion coefficients of the required orthogonal polynomials. Numerical results are also presented.

1. A CLASS OF REFINABLE FUNCTIONS

A refinable function ϕ is a solution of a two-scale difference equation

$$\phi(x) = \sum_{j\in\mathbb{Z}} a_j \phi(2x - j), \tag{1.1}$$

where a_j are real numbers satisfying

$$\sum_{j\in\mathbb{Z}} a_{k+2j} = 1, \qquad \text{all } k \in \mathbb{Z}. \tag{1.2}$$

Equation (1.1) is called a *refinement equation*, and $\mathbf{a} = \{a_j\}_{j\in\mathbb{Z}}$ the *mask*. Refinable functions occur in many different branches of analysis, notably in multiresolution approximation and wavelet analysis.

The existence of a solution of (1.1) is ensured under suitable assumptions on the mask $\mathbf{a}$ (see, for example, [2, 8] and references therein). In particular, the existence of a unique refinable function ϕ associated with a given mask $\mathbf{a}$ was proved in [4] in the case when $\mathbf{a}$ satisfies, in addition to (1.2), the following conditions, depending on an integer parameter $m \geq 2$:

(i) $\mathbf{a}$ is compactly supported on $j = 0, 1, \ldots, m+1$ (i.e., $a_j = 0$ for $j \notin [0, m+1]$, with $a_0 a_{m+1} \neq 0$);

(ii) $p_m(z) = \sum_{j=0}^{m+1} a_j z^j$ is a Hurwitz polynomial (i.e., has all its zeros in the left half-plane).

In [4] it was also proved that $\sum_{j\in\mathbb{Z}} \phi(x+j) = 1$ and $\phi \in C^k(\mathbb{R})$, $k \le m-1$, if and only if $p_m(z) = (z+1)^{k+1} q(z)$, where $q \in \mathbb{P}_{m-k}$ and $q(1) = 2^{-k}$.

This result for $k = m-2$ can be exploited to characterize all masks which satisfy (i) and (ii) and moreover are centrally symmetric (an important property in signal processing applications) [5]. To be precise, the function ϕ associated with this kind of mask is in $C^{m-2}(\mathbb{R})$ if and only if

$$a_{j,m}^{(h)} = 2^{-h}\left[\binom{m+1}{j} + 4(2^{h-m}-1)\binom{m-1}{j-1}\right], \qquad j \in \mathbb{Z}, \tag{1.3}$$

where $h > m-1$ is another parameter, and where by convention $\binom{r}{s} = 0$ if $s < 0$ or $s > r$. The associated refinement equation

$$\phi_{m,h}(x) = \sum_{j\in\mathbb{Z}} a_{j,m}^{(h)} \phi_{m,h}(2x-j) \tag{1.4}$$

allows one to compute $\phi_{m,h}$ recursively on any set of dyadic points,

$$X_r = \{x : x = k\cdot 2^{-r},\ k = 0, 1, 2, \ldots, (m+1)2^r\}, \qquad r = 0, 1, 2, \ldots, \tag{1.5}$$

starting with the values $\phi_{m,h}(j)$, $j = 0, 1, \ldots, m+1$.

We recall that for any compactly supported refinable function ϕ the values at the integers are the entries of the eigenvector of the matrix $A = [a_{2i-j}]_{i\in\mathbb{Z}, j\in\mathbb{Z}}$ corresponding to the eigenvalue 1 and normalized by the condition $\sum_{j\in\mathbb{Z}} \phi(j) = 1$.

The values of ϕ at dyadic points can also be computed by means of the cascade algorithm [2].

It is known that $\phi_{m,h}$ is compactly supported on the interval $[0, m+1]$, $\phi_{m,h}(x) > 0$ for $0 < x < m+1$, $\phi_{m,h}(0) = \phi_{m,h}(m+1) = 0$, and $\phi_{m,h}(x)$ is symmetric with respect to the midpoint $x = (m+1)/2$. If $h = m$, then (1.3) is the mask for the mth-degree cardinal B-spline.

Certain projection operators, for example in wavelet decompositions, as well as several applications such as the wavelet Galerkin method, lead to the problem of computing inner products of the form $(f, \phi) = \int_{\mathbb{R}} f(x)\phi(x)\,dx$, where ϕ is a refinable function. Such integrals have been dealt with, for example, in [1, 7, 10]. In certain applications, ϕ is of type $\phi_{m,h}$ defined in (1.4) (cf., e.g., [6]); in these cases, since $\phi_{m,h}$ is positive on its support, it is natural to think of it as a weight function and to compute the inner product by a weighted quadrature rule, specifically a Gaussian rule. To do this requires knowledge of the orthogonal polynomials that belong to the weight function $\phi_{m,h}$. In this note we show how these can be constructed and we present relevant numerical data.

2. CONSTRUCTION OF ORTHOGONAL POLYNOMIALS AND GAUSSIAN QUADRATURE RULES RELATIVE TO REFINABLE FUNCTIONS

To construct the desired orthogonal polynomials up to degree n, and with them the Gaussian rules with up to n points, it suffices to compute the recursion coefficients $\alpha_k =$

$\alpha_k(\phi_{m,h})$, $\beta_k = \beta_k(\phi_{m,h})$ in the three-term recurrence relation for the (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; \phi_{m,h})$ relative to the weight function $\phi_{m,h}$,

$$\begin{aligned} \pi_{k+1}(x) &= (x - \alpha_k)\pi_k(x) - \beta_k \pi_{k-1}(x), \qquad k = 0, 1, 2, \ldots, n-1, \\ \pi_{-1}(x) &= 0, \qquad \pi_0(x) = 1. \end{aligned} \tag{2.1}$$

The Gauss quadrature rules in question can then be computed by well-known eigenvalue/eigenvector techniques (cf. [3, Sect. 4]).

By symmetry, all α_k are constant equal to $(m+1)/2$, and we may as well shift the variable x so that $\alpha_k = 0$ for all k and the $\phi_{m,h}$ are supported on $[-(m+1)/2, (m+1)/2]$. Such a shift does not affect the coefficients β_k. The latter can be computed by a discretization method (cf. [3, Sect. 6]). Since $\phi_{m,h}$ is computable only at dyadic points, we choose the points x_k of the discrete inner product to be dyadic points

$$x_k = -(m+1)/2 + k \cdot 2^{-r}, \qquad k = 0, 1, 2, \ldots, (m+1)2^r, \tag{2.2}$$

in the shifted set X_r and the inner product itself to be the respective Simpson's quadrature sum,

$$(u, v)_r = \frac{1}{3 \cdot 2^r} \sum_{k=0}^{(m+1)2^r} w_k u(x_k) v(x_k) \phi_{m,h}(x_k), \qquad r = 1, 2, 3, \ldots, \tag{2.3}$$

where

$$w_k = \begin{cases} 1 & \text{if } k = 0 \text{ or } k = (m+1)2^r, \\ 2 & \text{if } k \text{ is even, } k \neq 0,\ k \neq (m+1)2^r, \\ 4 & \text{if } k \text{ is odd.} \end{cases} \tag{2.4}$$

The recursion coefficients $\beta_{k,r}$ for the discrete inner product, which approximate the desired coefficients β_k, are then computed by the Stieltjes procedure. (Alternatively, the Lanczos algorithm could be applied, which, however, was observed to take considerably longer.)

For given m and h the procedure is expected to converge as $r \to \infty$. Some relevant results (for double precision computations) are shown in Table 1.

The convergence test adopted was agreement of the coefficients $\beta_{k,r}, k = 0, 1, 2, \ldots, n-1$, for two successive values of r to within a relative error $\leq \varepsilon$. We chose $n = 17$ and $\varepsilon = \frac{1}{2} \cdot 10^{-10}$. Table 1 shows $r_{\min}$—the smallest value of r for which convergence is achieved when $h = m(1)m + 4$, $m = 2, 3, 4$, and the corresponding values of $N = (m+1)2^r$.

TABLE 1
Convergence Behavior of the Discretization Method

m	h	$r_{\min}$	N
2	2–6	14	49,152
3	3–7	13	32,768
4	4	11	10,240
	5–8	13	40,960

3. NUMERICAL RESULTS

The recursion coefficients $\beta_k(\phi_{m,h}), k = 0, 1, \ldots, 16$, obtained by the discretization method of Section 2 for the same values of m and h as in Table 1 are displayed in Table 2. Several observations can be made.

(i) When $m = 2$ and $h \to \infty$, the function $\phi_{m,h}$ tends to the unit step function supported on $[-\frac{1}{2}, \frac{1}{2}]$ (cf. (1.3) and the remarks in the penultimate paragraph of Section 1). One would expect, therefore, that the coefficients $\beta_k(\phi_{m,h})$ tend to the Legendre coefficients (relative to $[-\frac{1}{2}, \frac{1}{2}]$), that is,

$$\beta_k(\phi_{2,h}) \to \beta_k^L = \frac{1}{4}\frac{1}{4 - k^{-2}} \qquad \text{as } h \to \infty,$$

for each fixed $k \geq 1$. One would furthermore expect a similar limit behavior for the coefficients $\beta_{k,r}, r = r_{\min}$. A look at the last column of Table 2 (for $m = 2, h = m + 4$) does not seem to suggest this. The reason appears to be slow convergence, in fact, the slower convergence the larger k. We attempted to check this by running our procedure for $h = 20$; the resulting β-coefficients are shown in Table 3, together with the Legendre coefficients β_k^L in the last column. Both sets of coefficients are in reasonable agreement for about $k \leq 5$, but beyond this, the former coefficients become rather larger than the latter and also less regular. For much larger values of h (e.g., $h \geq 30$), we experienced near-singularity difficulties with our program for computing $\phi_{2,h}$.

(ii) In the case $m = h = 3$, the function $\phi_{m,h}$ coincides with the normalized cubic B-spline. The orthogonal polynomials relative to this B-spline and their recursion coefficients have been computed earlier by Phillips and Hanson [9]. Since these authors define B-splines on the interval $[-1, 1]$ and adopt normalized orthogonal polynomials on $[-1, 1]$, our coefficients must be compared with four times the squares of theirs. We found agreement to 10 decimal places in all of them [1].

(iii) When $m = 3$ and $h \to \infty$, the function $\phi_{m,h}$ tends to the hat function supported on $[-1, 1]$. Similarly as in (i), one observes relatively slow convergence of the coefficients $\beta_k(\phi_{m,h})$ to those of the hat function, $\hat{\beta}_k$. The latter are the squares of those tabulated in [9]. We were able, however, to use much larger values of h than in (i). The results for $h = 50$ are shown in Table 4 in a format analogous to that of Table 3. Increasing h further, we observed complete agreement to all 10 digits for all values of $k \leq 16$ beginning with $h = 70$.

(iv) A limit behavior similar to that in (iii) is observed when $m = 4$. In this case, the limit function as $h \to \infty$ is the normalized quadratic B-spline on $[-\frac{5}{2}, \frac{5}{2}]$ whose recursion coefficients are those in Table 2 (first column for $m = 2$). We found that exactly the same coefficients are obtained when $m = 4$ and $h = 65$.

4. EXAMPLES

The motivation for this work was to accurately evaluate integrals of the form $\int_{\mathbb{R}} f(x)\phi_{m,h}(x)\,dx$ by using Gaussian quadrature relative to the weight function $\phi_{m,h}$. We now present a few simple examples to illustrate this approach.

[1] It appears that the first coefficient b_0 in [9] is not p_0, as stated, but $1/p_0$.

TABLE 2

Beta Recursion Coefficients for $\phi_{m,h}$

k	$h=m$	$h=m+1$	$h=m+2$	$h=m+3$	$h=m+4$
			$m=2$		
0	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01
1	0.2500000000D+00	0.1666666667D+00	0.1250000000D+00	0.1041666667D+00	0.9375000000D−01
2	0.4000000000D+00	0.3083333333D+00	0.2250000000D+00	0.1608333333D+00	0.1187500000D+00
3	0.4690476190D+00	0.4265444015D+00	0.4013227513D+00	0.3613878608D+00	0.2972117794D+00
4	0.4926275079D+00	0.4131994186D+00	0.3612155402D+00	0.3602486522D+00	0.3894617800D+00
5	0.5164139087D+00	0.4889493219D+00	0.4057335794D+00	0.3089577065D+00	0.2577157643D+00
6	0.5260121260D+00	0.5124914898D+00	0.5341805666D+00	0.4983770790D+00	0.3835954907D+00
7	0.5337717704D+00	0.4775539694D+00	0.4525021293D+00	0.4964644418D+00	0.5446083654D+00
8	0.5405609927D+00	0.5219503079D+00	0.4573626341D+00	0.4090350284D+00	0.4160830123D+00
9	0.5432534143D+00	0.5378180443D+00	0.5139778763D+00	0.4648210629D+00	0.4317223413D+00
10	0.5472602761D+00	0.5378065265D+00	0.5302566016D+00	0.4715775550D+00	0.4216089322D+00
11	0.5492984861D+00	0.5274820118D+00	0.5585555467D+00	0.5675688928D+00	0.4591239192D+00
12	0.5509751767D+00	0.5149833923D+00	0.4820549575D+00	0.5516038182D+00	0.6192691428D+00
13	0.5529221428D+00	0.5594942772D+00	0.4956065998D+00	0.4428882444D+00	0.4978577650D+00
14	0.5536829341D+00	0.5546548375D+00	0.5617263587D+00	0.5119093536D+00	0.4603638949D+00
15	0.5549712966D+00	0.5412104303D+00	0.5309121931D+00	0.5190147724D+00	0.5115945171D+00
16	0.5557579663D+00	0.5554713583D+00	0.5575472787D+00	0.5154572813D+00	0.4668040403D+00
			$m=3$		
0	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01
1	0.3333333333D+00	0.2500000000D+00	0.2083333333D+00	0.1875000000D+00	0.1770833333D+00
2	0.5666666667D+00	0.4500000000D+00	0.3616666667D+00	0.3041666667D+00	0.2707107843D+00
3	0.7134453782D+00	0.6174603175D+00	0.5211784068D+00	0.4263046314D+00	0.3493264282D+00
4	0.7952707585D+00	0.7228390928D+00	0.6785401479D+00	0.6273778867D+00	0.5465934706D+00
5	0.8422226889D+00	0.7529745098D+00	0.6849577594D+00	0.6689368416D+00	0.6753586166D+00
6	0.8795817873D+00	0.8233008777D+00	0.7282730271D+00	0.6398576407D+00	0.6146982354D+00
7	0.9030410539D+00	0.8682915861D+00	0.8335415543D+00	0.7341908286D+00	0.6119073410D+00
8	0.9201183837D+00	0.8706958448D+00	0.8627011061D+00	0.8667957262D+00	0.7905098231D+00

TABLE 2—continued

k	$h=m$	$h=m+1$	$h=m+2$	$h=m+3$	$h=m+4$
9	0.9338358596D+00	0.8825547085D+00	0.8268930663D+00	0.8281263474D+00	0.8635648646D+00
10	0.9440898205D+00	0.9160350520D+00	0.8585407696D+00	0.8034660173D+00	0.7956929962D+00
11	0.9516519976D+00	0.9295438090D+00	0.8932013455D+00	0.8406906204D+00	0.8037908139D+00
12	0.9584565583D+00	0.9387358070D+00	0.9158471985D+00	0.8568094598D+00	0.8201732848D+00
13	0.9635375729D+00	0.9393682362D+00	0.9419111913D+00	0.9002870773D+00	0.8017840344D+00
14	0.9677464898D+00	0.9362132685D+00	0.9290173804D+00	0.9638541655D+00	0.9001209303D+00
15	0.9714182941D+00	0.9482919500D+00	0.9004785963D+00	0.9163884531D+00	0.9776423718D+00
16	0.9744405490D+00	0.9657892693D+00	0.9279858085D+00	0.8780208386D+00	0.9035867321D+00
			$m=4$		
0	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01
1	0.4166666667D+00	0.3333333333D+00	0.2916666667D+00	0.2708333333D+00	0.2604166667D+00
2	0.7333333333D+00	0.6041666667D+00	0.5154761905D+00	0.4618589744D+00	0.4320833333D+00
3	0.9603896104D+00	0.8285098522D+00	0.7095183108D+00	0.6145120147D+00	0.5503536989D+00
4	0.1113072188D+01	0.1003625315D+01	0.9011493335D+00	0.7898209370D+00	0.6844089076D+00
5	0.1212085693D+01	0.1113462600D+01	0.1046179645D+01	0.9839671488D+00	0.8925196922D+00
6	0.1280411106D+01	0.1178328005D+01	0.1091403254D+01	0.1053531136D+01	0.1037144514D+01
7	0.1333237569D+01	0.1254682840D+01	0.1150209200D+01	0.1059777451D+01	0.1034642882D+01
8	0.1371616323D+01	0.1312772180D+01	0.1244738258D+01	0.1129600896D+01	0.1022025588D+01
9	0.1400841814D+01	0.1341636122D+01	0.1308552918D+01	0.1253733344D+01	0.1129347034D+01
10	0.1424178377D+01	0.1362044143D+01	0.1315943841D+01	0.1308201088D+01	0.1272543020D+01
11	0.1442931032D+01	0.1389848000D+01	0.1324724898D+01	0.1290560223D+01	0.1296683563D+01
12	0.1457890762D+01	0.1417263596D+01	0.1358748789D+01	0.1301764461D+01	0.1275756157D+01
13	0.1470210353D+01	0.1435468376D+01	0.1387448684D+01	0.1328942794D+01	0.1294610510D+01
14	0.1480668945D+01	0.1449775269D+01	0.1415644740D+01	0.1348178509D+01	0.1303885554D+01
15	0.1489296163D+01	0.1457278763D+01	0.1441381736D+01	0.1388547588D+01	0.1297593523D+01
16	0.1496643616D+01	0.1462051780D+01	0.1445623971D+01	0.1441575476D+01	0.1353987666D+01

TABLE 3
Refinable vs Legendre Coefficients for $m = 2$, $h = 20$

k	$\beta_k(\phi_{2,20})$	β_k^L
0	0.1000000000D+01	0.1000000000D+01
1	0.8333396912D−01	0.8333333333D−01
2	0.6667022702D−01	0.6666666667D−01
3	0.6431584844D−01	0.6428571429D−01
4	0.6379615398D−01	0.6349206349D−01
5	0.6646081488D−01	0.6313131313D−01
6	0.9933788559D−01	0.6293706294D−01
7	0.3235789996D+00	0.6282051282D−01
8	0.4391642119D+00	0.6274509804D−01
9	0.1576157120D+00	0.6269349845D−01
10	0.1377001517D+00	0.6265664160D−01
11	0.3426699843D+00	0.6262939959D−01
12	0.3317378588D+00	0.6260869565D−01
13	0.1621446084D+00	0.6259259259D−01
14	0.2658907431D+00	0.6257982120D−01
15	0.4823743434D+00	0.6256952169D−01
16	0.3868745639D+00	0.6256109482D−01

EXAMPLE 1 (Partial sums of the exponential series). We take for f the partial sums s_p of the exponential series,

$$f(x) = s_p(x), \qquad s_p(x) = \sum_{j=0}^{p} x^j/j!, \qquad p = 3, 7, \text{ and } 11. \tag{4.1}$$

TABLE 4
Refinable vs Hat Coefficients for $m = 3$, $h = 50$

k	$\beta_k(\phi_{3,50})$	$\hat{\beta}_k$
0	0.1000000000D+01	0.1000000000D+01
1	0.1666666667D+00	0.1666666667D+00
2	0.2333333333D+00	0.2333333333D+00
3	0.2326530612D+00	0.2326530612D+00
4	0.2445399212D+00	0.2445399212D+00
5	0.2425328261D+00	0.2425328261D+00
6	0.2473404865D+00	0.2473404865D+00
7	0.2458445570D+00	0.2458445570D+00
8	0.2484370525D+00	0.2484370524D+00
9	0.2473524863D+00	0.2473524861D+00
10	0.2489746618D+00	0.2489746603D+00
11	0.2481652712D+00	0.2481652626D+00
12	0.2492769225D+00	0.2492768721D+00
13	0.2486536221D+00	0.2486533247D+00
14	0.2494649898D+00	0.2494632094D+00
15	0.2489800860D+00	0.2489693622D+00
16	0.2496512846D+00	0.2495860330D+00

TABLE 5
Results of n-point Gaussian Quadrature Applied to $\int_{-3/2}^{3/2} s_p(x)\phi_{2,4}(x)\,dx$

n	$p=3$	$p=7$	$p=11$
1	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01
2	0.1062500000D+01	0.1063153754D+01	0.1063153760D+01
3	0.1062500000D+01	0.1064344184D+01	0.1064344317D+01
4	...	0.1064359861D+01	0.1064360305D+01
5		0.1064359861D+01	0.1064360408D+01
6		...	0.1064360409D+01
7			0.1064360409D+01
8			...

Since these are polynomials of degree p, the n-point Gaussian quadrature rule should produce exact results for $n \geq (p+1)/2$. This is indeed the case and is illustrated in Table 5 for $m=2, h=4$. The ellipses at the bottom of each column are to indicate that the results remain exactly constant to the number of digits shown.

EXAMPLE 2 (Exponential function). Here, $f(x)=e^x$, and we take $m=3$, hence the interval $[-2,2]$, and $h=4(1)6$. The results are displayed in Table 6. As can be seen, convergence as $n\to\infty$ is quite fast. We do not know whether the exact answers are known explicitly.

EXAMPLE 3 (Cosine waves). In this final example, we take $m=4, h=8$, and for f three cosine waves

$$f(x)=c_k(x), \qquad c_k(x)=\cos(\tfrac{2k\pi}{5}(x+\tfrac{5}{2})), \qquad k=1,2,3$$

on the interval $[-\frac{5}{2},\frac{5}{2}]$. The results are shown in Table 7. Understandably, convergence of the quadrature formula slows down as the frequency of the cosine wave increases.

TABLE 6
Results of n-point Gaussian Quadrature Applied to $\int_{-2}^{2} e^x\phi_{3,h}(x)\,dx$

n	$h=4$	$h=5$	$h=6$
1	0.1000000000D+01	0.1000000000D+01	0.1000000000D+01
2	0.1127625965D+01	0.1105987721D+01	0.1095224030D+01
3	0.1132463949D+01	0.1109209557D+01	0.1097654654D+01
4	0.1132563961D+01	0.1109265738D+01	0.1097689281D+01
5	0.1132565253D+01	0.1109266420D+01	0.1097689670D+01
6	0.1132565264D+01	0.1109266425D+01	0.1097689673D+01
7	0.1132565264D+01	0.1109266425D+01	0.1097689673D+01
8	...	...	...

TABLE 7
Results of n-point Gaussian Quadrature Applied to $\int_{-5/2}^{5/2} \cos(\frac{2k\pi}{5}(x+\frac{5}{2}))\phi_{4,8}(x)\,dx$

n	$k=1$	$k=2$	$k=3$
1	−0.1000000000D+01	0.1000000000D+01	−0.1000000000D+01
2	−0.8013337327D+00	0.2842715025D+00	0.3457410443D+00
3	−0.8124511173D+00	0.4368769735D+00	−0.2478977458D+00
4	−0.8121304568D+00	0.4194894337D+00	−0.9850296578D−01
5	−0.8121366391D+00	0.4208268334D+00	−0.1242828114D+00
6	−0.8121365424D+00	0.4207434221D+00	−0.1206814510D+00
7	−0.8121365436D+00	0.4207475440D+00	−0.1210800305D+00
8	−0.8121365436D+00	0.4207473957D+00	−0.1210476809D+00
9	...	0.4207473998D+00	−0.1210496725D+00
10		0.4207473997D+00	−0.1210495661D+00
11		0.4207473997D+00	−0.1210495713D+00
12		...	−0.1210495710D+00
13			−0.1210495711D+00
14			−0.1210495711D+00
15			...

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High-order Gauss–Lobatto formulae

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Dedicated, in friendship and with high regard, to Richard S. Varga on the occasion of his 70th birthday

Currently, the method of choice for computing the $(n+2)$-point Gauss–Lobatto quadrature rule for any measure of integration is to first generate the Jacobi matrix of order $n+2$ for the measure at hand, then modify the three elements at the right lower corner of the matrix in a manner proposed in 1973 by Golub, and finally compute the eigenvalues and first components of the respective eigenvectors to produce the nodes and weights of the quadrature rule. In general, this works quite well, but when n becomes large, underflow problems cause the method to fail, at least in the software implementation provided by us in 1994. The reason is the singularity (caused by underflow) of the 2×2 system of linear equations that is used to compute the modified matrix elements. It is shown here that in the case of arbitrary Jacobi measures, these elements can be computed directly, without solving a linear system, thus allowing the method to function for essentially unrestricted values of n. In addition, it is shown that all weights of the quadrature rule can also be computed explicitly, which not only obviates the need to compute eigenvectors, but also provides better accuracy. Numerical comparisons are made to illustrate the effectiveness of this new implementation of the method.

1. Introduction

Given a positive measure $d\lambda$ supported on the interval $[-1, 1]$ of the real line $\mathbb{R}$, and assuming all its moments to exist, one can consider a quadrature rule of the form

$$\int_{-1}^{1} f(t)\,d\lambda(t) = \lambda_0 f(-1) + \sum_{k=1}^{n} \lambda_k f(t_k) + \lambda_{n+1} f(1) + R_n(f) \tag{1.1}$$

that is exact whenever f is a polynomial of degree $\leqslant 2n+1$,

$$R_n(f) = 0 \quad \text{if } f \in \mathbb{P}_{2n+1}. \tag{1.2}$$

It is called the ($(n+2)$-point) *Gauss–Lobatto rule* relative to the measure $d\lambda$. As is well known, the interior nodes t_k are the zeros of $\pi_n(\,\cdot\,; d\lambda_{\pm 1})$, the polynomial of degree n orthogonal with respect to the modified measure $d\lambda_{\pm 1}(t) = (1 - t^2)\,d\lambda(t)$, and the weights λ_j can be obtained by interpolation at the nodes $-1, t_1, \ldots, t_n, 1$.

A more elegant constructive procedure has been proposed by Golub [4]. It is based on a modified Jacobi matrix, the tridiagonal matrix of order $n+2$

$$J^*_{n+2}(\mathrm{d}\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \ddots & \ddots & & \\ & & \ddots & \alpha_{n-1} & \sqrt{\beta_n} & \\ & & & \sqrt{\beta_n} & \alpha_n & \sqrt{\beta^*_{n+1}} \\ 0 & & & & \sqrt{\beta^*_{n+1}} & \alpha^*_{n+1} \end{bmatrix}, \tag{1.3}$$

where α_k, β_k are the coefficients in the recurrence relation

$$\begin{aligned} &\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ &\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1 \end{aligned} \tag{1.4}$$

for the (monic) orthogonal polynomials $\pi_k(\cdot\,; \mathrm{d}\lambda)$, and α^*_{n+1}, β^*_{n+1} the solution of the 2×2 system of linear equations

$$\begin{bmatrix} \pi_{n+1}(-1) & \pi_n(-1) \\ \pi_{n+1}(1) & \pi_n(1) \end{bmatrix} \begin{bmatrix} \alpha^*_{n+1} \\ \beta^*_{n+1} \end{bmatrix} = \begin{bmatrix} -\pi_{n+1}(-1) \\ \pi_{n+1}(1) \end{bmatrix}. \tag{1.5}$$

The nodes of (1.1) (including ± 1) are then the eigenvalues of $J^*_{n+2}(\mathrm{d}\lambda)$, and the weights λ_j are obtainable in terms of the first components $v_{j,1}$ of the associated normalized eigenvectors v_j by means of

$$\lambda_j = \beta_0 v^2_{j,1}, \quad j = 0, 1, 2, \ldots, n, n+1, \tag{1.6}$$

where $\beta_0 = \int_{-1}^{1} \mathrm{d}\lambda(t)$ (cf. also [3]).

