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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 nonclassical 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] $\mathrm{d}\lambda$ on the real line $\mathbb{R}$ with respect to which polynomials can be integrated, that is, for which $\int_{\mathbb{R}} t^k \,\mathrm{d}\lambda(t)$ exists for each nonnegative integer $k \in \mathbb{N}_0$. A quadrature formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{0.1}$$

[1] For our purposes it suffices to assume that $\mathrm{d}\lambda$ is either a discrete measure, $\mathrm{d}\lambda(t) = \mathrm{d}\lambda_N(t)$, 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 $\mathrm{d}\lambda(t) = w(t)\,\mathrm{d}t$ 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,

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \begin{cases} \sum_{i=1}^{N} w_i f(t_i), & \mathrm{d}\lambda \text{ discrete}, \\ \int_{\mathrm{supp}(\mathrm{d}\lambda)} f(t)w(t)\,\mathrm{d}t, & \mathrm{d}\lambda \text{ absolutely continuous}, \end{cases}$$

where $\mathrm{supp}(\mathrm{d}\lambda)$ denotes the support of $\mathrm{d}\lambda$, 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 $\mathrm{d}\lambda$). 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

$$\int_{\mathbb{R}} \omega_n(t) p(t)\, \mathrm{d}\lambda(t) = 0 \qquad \text{for each } p \in \mathbb{P}_{m-1}. \tag{0.3}$$

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

$$(u, v)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t) v(t)\, \mathrm{d}\lambda(t), \qquad u, v \in \mathbb{P}, \tag{0.4}$$

in terms of which (0.3) can be stated as $(\omega_n, p)_{\mathrm{d}\lambda} = 0$ 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 $\int_{\mathbb{R}} \omega_n^2(t)\, \mathrm{d}\lambda(t) = 0$, which is impossible if $\mathrm{d}\lambda$ has more than n points of increase. (In the context of quadrature rules, $\mathrm{d}\lambda$ 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

$$(\omega_n, p)_{\mathrm{d}\lambda} = 0, \qquad \text{all } p \in \mathbb{P}_{n-1}. \tag{0.5}$$

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 $\omega_{n-1}(t) = \Pi_{\nu=2}^n(t-\tau_\nu)$, 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,

$$\int_{\mathbb{R}} \omega_n(t) p(t)\, d\lambda_\sigma(t) = 0, \quad \text{all } p \in \mathbb{P}_{m-1}, \quad \sigma = 1, 2, \ldots, s. \tag{0.8}$$

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

$$\pi_{k+1}(t) - t\pi_k(t) = -\alpha_k \pi_k(t) - \beta_k \pi_{k-1}(t) + \sum_{j=0}^{k-2} \gamma_{kj} \pi_j(t), \quad k = 0, 1, \ldots, N-1, \tag{0.10}$$

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 $\mathrm{d}\lambda$ 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 $\pi_k(\cdot\,; \mathrm{d}\lambda)$, both inside and outside the interval of orthogonality. For discrete measures $\mathrm{d}\lambda_N$, 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 $\mathrm{d}\lambda_N$ are equally spaced. As a consequence, the accuracy of the $\pi_k(\cdot\,; \mathrm{d}\lambda_N)$, 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

$$\| u \|_w^2 = \int_{-1}^{1} u^2(t) w(t)\, \mathrm{d}t, \tag{1.2}$$

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,

$$\lim_{n\to\infty} \int_{-1}^{1} [f(t) - (L_n f)(t)] w(t)\, \mathrm{d}t = 0 \qquad \text{for all } f \in C[-1, 1], \tag{1.3}$$

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).

$$\lambda_i = \frac{\pi}{3n}, \qquad i = 1, 2, \ldots, n,$$
$$\mu_j = \frac{2\pi/3}{n + \frac{3}{9 - 8\hat{\tau}_j^2}}, \qquad j = 1, 2, \ldots, n+1.$$