This works quite well as long as n is not too large. When n becomes large, the elements of the matrix in (1.5) become very small, and their products even smaller, so much so that when computing the determinant,

$$\Delta_n = \pi_{n+1}(-1)\pi_n(1) - \pi_{n+1}(1)\pi_n(-1), \tag{1.7}$$

both its terms underflow, creating a singular system. For the Legendre measure $\mathrm{d}\lambda(t) = \mathrm{d}t$, and single-precision IEEE arithmetic, this happens beginning with $n = 79$, and in double precision, beginning with $n = 543$.

One way of correcting the problem is to rescale the orthogonal polynomials. A better way is to compute the α^*_{n+1}, β^*_{n+1}, whenever possible, directly without solving a linear system. We show that this is indeed possible if $\mathrm{d}\lambda$ is the Jacobi measure

$$\mathrm{d}\lambda^{(\alpha,\beta)}(t) = (1-t)^\alpha (1+t)^\beta \, \mathrm{d}t, \quad \alpha > -1, \ \beta > -1. \tag{1.8}$$

In the case of the Legendre measure $d\lambda(t) = d\lambda^{(0,0)}$, it is known, furthermore, that the weights λ_j in (1.1) are expressible explicitly in terms of the Legendre polynomial P_{n+1} as follows (cf., e.g., [1, p. 104]):

$$\begin{aligned} \lambda_0 &= \lambda_{n+1} = \frac{2}{(n+1)(n+2)}, \\ \lambda_k &= \frac{2}{(n+1)(n+2)[P_{n+1}(t_k)]^2}, \quad k = 1, 2, \ldots, n \quad (d\lambda(t) = dt). \end{aligned} \tag{1.9}$$

We observed with our software [2] that the weights computed directly by (1.9) are, in general, rather more accurate than those produced via (1.6). We will show that analogous expressions for the weights, with similar advantages in accuracy, can be had for the Jacobi measure $d\lambda^{(\alpha,\beta)}$.

2. The modified Jacobi matrix

We denote the monic polynomials orthogonal with respect to the Jacobi measure (1.8) by $\pi_k = \pi_k^{(\alpha,\beta)}$, and the Jacobi polynomials, as conventionally defined (cf., e.g., [5]) by $P_k = P_k^{(\alpha,\beta)}$. It is well known that

$$P_n(t) = k_n \pi_n(t), \quad k_n = \frac{1}{2^n}\binom{2n+\alpha+\beta}{n}, \tag{2.1}$$

and that

$$P_n(1) = \binom{n+\alpha}{n}, \qquad P_n(-1) = (-1)^n \binom{n+\beta}{n}. \tag{2.2}$$

The determinant in (1.7) then becomes

$$\Delta_n = \frac{1}{k_n k_{n+1}} D_n, \tag{2.3}$$

where

$$D_n = \begin{vmatrix} P_{n+1}(-1) & P_n(-1) \\ P_{n+1}(1) & P_n(1) \end{vmatrix}. \tag{2.4}$$

Using (2.2), one finds

$$D_n = \frac{(-1)^{n+1}}{n+1}(2n+\alpha+\beta+2)\binom{n+\alpha}{n}\binom{n+\beta}{n}, \tag{2.5}$$

and from (1.5) and (2.1) one gets

$$\begin{aligned} \alpha_{n+1}^* &= \frac{-P_{n+1}(-1)P_n(1) - P_{n+1}(1)P_n(-1)}{D_n}, \\ \beta_{n+1}^* &= 2\frac{k_n}{k_{n+1}}\frac{P_{n+1}(-1)P_{n+1}(1)}{D_n}. \end{aligned}$$

Substituting (2.2) and (2.5) in these formulae yields

$$\begin{aligned}\alpha_{n+1}^{*} &= \frac{\alpha-\beta}{2n+\alpha+\beta+2},\\ \beta_{n+1}^{*} &= 4\,\frac{(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2}.\end{aligned} \tag{2.6}$$

Since the recursion coefficients α_k, β_k for the Jacobi measure $\mathrm{d}\lambda^{(\alpha,\beta)}$ are explicitly known, the Gauss–Lobatto formula for $\mathrm{d}\lambda^{(\alpha,\beta)}$ is now readily computable via eigenvalues and (first components of) eigenvectors of the matrix (1.3). Accuracy, however, is improved if the weights are computed separately, bypassing (1.6). The next two sections develop the necessary formulae.

3. The boundary weights

Our concern from now on is with the Gauss–Jacobi–Lobatto formula

$$\int_{-1}^{1} f(t)\,\mathrm{d}\lambda^{(\alpha,\beta)}(t) = \lambda_0 f(-1) + \sum_{k=1}^{n} \lambda_k f(t_k) + \lambda_{n+1} f(1) + R_n(f). \tag{3.1}$$

We first deal with the boundary weights $\lambda_0 = \lambda_0^{(\alpha,\beta)}$ and $\lambda_{n+1} = \lambda_{n+1}^{(\alpha,\beta)}$. Since the change of variable $t \mapsto -t$ converts $\mathrm{d}\lambda^{(\alpha,\beta)}$ into $\mathrm{d}\lambda^{(\beta,\alpha)}$, one easily sees that $\lambda_{n+1}^{(\alpha,\beta)} = \lambda_0^{(\beta,\alpha)}$. It suffices therefore to compute $\lambda_0^{(\alpha,\beta)}$.

We recall that the interior nodes $t_k = t_k^{(\alpha,\beta)}$ in (3.1) are the zeros of $\pi_n(\,\cdot\,;\mathrm{d}\lambda_{\pm1}^{(\alpha,\beta)})$, where $\mathrm{d}\lambda_{\pm1}^{(\alpha,\beta)}(t) = (1-t^2)\,\mathrm{d}\lambda^{(\alpha,\beta)}(t) = \mathrm{d}\lambda^{(\alpha+1,\beta+1)}(t)$, thus the zeros of $P_n^{(\alpha+1,\beta+1)}$,

$$P_n^{(\alpha+1,\beta+1)}(t_k) = 0, \quad k = 1, 2, \ldots, n. \tag{3.2}$$

Since [5, equation (4.21.7)]

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{P_{n+1}^{(\alpha,\beta)}(t)\right\} = \frac{1}{2}(n+\alpha+\beta+2)\,P_n^{(\alpha+1,\beta+1)}(t), \tag{3.3}$$

they are also the zeros of $P_{n+1}^{(\alpha,\beta)\prime}$,

$$P_{n+1}^{(\alpha,\beta)\prime}(t_k) = 0, \quad k = 1, 2, \ldots, n. \tag{3.4}$$

Now putting $f(t) = (1-t)P_n^{(\alpha+1,\beta+1)}(t)$ in (3.1), and observing (3.2), yields

$$2\lambda_0 P_n^{(\alpha+1,\beta+1)}(-1) = \int_{-1}^{1} P_n^{(\alpha+1,\beta+1)}(t)\,\mathrm{d}\lambda^{(\alpha+1,\beta)}(t). \tag{3.5}$$

The integrand on the right, by the second relation in [5, equation (4.5.4)] (with α replaced by $\alpha+1$), can be written as

$$P_n^{(\alpha+1,\beta+1)}(t) = \frac{2}{2n+\alpha+\beta+3}\,\frac{(n+1)P_{n+1}^{(\alpha+1,\beta)}(t) + (n+\beta+1)P_n^{(\alpha+1,\beta)}(t)}{t+1}. \quad (3.6)$$

Noting from the second relation in (2.2) that

$$n+1 = (-1)^n \frac{n+1}{\binom{n+\beta}{n}} P_n^{(\alpha+1,\beta)}(-1),$$

$$n+\beta+1 = -(-1)^n \frac{n+1}{\binom{n+\beta}{n}} P_{n+1}^{(\alpha+1,\beta)}(-1),$$

we can rewrite (3.6) as

$$P_n^{(\alpha+1,\beta+1)}(t) = \frac{2}{2n+\alpha+\beta+3}\,\frac{(-1)^n(n+1)}{\binom{n+\beta}{n}} \times \frac{P_{n+1}^{(\alpha+1,\beta)}(t)P_n^{(\alpha+1,\beta)}(-1) - P_n^{(\alpha+1,\beta)}(t)P_{n+1}^{(\alpha+1,\beta)}(-1)}{t+1}.$$

This calls for the application of the Christoffel–Darboux formula ([5, equation (4.5.2)] with α replaced by $\alpha+1$), which gives

$$P_n^{(\alpha+1,\beta+1)}(t) = \frac{2}{2n+\alpha+\beta+3}\,\frac{(-1)^n(n+1)}{\binom{n+\beta}{n}}\,c_n(\alpha,\beta) \times \sum_{\nu=0}^{n} \frac{1}{h_\nu^{(\alpha+1,\beta)}} P_\nu^{(\alpha+1,\beta)}(t)P_\nu^{(\alpha+1,\beta)}(-1), \quad (3.7)$$

where $h_\nu^{(\alpha+1,\beta)} = \int_{-1}^{1}[P_\nu^{(\alpha+1,\beta)}(t)]^2\,\mathrm{d}\lambda^{(\alpha+1,\beta)}(t)$ and

$$c_n(\alpha,\beta) = 2^{\alpha+\beta+1}(2n+\alpha+\beta+3)\,\frac{\Gamma(n+\alpha+2)\Gamma(n+\beta+1)}{\Gamma(n+2)\Gamma(n+\alpha+\beta+3)}. \quad (3.8)$$

Integration of (3.7) with the measure $\mathrm{d}\lambda^{(\alpha+1,\beta)}$ produces, by the orthogonality of the Jacobi polynomials,

$$\int_{-1}^{1} P_n^{(\alpha+1,\beta+1)}(t)\,\mathrm{d}\lambda^{(\alpha+1,\beta)}(t) = \frac{2}{2n+\alpha+\beta+3}\,\frac{(-1)^n(n+1)}{\binom{n+\beta}{n}}\,c_n(\alpha,\beta). \quad (3.9)$$

Therefore, the desired result now follows from (3.5) together with the second relation in (2.2) (with β replaced by $\beta+1$) and (3.9), (3.8), to read

$$\lambda_0^{(\alpha,\beta)} = 2^{\alpha+\beta+1}\,\frac{\Gamma(\alpha+2)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+3)}\,\frac{\binom{n+\alpha+1}{n}}{\binom{n+\beta+1}{n}\binom{n+\alpha+\beta+2}{n}}. \quad (3.10)$$

As mentioned at the beginning of this section,

$$\lambda_{n+1}^{(\alpha,\beta)} = \lambda_0^{(\beta,\alpha)}. \tag{3.11}$$

In the ultraspherical case, (3.10) and (3.11) simplify to

$$\lambda_0^{(\alpha,\alpha)} = \lambda_{n+1}^{(\alpha,\alpha)} = 2^{2\alpha+1}\,\frac{\Gamma^2(\alpha+2)}{(\alpha+1)\Gamma(2\alpha+3)}\,\frac{1}{\binom{n+2\alpha+2}{n}}, \tag{3.12}$$

recovering, for $\alpha = 0$, the first of (1.9).

4. The interior weights

We now put $f(t) = (1-t^2)P_n^{(\alpha+1,\beta+1)}(t)/(t-t_k)$ in (3.1) and take advantage of (3.2) to obtain

$$\big(1-t_k^2\big)\lambda_k P_n^{(\alpha+1,\beta+1)\prime}(t_k) = \int_{-1}^{1} \frac{P_n^{(\alpha+1,\beta+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha+1,\beta+1)}(t). \tag{4.1}$$

We first compute the coefficient $(1-t_k^2)P_n^{(\alpha+1,\beta+1)\prime}(t_k)$ on the left. By (3.3) we have

$$P_n^{(\alpha+1,\beta+1)\prime}(t) = \frac{2}{n+\alpha+\beta+2}\,P_{n+1}^{(\alpha,\beta)\prime\prime}(t),$$

and using the differential equation satisfied by the Jacobi polynomial $P_{n+1}^{(\alpha,\beta)}$ [5, equation (4.2.1)], we get

$$\begin{aligned}\big(1-t^2\big)P_n^{(\alpha+1,\beta+1)\prime}(t) = \frac{2}{n+\alpha+\beta+2}\Big\{\big[\alpha-\beta+(\alpha+\beta+2)t\big]P_{n+1}^{(\alpha,\beta)\prime}(t)\\ -(n+1)(n+\alpha+\beta+2)\,P_{n+1}^{(\alpha,\beta)}(t)\Big\}.\end{aligned}$$

Therefore, by (3.4),

$$\big(1-t_k^2\big)P_n^{(\alpha+1,\beta+1)\prime}(t_k) = -2(n+1)P_{n+1}^{(\alpha,\beta)}(t_k). \tag{4.2}$$

To compute the integral on the right of (4.1), we proceed similarly as in section 3, using the Christoffel–Darboux formula ([5, equation (4.5.2)] with n replaced by $n-1$, and α, β replaced by $\alpha+1$, $\beta+1$), but this time combining it with (3.2), to obtain

$$\int_{-1}^{1} \frac{P_n^{(\alpha+1,\beta+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha+1,\beta+1)}(t) = \frac{d_n(\alpha,\beta)}{P_{n-1}^{(\alpha+1,\beta+1)}(t_k)}, \tag{4.3}$$

where

$$d_n(\alpha,\beta) = 2^{\alpha+\beta+2}(2n+\alpha+\beta+2)\,\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+3)}. \tag{4.4}$$

On the other hand, by (3.3) with n replaced by $n-1$, we have

$$P_{n-1}^{(\alpha+1,\beta+1)}(t_k) = \frac{2}{n+\alpha+\beta+1} P_n^{(\alpha,\beta)\prime}(t_k), \tag{4.5}$$

and by the second relation in [5, equation (4.5.7)],

$$\begin{aligned}\big(1-t_k^2\big)P_n^{(\alpha,\beta)\prime}(t_k) = \frac{n+\alpha+\beta+1}{2n+\alpha+\beta+2}\big\{\big[(2n+\alpha+\beta+2)t_k+\alpha-\beta\big]P_n^{(\alpha,\beta)}(t_k)\\ -2(n+1)(n+\alpha+\beta+1)P_{n+1}^{(\alpha,\beta)}(t_k)\big\}.\end{aligned} \tag{4.6}$$

Recalling (3.4), we have from the first relation in [5, equation (4.5.7) with n replaced by $n+1$],

$$\begin{aligned}&(2n+\alpha+\beta+2)\big(1-t_k^2\big)P_{n+1}^{(\alpha,\beta)\prime}(t_k)\\ &\quad=-(n+1)\big[(2n+\alpha+\beta+2)t_k+\beta-\alpha\big]P_{n+1}^{(\alpha,\beta)}(t_k)\\ &\qquad+2(n+\alpha+1)(n+\beta+1)P_n^{(\alpha,\beta)}(t_k)=0,\end{aligned}$$

that is,

$$P_n^{(\alpha,\beta)}(t_k) = \frac{(n+1)[(2n+\alpha+\beta+2)t_k+\beta-\alpha]}{2(n+\alpha+1)(n+\beta+1)} P_{n+1}^{(\alpha,\beta)}(t_k).$$

Sustituting this into (4.6), and the result into (4.5), yields

$$\begin{aligned}&P_{n-1}^{(\alpha+1,\beta+1)}(t_k)\\ &\quad=\frac{2(n+1)}{2n+\alpha+\beta+2}\left[\frac{(2n+\alpha+\beta+2)^2t_k^2-(\alpha-\beta)^2}{2(n+\alpha+1)(n+\beta+1)}-2\right]\frac{P_{n+1}^{(\alpha,\beta)}(t_k)}{1-t_k^2}.\end{aligned}$$

Now (4.1) in combination with (4.2), (4.3), and (4.4) yields the desired formula,

$$\begin{aligned}\lambda_k^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+2)\Gamma(\beta+2)}{\Gamma(\alpha+\beta+3)(n+1)^2}\,\frac{\binom{n+\alpha+1}{n}\binom{n+\beta+1}{n}}{\binom{n+\alpha+\beta+2}{n}}\\ \times\frac{1}{\frac{4(n+\alpha+1)(n+\beta+1)+(\alpha-\beta)^2}{(2n+\alpha+\beta+2)^2}-t_k^2}\,\frac{1-t_k^2}{[P_{n+1}^{(\alpha,\beta)}(t_k)]^2}.\end{aligned} \tag{4.7}$$

In the ultraspherical case, this becomes

$$\lambda_k^{(\alpha,\alpha)} = \frac{2^{2\alpha+1}}{(n+1)^2}\,\frac{\Gamma^2(n+\alpha+2)}{\Gamma(n+1)\Gamma(n+2\alpha+3)}\,\frac{1}{[P_{n+1}^{(\alpha,\alpha)}(t_k)]^2}, \tag{4.8}$$

which, for $\alpha=0$, recovers

$$\lambda_k^{(0,0)} = \frac{2}{(n+1)(n+2)}\,\frac{1}{[P_{k+1}(t_k)]^2}, \tag{4.9}$$

the second relation in (1.9).

5. Numerical comparisons

In the numerical experiments described in this section, we used our software [2], in particular, the routines `recur` and `gauss` and their higher-precision companions. We are comparing the results of generating the Gauss–Lobatto formula by

(1) computing the modified Jacobi matrix (1.3) directly, using (2.6), and then computing the nodes as eigenvalues of (1.3) and the weights by means of (1.6);

(2) computing (1.3) and its eigenvalues as in (1), but computing the weights directly, using (3.10), (3.11), and (4.7).

We begin with the classical Gauss–Lobatto formula, i.e., with the case $\alpha = \beta = 0$. For each n being run, we determine the accuracy of the single-precision weights obtained by either (1) or (2) by comparing them with the double-precision results, and we record the respective relative errors $err1$, $err2$. We also record the number of times $err2$ is smaller, respectively larger, than $err1$, and by what amounts (i.e., calculating $r = err2/err1$). We denote by $err1b$, $err2b$ the larger of the relative errors of the two boundary weights obtained via (1) and (2), respectively. Similarly, $err1i$, $err2i$ will denote the maximum relative errors for the interior weights. The quantities *rmin* and *rmax* are the minimum respectively maximum ratio r taken over all interior weights.

In our first experiment, we take $n = 1(1)20$. An excerpt of the results is shown in table 1. (Integers in parentheses denote decimal exponents.) It is seen that the boundary weights obtained by (2) are considerably more accurate than those obtained by (1). The interior weights from (2) are also consistently more accurate than those from (1) in terms of their maximum errors. The same is true for all other values of n. Overall, the interior weights computed by (2) are more accurate (less accurate) than those computed by (1) in 165 [45] of the 210 cases, i.e., in 78.6% (21.4%) of all cases.

Our next experiment takes $n = 20(20)500$. Selected, but representative, results are shown in table 2. If anything, they reinforce the superiority of method (2), especially (though not surprisingly) for the boundary weights, but also, to a lesser degree, for the interior weights. As indicated by the column headed *rmin*, the gain in accuracy, even for the interior weights, is potentially more pronounced. It is now in 95.6% of all 6,500 cases, that the weights produced by (2) are more accurate than those produced by (1). Evidently, method (1) is pushing the limits of single-precision accuracy, and method (2), except for the boundary weights, is not far behind.

Table 1
Comparison of methods (1) and (2) for $n = 5(5)20$ in the case $\alpha = \beta = 0$.

n	$err1b$	$err2b$	$err1i$	$err2i$	*rmin*	*rmax*
5	0.26(–5)	0.19(–7)	0.76(–6)	0.36(–6)	0.18(0)	0.15(2)
10	0.26(–5)	0.32(–7)	0.30(–5)	0.68(–6)	0.20(0)	0.23(1)
15	0.24(–4)	0.60(–7)	0.99(–5)	0.98(–6)	0.34(–2)	0.43(1)
20	0.39(–4)	0.22(–6)	0.10(–4)	0.22(–5)	0.13(–1)	0.33(1)

Table 2
Comparison of methods (1) and (2) for $n = 100(100)500$ in the case $\alpha = \beta = 0$.

n	$err1b$	$err2b$	$err1i$	$err2i$	$rmin$	$rmax$
100	0.17(–2)	0.17(–6)	0.22(–3)	0.20(–4)	0.41(–2)	0.15(1)
200	0.26(–2)	0.86(–6)	0.95(–3)	0.78(–4)	0.75(–4)	0.25(2)
300	0.11(–1)	0.53(–6)	0.36(–2)	0.17(–3)	0.13(–2)	0.66(2)
400	0.23(–1)	0.57(–7)	0.34(–2)	0.29(–3)	0.12(–3)	0.17(2)
500	0.45(–1)	0.95(–6)	0.56(–2)	0.17(–2)	0.13(–3)	0.57(2)

Table 3
Comparison of methods (1) and (2) for $n = 1000(1000)5000$ in the case $\alpha = \beta = 0$.

n	$err1b$	$err2b$	$err1i$	$err2i$	$rmin$	$rmax$
1000	0.18(–9)	0.39(–14)	0.29(–10)	0.15(–11)	0.43(–4)	0.60(2)
2000	0.28(–8)	0.21(–14)	0.23(–9)	0.29(–11)	0.34(–4)	0.71(1)
3000	0.77(–8)	0.73(–14)	0.39(–9)	0.12(–10)	0.17(–5)	0.12(2)
4000	0.11(–9)	0.48(–14)	0.53(–9)	0.23(–10)	0.86(–5)	0.37(2)
5000	0.53(–8)	0.42(–14)	0.86(–9)	0.18(–10)	0.13(–5)	0.10(3)

To proceed to higher values of n, we adopt double and quadruple precision. Letting $n = 1000(1000)5000$ we find (at a considerable expense in computer time) the results in table 3. These, on the whole, are analogous to those in table 2, if not still more in favor of method (2); the latter indeed is more accurate than method (1) in 99% of all cases.

Other values of α and β were also tried. Specifically, we compared the two methods for α and β going through the values -0.9, -0.5, 0.5, 1.0, 2.0, 5.0, 10.0, independently from each other but with $\beta \leqslant \alpha$, and $n = 20(20)100$ for each α, β. The results are similar to those displayed for $\alpha = \beta = 0$ except for extremely poor accuracy in some of the interior weights computed by method (1) when α and β are both $\geqslant 5$ and $n \geqslant 80$. On the whole ensemble of 8,400 interior weights, those produced by method (2) are more accurate in 90% of all cases, by as much as a factor of 3.4×10^7, and never less accurate by more than a factor of 7.1×10^2.

The superiority of method (2) for generating the quadrature rule may or may not lead to more accurate quadrature results, the matter depending very much on the specific functions f involved.

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Gauss–Radau formulae for Jacobi and Laguerre weight functions

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Dedicated to John R. Rice, on the occasion of his 65th birthday

Abstract

Explicit expressions are obtained for the weights of the Gauss–Radau quadrature formula for integration over the interval $[-1, 1]$ relative to the Jacobi weight function $(1-t)^\alpha(1+t)^\beta$, $\alpha>-1$, $\beta>-1$. The nodes are known to be the eigenvalues of a symmetric tridiagonal matrix, which is also obtained explicitly. Similar results hold for Gauss–Radau quadrature over the interval $[0, \infty)$ relative to the Laguerre weight $t^\alpha e^{-t}$, $\alpha>-1$.

Keywords: Gauss–Radau formula; Jacobi weight function; Laguerre weight function

1. Introduction

For any positive measure $d\lambda$ supported on the interval $[a, b]$, with a a finite real number, and $d\lambda$ having moments of all orders, there exists a quadrature rule of the form

$$\int_a^b f(t)\,d\lambda(t) = \lambda_0 f(a) + \sum_{k=1}^{n} \lambda_k f(t_k) + R_n(f) \tag{1.1}$$

which is exact for polynomials of degree $\leq 2n$,

$$R_n(f) = 0, \quad \forall f \in \mathbb{P}_{2n}. \tag{1.2}$$

It is called the ($(n+1)$-point) Gauss–Radau rule for the measure $d\lambda$. Its interior nodes t_k are known to be the zeros of $\pi_n(\cdot; d\lambda_a)$, the polynomial of degree n orthogonal with respect to the modified measure $d\lambda_a(t)=(t-a)\,d\lambda(t)$. The weights are obtainable by interpolation at the nodes a, t_1, $t_2, \ldots, t_n$.

Golub [5] in 1973 observed that the formula can be obtained, more elegantly, via eigenvalues and eigenvectors of a modified Jacobi matrix of order $n+1$,

$$J_{n+1}^{*}(\mathrm{d}\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \sqrt{\beta_n} \\ 0 & & & \sqrt{\beta_n} & \alpha_n^{*} \end{bmatrix}. \tag{1.3}$$

Here, α_k and β_k are the coefficients in the recurrence relation

$$\pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \qquad \pi_{-1}(t) = 0, \qquad \pi_0(t) = 1 \tag{1.4}$$

satisfied by the (monic) orthogonal polynomials $\pi_k(\cdot)=\pi_k(\cdot; \mathrm{d}\lambda)$, and α_n^{*} is given by

$$\alpha_n^{*} = a - \beta_n \frac{\pi_{n-1}(a)}{\pi_n(a)}. \tag{1.5}$$

The nodes of Eq. (1.1) (including a) are then precisely the eigenvalues of $J_{n+1}^{*}(\mathrm{d}\lambda)$, whereas the weights λ_j are expressible in terms of the first components $v_{j,1}$ of the associated normalized eigenvectors v_j,

$$\lambda_j = \beta_0 v_{j,1}^2, \quad j = 0, 1, 2, \ldots, n, \tag{1.6}$$

where $\beta_0 = \int_a^b \mathrm{d}\lambda(t)$ (cf. also [2,3]).

We show here that in the case of the Jacobi measure on $[-1, 1]$,

$$\mathrm{d}\lambda^{(\alpha,\beta)}(t) = (1-t)^{\alpha}(1+t)^{\beta}\,\mathrm{d}t, \quad \alpha > -1, \ \beta > -1, \tag{1.7}$$

the quantity α_n^{*} in Eq. (1.5) as well as all the weights $\lambda_j = \lambda_j^{(\alpha,\beta)}$ in Eq. (1.1) can be computed explicitly in terms of n, α, and β, thus obviating the need of computing eigenvectors. Our results generalize well-known formulae for the Legendre measure $\mathrm{d}\lambda^{(0,0)}$ (cf., e.g. [1], p. 103),

$$\lambda_0^{(0,0)} = \frac{2}{(n+1)^2}, \qquad \lambda_k^{(0,0)} = \frac{1}{(1-t_k)[P_n'(t_k)]^2} = \frac{1}{(n+1)^2}\frac{1-t_k}{[P_n(t_k)]^2}, \quad k = 1, 2, \ldots, n, \tag{1.8}$$

where P_n is the Legendre polynomial of degree n. We obtain, in fact, an additional formula, which in the case of the Legendre measure becomes

$$\lambda_k^{(0,0)} = \left[\frac{2n+3}{(n+1)(n+2)}\right]^2 \frac{1-t_k}{[P_{n+1}^{(0,1)}(t_k)]^2}, \tag{1.9}$$

with $P_{n+1}^{(0,1)}$ the Jacobi polynomial of degree $n+1$ relative to the Jacobi parameters $\alpha=0$ and $\beta=1$. Similar techniques can be used to derive explicit Gauss–Lobatto formulae for general Jacobi weight functions (cf. [4]).

Analogous results hold for the Laguerre measure on $[0, \infty)$,

$$\mathrm{d}\lambda^{(\alpha)}(t) = t^{\alpha}\mathrm{e}^{-t}\,\mathrm{d}t, \quad \alpha > -1. \tag{1.10}$$

Sections 2–4 are dealing with the Jacobi measure (1.7). After the explicit formula for the modified element α_n^{*} in Eq. (1.3) is obtained in Section 2, the boundary weight $\lambda_0^{(\alpha,\beta)}$ will be developed in Section 3, and the interior weights $\lambda_k^{(\alpha,\beta)}$ in Section 4. Section 5 deals analogously with the Laguerre measure (1.10).

2. The modified Jacobi matrix

The monic polynomials orthogonal with respect to the Jacobi measure (1.7) will be denoted by $\pi_k = \pi_k^{(\alpha,\beta)}$, and the Jacobi polynomials, as conventionally defined (cf., e.g., [6]), by $P_k = P_k^{(\alpha,\beta)}$. They are related by

$$P_n(t) = k_n \pi_n(t), \quad k_n = \frac{1}{2^n}\binom{2n+\alpha+\beta}{n}. \tag{2.1}$$

It is well known, furthermore, that

$$P_n(-1) = (-1)^n \binom{n+\beta}{n}. \tag{2.2}$$

By Eq. (1.5), we have

$$\alpha_n^* = -1 - \beta_n \frac{\pi_{n-1}(-1)}{\pi_n(-1)} = -1 - \beta_n \frac{k_n}{k_{n-1}} \frac{P_{n-1}(-1)}{P_n(-1)},$$

which, in view of Eqs. (2.1) and (2.2), gives

$$\alpha_n^* = -1 + \frac{1}{2}\beta_n \frac{(2n+\alpha+\beta)(2n+\alpha+\beta-1)}{(n+\beta)(n+\alpha+\beta)}, \quad n \geq 1. \tag{2.3}$$

On the other hand,

$$\beta_n = \frac{\|\pi_n\|^2}{\|\pi_{n-1}\|^2} = \frac{k_{n-1}^2}{k_n^2}\frac{h_n}{h_{n-1}},$$

where

$$h_n = \left\|P_n^{(\alpha,\beta)}\right\|^2 = \int_{-1}^{1} [P_n^{(\alpha,\beta)}(t)]^2 \, \mathrm{d}\lambda^{(\alpha,\beta)}(t) = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}.$$

On substitution in Eq. (2.3), this yields

$$\alpha_n^* = -1 + \frac{2n(n+\alpha)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}, \quad n \geq 1. \tag{2.4}$$

The modified Jacobi matrix $J_{n+1}^*(\mathrm{d}\lambda^{(\alpha,\beta)})$ in Eq. (1.3) is now readily computable, the recursion coefficients α_k and β_k for the Jacobi measure $\mathrm{d}\lambda^{(\alpha,\beta)}$ being explicitly known. This yields the Gauss–Radau formula in terms of the eigenvalues and (first components of) the eigenvectors of the matrix (1.3). In the next two sections we develop explicit formulae for the weights $\lambda_j = \lambda_j^{(\alpha,\beta)}$, which allow us to bypass the formula (1.6).

3. The boundary weight

Our concern, in this and the next two sections, is with the Gauss–Jacobi–Radau formula

$$\int_{-1}^{1} f(t) \, \mathrm{d}\lambda^{(\alpha,\beta)}(t) = \lambda_0 f(-1) + \sum_{k=1}^{n} \lambda_k f(t_k) + R_n(f), \tag{3.1}$$

where $\mathrm{d}\lambda^{(\alpha,\beta)}$ is the Jacobi measure (1.7). We first deal with the boundary weight $\lambda_0 = \lambda_0^{(\alpha,\beta)}$.

For the Jacobi measure we have $d\lambda_{-1}(t)=(1+t)\,d\lambda^{(\alpha,\beta)}(t)=d\lambda^{(\alpha,\beta+1)}(t)$, so that the interior nodes $t_k = t_k^{(\alpha,\beta)}$ of Eq. (3.1) are the zeros of $P_n^{(\alpha,\beta+1)}$,

$$P_n^{(\alpha,\beta+1)}(t_k) = 0, \quad k = 1, 2, \ldots, n. \tag{3.2}$$

Putting $f(t)=P_n^{(\alpha,\beta+1)}(t)$ in Eq. (3.1) then yields

$$\lambda_0 P_n^{(\alpha,\beta+1)}(-1) = \int_{-1}^{1} P_n^{(\alpha,\beta+1)}(t)\,d\lambda^{(\alpha,\beta)}(t). \tag{3.3}$$

After replacing β by $\beta+1$ in Eq. (2.2), the coefficient on the left is given by

$$P_n^{(\alpha,\beta+1)}(-1) = (-1)^n \binom{n+\beta+1}{n}. \tag{3.4}$$

In order to compute the integral in Eq. (3.3), we begin writing, using the second relation in [6] (Eq. (4.5.4)),

$$P_n^{(\alpha,\beta+1)}(t) = \frac{2}{2n+\alpha+\beta+2}\,\frac{(n+1)P_{n+1}^{(\alpha,\beta)}(t) + (n+\beta+1)P_n^{(\alpha,\beta)}(t)}{1+t}. \tag{3.5}$$

Observing from (2.2) that

$$n+1 = (n+1)\frac{(-1)^n P_n^{(\alpha,\beta)}(-1)}{\binom{n+\beta}{n}},$$

and similarly

$$n+\beta+1 = \frac{(n+1)}{\binom{n+\beta}{n}}(-1)^{n+1} P_n^{(\alpha,\beta)}(-1),$$

we can write Eq. (3.5) as

$$P_n^{(\alpha,\beta+1)}(t) = \frac{2(-1)^n(n+1)}{(2n+\alpha+\beta+2)\binom{n+\beta}{n}}\,\frac{P_{n+1}^{(\alpha,\beta)}(t)P_n^{(\alpha,\beta)}(-1) - P_n^{(\alpha,\beta)}(t)P_{n+1}^{(\alpha,\beta)}(-1)}{1+t}. \tag{3.6}$$

On the other hand, by the Christoffel–Darboux formula ([6], Eq. (4.5.2)),

$$\frac{P_{n+1}^{(\alpha,\beta)}(t)P_n^{(\alpha,\beta)}(-1) - P_n^{(\alpha,\beta)}(t)P_{n+1}^{(\alpha,\beta)}(-1)}{1+t} = c_n(\alpha,\beta)\sum_{\nu=0}^{n}\frac{1}{h_\nu^{(\alpha,\beta)}}P_\nu^{(\alpha,\beta)}(t)P_\nu^{(\alpha,\beta)}(-1), \tag{3.7}$$

where

$$c_n(\alpha,\beta) = 2^{\alpha+\beta}\frac{(2n+\alpha+\beta+2)\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+2)\Gamma(n+\alpha+\beta+2)} \tag{3.8}$$

and $h_\nu^{(\alpha,\beta)} = \int_{-1}^{1}[P_\nu^{(\alpha,\beta)}(t)]^2\,\mathrm{d}\lambda^{(\alpha,\beta)}(t)$. Now integrating Eq. (3.6) with the measure $\mathrm{d}\lambda^{(\alpha,\beta)}$ gives, by Eq. (3.7) and the orthogonality of the Jacobi polynomials,

$$\int_{-1}^{1} P_n^{(\alpha,\beta+1)}(t)\,\mathrm{d}\lambda^{(\alpha,\beta)}(t) = \frac{2(-1)^n(n+1)c_n(\alpha,\beta)}{(2n+\alpha+\beta+2)\binom{n+\beta}{n}},$$

or by an elementary computation, using Eq. (3.8),

$$\int_{-1}^{1} P_n^{(\alpha,\beta+1)}(t)\,\mathrm{d}\lambda^{(\alpha,\beta)}(t) = (-1)^n 2^{\alpha+\beta+1}\Gamma(\beta+1)\frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha+\beta+2)}. \tag{3.9}$$

Combining Eqs. (3.3), (3.4), and (3.9) finally gives the desired result

$$\lambda_0^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(\beta+1)}{\binom{n+\beta+1}{n}}\frac{\Gamma(n+\alpha+1)}{\Gamma(n+\alpha+\beta+2)}. \tag{3.10}$$

In the case $\alpha=\beta=0$, we recover the first equation of (1.8).

In almost all cases computed, the boundary weight (3.10) turned out to be more accurate than the boundary weight computed by Eq. (1.6) (for $j=0$), often significantly so.

4. The interior weights

We now put $f(t) = (1+t)P_n^{(\alpha,\beta+1)}(t)/(t-t_k)$ in Eq. (3.1) and obtain, by virtue of Eq. (3.2),

$$(1+t_k)\lambda_k P_n^{(\alpha,\beta+1)\prime}(t_k) = \int_{-1}^{1}\frac{P_n^{(\alpha,\beta+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha,\beta+1)}(t).$$

Applying once more the Christoffel–Darboux formula ([6], Eq. (4.5.2) with n replaced by $n-1$, and β replaced by $\beta+1$), we get similarly as in Section 3, using Eq. (3.2),

$$\int_{-1}^{1}\frac{P_n^{(\alpha,\beta+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha,\beta+1)}(t) = \frac{d_n(\alpha,\beta)}{P_{n-1}^{(\alpha,\beta+1)}(t_k)},$$

where

$$d_n(\alpha,\beta) = \frac{2^{\alpha+\beta+1}(2n+\alpha+\beta+1)\Gamma(n+\alpha)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+2)}. \tag{4.1}$$

Thus,

$$\lambda_k^{(\alpha,\beta)} = \frac{d_n(\alpha,\beta)}{(1+t_k)P_n^{(\alpha,\beta+1)\prime}(t_k)P_{n-1}^{(\alpha,\beta+1)}(t_k)}. \tag{4.2}$$

4.1. The interior weights in terms of $P_{n+1}^{(\alpha,\beta+1)}(t_k)$

Here, we use the second relation in ([6], Eq. (4.5.7) with β replaced by $\beta+1$) in combination with Eq. (3.2) to obtain

$$(1+t_k)P_n^{(\alpha,\beta+1)\prime}(t_k)=\frac{1-t_k^2}{1-t_k}P_n^{(\alpha,\beta+1)\prime}(t_k)=-\frac{2(n+1)(n+\alpha+\beta+2)}{2n+\alpha+\beta+3}\frac{P_{n+1}^{(\alpha,\beta+1)}(t_k)}{1-t_k}. \tag{4.3}$$

The recurrence relation for the Jacobi polynomials $P_k^{(\alpha,\beta+1)}$ (cf. ([6], Eq. (4.5.1) with n replaced by $n+1$)), on the other hand, yields, again using Eq. (3.2),

$$\begin{aligned}&2(n+1)(n+\alpha+\beta+2)(2n+\alpha+\beta+1)P_{n+1}^{(\alpha,\beta+1)}(t_k)\\&\quad=-2(n+\alpha)(n+\beta+1)(2n+\alpha+\beta+3)P_{n-1}^{(\alpha,\beta+1)}(t_k),\end{aligned}$$

that is

$$P_{n-1}^{(\alpha,\beta+1)}(t_k)=-\frac{(n+1)(n+\alpha+\beta+2)(2n+\alpha+\beta+1)}{(n+\alpha)(n+\beta+1)(2n+\alpha+\beta+3)}P_{n+1}^{(\alpha,\beta+1)}(t_k). \tag{4.4}$$

It suffices now to insert Eqs. (4.1), (4.3), and (4.4) into Eq. (4.2) to obtain, after some computation,

$$\lambda_k^{(\alpha,\beta)}=2^{\alpha+\beta}\frac{(2n+\alpha+\beta+3)^2}{(n+1)(n+\alpha+\beta+2)}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+2)}{\Gamma(n+2)\Gamma(n+\alpha+\beta+3)}\frac{1-t_k}{[P_{n+1}^{(\alpha,\beta+1)}(t_k)]^2},\quad n\geq 1, \tag{4.5}$$

where $t_k=t_k^{(\alpha,\beta)}$ are the zeros of $P_n^{(\alpha,\beta+1)}$. This is Eq. (1.9) when $\alpha=\beta=0$.

4.2. The interior weights in terms of $P_n^{(\alpha,\beta)\prime}(t_k)$

We rewrite Eq. (4.2) by first noting from the first relation in ([6], Eq. (4.5.4) with n replaced by $n-1$, and β replaced by $\beta+1$), and also recalling Eq. (3.2), that

$$P_{n-1}^{(\alpha+1,\beta+1)}(t_k)=\frac{2(n+\alpha)}{2n+\alpha+\beta+1}\frac{P_{n-1}^{(\alpha,\beta+1)}(t_k)}{1-t_k}.$$

Furthermore, by ([6], Eq. (4.21.7)),

$$P_{n-1}^{(\alpha+1,\beta+1)}(t_k)=\frac{2}{n+\alpha+\beta+1}P_n^{(\alpha,\beta)\prime}(t_k).$$

Therefore,

$$P_{n-1}^{(\alpha,\beta+1)}(t_k)=(1-t_k)\frac{2n+\alpha+\beta+1}{(n+\alpha)(n+\alpha+\beta+1)}P_n^{(\alpha,\beta)\prime}(t_k). \tag{4.6}$$

On the other hand, using Eq. (4.3) and the relation

$$P_{n+1}^{(\alpha,\beta+1)}(t_k)=\frac{(n+\alpha)(n+\beta+1)(2n+\alpha+\beta+3)}{(n+1)(n+\alpha+\beta+2)(2n+\alpha+\beta+1)}P_{n-1}^{(\alpha,\beta+1)}(t_k),$$

which follows from the recurrence relation for $P_k^{(\alpha,\beta+1)}$ (cf. ([6], Eq. (4.5.1) with n replaced by $n+1$)) and from Eq. (3.2), we obtain

$$(1+t_k)P_n^{(\alpha,\beta+1)\prime}(t_k) = \frac{2(n+\alpha)(n+\beta+1)}{2n+\alpha+\beta+1}\frac{P_{n-1}^{(\alpha,\beta+1)}(t_k)}{1-t_k}.$$

This, together with Eq. (4.6), allows us to write Eq. (4.2) in the form

$$\lambda_k^{(\alpha,\beta)} = \frac{(n+\alpha)(n+\alpha+\beta+1)^2 d_n(\alpha,\beta)}{2(n+\beta+1)(2n+\alpha+\beta+1)}\frac{1}{(1-t_k)[P_n^{(\alpha,\beta)\prime}(t_k)]^2}.$$

Substituting the expression (4.1) for $d_n(\alpha,\beta)$ then gives

$$\lambda_k^{(\alpha,\beta)} = 2^{\alpha+\beta}\frac{n+\alpha+\beta+1}{n+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}\frac{1}{(1-t_k)[P_n^{(\alpha,\beta)\prime}(t_k)]^2}. \tag{4.7}$$

In the case of $\alpha=\beta=0$, we recover the second relation in Eq. (1.8). For computational purposes, one will probably want to replace $P_n^{(\alpha,\beta)\prime}(t_k)$ by $(1/2)(n+\alpha+\beta+1)P_{n-1}^{(\alpha+1,\beta+1)}(t_k)$ and compute $P_{n-1}^{(\alpha+1,\beta+1)}(t_k)$ from its recurrence relation.

4.3. *The interior weights in terms of* $P_n^{(\alpha,\beta)}(t_k)$

We now rewrite Eq. (4.7) by using the second relation in ([6], Eq. (4.5.7)),

$$(1-t_k^2)P_n^{(\alpha,\beta)\prime}(t_k) = \frac{1}{2n+\alpha+\beta+2}\{(n+\alpha+\beta+1)[(2n+\alpha+\beta+2)t_k + \alpha-\beta]P_n^{(\alpha,\beta)}(t_k) - 2(n+1)(n+\alpha+\beta+1)P_{n+1}^{(\alpha,\beta)}(t_k)\},$$

and combining it with the relation

$$0 = P_n^{(\alpha,\beta+1)}(t_k) = \frac{2}{2n+\alpha+\beta+2}\frac{(n+\beta+1)P_n^{(\alpha,\beta)}(t_k) + (n+1)P_{n+1}^{(\alpha,\beta)}(t_k)}{1+t_k},$$

which follows from Eq. (3.2) and the second relation in ([6], Eq. (4.5.4)), that is, with

$$P_{n+1}^{(\alpha,\beta)}(t_k) = -\frac{n+\beta+1}{n+1}P_n^{(\alpha,\beta)}(t_k).$$

The result is

$$\lambda_k^{(\alpha,\beta)} = \frac{2^{\alpha+\beta}}{n+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+2)}\frac{1-t_k}{[P_n^{(\alpha,\beta)}(t_k)]^2}. \tag{4.8}$$

In the Legendre case $\alpha=\beta=0$, this reduces to the last relation in Eq. (1.8).

Numerically, the three formulae (4.5), (4.7), and (4.8) behave similarly. They produce less accurate results than the formula (1.6) in about two-thirds of the cases computed, and more accurate results otherwise.

5. The Gauss–Radau formula for the Laguerre measure

Techniques similar to those in Sections 2–4, but much simpler, apply also to the Laguerre measure (1.10). The final results (Eqs. (5.5) and (5.9)) are in fact known (cf. [1], pp. 223–224)), but for completeness we re-derive them from scratch.

The monic and conventional Laguerre polynomials, $\pi_n^{(\alpha)}$ and $L_n^{(\alpha)}$, are related by

$$L_n^{(\alpha)}(t) = \frac{(-1)^n}{n!}\pi_n^{(\alpha)}(t),$$

and we have

$$L_n^{(\alpha)}(0) = \binom{n+\alpha}{n}, \qquad \beta_n = n(n+\alpha). \tag{5.1}$$

From Eq. (1.5), the modified element α_n^* in the matrix (1.3) is now

$$\alpha_n^* = -\beta_n \frac{\pi_{n-1}^{(\alpha)}(0)}{\pi_n^{(\alpha)}(0)} = \beta_n \frac{L_{n-1}^{(\alpha)}(0)}{nL_n^{(\alpha)}(0)},$$

which, by Eq. (5.1), becomes, surprisingly simply,

$$\alpha_n^* = n. \tag{5.2}$$

The Gauss–Laguerre–Radau formula to be considered is

$$\int_0^\infty f(t)\,\mathrm{d}\lambda^{(\alpha)}(t) = \lambda_0 f(0) + \sum_{k=1}^{n} \lambda_k f(t_k) + R_n(f), \tag{5.3}$$

where $\mathrm{d}\lambda^{(\alpha)}$ is the Laguerre measure (1.10), and, as before, $R_n(\mathbb{P}_{2n})=0$. Since $\mathrm{d}\lambda_0(t)=t\,\mathrm{d}\lambda^{(\alpha)}(t)=\mathrm{d}\lambda^{(\alpha+1)}(t)$, the interior nodes $t_k = t_k^{(\alpha)}$ are the zeros of $L_n^{(\alpha+1)}$,

$$L_n^{(\alpha+1)}(t_k) = 0. \tag{5.4}$$

The *boundary weight* is obtained by putting $f(t)=L_n^{(\alpha+1)}(t)$ in Eq. (5.3),

$$\lambda_0 L_n^{(\alpha+1)}(0) = \int_0^\infty L_n^{(\alpha+1)}(t)\,\mathrm{d}\lambda^{(\alpha)}(t).$$

The coefficient on the left can be computed by Eq. (5.1), and the integral on the right by noting from ([6], Eq. (5.1.13)) that

$$L_n^{(\alpha+1)}(t) = \sum_{\nu=0}^{n} L_\nu^{(\alpha)}(t),$$

and hence, by orthogonality,

$$\int_0^\infty L_n^{(\alpha+1)}(t)\,\mathrm{d}\lambda^{(\alpha)}(t) = \sum_{\nu=0}^{n}\int_0^\infty L_\nu^{(\alpha)}(t)\,\mathrm{d}\lambda^{(\alpha)}(t) = \int_0^\infty \mathrm{d}\lambda^{(\alpha)}(t) = \Gamma(\alpha+1).$$

There results

$$\lambda_0^{(\alpha)} = \frac{\Gamma(\alpha+1)}{\binom{n+\alpha+1}{n}}. \tag{5.5}$$

For the *interior weights* $\lambda_k = \lambda_k^{(\alpha)}$, we put $f(t) = t\,L_n^{(\alpha+1)}(t)/(t-t_k)$ in Eq. (5.3) to obtain

$$\lambda_k t_k L_n^{(\alpha+1)\prime}(t_k) = \int_0^\infty \frac{t\,L_n^{(\alpha+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha)}(t) = \int_0^\infty \frac{L_n^{(\alpha+1)}(t)}{t-t_k}\,\mathrm{d}\lambda^{(\alpha+1)}(t). \tag{5.6}$$

The Christoffel–Darboux formula ([6], Eq. (5.1.11) with α replaced by $\alpha+1$), similarly as in the beginning of Section 4, yields

$$\lambda_k^{(\alpha)} = \frac{\Gamma(\alpha+2)}{n+1}\binom{n+\alpha+1}{n}\frac{1}{t_k L_n^{(\alpha+1)\prime}(t_k) L_{n+1}^{(\alpha)}(t_k)}. \tag{5.7}$$

By ([6], Eq. (5.1.14) with α replaced by $\alpha+1$), and Eq. (5.4),

$$t_k L_n^{(\alpha+1)\prime}(t_k) = -(n+\alpha+1)L_{n-1}^{(\alpha+1)}(t_k),$$

where, by ([6], Eq. (5.1.13)) and Eq. (5.4),

$$L_{n-1}^{(\alpha+1)}(t_k) = -L_n^{(\alpha)}(t_k). \tag{5.8}$$

The recurrence relation for the Laguerre polynomials $L_k^{(\alpha+1)}$, (cf. [6], Eq. (5.1.10)), in combination with Eqs. (5.4) and (5.8), on the other hand, gives

$$L_{n+1}^{(\alpha+1)}(t_k) = -(n+\alpha+1)L_{n-1}^{(\alpha+1)}(t_k) = (n+\alpha+1)L_n^{(\alpha)}(t_k),$$

so that finally

$$\lambda_k^{(\alpha)} = \frac{\Gamma(\alpha+1)}{n+\alpha+1}\binom{n+\alpha}{n}\frac{1}{[L_n^{(\alpha)}(t_k)]^2}. \tag{5.9}$$

This is the analogue of Eq. (4.8). The analogue of Eq. (4.7) coincides with Eq. (5.9). This is because of the identities ([6], Eqs. (5.1.13) and (5.1.14))

$$L_n^{(\alpha)\prime}(t) = -L_{n-1}^{(\alpha+1)}(t) = L_n^{(\alpha)}(t) - L_n^{(\alpha+1)}(t),$$

which, for $t=t_k$, in view of Eq. (5.4), gives

$$L_n^{(\alpha)\prime}(t_k) = L_n^{(\alpha)}(t_k).$$

The numerical experience with these explicit formulae is much like in the case of the Jacobi measure, i.e., the boundary weight (5.5) is almost always considerably more accurate than the boundary weight obtained via eigenvectors, whereas for interior weights, the formula (1.6) involving eigenvectors is generally more accurate than the explicit formula (5.9).

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The use of rational functions in numerical quadrature

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Abstract

Quadrature problems involving functions that have poles outside the interval of integration can profitably be solved by methods that are exact not only for polynomials of appropriate degree, but also for rational functions having the same (or the most important) poles as the function to be integrated. Constructive and computational tools for accomplishing this are described and illustrated in a number of quadrature contexts. The superiority of such rational/polynomial methods is shown by an analysis of the remainder term and documented by numerical examples.

Keywords: Rational quadrature rules; Remainder term; Rational Fejér quadrature; Rational Gauss; Gauss–Kronrod, and Gauss–Turán quadrature; Rational quadrature rules for Cauchy principal value integrals

1. Introduction

Much of numerical analysis has been dominated by polynomial approximation, i.e., approximation procedures that yield exact answers if the function to be processed were a polynomial of some appropriate degree. This is particularly true in the area of numerical quadrature. Frequently, however, the functions to be integrated are not polynomial-like. They often have poles away from the interval of integration, in which case it would be more natural to make the integration exact for rational functions having the same, or at least the more important, poles (those closest to the interval of integration). It may be desirable to still have some low-degree polynomials, e.g., constants, integrated exactly. This suggests an approximation procedure that provides exact answers for a mixture of rational functions and polynomials. The constructive and computational tools for implementing this idea are described, not only for ordinary quadrature rules, but also for more sophisticated rules such as Gauss–Kronrod and Gauss–Turán rules, and quadrature procedures for Cauchy principal value integrals.

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An idea somewhat related to our's is to require exactness for a class of Laurent polynomials, which is meaningful if the underlying measure of integration is "strong", i.e., possesses moments of positive as well as negative orders. The approach is related to two-point Padé approximation, the two points being at the origin and at infinity. For this we refer to [4–8,29–31] and to [47–49] for specific examples. For rational quadrature over the unit circle, we refer to [9] and the references cited therein. Our results in Section 6 on rational Gauss-type quadrature formulae are closely related to multipoint Padé approximation. The convergence of such approximations and of related quadrature formulae has been studied in a series of papers by López Lagomasino and others; see, e.g., [24, 35–38,25,11]. Further convergence results, also for other rational quadrature formulae, can be found in [10].

There are other approaches, essentially different from those to be described, of incorporating the influence of poles outside (and particularly near) the interval of integration. One is to construct, in some way or another, a correction term to a standard, in particular Gaussian, quadrature rule. This is an approach taken by Lether, who in [33] uses the method of subtracting the singularity, and in [34] uses the principal part of the Laurent expansion at each pole to obtain the correction term. The latter approach, however, requires the evaluation of the regular part of the integrand at the pole(s). This is avoided in a method proposed by Hunter and Okecha [28]. Another entirely different approach is discussed in [3], where expansion in sinc functions is used.

2. The principle of exactness

We begin with a quadrature rule of the simplest kind,

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(t_\nu) + R_n(f), \tag{2.1}$$

where $\mathrm{d}\lambda$ is a given (usually positive) measure of integration all of whose moments exist. The general *principle of exactness* can be formulated as follows. Given a linear space $\mathbb{S}_d$ of functions (integrable with respect to $\mathrm{d}\lambda$), having dimension d, determine t_ν and λ_ν such that formula (2.1) is exact for all functions in $\mathbb{S}_d$, i.e.,

$$R_n(g) = 0 \quad \text{for all } g \in \mathbb{S}_d. \tag{2.2}$$

Such a formula may or may not exist, and if it does, may not be unique. Classical examples are the *Newton–Cotes formulae*, where the (distinct) nodes t_ν are prescribed, and one tries to determine the weights λ_ν such that (2.2) holds with $d = n$ and $\mathbb{S}_n = \mathbb{P}_{n-1}$, the space of polynomials of degree $\leqslant n-1$. This determines formula (2.1) uniquely. Alternatively, one could impose conditions on the weights λ_ν, for example, that they all be equal, and determine the nodes t_ν so as to have polynomial degree of exactness n. This gives rise to *quadrature rules of Chebyshev type*, which may or may not exist if one insists on reality of the nodes. Among all polynomial-based quadrature rules, the optimal one is the *Gauss–Christoffel rule*, or briefly the *Gaussian rule*, where one takes $d = 2n$ and $\mathbb{S}_{2n} = \mathbb{P}_{2n-1}$. In this case, both the nodes t_ν and the weights λ_ν are to be determined. It is well known that they exist uniquely, that all t_ν are contained in the support interval of the measure $\mathrm{d}\lambda$, and the λ_ν are all positive (if the measure $\mathrm{d}\lambda$ is positive).