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

$$q(t) > 0 \qquad \text{for } t \in \operatorname{supp}(\mathrm{d}\lambda); \qquad q(s_j) \neq 0, \qquad j = 0, 1, \ldots, m. \tag{2.14}$$

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 $\mathrm{d}\lambda_m$ in (2.31) admits a Gaussian quadrature formula

$$\int_0^\infty g(t)\,\mathrm{d}\lambda_m(t) = \sum_{\nu=1}^{n} \lambda_\nu^G g(t_\nu^G) + R_{n,m}^G(g), \qquad R_{n,m}^G(\mathbb{P}_{2n-1}) = 0, \tag{2.32}$$

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

$$\sum_{\nu=1}^{n} a_\nu \int_0^{\tau_\nu} t^j(\tau_\nu - t)^m\,\mathrm{d}t = \int_0^\infty t^j f(t)\,\mathrm{d}t, \qquad j = 0, 1, \ldots, 2n-1. \tag{2.35}$$

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

$$\begin{aligned} &m![(j+1)(j+2)\cdots(j+m)]^{-1}\sum_{\nu=1}^{n} a_\nu \int_0^{\tau_\nu} t^{j+m}\,\mathrm{d}t \\ &= m![(j+1)(j+2)\cdots(j+m)(j+m+1)]^{-1}\sum_{\nu=1}^{n} a_\nu \tau_\nu^{j+m+1}. \end{aligned} \tag{2.36}$$

On the right, we carry out the first integration by parts in detail to exhibit the reasonings involved. We have, for any $b > 0$,

$$\int_0^b t^j f(t)\,\mathrm{d}t = \frac{1}{j+1}\, t^{j+1} f(t)\Big|_0^b - \frac{1}{j+1}\int_0^b t^{j+1} f'(t)\,\mathrm{d}t. \tag{2.37}$$

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

$$\int_0^\infty t^j f(t)\,\mathrm{d}t = -\frac{1}{j+1}\int_0^\infty t^{j+1} f'(t)\,\mathrm{d}t.$$

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 $\int_0^\infty t^{j+\mu} f^{(\mu)}(t)\,\mathrm{d}t$ 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), Michelli (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 $\sqrt{(\pi_{k+1}, \pi_{k+1})\,d\lambda}$, 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,

$$t\tilde{\pi}_k(t) = \alpha_k\tilde{\pi}_k(t) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(t) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t), \qquad k = 0, 1, 2, \ldots, n-1. \tag{4.7}$$

In terms of the Jacobi matrix $J_n = J_n(d\lambda)$ 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

$$\operatorname{cond} G_n = \| \partial G_n \|, \tag{5.10}$$

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

$$\partial\Phi = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ t_1 & \cdots & t_n & \lambda_1 & \cdots & \lambda_n \\ t_1^2 & \cdots & t_n^2 & 2\lambda_1 t_1 & \cdots & 2\lambda_n t_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ t_1^{2n-1} & \cdots & t_n^{2n-1} & (2n-1)\lambda_1 t_1^{2n-2} & \cdots & (2n-1)\lambda_n t_n^{2n-2} \end{bmatrix} = T D_\lambda,$$

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 $t_1, t_2, \ldots, t_n$:

$$\begin{aligned} h_\nu(t_\mu) &= \delta_{\nu\mu}, \quad h_\nu'(t_\mu) = 0; \\ k_\nu(t_\mu) &= 0, \quad\quad k_\nu'(t_\mu) = \delta_{\nu\mu}, \end{aligned} \tag{5.21}$$

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

$$\begin{aligned} (D_\lambda^{-1} P^{-1} D_s)_{\nu\mu} &= s_{\mu-1} a_{\nu\mu}, & (D_\lambda^{-1} P^{-1} D_s)_{\nu+n,\mu} &= \lambda_\nu^{-1} s_{\mu-1} b_{\nu\mu}, \\ \nu &= 1, 2, \ldots, n; & \mu &= 1, 2, \ldots, 2n, \end{aligned}$$

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.