Here we are interested in a mixed rational/polynomial type of exactness. More precisely, given an integer parameter m with $0 \leqslant m \leqslant d$, we take $\mathbb{S}_d$ to be the direct sum of a space of rational functions and a space of polynomials,

$$\mathbb{S}_d = \mathbb{Q}_m \oplus \mathbb{P}_{d-1-m}, \quad 0 \leqslant m \leqslant d, \tag{2.3}$$

where

$$\mathbb{Q}_m = \operatorname{span}\left\{ g : g(t) = (1+\zeta_\mu t)^{-s};\ \mu = 1,2,\ldots,M;\right.$$

$$\left. s = 1,2,\ldots,s_\mu;\ \sum_{\mu=1}^{M} s_\mu = m \right\}. \tag{2.4}$$

The ζ_μ are given (in general complex) numbers satisfying

$$\zeta_\mu \neq 0, \quad 1+\zeta_\mu t \neq 0 \text{ on } \overline{\operatorname{supp}(d\lambda)}. \tag{2.5}$$

The rational component $\mathbb{Q}_m$ of $\mathbb{S}_d$ thus is made up of rational functions having poles $-1/\zeta_\mu$ of multiplicities up to s_μ outside the support of $d\lambda$. These poles are chosen to match the most important poles, if any, of the function f in (2.1). If f is an entire function, one might as well take $m = 0$, in which case $\mathbb{Q}_m$ is empty and $\mathbb{S}_d$ is a purely polynomial space. The other extreme is $m = d$, in which case $\mathbb{S}_d$ consists entirely of genuinely rational functions.

3. Characterization of quadrature rules of rational/polynomial exactness

The basic result concerning quadrature rules (2.1) exact on the space $\mathbb{S}_d$ of (2.2)–(2.4) was proved in [16] (for $d = 2n$) and, independently, in [50] for special choices of $\mathbb{Q}_m$. We state it as the following theorem.

Theorem 3.1. *Let* $0 \leqslant m \leqslant d$ *and*

$$\omega_m(t) = \prod_{\mu=1}^{M} (1+\zeta_\mu t)^{s_\mu} \tag{3.1}$$

(a polynomial of exact degree m). *Assume there exists an* n*-point quadrature rule of polynomial degree of exactness* $d-1$ *for the modified measure* $d\lambda/\omega_m$:

$$\int_{\mathbb{R}} p(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^* p(t_v^*), \quad p \in \mathbb{P}_{d-1}, \tag{3.2}$$

whose nodes t_v^* *are distinct and contained in the support of* $d\lambda$. *Define*

$$t_v = t_v^*, \quad \lambda_v = w_v^* \omega_m(t_v^*), \quad v = 1,2,\ldots,n. \tag{3.3}$$

Then

$$\int_{\mathbb{R}} g(t)\, d\lambda(t) = \sum_{v=1}^{n} \lambda_v g(t_v) + R_n(g), \tag{3.4}$$

where

$$R_n(g) = 0 \quad \textit{for all } g \in \mathbb{S}_d = \mathbb{Q}_m \oplus \mathbb{P}_{d-1-m}. \tag{3.5}$$

Conversely, if (3.4), (3.5) *hold for distinct* $t_v \in \operatorname{supp}(d\lambda)$, *then so does* (3.2) *with* t_v^*, w_v^* *as obtained from* (3.3).

The (rather elementary) proof is given in [16] for $d = 2n$, but holds equally well for arbitrary d.

The theorem says nothing about the existence or uniqueness of (3.2); it merely states an implication, namely that (3.2) implies (3.4), (3.5), with t_v, λ_v as defined in (3.3), and vice versa. Specific instances of existence and uniqueness will be given later.

4. The remainder term

Assume that $d\lambda$ has compact support and formula (3.2) exists. It then follows by (3.3) and (3.2) that

$$\int_{\mathbb{R}} \frac{p(t)}{\omega_m(t)}\, d\lambda(t) = \sum_{v=1}^{n} \lambda_v \frac{p(t_v)}{\omega_m(t_v)}, \quad p \in \mathbb{P}_{d-1}. \tag{4.1}$$

Now define

$$\mathscr{E}_{d,m}(g) := \inf_{p\in\mathbb{P}_{d-1}} \left\| \frac{p}{\omega_m} - g \right\|_\infty = \left\| \frac{p^*}{\omega_m} - g \right\|_\infty \tag{4.2}$$

to be the best approximation of g by rational functions of the form p/ω_m in the maximum norm $\|\cdot\|_\infty$ on the support of $d\lambda$. Then by a standard argument in the theory of approximation, using (4.1), we have (cf. also [45])

$$\begin{aligned} |R_n(g)| &= \left| \int_{\mathbb{R}} g(t)\, d\lambda(t) - \sum_{v=1}^{n} \lambda_v g(t_v) \right| \\ &= \left| \int_{\mathbb{R}} \left[g(t) - \frac{p^*(t)}{\omega_m(t)} \right] d\lambda(t) - \sum_{v=1}^{n} \lambda_v \left[g(t_v) - \frac{p^*(t_v)}{\omega_m(t_v)} \right] \right| \\ &\leqslant \mathscr{E}_{d,m}(g) \left\{ \int_{\mathbb{R}} d\lambda(t) + \sum_{v=1}^{n} |\lambda_v| \right\}, \end{aligned}$$

that is,

$$|R_n(g)| \leqslant \mathscr{E}_{d,m}(g) \left\{ \int_{\mathbb{R}} d\lambda(t) + \sum_{v=1}^{n} |\lambda_v| \right\}. \tag{4.3}$$

If $\lambda_v > 0$ and formula (3.4) is exact for a constant, i.e., $d - 1 - m \geqslant 0$, then (4.3) simplifies to

$$|R_n(g)| \leqslant 2\mathscr{E}_{d,m}(g) \int_{\mathbb{R}} d\lambda(t), \quad m \leqslant d - 1. \tag{4.4}$$

The significance of (4.3) is as follows: if g can be well approximated on $\operatorname{supp}(d\lambda)$ by a function p/ω_m, where p is a polynomial, that is, $g\omega_m$ can be well approximated by a polynomial, then the

quadrature error $R_n(g)$ is small. By our choice of ω_m, multiplying g into ω_m removes the more important poles of g, and the resulting function $\omega_m g$, whose (remaining, if any) poles are now further away from the real axis, can indeed be well approximated by polynomials, certainly better than the original function g.

5. The rational Fejér quadrature rule

The classical Fejér quadrature rule is the interpolatory rule for $d\lambda(t) = dt$ on $[-1,1]$,

$$\int_{-1}^{1} f(t)\,dt = \sum_{v=1}^{n} \lambda_v f(t_v) + R_n(f), \quad R_n(\mathbb{P}_{n-1}) = 0, \tag{5.1}$$

where the nodes t_v are the Chebyshev points, or, as we call them now, the *Fejér nodes*

$$t_v^{\mathrm{F}} = \cos\theta_v, \quad \theta_v = \frac{2v-1}{2n}\pi, \quad v = 1,2,\ldots,n. \tag{5.2}$$

Fejér [13] showed that the weights λ_v in (5.1) can be computed explicitly as

$$\lambda_v = \frac{2}{n}\left(1 - 2\sum_{\mu=1}^{\lfloor n/2\rfloor} \frac{\cos(2\mu\theta_v)}{4\mu^2-1}\right), \quad v = 1,2,\ldots,n, \tag{5.3}$$

and that $\lambda_v > 0$ for all v. Similar results hold for Chebyshev points of the second kind, as was already shown by Fejér, and also for Chebyshev points of the third and fourth kind, with or without one or both of the endpoints ± 1 included, as was shown more recently in [43,44]. We consider here only Chebyshev nodes of the first kind, (5.2), and want to make the quadrature rule (5.1) exact on $\mathbb{S}_n = \mathbb{Q}_m \oplus \mathbb{P}_{n-1-m}$ (i.e., $d = n$ in (2.3)). According to our theorem (cf. (3.2), where we write $t_v^* = t_v^{\mathrm{F}}$, $w_v^* = w_v^{\mathrm{F}}$ and let $d = n$), we need to determine w_v^{F} such that

$$\sum_{v=1}^{n} w_v^{\mathrm{F}} T_k(t_v^{\mathrm{F}}) = \int_{-1}^{1} \frac{T_k(t)}{\omega_m(t)}\,dt, \quad k = 0,1,\ldots,n-1, \tag{5.4}$$

where T_k is the Chebyshev polynomial of degree k. Letting

$$\mu_k = \int_{-1}^{1} \frac{T_k(t)}{\omega_m(t)}\,dt, \quad k = 0,1,2,\ldots \tag{5.5}$$

and making use of the "orthogonality" relation

$$\sum_{k=0}^{n-1}{}' T_k(t_v^{\mathrm{F}}) T_k(t_\mu^{\mathrm{F}}) = \frac{n}{2}\delta_{v\mu}, \tag{5.6}$$

which is a consequence of the Christoffel–Darboux formula for Chebyshev polynomials (the prime on the summation sign means that the first term has to be multiplied by $\frac{1}{2}$), we find from (5.4) immediately that [51]

$$w_v^{\mathrm{F}} = \frac{2}{n}\sum_{k=0}^{n-1}{}' \mu_k T_k(t_v^{\mathrm{F}}), \quad v = 1,2,\ldots,n. \tag{5.7}$$

It is easily seen that (5.7) reduces to (5.3) when $m = 0$. The computational challenge lies in the computation of the quantities μ_k in (5.5); for these, Weideman and Laurie [51] developed recursive algorithms that allow their stable and efficient computation.

Similar techniques have been employed earlier by Monegato [41], who uses as nodes the zeros of orthogonal polynomials, and have been applied in [42] to Fredholm integral equations with rational kernels. Hasegawa and Torii [27] and Hasegawa [26], instead, use Clenshaw–Curtis nodes. Schneider [46] constructs quadrature rules by integrating rational Hermite interpolants.

6. The rational Gauss quadrature rule

Here, $d = 2n$ in (3.2), and the space of rational/polynomial gauge functions is $\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m}$, where $0 \leqslant m \leqslant 2n$. The existence of the rational Gauss formula which is exact on $\mathbb{S}_{2n}$ now hinges on the existence of the (polynomial) Gauss formula

$$\int_{\mathbb{R}} p(t)\frac{d\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^G p(t_v^G), \quad p \in \mathbb{P}_{2n-1} \tag{6.1}$$

(cf. (3.2), with $t_v^* = t_v^G$, $w_v^* = w_v^G$ and $d = 2n$). Since the ζ_μ in (2.4) may well be complex, hence ω_m a complex-valued polynomial, the existence of (6.1) is by no means guaranteed. There are, however, a number of special cases, of interest in applications, in which the existence and uniqueness of the Gauss formula (6.1) is assured. Some of these are as follows:

(i) *Simple real poles*: Here all $s_\mu = 1$, hence $M = m$, and we write

$$\zeta_\mu = \xi_\mu \in \mathbb{R}, \quad \xi_\mu \neq 0, \quad \mu = 1,2,\ldots,m, \tag{6.2}$$

where ξ_μ are distinct real numbers. The corresponding polynomial ω_m becomes

$$\omega_m(t) = \prod_{\mu=1}^{m}(1 + \xi_\mu t), \tag{6.3}$$

which by the assumption $1 + \xi_\mu t \neq 0$ on $\operatorname{supp}(d\lambda)$ (cf. (2.5)) has constant sign on the support of $d\lambda$ if the support is connected. Furthermore, if $d\lambda$ has finite moments, as we assumed, then so does $d\lambda/\omega_m$. Hence, the Gauss formula (6.1) exists for each n and m and is unique. According to (3.3), the nodes and weights of the rational Gauss formula (2.1) are given by

$$t_v = t_v^G, \quad \lambda_v = w_v^G \omega_m(t_v^G), \quad v = 1,2,\ldots,n. \tag{6.4}$$

Since all w_v^G have the same sign, namely the sign of ω_m on $\operatorname{supp}(d\lambda)$, it follows that all λ_v are positive.

(ii) *Simple conjugate complex poles*: It is natural, in this case, to take m even, and thus

$$\zeta_\mu = \xi_v + i\eta_v, \quad \zeta_{\mu+1} = \xi_v - i\eta_v \quad (v = 1 + \lfloor \mu/2 \rfloor), \quad \mu \text{ (odd)} = 1,3,\ldots,m-1. \tag{6.5}$$

Here, the polynomial

$$\omega_m(t) = \prod_{v=1}^{m/2}[(1 + \xi_v t)^2 + \eta_v^2 t^2] \tag{6.6}$$

is strictly positive on all of $\mathbb{R}$, and the Gauss formula (6.1) again exists and is unique for each n and m.

(iii) *Simple conjugate complex poles plus a real pole*: This is the case where in addition to pairs of conjugate complex poles there is one simple real pole, i.e., m is odd and

$$\zeta_\mu = \xi_\nu + i\eta_\nu, \quad \zeta_{\mu+1} = \xi_\nu - i\eta_\nu \quad (\nu = 1 + \lfloor \mu/2 \rfloor), \quad \zeta_m = \xi_m \in \mathbb{R}, \quad \mu \text{ (odd)} = 1, 3, \ldots, m-2. \tag{6.7}$$

The polynomial ω_m is now

$$\omega_m(t) = (1 + \xi_m t) \prod_{\nu=1}^{(m-1)/2} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2] \tag{6.8}$$

and is of constant sign on the support of $d\lambda$. Here again, formula (6.1) exists uniquely for all n and m, and is positive.

Some, or all, of the above poles could have multiplicity 2 or higher.

For rational Gauss and Gauss–Lobatto formulae on $[-1, 1]$, with $d\lambda(t) = (1 - t^2)^{-1/2}\, dt$, and with poles distributed as in (i) and (ii), see also [39,40].

7. Spectral characterization of the Gauss formula (6.1)

We assume that $d\hat{\lambda} = d\lambda/\omega_m$ is a positive measure. The connection between Gaussian quadrature and orthogonal polynomials is well known. The polynomials we need are those orthogonal with respect to $d\hat{\lambda}$; we assume them to be monic and denote them by $\hat{\pi}_k(\cdot) = \pi_k(\cdot; d\hat{\lambda})$, $k = 0, 1, 2, \ldots$. They satisfy a three-term recurrence relation

$$\begin{aligned} &\hat{\pi}_{k+1}(t) = (t - \hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k \hat{\pi}_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ &\hat{\pi}_{-1}(t) = 0, \quad \hat{\pi}_0(t) = 1, \end{aligned} \tag{7.1}$$

where $\hat{\alpha}_k \in \mathbb{R}$ and $\hat{\beta}_k > 0$. Associated with the recurrence relation is the *Jacobi matrix*

$$\hat{J} = J(d\hat{\lambda}) = \begin{bmatrix} \hat{\alpha}_0 & \sqrt{\hat{\beta}_1} & & & \\ \sqrt{\hat{\beta}_1} & \hat{\alpha}_1 & \sqrt{\hat{\beta}_2} & & \\ & \sqrt{\hat{\beta}_2} & \hat{\alpha}_2 & \sqrt{\hat{\beta}_3} & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{7.2}$$

an infinite symmetric tridiagonal matrix. Although $\hat{\beta}_0$ is arbitrary (it multiplies $\hat{\pi}_{-1} = 0$ in (7.1)), it is customary to define it as

$$\hat{\beta}_0 = \int_{\mathbb{R}} d\hat{\lambda}(t). \tag{7.3}$$

If we are interested in the n-point quadrature rule (6.1), we need only the first $n + 1$ orthogonal polynomials $\hat{\pi}_0, \hat{\pi}_1, \ldots, \hat{\pi}_n$, hence the truncated Jacobi matrix $\hat{J}_n$ — the $n \times n$ leading principal minor matrix of (7.2). The quadrature rule can then be characterized in terms of the eigenvalues and eigenvectors of $\hat{J}_n$ [23]. Indeed, the Gauss nodes t_ν^G are the eigenvalues of $\hat{J}_n$, and the Gauss weights

w_v^G expressible in terms of the first components $v_{v,1}$ of the corresponding normalized eigenvectors v_v; more precisely,

$$\hat{J}_n v_v = t_v^G v_v, \quad v_v^T v_v = 1,$$
$$w_v^G = \hat{\beta}_0 v_{v,1}^2. \tag{7.4}$$

To compute the Gauss formula, it suffices therefore to solve an eigenvalue/eigenvector problem for a real symmetric tridiagonal matrix. This, nowadays, is a routine problem, and there are fast and accurate methods available for its solution, including appropriate software (cf., e.g., [18, Section 6]). The major challenge is the computation of the recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$, since $d\hat{\lambda} = d\lambda/\omega_m$ is not a standard classical measure. For these, one can use a simple discretization procedure and special techniques for "difficult" poles, i.e., poles very close to the support interval of the measure $d\lambda$. These latter techniques are somewhat technical and will not be described here in detail. Basically, one first applies the discretization procedure to the "reduced" measure $d\tilde{\lambda} = d\lambda/\tilde{\omega}_m$, where $\tilde{\omega}_m$ is the polynomial ω_m with the difficult poles removed, and then incorporates the difficult poles by special techniques; see [19]. The discretization procedure is described in the next section.

8. The discretization procedure

If the inner product underlying the measure $d\hat{\lambda}$ is denoted by

$$(u,v) = \int_{\mathbb{R}} u(t)v(t)\,d\hat{\lambda}(t), \quad d\hat{\lambda}(t) = \frac{d\lambda(t)}{\omega_m(t)}, \tag{8.1}$$

then, as is well known, the desired coefficients can be expressed in terms of this inner product and the orthogonal polynomials $\hat{\pi}_k(\cdot) = \pi_k(\cdot; d\hat{\lambda})$ as

$$\hat{\alpha}_k = \frac{(t\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_k, \hat{\pi}_k)}, \quad 0 \leqslant k \leqslant n-1,$$
$$\hat{\beta}_0 = (\hat{\pi}_0, \hat{\pi}_0), \quad \hat{\beta}_k = \frac{(\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_{k-1}, \hat{\pi}_{k-1})}, \quad k = 1,2,\ldots n-1. \tag{8.2}$$

This suggests, as already noted by Stieltjes, a simple "bootstrapping" procedure, which is now known as *Stieltjes procedure*: Since $\hat{\pi}_0 = 1$ is known, one computes $\hat{\alpha}_0$, $\hat{\beta}_0$ by (8.2) for $k = 0$. With $\hat{\alpha}_0$, $\hat{\beta}_0$ at hand, the recurrence relation (7.1), with $k = 0$, yields $\hat{\pi}_1$. This allows us to apply (8.2) with $k = 1$ to get $\hat{\alpha}_1$, $\hat{\beta}_1$, which by (7.1) for $k = 1$ yields $\hat{\pi}_2$, and so forth. The major difficulty with this procedure is the computation of the inner products in (8.2); this requires integration with respect to the measure $d\hat{\lambda}$, which is not straightforward.

However, already in 1968, and later in 1994, we proposed a simple modification of Stieltjes's procedure [14,18], which consists in applying it to a discrete inner product

$$(u,v)_N = \sum_{k=1}^{N} \omega_k^{(N)} u(t_k^{(N)}) v(t_k^{(N)}), \quad N > n, \tag{8.3}$$

which approximates (u,v) in such a way that

$$\lim_{N\to\infty}(u,v)_N=(u,v) \quad \text{for all } u,v\in\mathbb{P}. \tag{8.4}$$

Here, $\mathbb{P}$ is the space of polynomials. If $\hat{\pi}_{k,N}$ denote the discrete orthogonal polynomials associated with the inner product (8.3), and $\hat{\alpha}_{k,N}$, $\hat{\beta}_{k,N}$ the respective recursion coefficients, it can be shown [14, Section 4] that for any fixed k,

$$\lim_{N\to\infty}\hat{\alpha}_{k,N}=\hat{\alpha}_k, \quad \lim_{N\to\infty}\hat{\beta}_{k,N}=\hat{\beta}_k. \tag{8.5}$$

There is no difficulty in computing the $\hat{\alpha}_{k,N}$, $\hat{\beta}_{k,N}$ by a procedure analogous to Stieltjes's procedure — now known as the *discrete Stieltjes procedure* — since all inner products required are finite sums.

A natural way of obtaining a discretization (8.3) is by applying the Gaussian quadrature rule for the measure $\mathrm{d}\lambda$ to (8.1), i.e., by taking

$$t_k^{(N)}=t_k^{(N)}(\mathrm{d}\lambda), \quad \omega_k^{(N)}=\frac{w_k^{(N)}(\mathrm{d}\lambda)}{\omega_m(t_k^{(N)})}, \quad k=1,2,\ldots,N, \tag{8.6}$$

where $t_k^{(N)}(\mathrm{d}\lambda)$ and $w_k^{(N)}(\mathrm{d}\lambda)$ are the nodes and weights of the N-point Gaussian quadrature rule for $\mathrm{d}\lambda$. Since $\mathrm{d}\lambda$ is usually one of the classical measures, these quantities are easily computed; for related software, see, e.g., [18, Section 2]. Also, the procedure converges relatively fast as $N\to\infty$, unless there are poles very close to the support interval of $\mathrm{d}\lambda$. It is for this reason that special techniques are required for incorporating these "difficult" poles.

9. Examples

We present four examples for the application of rational Gauss formulae, illustrating the three configurations (i)–(iii) of poles described in Section 6 and a case of a single pole with high multiplicity. The numerical results shown were obtained with the help of software described in [19].

Example 1.

$$I(\omega)=\int_0^1\frac{t^{-1/2}\Gamma(1+t)}{t+\omega}\,\mathrm{d}t, \quad \omega>0.$$

Here, the appropriate measure is $\mathrm{d}\lambda(t)=t^{-1/2}\,\mathrm{d}t$, a Jacobi measure on $[0,1]$ with parameters $\alpha=0$, $\beta=-\frac{1}{2}$. The poles of the integrand are all real; those of the gamma function are located at $-1,-2,-3,\ldots$ and the remaining pole is at $-\omega$. This suggests the choices

$$\xi_\mu=\frac{1}{\mu}, \quad \mu=1,2,\ldots,m-1; \quad \xi_m=\frac{1}{\omega} \tag{9.1}$$

in (6.2) and thus the polynomial ω_m in (6.3). (Note that $\xi_\mu=\xi_m$ if ω is an integer μ with $1\leqslant\mu\leqslant m-1$. In this case, $1/\omega_m$ has a pole of multiplicity 2 at $-1/\xi_\mu$.) The rational n-point Gauss formula applied to $I(\omega)$ then becomes

$$I(\omega)\approx I_n(\omega)=\sum_{v=1}^{n}\lambda_v\frac{\Gamma(1+t_v)}{t_v+\omega}. \tag{9.2}$$

Table 1
Numerical results for Example 1

$n \setminus m$	$2n$	n	1	0
2	0.995E−03	0.331E−03	0.104E−02	0.143E−01
4	0.258E−06	0.372E−07	0.877E−06	0.819E−04
6	0.153E−10	0.120E−11	0.769E−09	0.431E−06
8	0.377E−13	0.398E−13	0.571E−12	0.223E−08
13				0.419E−13

The discretization method for computing the recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$, and hence the nodes t_v and weights λ_v (in terms of the eigenvalues and eigenvectors of the Jacobi matrix $\hat{J}_n$) works rather well if ω is not exceptionally small. For $\omega = \frac{1}{2}$, for example, it yields essentially machine accuracy (in IEEE standard double precision) with $N = 45$ in (8.6) when $n \leqslant 10$. Some numerical results in this case are shown in Table 1, which lists the relative errors $|[I(\omega) - I_n(\omega)]/I(\omega)|$ for the choices $m = 2n, n, 1$, and 0. The last choice corresponds to applying the ordinary Gauss rule for the measure $d\lambda$. Curiously, the results for $m = n$ are slightly more accurate than those for $m = 2n$, a phenomenon also observed in the subsequent examples.

For $\omega = 0.001$, the discretization method must work hard to get comparable accuracy; typically, $N = 350$ in this case.

Example 2. Generalized Fermi–Dirac integral

$$F_k(\eta, \theta) = \int_0^\infty \frac{t^k \sqrt{1 + \frac{1}{2}\theta t}}{e^{-\eta + t} + 1} \, dt, \quad \eta \in \mathbb{R}, \ \theta \geqslant 0. \tag{9.3}$$

Integrals of this type are of interest in solid-state physics, where the parameter k assumes half-integer values $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, and θ is a small parameter; cf. [17] and the literature cited therein.

To prepare the integral (9.3) for the application of our method, we write it in the form

$$F_k(\eta, \theta) = \int_0^\infty \frac{\sqrt{1 + \frac{1}{2}\theta t}}{e^{-\eta} + e^{-t}} t^k e^{-t} \, dt, \tag{9.4}$$

suggesting the integration measure $d\lambda(t) = t^k e^{-t} \, dt$ on $[0, \infty]$ — a generalized Laguerre measure. The integrand in (9.4) has poles at $t = \eta \pm \mu i\pi$, μ (odd) $= 1, 3, 5, \ldots$. The pairs of poles closest to the interval $[0, \infty]$ are captured by taking m even and

$$\zeta_\mu = -\frac{1}{\eta + \mu i\pi}, \qquad \zeta_{\mu+1} = -\frac{1}{\eta - \mu i\pi}, \quad \mu \text{ (odd)} = 1, 3, \ldots, m - 1. \tag{9.5}$$

The discretization method works well for all η and for θ not too large. Numerical results analogous to those in Table 1, for $k = \frac{1}{2}$, $\eta = -1$, $\theta = 10^{-4}$, are shown in Table 2.

For larger values of θ, one should include the square root $\sqrt{1 + \frac{1}{2}\theta t}$ in the measure $d\lambda$ and proceed as before.

Table 2
Numerical results for Example 2

$n \setminus m$	$2n$	n	2	0
2	0.134E−02	0.414E−03	0.414E−03	0.377E−02
4	0.487E−06	0.861E−07	0.935E−06	0.241E−03
6	0.127E−09	0.374E−12	0.118E−07	0.262E−05
8	0.220E−13	0.111E−13	0.423E−09	0.250E−05
10	0.726E−14	0.669E−14	0.221E−10	0.158E−06
15			0.304E−13	0.407E−08
20			0.707E−14	0.205E−09
40				0.745E−14

Example 3. Generalized Bose–Einstein integral

$$G_k(\eta,\theta)=\int_0^\infty \frac{t^k\sqrt{1+\frac{1}{2}\theta t}}{\mathrm{e}^{-\eta+t}-1}\,\mathrm{d}t, \quad \eta<0,\ \theta\geqslant 0. \tag{9.6}$$

This is conveniently rewritten as

$$G_k(\eta,\theta)=\int_0^\infty \frac{t\sqrt{1+\frac{1}{2}\theta t}}{\mathrm{e}^{-\eta}-\mathrm{e}^{-t}}t^{k-1}\mathrm{e}^{-t}\,\mathrm{d}t, \tag{9.7}$$

where a factor t was split off in order for the integrand to remain regular as $t\to 0$, even if η were zero. The measure of integration therefore is $\mathrm{d}\lambda(t)=t^{k-1}\mathrm{e}^{-t}\,\mathrm{d}t$ on $[0,\infty]$. The poles of the integrand are at $t=\eta+2\nu\mathrm{i}\pi$, $\nu=0,\pm1,\pm2,\ldots$, which include a real pole at η. We thus take m odd and let

$$\zeta_\mu=-\frac{1}{\eta+(\mu+1)\mathrm{i}\pi}, \qquad \zeta_{\mu+1}=-\frac{1}{\eta-(\mu+1)\mathrm{i}\pi}, \quad \mu\ (\text{odd})=1,3,\ldots,m-2, \tag{9.8}$$

$$\zeta_m=-\frac{1}{\eta}.$$

Again, as in the preceding example, the discretization works well for $|\eta|$ not too small and θ not too large. Numerical results for $k=\frac{1}{2}$, $\eta=-1$, $\theta=10^{-4}$ are shown in Table 3.

It can be seen that the rational methods here perform significantly better than the polynomial method (for $m=0$) as far as accuracy is concerned.

Example 4. A radiation transfer integral[1]

$$G_m(c)=2\int_0^1 P_m(x)[\sin(2\pi x)]^2\mathrm{e}^{-c/x}\,\mathrm{d}x, \quad c>0. \tag{9.9}$$

Here, P_m is the Legendre polynomial of degree m, and interest rests in large values of m.

[1] This example was kindly communicated to the author by Dr. Martin Gander.

Table 3
Numerical results for Example 3

$n \setminus m$	$2n-1$	$n-1$	1	0
2	0.783E−02	0.362E−02	0.362E−02	0.357E−01
4	0.317E−05	0.831E−06	0.262E−04	0.398E−02
6	0.859E−09	0.122E−10	0.720E−06	0.700E−03
8	0.197E−12	0.482E−13	0.202E−07	0.160E−03
10	0.132E−14	0.585E−15	0.115E−08	0.430E−04
15			0.837E−11	0.261E−05
20			0.924E−13	0.243E−06
40				0.154E−09
80				0.219E−14

Although the following is not necessarily the best way to proceed, it nicely illustrates the case of a pole of high multiplicity. The change of variables

$$x = \frac{1}{1+t/c}, \quad 0 \leqslant t \leqslant \infty$$

yields

$$G_m(c) = \frac{2e^{-c}}{(2\pi)^2 c} \int_0^\infty P_m\left(\frac{1}{1+t/c}\right) \left[\frac{2\pi}{1+t/c} \sin \frac{2\pi}{1+t/c}\right]^2 e^{-t}\, dt.$$

We choose to use n-point rational Gauss quadrature with

$$n \geqslant 1 + \lfloor m/2 \rfloor,$$

$$d\lambda(t) = \left[\frac{2\pi}{1+t/c} \sin \frac{2\pi}{1+t/c}\right]^2 e^{-t}\, dt \quad \text{on } [0,\infty]$$

and

$$\mathbb{Q}_m = \text{span}\{g\colon g(t) = (1+t/c)^{-s},\ s = 1,2,\ldots,m\}.$$

Since, by the choice of n, we have

$$\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m} \supset \mathbb{Q}_m \oplus \mathbb{P}_0$$

and clearly $P_m(1/(1+t/c)) \in \mathbb{Q}_m \oplus \mathbb{P}_0$, the rational Gauss formula so constructed should give the exact answer for $G_m(c)$ except for rounding errors. The latter, unfortunately, are somewhat bothersome because of the highly oscillatory behavior of the integrand $f(t) = P_m(1/(1+t/c))$ when m is large. For example, if $m = 50$ and $c = 2$, we find (in IEEE double precision)

$$G_{50}(2) = \begin{cases} \textbf{0.29351229}600590\text{E}-07 & \text{if } n = 26, \\ \textbf{0.29351229}563622\text{E}-07 & \text{if } n = 27. \end{cases}$$

Theoretically, the results should be identical, but cancellation errors in the evaluation of the quadrature sum wipe out about 5 of the 14 decimal digits.

10. Other types of integrals

Similar techniques apply, with similar success, to other types of integrals (cf. [21]).

10.1. Rational Gauss–Kronrod quadrature

The theorem of Section 3 holds also for Gauss–Kronrod quadrature, where the polynomial formula (3.2) is now

$$\int_{\mathbb{R}} p(t)\frac{d\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^{K}\, p(t_v^{G}) + \sum_{\mu=1}^{n+1} w_\mu^{*K}\, p(t_\mu^{K}), \quad p \in \mathbb{P}_{3n+1}. \tag{10.1}$$

Here, t_v^{G} are the nodes of the n-point Gauss formula for the measure $d\lambda/\omega_m$, and w_v^{K}, w_μ^{*K}, t_μ^{K} are determined so as to have maximum polynomial degree of exactness $3n+1$. Assuming that this formula exists with distinct "Kronrod" nodes t_μ^{K} on the support of $d\lambda$, all different from the Gauss nodes t_v^{G}, the corresponding rational Gauss–Kronrod formula is given by

$$\int_{\mathbb{R}} g(t)\,d\lambda(t) = \sum_{v=1}^{n} \lambda_v^{K} g(\tau_v^{G}) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} g(\tau_\mu^{K}) + R_n^{K}(g), \tag{10.2}$$

where

$$R_n^{K}(g) = 0 \quad \text{for } g \in \mathbb{S}_{3n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{3n+1-m}, \quad 0 \leqslant m \leqslant 3n+2, \tag{10.3}$$

provided that

$$\tau_v^{G} = t_v^{G}, \quad \tau_\mu^{K} = t_\mu^{K}; \quad \lambda_v^{K} = w_v^{K}\omega_m(t_v^{G}), \quad \lambda_\mu^{*K} = w_\mu^{*K}\omega_m(t_\mu^{K}). \tag{10.4}$$

We recall (see, e.g., [15]) that t_v^{G} in (10.1) are the zeros of $\hat{\pi}_n(\,\cdot\,) = \pi_n(\cdot; d\lambda/\omega_m)$, and t_μ^{K} the zeros of $\pi_{n+1}^{*}(\,\cdot\,) = \pi_{n+1}(\cdot; \hat{\pi}_n\, d\lambda/\omega_m)$. Constructive procedures for computing Gauss–Kronrod formulae that, like the Golub–Welsch procedure, are based on eigenvalues and eigenvectors of a Jacobi-like matrix of order $2n+1$, have recently been developed by Laurie [32], Ammar et al. [1], and Calvetti et al. [12]; see also [20]. Rational Gauss–Kronrod rules are also considered in [2, Section 4.2], where an asymptotic error estimate is given for analytic functions.

10.2. Rational Gauss–Turán quadrature

These are Gauss-type formulae in which not only function values, but also derivative values up to some even order, occur in the quadrature sum. The polynomial formula (analogous to (3.2)) has the form

$$\int_{\mathbb{R}} p(t)\frac{d\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n}\sum_{\sigma=0}^{2s} w_v^{(\sigma)T}\, p^{(\sigma)}(t_v^{T}), \quad p \in \mathbb{P}_{2(s+1)n-1}, \tag{10.5}$$

whereas the rational counterpart is

$$\int_{\mathbb{R}} g(t)\,d\lambda(t) = \sum_{v=1}^{n}\sum_{\sigma=0}^{2s} \lambda_v^{(\sigma)} g^{(\sigma)}(\tau_v) + R_n^{T}(g) \tag{10.6}$$

with the exactness property

$$R_n^{\mathrm{T}}(g) = 0 \quad \text{for } g \in \mathbb{S}_{2(s+1)n} = \mathbb{Q}_m \oplus \mathbb{P}_{2(s+1)n-m-1}, \quad 0 \leqslant m \leqslant 2(s+1)n, \tag{10.7}$$

provided that

$$\tau_v = t_v^{\mathrm{T}}, \quad v = 1, 2, \ldots, n,$$

$$\lambda_v^{(\sigma)} = \sum_{\rho=\sigma}^{2s} w_v^{(\rho)\mathrm{T}} \binom{\rho}{\sigma} \omega_m^{(\rho-\sigma)}(t_v^{\mathrm{T}}), \quad v = 1, 2, \ldots, n, \quad \sigma = 0, 1, \ldots, 2s. \tag{10.8}$$

We recall that t_v^{T} in (10.5) are the zeros of the nth-degree s-orthogonal polynomial $\pi_{n,s}$ for the measure $\mathrm{d}\lambda/\omega_m$, i.e., the polynomial of degree n which satisfies the power orthogonality relation

$$\int_{\mathbb{R}} [\pi_{n,s}(t)]^{2s+1} p(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}. \tag{10.9}$$

Constructive procedures for generating Gauss–Turán formulae (10.5) are discussed in [22].

10.3. Rational Cauchy principal value quadrature

Here the object is to construct a quadrature rule of the form

$$\int\!\!\!\!\!\!-_{\mathbb{R}} \frac{g(t)}{t-x} \mathrm{d}\lambda(t) = \sum_{v=1}^{n} \frac{\lambda_v}{\tau_v - x} g(\tau_v) + \lambda_0(x) g(x) + R_n^{\mathrm{C}}(g), \tag{10.10}$$

where

$$\lambda_0(x) = \int\!\!\!\!\!\!-_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{t-x} - \sum_{v=1}^{n} \frac{\lambda_v}{\tau_v - x} \tag{10.11}$$

and where we require the exactness condition

$$R_n^{\mathrm{C}}(g) = 0 \quad \text{for all } g \in \mathbb{S}_{2n+1} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-m}, \quad 0 \leqslant m \leqslant 2n. \tag{10.12}$$

Note that x is assumed to be inside the support of $\mathrm{d}\lambda$, so that the integrals in (10.10) and (10.11) are Cauchy principal value integrals.

It turns out that the exactness property (10.12) can be achieved for the formula (10.10) if we choose

$$\tau_v = t_v^{\mathrm{G}}, \quad \lambda_v = w_v^{\mathrm{G}} \omega_m(t_v^{\mathrm{G}}), \quad v = 1, 2, \ldots, n, \tag{10.13}$$

where t_v^{G} and w_v^{G} are the Gauss nodes and weights for the measure $\mathrm{d}\lambda/\omega_m$,

$$\int_{\mathbb{R}} p(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^{\mathrm{G}} p(t_v^{\mathrm{G}}), \quad p \in \mathbb{P}_{2n-1}, \tag{10.14}$$

provided that none of the t_v^{G} equals x. Formula (10.14) can be constructed as described in Sections 7 and 8.

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GENERALIZED GAUSS–RADAU AND GAUSS–LOBATTO FORMULAE

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Abstract.

Computational methods are developed for generating Gauss-type quadrature formulae having nodes of arbitrary multiplicity at one or both end points of the interval of integration. Positivity properties of the boundary weights are investigated numerically, and related conjectures are formulated. Applications are made to moment-preserving spline approximation.

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1 Introduction.

Gauss–Radau and Gauss–Lobatto formulae, as is well known, are quadrature formulae of Gauss type involving function values not only at interior points of the interval of integration, but also at one or both end points of this interval. The phrase "of Gauss type" means that the polynomial degree of exactness of these formulae is as large as possible subject to the constraints on the nodes. Similarly, one can define *generalized* Gauss–Radau and Gauss–Lobatto formulae in which not only function values at one or both end points appear, but also consecutive derivative values up to an arbitrary finite order $r-1$. These are of interest, e.g., in moment-preserving spline approximation on a compact interval (cf. Section 4). Thus, in the case of Gauss–Radau formulae, they have the form

$$\int_a^\infty f(t)\,\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(a) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_{n,r}^R(f), \tag{1.1}$$

where $r > 1$ is the multiplicity of the end point a and $\mathrm{d}\lambda$ a positive measure with (bounded or unbounded) support contained in $[a,\infty]$. The degree of exactness is $2n-1+r$,

$$R_{n,r}^R(f) = 0 \quad \text{for all } f \in \mathbb{P}_{2n-1+r}. \tag{1.2}$$

Here and in the following, $\mathbb{P}_m$ denotes the space of real polynomials of degree $\le m$. The internal nodes τ_ν^R and weights λ_ν^R, as well as the weights $\lambda_0^{(\rho)}$, although not expressed in our notation, all depend on n and r.

Naturally, there is an analogous formula for $\int_{-\infty}^{b} f(t)\,\mathrm{d}\lambda(t)$ with fixed multiple node at $t=b$.

In the case of the generalized Gauss–Lobatto formula, the support of $\mathrm{d}\lambda$ is assumed to be contained in a finite interval $[a,b]$, $a<b$, and the formula takes the form

$$\int_a^b f(t)\,\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1}\lambda_0^{(\rho)}f^{(\rho)}(a)+\sum_{\nu=1}^{n}\lambda_\nu^L f(\tau_\nu^L)+ \\ +\sum_{\rho=0}^{r-1}(-1)^\rho\lambda_{n+1}^{(\rho)}f^{(\rho)}(b)+R_{n,r}^L(f), \tag{1.3}$$

where

$$R_{n,r}^L(f)=0 \quad \text{for all } f\in\mathbb{P}_{2n-1+2r}. \tag{1.4}$$

We have included signs $(-1)^\rho$ in the weights of the derivative values at $t=b$ in anticipation of the fact that $\lambda_0^{(\rho)}=\lambda_{n+1}^{(\rho)}$ in the case of symmetric formulae, that is, formulae with $a+b=0$ and $\mathrm{d}\lambda(-t)=\mathrm{d}\lambda(t)$.

The characterization of the internal nodes and weights of generalized Gauss–Radau and Gauss–Lobatto formulae is well known; see, e.g., [1, Theorems 3.9 and 3.12]. In the former case,

$$\tau_\nu^R=\tau_\nu^{[r]},\qquad \lambda_\nu^R=\frac{\lambda_\nu^{[r]}}{(\tau_\nu^R-a)^r},\quad \nu=1,2,\dots,n, \tag{1.5}$$

where $\tau_\nu^{[r]}$, $\lambda_\nu^{[r]}$ are the nodes and weights of the n-point Gauss quadrature formula for the measure

$$\mathrm{d}\lambda^{[r]}(t)=(t-a)^r\,\mathrm{d}\lambda(t)\quad\text{(Radau)}, \tag{1.6}$$

while in the latter case,

$$\tau_\nu^L=\tau_\nu^{[r]},\qquad \lambda_\nu^L=\frac{\lambda_\nu^{[r]}}{[(\tau_\nu^L-a)(b-\tau_\nu^L)]^r},\quad \nu=1,2,\dots,n, \tag{1.7}$$

with $\tau_\nu^{[r]}$, $\lambda_\nu^{[r]}$ the Gaussian nodes and weights of

$$\mathrm{d}\lambda^{[r]}(t)=[(t-a)(b-t)]^r\,\mathrm{d}\lambda(t)\quad\text{(Lobatto)}. \tag{1.8}$$

All internal weights are therefore positive, and the same is true for the boundary weights if $r=2$ (cf. Sections 2.2 and 3.2). In this latter case, explicit formulae are known for the Legendre measure $\mathrm{d}\lambda(t)=\mathrm{d}t$ on $[-1,1]$ ([1, Examples 3.10 and 3.13]) and for all four Chebyshev measures [2]. Other than that, little is known about generalized Gauss–Radau and Gauss–Lobatto formulae.

In this paper, we develop a procedure for computing such formulae for arbitrary r. Respective Matlab routines `gradau.m` and `globatto.m` are downloadable

from the Web site `http://www.cs.purdue.edu/archives/2002/wxg/codes/` which contains a suite of many other useful routines, in part assembled as a companion piece to the book in [1]. All Matlab routines referred to in this paper are downloadable individually from this site, in particular also routines developed for testing `gradau.m` and `globatto.m`. Both routines are used to investigate (numerically) the positivity of the boundary weights. In Section 4 we illustrate the use of these routines in the context of moment-preserving spline approximation.

2 The generalized Gauss–Radau formula.

2.1 Computational method.

The measure relevant for the internal nodes and weights, by (1.6), is obtained by r successive modifications of the measure $\mathrm{d}\lambda(t)$ by the linear factor $t-a$. The respective orthogonal polynomials can thus be generated by r applications of the routine `chri1.m` (cf. [1, §2.4.2]). For the computation of $\tau_\nu^{[r]}$ and $\lambda_\nu^{[r]}$ in (1.5) one then applies the Gauss quadrature routine `gauss.m`.

In order to compute the boundary weights $\lambda_0^{(\rho)}$ in (1.1), we use (1.1) with $f(t) = (t-a)^{i-1}\pi_n^2(t)$, $i = 1, 2, \ldots, r$, where $\pi_n(t) = \prod_{\nu=1}^{n}(t-\tau_\nu^R)$, and note, since $f \in \mathbb{P}_{2n-1+r}$, that the remainder is zero, and by the choice of f, that all terms in the quadrature sum are zero except the boundary terms with $\rho \geq i-1$. Therefore,

$$\sum_{\rho=i-1}^{r-1} \lambda_0^{(\rho)}[(t-a)^{i-1}\pi_n^2(t)]_{t=a}^{(\rho)} = b_i, \tag{2.1}$$

$$b_i = \int_a^\infty (t-a)^{i-1}\pi_n^2(t)\,\mathrm{d}\lambda(t),\ i = 1, 2, \ldots, r.$$

Here, the integrals on the right are computable (exactly) by $(n + \lfloor (r+1)/2 \rfloor)$-point Gauss quadrature with respect to the measure $\mathrm{d}\lambda$. Writing $\rho = j-1$, $j = i, i+1, \ldots, r$, Equations (2.1) represent an upper triangular system of linear algebraic equations

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \quad \boldsymbol{A} \in \mathbb{R}^{r\times r},\ \boldsymbol{x}, \boldsymbol{b} \in \mathbb{R}^r, \tag{2.2}$$

where

$$\boldsymbol{A} = [a_{ij}], \quad a_{ij} = [(t-a)^{i-1}\pi_n^2(t)]_{t=a}^{(j-1)}, \quad j \geq i; \qquad a_{ij} = 0,\ j < i, \tag{2.3}$$

$$\boldsymbol{x} = [x_j], \quad x_j = \lambda_0^{(j-1)}; \qquad \boldsymbol{b} = [b_i].$$

When applying Leibniz's rule to compute a_{ij}, only one term survives, namely the one in which the first factor $(t-a)^{i-1}$ is differentiated $i-1$ times and the other factor $j-1-(i-1) = j-i$ times. Thus,

$$a_{ij} = \binom{j-1}{j-i}(i-1)![\pi_n^2(t)]_{t=a}^{(j-i)}, \quad j \geq i. \tag{2.4}$$

It remains to compute the derivatives $[\pi_n^2(t)]_{t=a}^{(s)}$. Since $\pi_n^2(t) = \prod_{\nu=1}^n (\tau_\nu^R - t)^2$, we have

$$[\pi_n^2(t)]' = -2\sum_{\nu=1}^n (\tau_\nu^R - t) \prod_{\mu\neq\nu} (\tau_\mu^R - t)^2 = -2\pi_n^2(t) \sum_{\nu=1}^n (\tau_\nu^R - t)^{-1}.$$

Differentiating this $j-i-1$ times by Leibniz's rule, and then putting $t=a$, yields, for $j > i$,

$$[\pi_n^2(t)]_{t=a}^{(j-i)} = -2 \sum_{\sigma=0}^{j-i-1} \binom{j-i-1}{\sigma} [\pi_n^2(t)]_{t=a}^{(j-i-1-\sigma)} \cdot \sigma! \sum_{\nu=1}^n (\tau_\nu^R - a)^{-(\sigma+1)}.$$

With (2.4) used both on the left and on the right, this gives, for $i = r-1$, $r-2, \ldots, 1$,

$$a_{ij} = -\frac{2}{j-i} \sum_{\sigma=0}^{j-i-1} a_{i+1+\sigma,j} \sum_{\nu=1}^n (\tau_\nu^R - a)^{-(\sigma+1)}, \quad j = i+1, i+2, \ldots, r, \tag{2.5}$$

while for $j = i$,

$$a_{ii} = (i-1)!\pi_n^2(a), \quad i = r, r-1, \ldots, 1. \tag{2.6}$$

This allows us to compute the elements of the upper triangular matrix $\boldsymbol{A}$ from the bottom up, and then to solve the system (2.2) by backward substitution. The procedure is implemented in the routine `gradau.m`.

Tests against the known formulae for $r = 2$ in the case of the Legendre and Chebyshev measures turned out to be satisfactory, even for values of n as large as $n = 160$; see the routine `test_gradau_req2.m`. A meaningful test for $r \geq 1$ is to have the generalized Gauss–Radau formula for arbitrary r, say $r = 1{:}10$, and with n internal points, compute (exactly) all moments of orders up to $2n-1+r$ for relatively small values of n, say $n = 1{:}5$. This, too, turned out very satisfactory; see the routine `test_gradau_rgt0.m`. Finally, for $r = 1$, the generalized Gauss–Radau formula reduces to the ordinary Gauss–Radau formula, so that `gradau.m` can be tested against `radau.m`. This is done successfully in the routine `test_gradau_radau.m`.

2.2 Positivity.

It is clear from (2.6) that all diagonal elements of $\boldsymbol{A}$ are positive, and from (2.1) that the same is true for the elements of $\boldsymbol{b}$. In particular, $x_r = b_r/a_{rr} > 0$. From (2.5) it can also be seen that $a_{r-1,r} < 0$, from which $x_{r-1} = (b_{r-1} - a_{r-1,r}x_r)/a_{r-1,r-1} > 0$. There follows

$$\lambda_0^{(r-1)} > 0, \qquad \lambda_0^{(r-2)} > 0. \tag{2.7}$$

Thus, if $r = 2$, the boundary weights of the generalized Gauss–Radau formula are positive. Whether or not the same is true for arbitrary $r > 2$ is an open

question. Using the routine `gradau.m`, we found numerically that positivity holds for Jacobi measures with parameters $\alpha = -.9{:}.2{:}.9$, $\beta = \alpha{:}.2{:}.9$ and with $\alpha = -.75{:}.25{:}1$, $\beta = 1, 1.5, 2, 5, 10$, each time for values of $n = 2{:}20$, $n = 25{:}5{:}40$ and $r = 2{:}10$. For the same values of α, n, and r, positivity was also observed for generalized Laguerre measures. For these two measures, therefore, it seems safe to conjecture that the generalized Gauss–Radau formula has positive boundary weights. Additional tests involving the "elliptic" Chebyshev measure ([1, Example 2.29]) and the half-range Hermite measure ([1, Example 2.31]) suggest that positivity may hold for arbitrary measures. At any rate, the situation appears to be rather different from what is known in the case of Gauss–Turán formulae, which also involve derivative values, but at internal nodes. Here one can prove positivity of the weights only for derivative terms of *even* order (cf. [1, §3.1.3.1]), whereas those of odd order may have weights of either sign.

3 The generalized Gauss–Lobatto formula.

3.1 Computational method.

The measure (1.8) determining the internal nodes and weights of the generalized Gauss–Lobatto formula is now obtained by $2r$ consecutive modifications of the measure $\mathrm{d}\lambda$, half of them with the shift a, and the other half with shift b. When r is odd, the resulting measure is negative definite, which is easily corrected by changing the sign of the coefficient β_0 produced by `chri1.m`.

The boundary weights are computed similarly as in the case of generalized Gauss–Radau formulae except for some special attention being required when r is odd. The formula (1.3) is applied once to $f(t) = (t-a)^{i-1}\pi_n^2(t)(b-t)^r$ to find the weights $\lambda_0^{(\rho)}$, and once to $f(t) = (t-b)^{i-1}\pi_n^2(t)(a-t)^r$ to determine the weights $(-1)^\rho \lambda_{n+1}^{(\rho)}$, where now $\pi_n(t) = \prod_{\nu=1}^n (t-\tau_\nu^L)$. In both cases, the remainder is zero, since $f \in \mathbb{P}_{2n-1+2r}$. Suppose first that $r \geq 2$ is even. The first choice of f then yields for $x_j = \lambda_0^{(j-1)}$ the upper triangular system (2.2) with

$$\boldsymbol{A} = [a_{ij}], \quad a_{ij} = ((t-a)^{i-1}[\pi_n^2(t)(b-t)^r])_{t=a}^{(j-1)},$$

$$\boldsymbol{b} = [b_i], \quad b_i = \int_a^b (t-a)^{i-1}\pi_n^2(t)(b-t)^r \,\mathrm{d}\lambda(t).$$

The integrals defining b_i can all be evaluated (exactly) by $(n+r)$-point Gauss quadrature relative to the measure $\mathrm{d}\lambda$.

To compute a_{ij}, we proceed similarly as in Section 2.1, writing

$$\pi_n^2(t)(b-t)^r = \prod_{\nu=1}^{n+r/2} (\tau_\nu - t)^2 \quad (r \text{ even}),$$

where $\tau_\nu = \tau_\nu^L$ for $1 \le \nu \le n$, and $\tau_\nu = b$ for $n+1 \le \nu \le n + r/2$. Then, exactly as before, one gets for $i = r, r-1, \ldots, 1$,

$$a_{ii} = (i-1)!\pi_n^2(a)(b-a)^r,$$

$$a_{ij} = -\frac{2}{j-i} \sum_{\sigma=0}^{j-i-1} a_{i+1+\sigma,j} \sum_{\nu=1}^{n+r/2} (\tau_\nu - a)^{-(\sigma+1)}, \quad j = i+1, i+2, \ldots, r, \tag{3.1}$$

and the computation is the same as in Section 2.1, except for the extended summation on the right.

When r is odd, one defines as before $\tau_\nu = \tau_\nu^L$ for $1 \le \nu \le n$ and $\tau_\nu = b$, but now for $n+1 \le \nu \le n + \lfloor (r+1)/2 \rfloor$ (which is valid also when r is even). Then

$$\pi_n^2(t)(b-t)^r = \left[\prod_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t)^2 \right] (b-t) \quad (b = \tau_{n+(r+1)/2}),$$

and one obtains

$$\begin{aligned}
&[\pi_n^2(t)(b-t)^r]' \\
&\quad = -2 \sum_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t) \prod_{\mu \ne \nu} (\tau_\mu - t)^2 \cdot (b-t) - \prod_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t)^2 \\
&\quad = -2 \sum_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t)^{-1} \prod_{\mu=1}^{n+(r-1)/2} (\tau_\mu - t)^2 \cdot (b-t) - \prod_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t)^2 \\
&\quad = -2\pi_n^2(t)(b-t)^r \left\{ \sum_{\nu=1}^{n+(r-1)/2} (\tau_\nu - t)^{-1} + \frac{1}{2}(b-t)^{-1} \right\}.
\end{aligned}$$

Thus,

$$[\pi_n^2(t)(b-t)^r]' = -2\pi_n^2(t)(b-t)^r \sum_{\nu=1}^{n+(r+1)/2}{}' (\tau_\nu - t)^{-1},$$

where the prime on the summation sign indicates that the last term in the summation is to be halved. In the same manner as in Section 2.1, differentiating $j-i-1$ times, one obtains for $j > i$

$$a_{ij} = -\frac{2}{j-i} \sum_{\sigma=0}^{j-i-1} a_{i+1+\sigma,j} \sum_{\nu=1}^{n+(r+1)/2}{}' (\tau_\nu - a)^{-(\sigma+1)}, \quad j = i+1, i+2, \ldots, r,$$

while for $j = i$, as before,

$$a_{ii} = (i-1)!\pi_n^2(a)(b-a)^r.$$

For the choice $f(t) = (t-b)^{i-1}\pi_n^2(t)(a-t)^r$, the same procedure applies, with the roles of a and b in (3.1) interchanged. The routine implementing all of this is `globatto.m`.

Tests analogous to those in Section 2.1 were performed on the routine `globatto.m` with equal success; see the routines `test_globatto_req2.m`, `test_globatto_rgt0.m`, and `test_globatto_lobatto.m`.

3.2 Positivity.

As in Section 2.2, one shows from (3.1) that

$$\lambda_0^{(r-1)} > 0, \qquad \lambda_0^{(r-2)} > 0.$$

With regard to the boundary weights at the point b, one must interchange a and b both in (3.1) and in the integrand of b_i. One then has $\operatorname{sign} a_{ii} = (-1)^r$, $\operatorname{sign} b_i = (-1)^{i-1+r}$, hence $\operatorname{sign} x_r = \operatorname{sign}(b_r/a_{rr}) = (-1)^{r+1}$, so that $\operatorname{sign}((-1)^{r-1}\lambda_{n+1}^{(r-1)}) = (-1)^{r+1}$, that is, $\lambda_{n+1}^{(r-1)} > 0$. Similarly, $\operatorname{sign} a_{r-1,r} = (-1)^r$, $\operatorname{sign} x_{r-1} = \operatorname{sign}[(b_{r-1} - a_{r-1,r}x_r)/a_{r-1,r-1}] = \operatorname{sign} a_{r-1,r-1} = (-1)^r$, so that $\operatorname{sign}[(-1)^{r-2}\lambda_{n+1}^{(r-2)}] = (-1)^r$, and $\lambda_{n+1}^{(r-2)} > 0$. Thus, generalized Gauss–Lobatto formulae, when $r = 2$, have boundary weights satisfying

$$\lambda_0^{(\rho)} > 0, \qquad \lambda_{n+1}^{(\rho)} > 0, \quad \rho = 0, 1, \ldots, r-1 \ (r = 2). \tag{3.2}$$

Positivity in the case $r > 2$ is still an open question. Numerical tests with `globatto.m` for the same Jacobi measures as in Section 2.2, and for the same values of $n \geq 3$ and r, revealed positivity in all cases (cf. the routine `globatto_pos.m`). We therefore conjecture that the generalized Gauss–Lobatto formula for Jacobi measures has boundary weights satisfying (3.2) for arbitrary $r > 2$. Judging from additional tests with the elliptic Chebyshev measure, we believe that positivity holds for other, if not all, measures as well.

4 Examples.

It is known (cf. [1, §3.3]) that Gauss-type quadrature formulae, and in particular generalized Gauss–Lobatto and Gauss–Radau formulae, are useful in generating spline approximations to functions f that reproduce as many consecutive moments of f as possible. For approximation on the positive real line $\mathbb{R}_+$, the measure involved is

$$\mathrm{d}\lambda^{[m]}(t) = \frac{(-1)^{m+1}}{m!} t^{m+1} f^{(m+1)}(t)\,\mathrm{d}t, \quad t \in \mathbb{R}_+, \tag{4.1}$$

where m is the degree of the spline. The spline, in this case, has the form

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (t_\nu - t)_+^m, \quad t \in \mathbb{R}_+, \tag{4.2}$$

where $u_+(t) = \max(0, u(t))$ and $0 < t_1 < t_2 < \cdots < t_n < \infty$ are the knots of the spline. These are assumed freely variable (subject to ordering), and so

are the coefficients $a_\nu \in \mathbb{R}$. Given the first $2n$ moments $\mu_j = \int_{\mathbb{R}_+} f(t)t^j \, \mathrm{d}t$, $j = 0, 1, \ldots, 2n-1$, of f, the problem on $\mathbb{R}_+$ is to find $s_{n,m}$ such that

$$\int_{\mathbb{R}_+} s_{n,m}(t)t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n-1. \tag{4.3}$$

This has a unique solution precisely if the measure (4.1) admits a Gaussian quadrature formula

$$\int_{\mathbb{R}_+} g(t) \, \mathrm{d}\lambda^{[m]}(t) = \sum_{\nu=1}^{n} \lambda_\nu^G g(\tau_\nu^G), \quad g \in \mathbb{P}_{2n-1}, \tag{4.4}$$

satisfying $0 < \tau_1^G < \tau_2^G < \cdots < \tau_n^G$, in which case

$$t_\nu = \tau_\nu^G, \qquad a_\nu = \frac{\lambda_\nu^G}{[\tau_\nu^G]^{m+1}}, \quad \nu = 1, 2, \ldots, n, \tag{4.5}$$

yields the desired spline approximant (cf. [1, Theorem 3.57]).

On a compact interval $[0, 1]$, the measure involved is

$$\mathrm{d}\lambda^{[m]}(t) = \frac{(-1)^{m+1}}{m!} f^{(m+1)}(t) \, \mathrm{d}t, \quad t \in [0, 1]. \tag{4.6}$$

In this case, a polynomial $p \in \mathbb{P}_m$ may be added to the spline in (4.2), so that

$$s_{n,m}(t) = p(t) + \sum_{\nu=1}^{n} a_\nu (t_\nu - t)_+^m, \quad t \in [0, 1], \tag{4.7}$$

where $0 < t_1 < t_2 < \cdots < t_n < 1$. Two problems are then of interest:

PROBLEM I. Determine $s_{n,m}$ in (4.7) such that

$$\int_0^1 s_{n,m}(t)t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n+m. \tag{4.8}$$

Since we have $m+1$ more parameters at our disposal (the coefficients of p), we can impose $m+1$ additional moment conditions compared to (4.3).

PROBLEM II. Determine $s_{n,m}$ in (4.7) such that

$$\int_0^1 s_{n,m}(t)t^j \, \mathrm{d}t = \mu_j, \quad j = 0, 1, \ldots, 2n-1, \tag{4.9}$$

and

$$s_{n,m}^{(\mu)}(1) = f^{(\mu)}(1), \quad \mu = 0, 1, \ldots, m. \tag{4.10}$$

Here the extra $m+1$ parameters are used to enforce the derivative conditions (4.10), which, incidentally, immediately determine p, since $s_{n,m}^{(\mu)}(1) = p^{(\mu)}(1)$.

4.1 Solution of Problem I.

By [1, Theorem 3.61], Problem I has a unique solution if and only if the measure $\mathrm{d}\lambda^{[m]}$ in (4.6) admits a generalized Gauss–Lobatto formula (1.3), with $[a,b] = [0,1]$, satisfying $0 < \tau_1^L < \tau_2^L < \cdots < \tau_n^L < 1$ and having boundary points of multiplicity $r = m+1$. The solution of Problem I is then given by

$$t_\nu = \tau_\nu^L, \qquad a_\nu = \lambda_\nu^L, \quad \nu = 0,1,\ldots,n, \tag{4.11}$$

with the polynomial p uniquely determined by its derivative values at $t = 1$,

$$p^{(\mu)}(1) = f^{(\mu)}(1) + (-1)^m m! \lambda_{n+1}^{(m-\mu)}, \quad \mu = 0,1,\ldots,m. \tag{4.12}$$

Even though the emphasis of these approximations is on preserving as many moments as possible, it is still interesting to observe how well they do with regard to pointwise approximation.

EXAMPLE 4.1. The exponential function $f(t) = \mathrm{e}^{-t}$.

This example was solved in [1, Example 3.59] on the interval $\mathbb{R}_+$ using the Gauss formula (4.4) for the measure (4.1), and (4.5). We now compare the restriction of that solution to the interval $[0,1]$ with direct solution on $[0,1]$ via (4.11) and (4.12).

Note, first of all, that the measure (4.6) in this case is

$$\mathrm{d}\lambda^{[m]}(t) = \frac{1}{m!}\,\mathrm{e}^{-t}\,\mathrm{d}t, \quad 0 < t < 1, \tag{4.13}$$

the Laguerre measure on the finite interval $[0,1]$. Its first $n+2m+2$ recurrence coefficients needed in the $2r = 2m+2$ applications of the routine `chri1.m` to the measure $\mathrm{d}\lambda^{[m]}$ (cf. the first paragraph of Section 3.1) are not known explicitly, but can easily be computed by a discretization procedure using Gauss–Legendre quadrature on $[0,1]$ to discretize the inner product for $\mathrm{d}\lambda^{[m]}$ (cf. [1, §2.2.4]). This, together with the procedure in Section 3.1, is implemented in the routine `ex3_3.m`, which also computes the restriction to $[0,1]$ of the spline approximation on $\mathbb{R}_+$ for comparison. The results are shown in the first four columns of Table 4.1, where the third column contains the maximum errors on $[0,1]$ of the spline approximation (4.2), (4.5), and the fourth column the analogous information for the spline (4.7), (4.11)–(4.12). (The maximum errors are computed on a set of 100 equally spaced points on $[0,1]$.) It is seen, not surprisingly, that the latter are significantly smaller than the former.

4.2 Solution of Problem II.

By [1, Theorem 3.62], the solution, if it exists, is now provided by the generalized Gauss–Radau formula (1.1) for the measure $\mathrm{d}\lambda^{[m]}$ in (4.6), where $[a,\infty]$ is to be replaced by $[0,1]$. Indeed,

$$t_\nu = \tau_\nu^R, \qquad a_\nu = \lambda_\nu^R, \quad \nu = 1,2,\ldots,n, \tag{4.14}$$

Table 4.1: Maximum errors in Examples 4.1 and 4.2

m	n	err	err	err
1	5	5.0419e−02	2.3346e−03	2.9070e−03
1	10	2.8150e−02	7.5711e−04	9.5130e−04
1	20	1.4824e−02	2.5198e−04	2.4060e−04
1	40	7.1401e−03	6.4979e−05	7.2096e−05
1	80	3.7475e−03	1.5633e−05	1.9889e−05
2	5	1.7857e−02	3.9962e−05	6.8379e−05
2	10	3.4965e−03	8.5681e−06	1.1922e−05
2	20	1.0938e−03	1.5137e−06	1.8741e−06
2	40	3.6171e−04	2.3831e−07	2.6307e−07
2	80	1.2197e−04	3.3245e−08	3.5524e−08
3	5	7.9365e−03	9.6683e−07	2.4463e−06
3	10	9.9900e−04	1.4155e−07	2.4701e−07
3	20	1.3962e−04	1.5061e−08	2.1292e−08
3	40	3.0058e−05	1.3686e−09	1.6194e−09
3	80	7.8536e−06	9.9495e−11	1.1154e−10

in (4.7), and p is given (trivially) by

$$p(t) = \sum_{\mu=0}^{m} \frac{f^{(\mu)}(1)}{\mu!}(t-1)^{\mu}. \tag{4.15}$$

EXAMPLE 4.2. The exponential function $f(t) = \mathrm{e}^{-t}$.

We now need only $r = m + 1$ applications of the routine `chri1.m` to the measure (4.13) (cf. the first paragraph of Section 2.1), which is done analogously as in Example 4.1. The results, also produced by the routine `ex3_3.m`, are shown in the last column of Table 4.1. They are very similar, and only slightly worse, than those in the fourth column.

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THE CIRCLE THEOREM AND RELATED THEOREMS FOR GAUSS-TYPE QUADRATURE RULES*

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Dedicated to Ed Saff on the occasion of his 60th birthday

Abstract. In 1961, P.J. Davis and P. Rabinowitz established a beautiful "circle theorem" for Gauss and Gauss–Lobatto quadrature rules. They showed that, in the case of Jacobi weight functions, the Gaussian weights, suitably normalized and plotted against the Gaussian nodes, lie asymptotically for large orders on the upper half of the unit circle centered at the origin. Here analogous results are proved for rather more general weight functions—essentially those in the Szegö class—, not only for Gauss and Gauss–Lobatto, but also for Gauss–Radau formulae. For much more restricted classes of weight functions, the circle theorem even holds for Gauss–Kronrod rules. In terms of potential theory, the semicircle of the circle theorem can be interpreted as the reciprocal density of the equilibrium measure of the interval $[-1,1]$. Analogous theorems hold for weight functions supported on any compact subset Δ of $(-1,1)$, in which case the (normalized) Gauss points approach the reciprocal density of the equilibrium measure of Δ. Many of the results are illustrated graphically.

Key words. Gauss quadrature formulae, circle theorem, Gauss–Radau, Gauss–Lobatto and Gauss–Kronrod formulae, Christoffel function, potential theory, equilibrium measure

AMS subject classifications. 65D32, 42C05

1. Introduction. One of the gems in the theory of Gaussian quadrature relates to the distribution of the Gaussian weights. In fact, asymptotically for large orders, the weights, when suitably normalized and plotted against the Gaussian nodes, come to lie on a half circle drawn over the support interval of the weight function under consideration. This geometric view of Gauss quadrature rules was first taken by Davis and Rabinowitz [2, §II], who established the asymptotic property described—a "circle theorem", as they called it—in the case of Jacobi weight functions $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha > -1$, $\beta > -1$, not only for the Gauss formula, but also for the Gauss-Lobatto formula. For the Gauss-Radau formula, they only conjectured it "with meager numerical evidence at hand". It should be mentioned, however, that the underlying asymptotic formula (see eqn (2.2) below) has previously been obtained by Erdös and Turán [4, Theorem IX], and even earlier by Akhiezer [1, p. 81, footnote 9], for weight functions $w(t)$ on $[-1,1]$ such that $w(t)\sqrt{1-t^2}$ is continuous and $w(t)\sqrt{1-t^2} \geq m > 0$ on $[-1,1]$. This answers, in part, one of the questions raised in [2, last paragraph of §IV] regarding weight functions other than those of Jacobi admitting a circle theorem. In §§2–4 we show that the circle theorem, not only for Gaussian quadrature rules, but also for Gauss–Radau and Gauss–Lobatto rules, holds essentially for all weight functions in the Szegö class, i.e., weight functions w on $[-1,1]$ for which

$$\frac{\ln w(t)}{\sqrt{1-t^2}} \in L_1(-1,1). \tag{1.1}$$

We say "essentially", since an additional, mild condition, viz.

$$1/w(t) \in L_1(\Delta),$$

must also be satisfied, where Δ is any compact subinterval of $(-1,1)$. In §5, we show, moreover, that circle theorems, under suitable assumptions, hold also for Gauss–Kronrod

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formulae. In §6 we give a potential-theoretic interpretation of the circle theorem, namely that the semicircle in question is the reciprocal density of the equilibrium measure of the interval $[-1,1]$. This is true in more general situations, where the support of the given weight function is any compact subset Δ of $(-1,1)$, in which case the (normalized) Gauss points come to lie on the reciprocal density of the equilibrium measure of Δ. This is illustrated in the case of Δ being the union of two disjoint symmetric subintervals of $[-1,1]$. The equation of the limiting curve can be written down in this case and answers in the affirmative another question raised in [2, last sentence of §IV].

2. Gaussian quadrature. We write the Gaussian quadrature formula for the weight function w in the form

$$\int_{-1}^{1} f(t)w(t)\mathrm{d}t = \sum_{\nu=1}^{n} \lambda_\nu^G f(\tau_\nu^G) + R_n^G(f), \tag{2.1}$$

where τ_ν^G are the *Gaussian nodes* and λ_ν^G the *Gaussian weights*; cf., e.g., [7, §1.4.2]. (Their dependence on n is suppressed in our notation.) The remainder satisfies

$$R_n^G(p) = 0 \quad \text{for any } p \in \mathbb{P}_{2n-1},$$

where $\mathbb{P}_{2n-1}$ is the class of polynomials of degree $\leq 2n-1$. Without loss of generality we have assumed that the support of the weight function w is the interval $[-1,1]$. The circle theorem can then be formulated as follows.

THEOREM 2.1. *(Circle theorem) Let w be a weight function in the Szegö class (cf. §1, (1.1)) satisfying $1/w(t) \in L_1(\Delta)$ for any compact interval $\Delta \subset (-1,1)$. Then*

$$\frac{n\lambda_\nu^G}{\pi w(\tau_\nu^G)} \sim \sqrt{1-(\tau_\nu^G)^2} \quad \text{as } n \to \infty, \tag{2.2}$$

for all nodes τ_ν^G (and corresponding weights) that lie in Δ. (The relation $a_n \sim b_n$ here means that $\lim_{n\to\infty} a_n/b_n = 1$.)

As mentioned in §1, this was shown to be true by Davis and Rabinowitz [2] in the case of the Jacobi weight function $w(t) = (1-t)^\alpha(1+t)^\beta$ on $[-1,1]$, $\alpha > -1$, $\beta > -1$. We illustrate the theorem in Fig. 2.1 by plotting all quantities on the left of (2.2) for $\alpha,\beta = -0.75 : 0.25 : 1.0, 1.5 : 0.5 : 3.0$, $\beta \geq \alpha$, and for $n = 20 : 5 : 40$ in the plot on the left, and for $n = 60 : 5 : 80$ in the plot on the right.

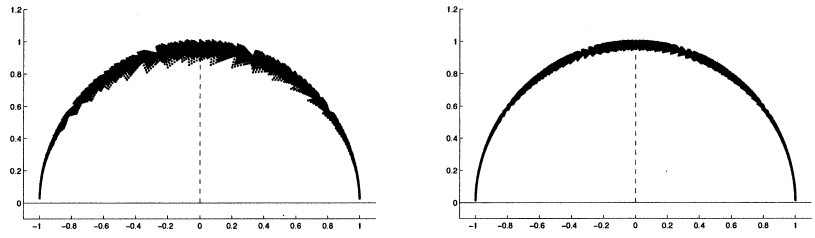

FIG. 2.1. *The circle theorem for Jacobi weight functions*

The circle theorem for the more general weight function indicated in Theorem 2.1 has been around implicitly for some time. Indeed, it is contained in an important asymptotic result for Christoffel functions $\lambda_n(t;w)$ due to Nevai [12, Theorem 34]. According to this

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result, one has

$$\frac{n\lambda_n(t;w)}{\pi w(t)} \sim \sqrt{1-t^2} \quad \text{as } n \to \infty, \tag{2.3}$$

uniformly for $t \in \Delta$. Recalling that $\lambda_n(\tau_\nu^G; w) = \lambda_\nu^G$ (cf. [5, Theorem 3.2 and last paragraph of §I.3]) yields Theorem 2.1.

COROLLARY TO THEOREM 2.1. *If* $w(t) = (1-t^2)^{-1/2}$ *on* $(-1,1)$, *then*

$$\frac{n\lambda_\nu^G}{\pi w(\tau_\nu^G)} = \sqrt{1-(\tau_\nu^G)^2}, \quad \nu = 1,2,\ldots,n.$$

Proof. This follows from the well-known fact that $\lambda_\nu^G = \pi/n$, $\nu = 1,2,\ldots,n$, in this case. □

REMARK 2.2. *Theorem 2.1 in a weaker form (pointwise convergence almost everywhere) holds also when* w *is locally in Szegö's class, i.e.,* w *has support* $[-1,1]$ *and satisfies*

$$\int_\Delta \ln w(t)\mathrm{d}t > -\infty, \tag{2.4}$$

where Δ *is an open subinterval of* $[-1,1]$. *Then (2.2) holds for almost all* $\tau_\nu \in \Delta$ *([11, Theorem 8]).*

EXAMPLE 1. The Pollaczek weight function $w(t;a,b)$ on $[-1,1]$, $a \geq |b|$ (cf. [14]).

The weight function is given explicitly by (*ibid.*, eqn (3), multiplied by 2)

$$w(t;a,b) = \frac{2\exp(\omega\cos^{-1}(t))}{1+\exp(\omega\pi)}, \quad |t| \leq 1, \tag{2.5}$$

where $\omega = \omega(t) = (at+b)(1-t^2)^{-1/2}$. It is not in Szegö's class, but is so locally. The recurrence coefficients are known explicitly (*ibid.*, eqn (14)),

$$\begin{aligned} \alpha_k &= \frac{-b}{2k+a+1}, \quad k \geq 0, \\ \beta_0 &= \frac{2}{a+1}, \quad \beta_k = \frac{k^2}{(2k+a)^2-1}, \quad k \geq 1. \end{aligned} \tag{2.6}$$

From (2.5) and (2.6), it is straightforward to compute the ratios $n\lambda_\nu^G/\pi w(\tau_\nu^G;a,b)$. Their behavior, when $n = 380 : 5 : 400$, is shown in Fig. 2.2 for $a = b = 0$ on the left, and for $a = 4$, $b = 1$ on the right. The circle theorem obviously holds when $a = b = 0$ (i.e., $w = 1$), but also, as expected from the above remark, with possible isolated exceptions, for other values of a and b.

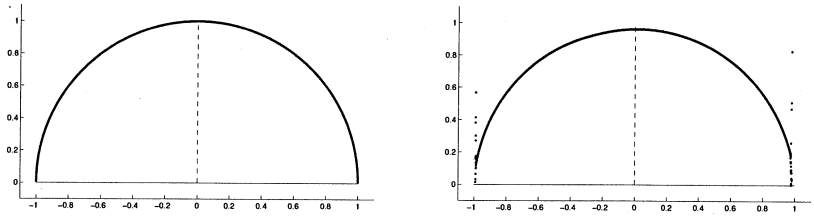

FIG. 2.2. *The circle theorem for Pollaczek weight functions*

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3. Gauss–Radau formula. Our analysis of the Gauss–Radau formula (and also the Gauss–Lobatto formula in §4) seeks to conclude from the validity of the circle theorem for the Gauss formula (2.1) the same for the corresponding Gauss–Radau formula,

$$\int_{-1}^{1} f(t)w(t)\mathrm{d}t = \lambda_0^R f(-1) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_n^R(f), \tag{3.1}$$

where $R_n^R(\mathbb{P}_{2n}) = 0$. (Here, as in (2.1), the nodes and weights depend on n.)

THEOREM 3.1. *Let the weight function w satisfy the conditions of Theorem 2.1. Then not only the Gaussian quadrature rule (2.1) for w, but also the Gauss–Radau rule (3.1) for w admits a circle theorem.*

Proof. It is known that τ_ν^R are the zeros of $\pi_n(\cdot\,; w_{-1})$, the polynomial of degree n orthogonal with respect to the weight function $w_{-1}(t) = (t+1)w(t)$ (cf. [7, §1.4.2, p. 25]). Let

$$\ell_\nu^*(t) = \prod_{\mu\neq\nu} \frac{t-\tau_\mu^R}{\tau_\nu^R - \tau_\mu^R}, \quad \nu = 1, 2, \ldots, n, \tag{3.2}$$

be the elementary Lagrange interpolation polynomials for the nodes $\tau_1^R, \tau_2^R, \ldots, \tau_n^R$. Since the Gauss–Radau formula is interpolatory, there holds

$$\begin{aligned} \lambda_\nu^R &= \int_{-1}^{1} \frac{(t+1)\pi_n(t; w_{-1})}{(\tau_\nu^R+1)(t-\tau_\nu^R)\pi_n'(\tau_\nu^R; w_{-1})} w(t)\mathrm{d}t \\ &= \int_{-1}^{1} \frac{(t+1)\ell_\nu^*(t)}{\tau_\nu^R+1} w(t)\mathrm{d}t. \end{aligned} \tag{3.3}$$

If λ_ν^* are the n Gaussian weights for the weight function w_{-1}, we have, again by the interpolatory nature of the Gaussian quadrature formula, and by (3.3),

$$\lambda_\nu^* = \int_{-1}^{1} \ell_\nu^*(t)(t+1)w(t)\mathrm{d}t = (\tau_\nu^R+1)\lambda_\nu^R.$$

By assumption, the Gauss formula for the weight function w, and hence also the one for the weight function w_{-1} (which satisfies the same conditions as those imposed on w) admits a circle theorem. Therefore,

$$\frac{n\lambda_\nu^R}{\pi w(\tau_\nu^R)} = \frac{n\lambda_\nu^*}{\pi(\tau_\nu^R+1)w(\tau_\nu^R)} = \frac{n\lambda_\nu^*}{\pi w_{-1}(\tau_\nu^R)} \sim \sqrt{1-(\tau_\nu^R)^2}, \quad n\to\infty.$$

□

EXAMPLE 2. The logarithmic weight function $w(t) = t^\alpha \ln(1/t)$ on $[0,1]$, $\alpha > -1$. Here, Gauss–Radau quadrature is over the interval $[0,1]$,

$$\int_0^1 f(t)t^\alpha \ln(1/t)\mathrm{d}t = \lambda_0 f(0) + \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f).$$

A linear transformation of variables, mapping $[0,1]$ onto $[-1,1]$, yields the Gauss–Radau quadrature formula over $[-1,1]$, to which Theorem 3.1 is applicable. The circle theorem, therefore, by a simple computation, now assumes the form

$$\frac{n\lambda_\nu}{\pi\tau_\nu^\alpha \ln(1/\tau_\nu)} \sim \sqrt{(\tfrac{1}{2})^2 - (\tau_\nu - \tfrac{1}{2})^2}, \quad n\to\infty.$$

This is illustrated in Fig. 3.1, on the left for $n = 20:5:40$, on the right for $n = 60:5:80$, and $\alpha = -0.75:0.25:1.0, 1.5:0.5:3$ in both cases.

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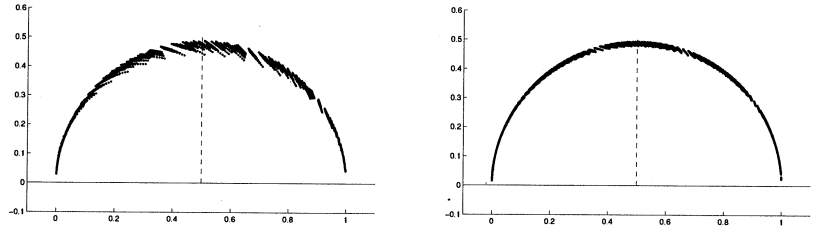

FIG. 3.1. *The circle theorem for Gauss–Radau quadrature*

4. Gauss–Lobatto formula. The argumentation, in this case, is quite similar to the one in §3 for Gauss–Radau formulae. We recall that the Gauss–Lobatto formula for the weight function w is

$$\int_{-1}^{1} f(t)w(t)\mathrm{d}t = \lambda_0^L f(-1) + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + \lambda_{n+1}^L f(1) + R_n^L(f), \tag{4.1}$$

where $R_n^L(\mathbb{P}_{2n+1}) = 0$ and τ_ν^L are the zeros of $\pi_n(\cdot\,; w_{\pm 1})$, the polynomial of degree n orthogonal with respect to the weight function $w_{\pm 1}(t) = (1-t^2)w(t)$ (cf. [7, §1.4.2, p. 26]).

THEOREM 4.1. *Let the weight function w satisfy the conditions of Theorem 2.1. Then the Gauss–Lobatto rule (4.1) for w admits a circle theorem.*

Proof. In analogy to (3.2), we define

$$\ell_\nu^*(t) = \prod_{\mu \neq \nu} \frac{t - \tau_\mu^L}{\tau_\nu^L - \tau_\mu^L}, \quad \nu = 1, 2, \ldots, n,$$

and denote by λ_ν^* the n Gaussian weights for the weight function $w_{\pm 1}$. Then we have

$$\lambda_\nu^L = \int_{-1}^{1} \frac{(1-t^2)\ell_\nu^*(t)}{1-(\tau_\nu^L)^2} w(t)\mathrm{d}t,$$

while, on the other hand,

$$\lambda_\nu^* = \int_{-1}^{1} \ell_\nu^*(t)(1-t^2)w(t)\mathrm{d}t = (1-(\tau_\nu^L)^2)\lambda_\nu^L.$$

Consequently,

$$\frac{n\lambda_\nu^L}{\pi w(\tau_\nu^L)} = \frac{n\lambda_\nu^*}{\pi(1-(\tau_\nu^L)^2)w(\tau_\nu^L)} = \frac{n\lambda_\nu^*}{\pi w_{\pm 1}(\tau_\nu^L)} \sim \sqrt{1-(\tau_\nu^L)^2}, \quad n \to \infty,$$

by Theorem 2.1 and the fact that $w_{\pm 1}$ satisfies the same conditions as those imposed on w. □

5. Gauss–Kronrod formula. While the quadrature rules discussed so far are products of the 19th century, the rules to be considered now are brainchilds of the 20th century ([10]). The idea[1] is to expand the Gaussian n-point quadrature formula (2.1) into a $(2n+1)$-point formula by inserting $n+1$ additional nodes and redefining all weights in such a manner as to achieve maximum degree of exactness. It turns out, as one expects, that this optimal degree

[1] In a germinal form, the idea can already be found in work of Skutsch [16]; see [8].

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of exactness is $3n+1$; it comes at an expenditure of only $n+1$ new function evaluations, but at the expense of possibly having to confront complex-valued nodes and weights.

The quadrature formula described, called *Gauss–Kronrod formula*, thus has the form

$$\int_{-1}^{1} f(t)w(t)\mathrm{d}t = \sum_{\nu=1}^{n} \lambda_\nu^K f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} f(\tau_\mu^K) + R_n^K(f), \tag{5.1}$$

where τ_ν^G are the Gaussian nodes for the weight function w and

$$R_n^K(p) = 0 \quad \text{for all } p \in \mathbb{P}_{3n+1}. \tag{5.2}$$

The formula (5.1) is uniquely determined by the requirement (5.2); indeed (cf. [7, §3.1.2]), the inserted nodes τ_μ^K—the *Kronrod nodes*—must be the zeros of the polynomial π_{n+1}^K of degree $n+1$ orthogonal to all lower-degree polynomials with respect to the "weight function" $\pi_n(t)w(t)$, where π_n is the orthogonal polynomial of degree n relative to the weight function w,

$$\int_{-1}^{1} \pi_{n+1}^K(t)p(t)\pi_n(t)w(t)\mathrm{d}t = 0, \quad \text{all } p \in \mathbb{P}_n. \tag{5.3}$$

The weights in (5.1) are then determined "by interpolation".

Interestingly, in the simplest case $w(t) = 1$, the polynomial π_{n+1}^K has already been considered by Stieltjes in 1894, though not in the context of quadrature. It is nowadays, for arbitrary w, called the *Stieltjes polynomial* for the weight function w.

Orthogonality in the sense (5.3) is problematic for two reasons: the "weight function" $w_n^K = \pi_n w$ is oscillatory and sign-varying on the interval $[-1,1]$, and it depends on n. The zeros of π_{n+1}^K, therefore, are not necessarily contained in $(-1,1)$, or even real, although in special cases they are. A circle theorem for Gauss–Kronrod formulae is therefore meaningful only if all Kronrod nodes are real, distinct, contained in $(-1,1)$, and different from any Gaussian node. If that is the case, and moreover, w is a weight function of the type considered in Theorem 2.1, there is a chance that a circle theorem will hold. The best we can prove is the following theorem.

THEOREM 5.1. *Assume that the Gauss–Kronrod formula (5.1) exists with τ_μ^K distinct nodes in $(-1,1)$ and $\tau_\mu^K \neq \tau_\nu^G$ for all μ and ν. Assume, moreover, that*

(i) the Gauss quadrature formula for the weight function w admits a circle theorem;

(ii) the $(n+1)$-point Gaussian quadrature formula for $w^K(t) = \pi_n(t)w(t)$, with Gaussian weights λ_μ^*, admits a circle theorem in the sense

$$\frac{2n\lambda_\mu^*}{\pi w^K(\tau_\mu^K)} \sim \sqrt{1-(\tau_\mu^K)^2} \quad \text{as } n \to \infty$$

for all μ such that $\tau_\mu^K \in \Delta$, where Δ is any compact subinterval of $(-1,1)$;

(iii) $\lambda_\nu^K \sim \frac{1}{2}\lambda_\nu^G$ as $n \to \infty$ for all ν such that $\tau_\nu^G \in \Delta$.

Then the Gauss–Kronrod formula (5.1) admits a circle theorem in the sense

$$\frac{2n\lambda_\nu^K}{\pi w(\tau_\nu^G)} \sim \sqrt{1-(\tau_\nu^G)^2}, \quad \frac{2n\lambda_\mu^{*K}}{\pi w(\tau_\mu^K)} \sim \sqrt{1-(\tau_\mu^K)^2}, \quad n \to \infty, \tag{5.4}$$

for all ν, μ as defined in assumptions (ii) and (iii).

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Proof. The first relation in (5.4) is an easy consequence of assumptions (i) and (iii):

$$\frac{2n\lambda_\nu^K}{\pi w(\tau_\nu^G)} \sim \frac{n\lambda_\nu^G}{\pi w(\tau_\nu^G)} \sim \sqrt{1-(\tau_\nu^G)^2}, \quad n \to \infty.$$

To prove the second relation in (5.4), we first note that the $n+1$ Gaussian nodes for $w^K = \pi_n w$ are precisely the Kronrod nodes τ_μ^K. By assumption (ii),

$$\frac{2n\lambda_\mu^*}{\pi\pi_n(\tau_\mu^K)w(\tau_\mu^K)} \sim \sqrt{1-(\tau_\mu^K)^2}, \quad n \to \infty. \tag{5.5}$$

Since the Gauss formula for w^K is certainly interpolatory, we have

$$\lambda_\mu^* = \int_{-1}^{1} \ell_\mu^*(t) w_K(t)\mathrm{d}t = \int_{-1}^{1} \ell_\mu^*(t)\pi_n(t)w(t)\mathrm{d}t$$

with

$$\ell_\mu^*(t) = \prod_{\kappa\neq\mu} \frac{t-\tau_\kappa^K}{\tau_\mu^K - \tau_\kappa^K}, \quad \mu = 1, 2, \ldots, n+1,$$

denoting the elementary Lagrange interpolation polynomials for the nodes $\tau_1^K, \tau_2^K, \ldots, \tau_{n+1}^K$. On the other hand, by the interpolatory nature of (5.1), we have similarly

$$\lambda_\mu^{*K} = \int_{-1}^{1} \frac{\pi_n(t)}{\pi_n(\tau_\mu^K)} \ell_\mu^*(t)w(t)\mathrm{d}t = \frac{1}{\pi_n(\tau_\mu^K)}\lambda_\mu^*. \tag{5.6}$$

By (5.5) and (5.6), therefore,

$$\frac{2n\lambda_\mu^{*K}}{\pi w(\tau_\mu^K)} \sim \frac{2n\lambda_\mu^*}{\pi\pi_n(\tau_\mu^K)w(\tau_\mu^K)} \sim \sqrt{1-(\tau_\mu^K)^2}, \quad n \to \infty.$$

□

EXAMPLE 3. Jacobi weight function $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha, \beta \in [0, \frac{5}{2})$.

For these weight functions, (5.4) has been proved by Peherstorfer and Petras [13, Theorem 2], from which assumptions (ii) and (iii) can be recovered by "inverse implication". Assumption (i), of course, is satisfied for these weight functions by virtue of Theorem 2.1.

The circle theorem, in this case, is illustrated in Fig. 5.1, on the left for $n = 20:5:40$, on the right for $n = 60:5:80$, with $\alpha, \beta = 0:0.4:2$, $\beta \geq \alpha$, in both cases.

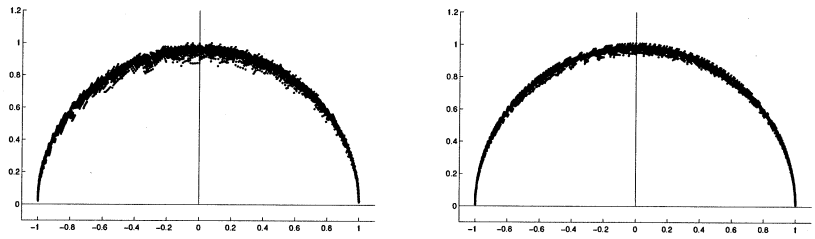

FIG. 5.1. *The circle theorem for Gauss–Kronrod quadrature*

We remark that asymptotic results of Ehrich [3, Corollary 3] imply the circle theorem also for negative values of $\alpha = \beta > -\frac{1}{2}$.

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6. Potential-theoretic interpretation and extension of the circle theorem. There is a deep connection between Christoffel functions (and hence Gaussian weights) and equilibrium measures in potential theory. For the necessary potential-theoretic concepts, see [15]. Thus, for example, the density of the equilibrium measure $\omega_{[-1,1]}$ of the interval $[-1,1]$ is $\omega'_{[-1,1]}(t) = 1/(\pi\sqrt{1-t^2})$, showing that (2.3) can be interpreted by saying that as $n \to \infty$ the ratio $n\lambda_n(t;w)/w(t)$ converges to the reciprocal of the density of the equilibrium measure of $[-1,1]$. Here we consider a weight function w that is compactly supported on a (regular) set $E \subset \mathbb{R}$ and $\Delta \subset E$ an interval on which w satisfies the Szegö condition (2.4). Then, for almost all ν,

$$\frac{n\lambda_\nu^G}{w(t)} \sim \frac{1}{\omega'_E}, \quad n \to \infty, \tag{6.1}$$

where ω'_E is the density of the equilibrium measure of E (cf. [17, Theorem 1]).

EXAMPLE 4. A weight function supported on two intervals,

$$w(t) = \begin{cases} |t|^\gamma (t^2-\xi^2)^p (1-t^2)^q, & t \in [-1,-\xi] \cup [\xi,1], \\ 0 \quad \text{elsewhere}, \end{cases}$$

where $0 < \xi < 1$, $p > -1$, $q > -1$ and $\gamma \in \mathbb{R}$.

The recursion coefficients for the weight function w are explicitly known if $\gamma = \pm 1$ and $p = q = \pm 1/2$ (see [6, §5]). The quantities $n\lambda_\nu^G/(\pi w(\tau_\nu^G))$ in these cases are therefore easily computable; plotting them for $\xi = \frac{1}{2}$, and $n = 60 : 5 : 80$, yields the graph in Fig. 6.1.

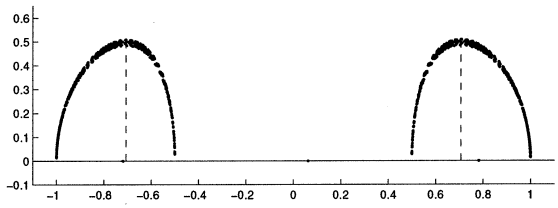

FIG. 6.1. *Analogue of the circle theorem for the weight function of Example 4*

The limiting curve for general ξ must be related to the reciprocal density $\omega'_{[-1,-\xi]\cup[\xi,1]}$ of the two support intervals. We can find its equation by using the known fact [6, §6] that for $\gamma = 1$ and $p = q = -1/2$, when n is even, the Gauss weights λ_ν^G are all equal to π/n. Consequently, for these n, and $\tau_\nu^G \in [\xi,1]$,

$$\frac{n\lambda_\nu^G}{\pi w(\tau_\nu^G)} = \frac{1}{w(\tau_\nu^G)} = |\tau_\nu^G|^{-1}[(\tau_\nu^G)^2 - \xi^2]^{1/2}[1-(\tau_\nu^G)^2]^{1/2}, \tag{6.2}$$

so that the right branch of the limiting curve, and by symmetry the curve itself, has the equation $y = \varphi(t)$, where

$$\varphi(t) = |t|^{-1}(t^2-\xi^2)^{1/2}(1-t^2)^{1/2}.$$

The extrema of φ are attained at $t_0 = \pm\sqrt{\xi}$ and have the value $\varphi_0 = 1-\xi$. For $\xi = \frac{1}{2}$, therefore, $t_0 = \pm\sqrt{1/2} = \pm 0.7071\ldots$, $\varphi_0 = \frac{1}{2}$.

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We conclude from (6.1) and (6.2) that

$$\omega'_{[-1,-\xi]\cup[\xi,1]}(t) = \pi^{-1}|t|(t^2-\xi^2)^{-1/2}(1-t^2)^{-1/2}, \quad t \in [-1,-\xi]\cup[\xi,1]. \tag{6.3}$$

Actually, the equilibrium measure is known for any set E whose support consists of several intervals and is an inverse polynomial image of $[-1,1]$,

$$E = \mathcal{T}_N^{-1}([-1,1]),$$

where $\mathcal{T}_N$ is a polynomial of degree N. Then indeed [9, p. 577],

$$\omega'_E(t) = \frac{|\mathcal{T}'_N(t)|}{N\pi\sqrt{1-\mathcal{T}_N^2(t)}}, \quad t \in E. \tag{6.4}$$

In the case at hand, $E = [-1,-\xi]\cup[\xi,1]$, $0<\xi<1$, we have

$$\mathcal{T}_2(t) = \frac{2t^2-\xi^2-1}{1-\xi^2},$$

and (6.4) becomes (6.3).

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ORIGINAL PAPER

High-order generalized Gauss–Radau and Gauss–Lobatto formulae for Jacobi and Laguerre weight functions

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Abstract The generation of generalized Gauss–Radau and Gauss–Lobatto quadrature formulae by methods developed by us earlier breaks down in the case of Jacobi and Laguerre measures when the order of the quadrature rules becomes very large. The reason for this is underflow resp. overflow of the respective monic orthogonal polynomials. By rescaling of the polynomials, and other corrective measures, the problem can be circumvented, and formulae can be generated of orders as high as 1,000.

Keywords High-order generalized Gauss–Radau and Gauss–Lobatto quadrature formulae · Jacobi weight functions · Laguerre weight functions

1 Introduction

Generalized Gauss–Radau and Gauss–Lobatto formulae are quadrature formulae of Gauss type, i.e. of maximum polynomial degree of exactness, that involve boundary points of arbitrary multiplicity $r \geq 2$ (those with $r = 1$ being the ordinary Gauss–Radau resp. Gauss–Lobatto formualae). The computation of these formulae for arbitrary weight functions has been discussed in [3], where reference is also made to respective Matlab routines `gradau.m` and `globatto.m`. It has recently been noted by B.D. Welfert (unpublished manuscript, Section 3.1.2) that `gradau.m` (in the case of the Jacobi measure with parameter $\alpha = 1$, $\beta = 0$ and $r = 2$) breaks down for very large order

In memoriam Gene H. Golub.

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$N \gtrsim 400$ "because of the ill-conditioning of the 2×2 linear system" used to compute the boundary weights. Here we observe that the breakdown is due to underflow, causing division by zero, similarly as noted for Gauss–Lobatto formulae in [1, p. 214].[1] The routine `gradau.m` experiences similar problems also for the generalized Laguerre weight functions, except this time it is overflow, not underflow, that causes breakdown. There are, however, additional numerical complications that have to do with the underlying range of integration being unbounded.

The remedy proposed in [1] for Jacobi weight functions—Golub's modified Jacobi matrix [5] with explicit formulae for the modified elements in the lower right-hand corner of the matrix—is no longer available in the present context, but another remedy also mentioned in [1] is, namely appropriate rescaling. The same remedy works also for generalized Laguerre weight functions, but as noted above, additional complications need to be dealt with.

The problems for high-order generalized Gauss–Radau formulae are discussed in Section 2, both for Jacobi and generalized Laguerre weight functions. The analogous problems for high-order generalized Gauss–Lobatto formulae and Jacobi weight functions are discussed in Section 3. In Section 4, we report on numerical experiments.

2 Generalized Gauss–Radau formulae

The problems mentioned in Section 1 can be resolved, at least in the case of Jacobi measures, in an embarrassingly simple manner. The same resolution, with additional precautions, works also for generalized Laguerre measures. This will be discussed respectively in Sections 2.1 and 2.2.

2.1 Jacobi measures

Here, the generalized Gauss–Radau formula has the form

$$\int_{-1}^{1} f(t)\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(-1) + \sum_{\nu=1}^{n} \lambda_\nu^R f\left(\tau_\nu^R\right) + R_{n,r}^R(f), \tag{1}$$

where

$$\mathrm{d}\lambda(t) = (1-t)^\alpha (1+t)^\beta, \quad t \in (-1,1), \quad \alpha > -1,\ \beta > -1. \tag{2}$$

[1] We take the opportunity here to point out a simplification in Eq. 4.7 of [1]. As already noted by B.D. Welfert (unpublished manuscript, Section 1), one has $4(n+\alpha+1)(n+\beta+1)+(\alpha-\beta)^2 = (2n+\alpha+\beta+2)^2$, so that the expression for $\lambda_k^{(\alpha,\beta)}$ in [1, Eq. 4.7], after additional simplifications in the products and ratios of the binomial coefficients and gamma functions, becomes $\lambda_k^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+2)\Gamma(n+\beta+2)}{(n+1)\Gamma(n+2)\Gamma(n+n+\alpha+\beta+3)} \frac{1}{\left[P_{n+1}^{(\alpha,\beta)}(t_k)\right]^2}$.

Expressions for the interior nodes and weights, τ_ν^R and λ_ν^R, are well known (cf. [3, Eq. 1.5]), and are unproblematic, numerically. On the other hand, the boundary weights $\lambda_0^{(\rho)}$, according to [3, Eq. 2.2], are the solution $\boldsymbol{x} = [x_j]$, $x_j = \lambda_0^{(j-1)}$, $j = 1, 2, \ldots, r$, of an upper triangular $r \times r$ system of linear equations

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \tag{3}$$

in which the elements b_i of the vector $\boldsymbol{b}$ are

$$b_i = \int_{-1}^{1} (t+1)^{i-1} \pi_n^2(t) \mathrm{d}\lambda(t), \quad i = 1, 2, \ldots, r, \tag{4}$$

and the diagonal elements a_{ii} of the matrix $\boldsymbol{A}$ are given by (cf. [3, eq (2.6)])

$$a_{ii} = (i-1)! \pi_n^2(-1), \quad i = 1, 2, \ldots, r. \tag{5}$$

Here, π_n is the monic polynomial of degree n orthogonal on $[-1, 1]$ with respect to the measure

$$\mathrm{d}\lambda^{[r]}(t) = (t+1)^r \mathrm{d}\lambda(t) = (1-t)^\alpha (1+t)^{\beta+r} \, \mathrm{d}t. \tag{6}$$

The problem, as n grows very large, consists in $|\pi_n|$, and even more so, π_n^2, becoming extremely small and eventually underflowing to zero. Then $\pi_n^2(-1)$ in (5) is zero, causing division by zero in the very first step of the back substitution process for solving the upper triangular system (3). The remedy is simple enough: Rescale the orthogonal polynomial π_n; i.e., do not use the monic Jacobi polynomial π_n, but instead the conventional Jacobi polynomial $P_n^{(\alpha,\beta+r)} = k_n \pi_n$, where for large n the constant k_n is of the order 2^n. More precisely, we multiply both sides of (3) by k_n^2, which in view of (4) and (5) can be effected by replacing π_n at every occurrence by $P_n^{(\alpha,\beta+r)}$ (cf. also (2.5) and (2.6) in [3] for the remaining elements a_{ij} of $\boldsymbol{A}$). In particular, instead of $\pi_n(-1)$ in (5), we use

$$P_n^{(\alpha,\beta+r)}(-1) = (-1)^n \binom{n+\beta+r}{n},$$

and in (4) we use $P_n^{(\alpha,\beta+r)}$ instead of π_n, computing it by means of the standard recurrence relation for the Jacobi polynomials (see, e.g., [2, p. 30]). This has been implemented in the Matlab routine `gradau_jacobi.m`, which, like all the other routines referenced in this paper, can be downloaded from the web site http://www.cs.purdue.edu/archives/2002/wxg/codes. This new routine works well for values of n as large as 1,000.

2.2 Generalized Laguerre measures

The generalized Gauss–Radau formula now takes the form

$$\int_0^\infty f(t) \mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(0) + \sum_{\nu=1}^{n} \lambda_\nu^R f\left(\tau_\nu^R\right) + R_{n,r}^R(f), \tag{7}$$

where

$$\mathrm{d}\lambda(t) = t^{\alpha} e^{-t}, \quad t \in (0, \infty), \quad \alpha > -1, \tag{8}$$

and the numerical values of the nodes and weights in (7) are of course different from those in (1), even though we use the same notation. Again, the problem is with the boundary weights $\lambda_0^{(\rho)}$ only, the interior nodes and weights being computable safely from known formulae ([3, eq (1.5)]).

The linear system for the boundary weights is again (3), with a_{ii} as in (5), and

$$b_i = \int_0^{\infty} t^{i-1} \pi_n^2(t) \mathrm{d}\lambda(t), \quad i = 1, 2, \ldots, r. \tag{9}$$

Here, π_n is now the monic generalized Laguerre polynomial $\pi_n = k_n^{-1} L_n^{(\alpha+r)}$, where $L_n^{(\alpha+r)}$ is the conventional generalized Laguerre polynomial, and $k_n^{-1} = (-1)^n n!$. In particular (cf. [2, p. 31]),

$$L_n^{(\alpha+r)}(0) = \binom{n+\alpha+r}{n}.$$

Evidently, $|\pi_n|$, with growing n, becomes rapidly very large, causing overflow both in (5) and (9). Hence, we multiply both sides of (3) by k_n^2, which can be effected as explained in Section 2.1. This takes care completely of the overflow problem as it regards the matrix $\boldsymbol{A}$. Unfortunately, the same is not necessarily the case for the vector $\boldsymbol{b}$, which after rescaling is computed (exactly, in theory) by $(n + \lfloor (r+1)/2 \rfloor)$-point Gauss–Laguerre quadrature of

$$k_n^2 b_i = \int_0^{\infty} t^{i-1} \left[L_n^{(\alpha+r)}(t) \right]^2 \mathrm{d}\lambda(t),$$

that is,

$$k_n^2 b_i = \sum_{\nu=1}^{n_g} w_\nu \tau_\nu^{i-1} \left[L_n^{(\alpha+r)}(\tau_\nu) \right]^2, \quad n_g = n + \left\lfloor \frac{r+1}{2} \right\rfloor, \tag{10}$$

where $\tau_\nu = \tau_\nu^{(n_g)}$, $w_\nu = w_\nu^{(n_g)}$ are the nodes (ordered increasingly) and weights of the n_g-point Gauss–Laguerre quadrature rule.

What is happening here, when n grows very large, is the following: Some of the Gauss nodes τ_ν at the upper end of their spectrum become quite large, and since $|L_n^{(\alpha+r)}(t)|$ when n is large grows exponentially with t (cf. Fejér's theorem in [6, Section 8.22]), the quantities $|L_n^{(\alpha+r)}(\tau_\nu)|$, and even more so, their squares, become extremely large to the point of overflowing. While it is true that the Gauss weights w_ν corresponding to those large nodes τ_ν become extremely small (some may even underflow to zero), so much so that the terms in the quadrature sum (10) remain of moderate size, once $[L_n^{(\alpha+r)}(\tau_\nu)]^2$ overflows, the damage is done, and the computation breaks down.

The way we overcome this difficulty is in (10) to recursively generate, before squaring, not the Laguerre polynomial $L_n^{(\alpha+r)}(\tau_\nu)$ itself, but $c_\nu L_n^{(\alpha+r)}(\tau_\nu)$, where $c_\nu = w_\nu \tau_\nu^{i-1}$, and after squaring compute the νth term of the sum by dividing

the result by c_ν. The recursion is easily done by multiplying both $L_0^{(\alpha+r)}(\tau_\nu) = 1$ and $L_1^{(\alpha+r)}(\tau_\nu) = \alpha + r + 1 - \tau_\nu$ by c_ν and then applying the standard recurrence relation for the Laguerre polynomials. The only additional precaution is to omit all those terms in the sum of (10) for which $w_\nu = 0$ (by underflow). This idea is implemented in the routine `gradau_laguerre.m`, which again works well for values of n as large as $n = 1,000$.

3 Generalized Gauss–Lobatto formulae

The generalized Gauss–Lobatto formula for the Jacobi measure $\mathrm{d}\lambda$ in (2) is given by (cf. [3, Eq. 1.3])

$$\int_{-1}^{1} f(t)\mathrm{d}\lambda(t) = \sum_{\rho=0}^{r-1} \lambda_0^{(\rho)} f^{(\rho)}(-1) + \sum_{\nu=1}^{n} \lambda_\nu^L f\left(\tau_\nu^L\right) + \sum_{\rho=0}^{r-1} (-1)^\rho \lambda_{n+1}^{(\rho)} f^{(\rho)}(1) + R_{n,r}^L(f). \tag{11}$$

The interior nodes τ_ν^L and weights λ_ν^L can be computed safely, even for very large n, from well-known expressions (cf. [3, Eq. 1.7]). The problem, as in the case of generalized Gauss–Radau formulae, is with the boundary weights $\lambda_0^{(\rho)}$ and $(-1)^\rho \lambda_{n+1}^{(\rho)}$. Both are again computed from an upper triangular $r \times r$ system of linear equations (3), where in the case of the first boundary weights we have $\boldsymbol{b} = [b_i]$ with

$$b_i = \int_{-1}^{1} (t+1)^{i-1} \pi_n^2(t)(1-t)^r \mathrm{d}\lambda(t), \quad i = 1, 2, \ldots, r, \tag{12}$$

and π_n the monic polynomial of degree n orthogonal on $[-1, 1]$ with respect to the measure

$$\mathrm{d}\lambda^{[r]}(t) = (1-t)^{\alpha+r}(1+t)^{\beta+r}\mathrm{d}t. \tag{13}$$

The computation of both sets of boundary weights is virtually the same, except for an interchange of the roles of the boundary points -1 and $+1$ when computing the second set of boundary weights (cf. [3, Section 3.1]). The diagonal elements of the matrix $\boldsymbol{A}$ are

$$a_{ii} = (i-1)!\pi_n^2(-1)2^r \quad \text{resp.} \quad a_{ii} = (i-1)!\pi_n^2(1)(-2)^r \tag{14}$$

for the first resp. second set of boundary weights.

The problem for very large n is the same as before: underflow of π_n. So is the remedy: replacement of π_n by $P_n^{(\alpha+r,\beta+r)}$ in (12), and use of

$$P_n^{(\alpha+r,\beta+r)}(-1) = (-1)^n \binom{n+\beta+r}{n}, \quad P_n^{(\alpha+r,\beta+r)}(1) = \binom{n+\alpha+r}{n}$$

in (14). This is implemented in the Matlab routine `globatto_jacobi.m`, which works without any breakdown for n as large as 1,000.

4 Numerical results

4.1 Generalized Gauss–Radau formulae

We ran tests for the Jacobi weight function with parameters $\alpha = 1$, $\beta = 0$, and for the generalized Laguerre weight function with $\alpha = 1$. We are especially interested in finding out if, and when, the routines `gradau.m` and `gradau_jacobi.m` resp. `gradau_laguerre.m` break down. In all tests we let r vary in the range $2 \le r \le 5$.

In the case of the Jacobi weight function, the routine `gradau.m` works flawlessly for n up to $n = 421$, but breaks down, first when $n = 422$ and $r = 2$, and then for all r when $n \ge 435$. In contrast, `gradau_jacobi.m` never breaks down, even for n as large as $n = 1024$. Comparing the results with exact values of the boundary weights, available for $r = 2$ and arbitrary α, β in Welfert (unpublished manuscript, Eqs. 34, 35), it also transpires that `gradau.m` for values of n approaching the critical value $n = 422$ gradually deteriorates in relative accuracy to the point of incurring 100% error shortly before breakdown. In contrast, `gradau_jacobi.m` for $r = 2$ maintains good relative accuracy up to $n = 1024$, and this in spite of the fact that the matrix $\boldsymbol{A}$ in (3) becomes quite ill-conditioned with increasing n, the condition number being 1.23×10^{11} when $n = 1024$.

In the case of the Laguerre weight function, both routines `gradau.m` and `gradau_laguerre.m` work well up to $n = 67$. When $68 \le n \le 69$, the former breaks down for one or several values of r, and when $n \ge 70$ for all values of r. The accuracy, at least when $r = 2$ (in which case exact values are available from Welfert (unpublished manuscript)) remains excellent up to immediately before breakdown. In contrast, the routine `gradau_laguerre.m` works well and accurately for n up to 1024.

4.2 Generalized Gauss–Lobatto formulae

Breakdowns of `globatto.m` in the case of Jacobi measures with $\alpha = 1$, $\beta = 0$ begin to occur, similarly as with `gradau.m`, when $n = 421$. In contrast, `globatto_jacobi.m` produces results for all $2 \le r \le 5$ up to $n = 1024$. Comparing the boundary weights with exact values (from [4]) in the case of $r = 2$ and Chebyshev weight functions of all four kinds reveals that the routine maintains good accuracy all the way up to $n = 1024$.

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ORIGINAL PAPER

Gauss quadrature routines for two classes of logarithmic weight functions

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Abstract By means of the Matlab symbolic/variable-precision facilities, routines are developed that generate an arbitrary number of recurrence coefficients to any given precision for polynomials orthogonal with respect to weight functions of Laguerre and Jacobi type containing logarithmic factors. The vehicle used is a symbolic modified Chebyshev algorithm based on ordinary as well as modified moments, executed with sufficiently high precision. The results are applied to Gaussian quadrature of integrals involving weight functions of the type mentioned.

Keywords Gaussian quadrature · Logarithmic weight functions · Orthogonal polynomials · Modified Chebyshev algorithm · Variable-precision arithmetic

1 Introduction

In [1], the authors construct quadrature rules for dealing with integrals of either the form

$$I = \int_0^\infty x^\alpha \mathrm{e}^{-x} \ln x \, f(x)\mathrm{d}x, \quad \alpha > -1, \tag{1}$$

or the form

$$K = \int_{-1}^1 (1-x)^\alpha (1+x)^\beta \ln(1+x) \, f(x)\mathrm{d}x, \quad \alpha > -1, \ \beta > -1. \tag{2}$$

In memoriam Borislav Bojanov.

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Notice that in both cases the logarithm is not of one sign on the interval of integration, thus precluding direct use of Gaussian quadrature. Instead, the authors introduce related *positive* weight functions, also involving logarithms, construct the corresponding Gaussian quadrature rules and combine them with the classical Gauss–Laguerre resp. Gauss–Jacobi rules to obtain quadrature rules for the integrals in (1) resp. (2). These involve $2n$ function values and corresponding $2n$ weights and are exact if the function f is a polynomial of degree $2n-2$ in the case of (1), and of degree $2n-1$ in the case of (2).

For (1), the related (positive) weight function is

$$v(x) = x^{\alpha} e^{-x}(x - 1 - \ln x), \quad x \in \mathbb{R}_+, \tag{3}$$

while for (2), it is

$$w(x) = (1-x)^{\alpha}(1+x)^{\beta} \ln(2/(1+x)), \quad x \in (-1, 1). \tag{4}$$

To deal with (1), suppose that $\{x_k^0, w_k^0\}_{k=1}^n$ are the nodes and weights of the n-point Gauss–Laguerre quadrature rule (associated with the weight function $x^{\alpha}e^{-x}$ on $\mathbb{R}_+$), and $\{x_k, w_k\}_{k=1}^n$ those for the n-point Gaussian quadrature rule associated with the weight function v. Then, since

$$I = \int_0^{\infty} \left[x^{\alpha} e^{-x}(x-1) - v(x)\right] f(x) \mathrm{d}x,$$

the desired quadrature rule for I is

$$I = \sum_{k=1}^{n} \left[w_k^0 \left(x_k^0 - 1\right) f\left(x_k^0\right) - w_k f(x_k)\right], \quad f \in \mathbb{P}_{2n-2}. \tag{5}$$

Similarly, in the case of (2), let $\{x_k^0, w_k^0\}_{k=1}^n$ be the nodes and weights of the n-point Gauss–Jacobi rule, and $\{x_k, w_k\}_{k=1}^n$ those of the n-point Gaussian quadrature rule associated with the weight function w. Then, since

$$K = \int_{-1}^{1} \left[(1-x)^{\alpha}(1+x)^{\beta} \ln 2 - w(x)\right] f(x) \mathrm{d}x,$$

the desired quadrature rule for K is

$$K = \sum_{k=1}^{n} \left[w_k^0 f\left(x_k^0\right) \ln 2 - w_k f(x_k)\right], \quad f \in \mathbb{P}_{2n-1}. \tag{6}$$

The same procedure applies to integrals I in (1) where the logarithmic term is $\ln(cx)$. The classical part of the quadrature sum in (5) simply has to be extended to include a term $w_k^0 f(x_k^0) \ln c$, i.e., changing $x_k^0 - 1$ to $x_k^0 - 1 + \ln c$. Similarly in the case of K in (2) when the logarithmic term is $\ln c(1+x)$; it suffices to change $\ln 2$ in (6) to $\ln(2c)$.

Generation of the quadrature nodes and weights x_k^0, w_k^0 for the two classical weight functions—generalized Laguerre and Jacobi—is straightforward, for example by using the `OPQ` Matlab package[1] for orthogonal polynomials and

[1] Accessible at the Web site http://www.cs.purdue.edu/archives/2002/wxg/codes/OPQ.html.

quadrature formulae. For the nonclassical weight functions in (3) and (4), the authors of [1] generate $2n$-point quadrature rules involving n function values and n derivative values and use them, as indicated above, to deal with the integrals (1) and (2). Alternatively, they use these Hermite-type quadrature rules as a tool of integration in Stieltjes's procedure for generating the recurrence coefficients of the orthogonal polynomials for the weight functions v and w. In the present paper, in order to produce these recurrence coefficients, we use the moments, or modified moments, of the weight functions in combination with the modified Chebyshev algorithm, executed in variable-precision arithmetic. This has the advantage of being able to obtain an arbitrary number of recurrence coefficients to any prescribed precision. The disadvantage is a possibly large amount of computing time, which, however, has to be expended only once for any given α or β. Numerical results in Section 4 will illustrate our approach.

2 The weight function v

2.1 The moments of v

Since

$$\int_0^\infty x^\omega \mathrm{e}^{-x}\mathrm{d}x = \Gamma(\omega+1),$$

differentiating with respect to ω, we get

$$\int_0^\infty x^\omega \mathrm{e}^{-x}\ln x\,\mathrm{d}x = \Gamma'(\omega+1).$$

Therefore, for the kth moment of v,

$$\mu_k = \int_0^\infty x^{\alpha+k}\mathrm{e}^{-x}(x-1-\ln x)\mathrm{d}x,$$

we find that

$$\begin{aligned}\mu_k &= \Gamma(\alpha+k+2)-\Gamma(\alpha+k+1)-\Gamma'(\alpha+k+1)\\ &= (\alpha+k+1)\Gamma(\alpha+k+1)-\Gamma(\alpha+k+1)-\Gamma'(\alpha+k+1)\\ &= (\alpha+k)\Gamma(\alpha+k+1)-\Gamma'(\alpha+k+1),\end{aligned}$$

hence

$$\mu_k = \Gamma(\alpha+k+1)[\alpha+k-\psi(\alpha+k+1)], \quad k=0,1,2,\ldots, \tag{7}$$

where $\psi(x)=\Gamma'(x)/\Gamma(x)$ is the logarithmic derivative of the gamma function. This is implemented in the symbolic/variable-precision Matlab routine

`momlaglog.m`,[2] which produces the first `2N` moments of v to `dig` decimal digits (the parameter α is input via the variable `a`):[3]

```
function mom=momlaglog(dig,N,a)
digits(dig);
for k=1:2*N
   mom(k)=gamma(vpa(a+k))*(a+k-1-psi(vpa(a+k)));
end
```

2.2 Modified moments of v

Let $\hat{L}_k^{(\alpha)}(x)$ be the monic generalized Laguerre polynomial of degree k. Then, from [2, eq (4.1)] it follows that the modified moments of the weight function $x^\alpha e^{-x} \ln x$ on $\mathbb{R}_+$ relative to the system of monic generalized Laguerre polynomials are

$$\int_0^\infty x^\alpha e^{-x} \ln x \, \hat{L}_k^{(\alpha)}(x)\mathrm{d}x = \begin{cases} \Gamma(\alpha+1)\psi(\alpha+1) \text{ if } k=0, \\ (-1)^{k+1}\Gamma(\alpha+1)(k-1)! \text{ if } k>0. \end{cases} \tag{8}$$

If m_k, $k = 0, 1, 2, \ldots$, denote the modified moments of the weight function v in (3), then

$$\begin{aligned} m_0 &= \int_0^\infty x^\alpha e^{-x}(x - 1 - \ln x)\mathrm{d}x \\ &= \Gamma(\alpha+2) - \Gamma(\alpha+1) - \Gamma(\alpha+1)\psi(\alpha+1) = \Gamma(\alpha+1)[\alpha - \psi(\alpha+1)]. \end{aligned}$$

Furthermore, since

$$x\hat{L}_1^{(\alpha)}(x) = \hat{L}_2^{(\alpha)}(x) + (\alpha+3)\hat{L}_1^{(\alpha)}(x) + (\alpha+1)\hat{L}_0^{(\alpha)}(x),$$

and using orthogonality,

$$\begin{aligned} m_1 &= \int_0^\infty x^\alpha e^{-x}(x - 1 - \ln x)\hat{L}_1^{(\alpha)}(x)\mathrm{d}x \\ &= (\alpha+1)\Gamma(\alpha+1) - \Gamma(\alpha+1) = \alpha\Gamma(\alpha+1). \end{aligned}$$

Finally, for $k \geq 2$, by orthogonality and (8),

$$m_k = \int_0^\infty x^\alpha e^{-x}(x - 1 - \ln x)\hat{L}_k^{(\alpha)}(x)\mathrm{d}x = (-1)^k\Gamma(\alpha+1)(k-1)!, \quad k \geq 2.$$

[2] All Matlab routines referenced in this paper can be downloaded from the Web site http://www.cs.purdue.edu/archives/2002/wxg/codes/GQLOG.html.

[3] The symbolic Matlab toolbox does not currently support `psi` for variable-precision arguments. Release 5.1 (R2008b) of the Symbolic Math Toolbox and later releases, however, allow the calculation of the ψ-function to `dig` decimal digits by the commands `digits(dig)`, `y=feval(symengine,'psi',x)`, `y=vpa(y)`.

The first 2N modified moments of v can thus be computed to dig decimal places by the following Matlab routine,[4]

```
function mom=mmomlaglog(dig,N,a)
digits(dig);
mom(1)=gamma(vpa(a+1))*(a-psi(vpa(a+1)));
mom(2)=a*gamma(vpa(a+1));
sgn=-1;
for k=3:2*N
   sgn=-sgn;
   mom(k)=sgn*gamma(vpa(a+1))*gamma(vpa(k-1));
end
```

2.3 Recurrence coefficients for v

With the moments resp. modified moments of v at our disposal, we can now call upon the modified Chebyshev algorithm (cf. [4, §2.1.7]), implemented in the variable-precision Matlab routine

$$\mathtt{ab} = \mathtt{schebyshev(dig, N, mom, abm)}, \tag{9}$$

to generate in dig-decimal digit arithmetic the first N recurrence coefficients α_k and β_k of the weight function v, which are stored in the two columns of the N×2 array ab. In the case of ordinary moments, mom in (9) has to be identified with momlaglog and abm omitted or assigned the zero array of dimension (2N−1)×2, whereas in the case of modified moments, mom has to be identified with mmomlaglog and the (2N−1)×2 array abm filled in the first resp. second column with the first 2N−1 recurrence coefficients a_k resp. b_k of the (monic) generalized Laguerre polynomials. They are

$$\begin{aligned} a_k &= 2k+\alpha+1, \quad k = 0, 1, 2, \ldots, 2\mathtt{N}-2, \\ b_0 &= \Gamma(\alpha+1), \quad b_k = k(k+\alpha), \quad k = 1, 2, \ldots, 2\mathtt{N}-2. \end{aligned}$$

Because of possible ill-conditioning, the number dig of digits required in (9) will in general be much larger than the number nofdig of desired digits in the recurrence coefficients. There is a simple routine (for details, see [5, §2]) that determines the number dig iteratively by doing the computation repeatedly, with increasing precisions, until two successive results for ab agree to nofdig digits in terms of either absolute or relative accuracy. In the present case, this is accomplished by the routines sr_laguerrelog0.m and sr_laguerrelog1.m, which are called by

$$\begin{aligned} &\mathtt{[ab, dig] = sr\_laguerrelog0(N, a, nofdig)}, \\ &\mathtt{[ab, dig] = sr\_laguerrelog1(N, a, nofdig)}, \end{aligned} \tag{10}$$

[4]See footnote 3.

the former using ordinary moments, the latter modified moments. Both employ a relative accuracy criterion to control termination of the iterations involved.

3 The weight function w

In dealing with the weight function w in (4), it is convenient to pass from the interval $[-1, 1]$ to the interval $[0, 1]$ by letting $x = 2t - 1, 0 \le t \le 1$. The weight function $w(x)$ then becomes, up to a constant factor,

$$w^0(t) = (1-t)^\alpha t^\beta \ln(1/t), \quad 0 < t < 1. \tag{11}$$

If α_k^0, β_k^0, $k = 0, 1, 2, \ldots$, denote the recurrence coefficients of the (monic) polynomials orthogonal with respect to w^0, then those for the orthogonal polynomials with respect to w are

$$\begin{aligned} &\alpha_k = 2\alpha_k^0 - 1, \quad k \ge 0, \\ &\beta_0 = 2^{\alpha+\beta+1}\beta_0^0, \quad \beta_k = 4\beta_k^0, \quad k > 0. \end{aligned} \tag{12}$$

We may therefore, from now on, restrict ourselves to the "shifted" weight function w^0 in (11).

3.1 The moments of w^0

The moments

$$\mu_k^0 = \int_0^1 t^{k+\beta}(1-t)^\alpha \ln(1/t)\mathrm{d}t \tag{13}$$

can be obtained from the known Beta integral

$$\int_0^1 t^{k+\beta}(1-t)^\alpha \mathrm{d}t = \frac{\Gamma(k+\beta+1)\Gamma(\alpha+1)}{\Gamma(k+\alpha+\beta+2)} \tag{14}$$

by differentiating both sides partially with respect to β,

$$-\int_0^1 t^{k+\beta}(1-t)^\alpha \ln(1/t)\mathrm{d}t = \Gamma(\alpha+1)\frac{\partial}{\partial\beta}\left\{\frac{\Gamma(k+\beta+1)}{\Gamma(k+\alpha+\beta+2)}\right\}.$$

An elementary calculation yields

$$\begin{aligned} \mu_k^0 = &\frac{\Gamma(\alpha+1)\Gamma(k+\beta+1)}{\Gamma(k+\alpha+\beta+2)}\{\psi(k+\alpha+\beta+2) - \psi(k+\beta+1)\}, \\ &k = 0, 1, 2, \ldots . \end{aligned} \tag{15}$$

The following Matlab routine `momjaclog.m`[5] generates the first `2N` moments of w^0 to `dig` decimal digits.

```
function mom=momjaclog(dig,N,a,b)
digits(dig);
for k=1:2*N
   mom(k)=gamma(vpa(a+1))*gamma(vpa(k+b))* ...
      (psi(vpa(k+a+b+1))-psi(vpa(k+b)))/ ...
      gamma(vpa(k+a+b+1));
end
```

3.2 Modified moments of w^0

If $P_n^{*(\alpha,\beta)}(t) = P_n^{(\alpha,\beta)}(2t-1)$ is the shifted Jacobi polynomial of degree n, then the corresponding modified moments of w^0, by [2, eq (2.2)], are

$$\int_0^1 t^\beta (1-t)^\alpha \ln(1/t) P_k^{*(\alpha,\beta)}(t)\mathrm{d}t = \begin{cases} \dfrac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}\{\psi(\alpha+\beta+2)-\psi(\beta+1)\} & \text{if } k=0, \\ \dfrac{(-1)^k}{k}\dfrac{\Gamma(k+\alpha+1)\Gamma(\beta+1)}{\Gamma(k+\alpha+\beta+2)} & \text{if } k\geq 1. \end{cases} \tag{16}$$

For the application of the modified Chebyshev algorithm we need the modified moments m_k relative to the *monic* shifted Jacobi polynomials, $\hat{P}_k^{*(\alpha,\beta)}$. Since

$$\hat{P}_k^{*(\alpha,\beta)}(t) = \frac{\Gamma(k+\alpha+\beta+1)k!}{\Gamma(2k+\alpha+\beta+1)} P_k^{*(\alpha,\beta)}(t),$$

these are, by (16),

$$m_k = \begin{cases} \dfrac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}\{\psi(\alpha+\beta+2)-\psi(\beta+1)\} & \text{if } k=0, \\ \dfrac{(-1)^k(k-1)!}{k+\alpha+\beta+1}\dfrac{\Gamma(k+\alpha+1)\Gamma(\beta+1)}{\Gamma(2k+\alpha+\beta+1)} & \text{if } k\geq 1. \end{cases} \tag{17}$$

The first $2N$ of them are generated to `dig` decimal places by the following Matlab routine.[6]

[5] See footnote 3.
[6] See footnote 3.

```
function mom=mmomjaclog(dig,N,a,b)
digits(dig);
mom(1)=gamma(vpa(a+1))*gamma(vpa(b+1))* ...
   (psi(vpa(a+b+2))-psi(vpa(b+1)))/ ...
   gamma(vpa(a+b+2));
sgn=1;
for k=2:2*N
   sgn=-sgn;
   mom(k)=sgn*gamma(vpa(k-1))*gamma(vpa(k+a))* ...
      gamma(vpa(b+1))/((k+a+b)*gamma(vpa(2*k+a+b-1)));
end
```

3.3 Recurrence coefficients for w^0

Similarly as in Section 2.3, we can use the routines `momjaclog.m` and `mmomjaclog.m`, in combination with the routine `schebyshev.m` in (9) to generate the `N` recurrence coefficients α_k, β_k, $k = 0, 1, \ldots, \mathtt{N}-1$, to `nofdig` decimal digits, using either moments or modified moments of w^0. When using modified moments, the routine `schebyshev.m` requires, in addition to the modified moments, also the recurrence coefficients a_k, b_k of the monic shifted Jacobi polynomials, which in terms of the recurrence coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ for the monic Jacobi polynomials are

$$a_k = (\hat{\alpha}_k + 1)/2, \quad b_k = \hat{\beta}_k/4, \quad k = 0, 1, 2, \ldots .$$

(The coefficient b_0 is immaterial, since it is not used in the modified Chebyshev algorithm.) The respective routines are called via

$$\begin{aligned} &[\mathtt{ab}, \mathtt{dig}] = \mathtt{sr\_jacobilog0}(\mathtt{N}, \mathtt{a}, \mathtt{b}, \mathtt{nofdig}), \\ &[\mathtt{ab}, \mathtt{dig}] = \mathtt{sr\_jacobilog1}(\mathtt{N}, \mathtt{a}, \mathtt{b}, \mathtt{nofdig}). \end{aligned} \tag{18}$$

Both use an absolute error criterion to control termination of the iterations involved.

4 Numerical results

4.1 Logarithmic Gauss–Laguerre quadrature

We have noted in Section 2.3 that the number `dig` of digits required to obtain recurrence coefficients to `nofdig` digits is usually much larger than `nofdig` because of ill-conditioning. We document this in the case of the two routines in (10) by letting $\mathtt{N} = 20$, $\mathtt{nofdig} = 16$, and $\mathtt{a} = -1/2, 0, 1/2$. The respective output `dig` for the first routine is found to be 35 in all three cases, while for the second routine it is 32, 31, and 31. This indicates severe ill-conditioning, both for ordinary as well as for modified moments, suggesting condition numbers of the order 10^{19} in the former case, and 10^{16} in the latter. The matter becomes

Table 1 Numerical results for Example 4.1

α	N	I
$-1/2$	93	2.523864212300172075250265713988 3
0	95	0.565882809536091407557552758692 02
1/2	97	0.407012665469387057879432265854 98

rapidly worse with increasing N. When N = 40, for example, the first routine returns dig = 53, 54, 53, and the second routine dig = 50 for all three values of a.

We used the second routine to compute the first N = 100 recurrence coefficients to 32 decimal places for the weight function v in (3) with $\alpha = -1/2, 0, 1/2$. The results are stored in the files coefflaglog$i$, $i = 1:3$.[7] Each file took over 10 hours to compute on the Sun Ultra workstation and required precisions of up to about 130 digits. The files, however, allow us, in conjunction with the routine gauss.m or its symbolic counterpart sgauss.m, to generate Gaussian quadrature rules for the weight function v with $\alpha = -1/2, 0, 1/2$ of orders up to 100 and precisions up to 32 decimal digits.

Example 4.1 Compute

$$I = \int_0^\infty \frac{x^\alpha e^{-x}(x - 1 - \ln x)}{1 + e^{-(x+7/2)}}\,\mathrm{d}x, \quad \alpha = -1/2, 0, 1/2.$$

Not knowing exact results, we use N-point Gaussian rules, starting with some appropriately large value of N and incrementing it in steps of 1 until two successive results agree to within a tolerance of 1.5×10^{-32}. This is done in the routine GLExample.m, an excerpt of which (for $\alpha = -1/2$) is shown below[8]

```
digits(32); dig=digits;
ab1=vpaconvert('coefflaglog1');
derr=1; N=89; I=vpa(1);
while derr>1.5e-32
   I0=I; N=N+1
   ab=ab1(1:N,:);
   xw=sgauss(dig,N,ab);
   I=sum(xw(:,2)./(1+exp(-xw(:,1)-7/2)));
   err=abs(I-I0); derr=subs(err);
end
I=vpa(I)
```

The results are shown in Table 1. As can be seen, Gauss quadrature has to work hard to achieve the requested accuracy. The reason for this are the poles

[7] Accessible at the Web site http://www.cs.purdue.edu/archives/2001/wxg/tables.

[8] vpaconvert.m in the second line is a nonstandard routine that loads columns of variable-precision numbers into a corresponding Matlab array. It uses the perl script vpaconvert.pl.

Table 2 Numerical results for Example 4.1, modified

α	N	I
$-1/2$	35	2.66616486982777464899394494941 25
0	35	0.58884713601088713559014872249026
1/2	36	0.41462273453688846429076235114236

of the integrand, those closest to the real axis being located at $-7/2 \pm i\pi$. Indeed, reciprocating the integrand, i.e., multiplying instead of dividing by $1 + e^{-(x+7/2)}$, we get the results shown in Table 2.

Example 4.2 Compute

$$I = \int_0^\infty \frac{x^\alpha e^{-x} \ln x}{1 + e^{-(x+7/2)}} \, dx, \quad \alpha = -1/2, 0, 1/2.$$

Here we use (5) and the results of Example 4.1. The required N-point Gauss–Laguerre quadrature rules are generated by means of

```
ab0 = sr_laguerre(dig, N, a);  xw0 = sgauss(dig, N, ab0);
```

where dig = 32 and N as in Table 1. The results are shown in Table 3.

4.2 Logarithmic Gauss–Jacobi quadrature

We first discuss the performance of the two routines in (18). The use of ordinary moments, when the interval of orthogonality is finite, invariably gives rise to severe ill-conditioning, in contrast to modified moments, which usually lead to rather well-conditioned problems. Thus, the use of the first routine in (18) is discouraged. To illustrate, let N=20, nofdig=16, a=0, and b= $-1/2$. Then dig, the number of digits required to obtain ab to nofdig decimal digits, is found to be 44 for the first routine, and 19 for the other, showing that ill-conditioning in the first case is so bad that 28 more digits are required to overcome it, whereas in the second case, three additional digits suffice to deal with the little ill-conditioning there is. (The condition number is indeed of the order 400 at most, judging from Table 2.6 in [4].)

The parameters α, β in the weight function w^0 of (11) that are of most interest are likely to be those in the set $\{-1/2, 0, 1/2\}$. We therefore computed the first N=100 recurrence coefficients to 32 decimal digits for all nine combinations of these parameters, using the routine sr_jacobilog1.m. The

Table 3 Numerical results for Example 4.2

α	N	I
$-1/2$	93	$-3.38246288364444518111145833447731$
0	95	$-0.55853107068055456953552519830935$
1/2	97	0.03839032146080956123838601301 5731

Table 4 Numerical results for Example 4.3

β	N	K	err
−1/2	21	14.655449506835504240873656238918	2.455e–33
0	21	3.289868133696452872944830333292O	6.010e–33
1/2	22	1.344550493164495759126343761O818	1.035e–32

results are stored in the files `coeffjaclog`ij, $i = 1:3$, $j = 1:3$,[9] where the index i refers to the parameter α and the index j to the parameter β, and where the three values of the indices correspond to the values $-1/2, 0, 1/2$ of the parameters. Thus, the files `coeffjaclog2`j, $j = 1:3$, for example, contain the recurrence coefficients for the weight functions $x^\beta \ln(1/x)$, $\beta = -1/2, 0, 1/2$, which have previously been computed to 25 digits in [3, Table III]. Our new, more accurate computation confirms the accuracy of the earlier results except for occasional end-figure discrepancies. Each file took about three hours or less to compute on our Sun Ultra workstation and required precisions of the order of 50 decimal digits.

Example 4.3 Compute

$$K = 4\int_0^1 \frac{x^\beta \ln(1/x)}{1+x}\,\mathrm{d}x, \quad \beta = -1/2, 0, 1/2.$$

It is known that (cf. [6, 4.251(3)])[10]

$$K = \begin{cases} \psi'\left(\frac{1}{4}\right) - \psi'\left(\frac{3}{4}\right) & \text{if } \beta = -1/2, \\ \psi'\left(\frac{1}{2}\right) - \psi'(1) = 2\zeta(2) & \text{if } \beta = 0, \\ \psi'\left(\frac{3}{4}\right) - \psi'\left(\frac{5}{4}\right) & \text{if } \beta = 1/2. \end{cases} \tag{19}$$

We use the recurrence coefficients in the files `coeffjaclog2`j, $j = 1:3$, to generate Gaussian quadrature rules for the integral in Example 4.3 by means of the routine `sgauss.m` and determine the smallest number `N` of quadrature nodes such that the relative errors are $\le 1.5 \times 10^{-32}$. This is done in the routine `GJExample1.m`, an excerpt of which (for $\beta = -1/2$) is shown below.[11]

[9] See footnote 7.

[10] There is a typographical error in this formula: β should read β'. The formula is given correctly in the cited source.

[11] See footnote 8 for `vpaconvert`. The evaluation of $\psi'(x)$ in the 3rd line is currently to be done as indicated in footnote 3, except that `x` has to be replaced by `x,1`.

Table 5 Numerical results for Example 4.4

α	N	K	err
−1/2	21	4.11871837492687201436674014469 73	7.864–33
0	22	3.82080722592471875024200170724 60	
1/2	22	3.60447218516353104232409970731 29	

```
digits(32); dig=digits;
ab1=vpaconvert('coeffjaclog21');
dpsi1=psi(vpa(1/4),1); dpsi3=psi(vpa(3/4),1);
derr=1; N=18;
while derr>1.5e-32
   N=N+1
   ab=ab1(1:N,:);
   xw=sgauss(dig,N,ab);
   K1=4*sum(xw(:,2)./(1+xw(:,1)));
   err=abs((K1-dpsi1+dpsi3)/(dpsi1-dpsi3));
   derr=subs(err);
end
K1=vpa(K1), derr
```

Numerical results are shown in Table 4. Remarkably, Gaussian rules of order $\texttt{N} \approx 20$ already yield answers accurate to 32 digits, even though the integrand has a pole at $x = -1$, a distance of 1 away from the end point of the interval of integration.

Example 4.4 Compute

$$K = \int_0^1 \frac{x^{-1/2}(1-x)^{\alpha}\,\ln(1/x)}{\sqrt{1+x}}\,\mathrm{d}x, \quad \alpha = -1/2,\, 0,\, 1/2.$$

It appears that an exact answer is known only for $\alpha = -1/2$, in which case $K = \frac{\sqrt{2\pi}}{8}\,[\Gamma(1/4)]^2$ (cf. [6, 4.241(11)]). The routine `GJExample2.m` now uses the files `coeffjaclog`$i1, i = 1:3$, in conjunction with the routine `sgauss.m`, to obtain the results displayed in Table 5. Here, too, convergence of Gauss quadrature is quite fast, in spite of the square-root singularity at $x = -1$.

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