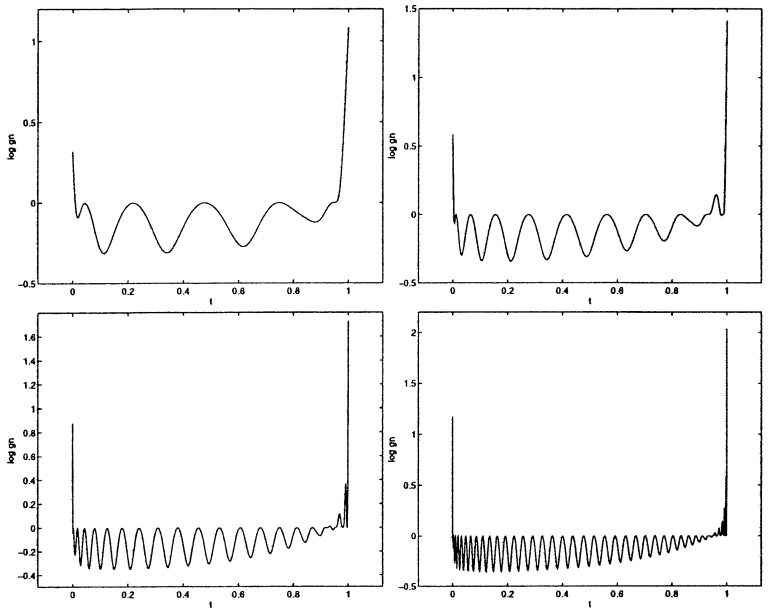

Fig. 1. The polynomial g_n, $n = 5, 10, 20, 40$, for the Maxwell measure with $c = 1$

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

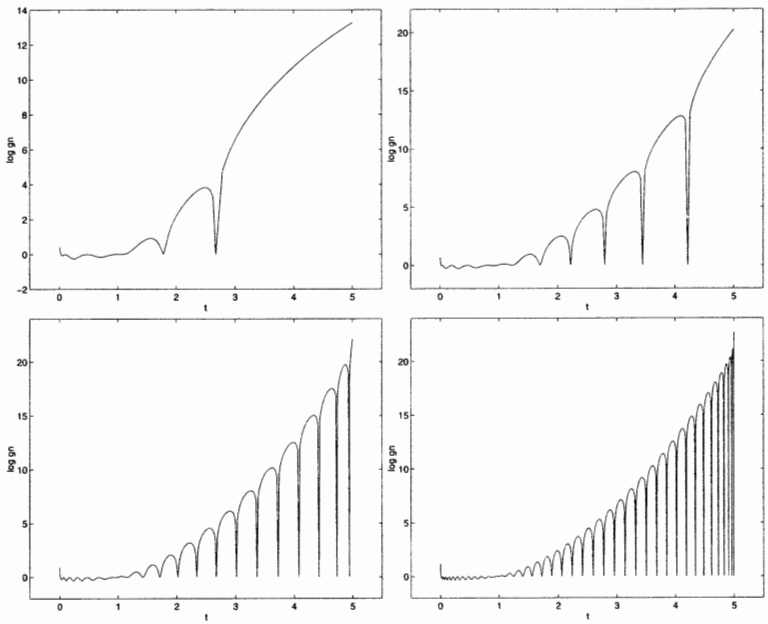

Fig. 2. The polynomial g_n, $n = 5, 10, 20, 40$, for the Maxwell measure with $c = 5$

(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 $t p_k(t) = p_{k+1}(t) + a_k p_k(t) + b_k p_{k-1}(t)$, 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

$$\begin{aligned} &\sigma_{-1,\ell} = 0, \qquad \ell = 1, 2, \ldots, 2n-2, \\ &\sigma_{0,\ell} = m_\ell, \qquad \ell = 0, 1, \ldots, 2n-1, \\ &\alpha_0(\,\mathrm{d}\lambda) = a_0 + \frac{m_1}{m_0}, \qquad \beta_0(\,\mathrm{d}\lambda) = m_0, \end{aligned} \tag{5.33}$$

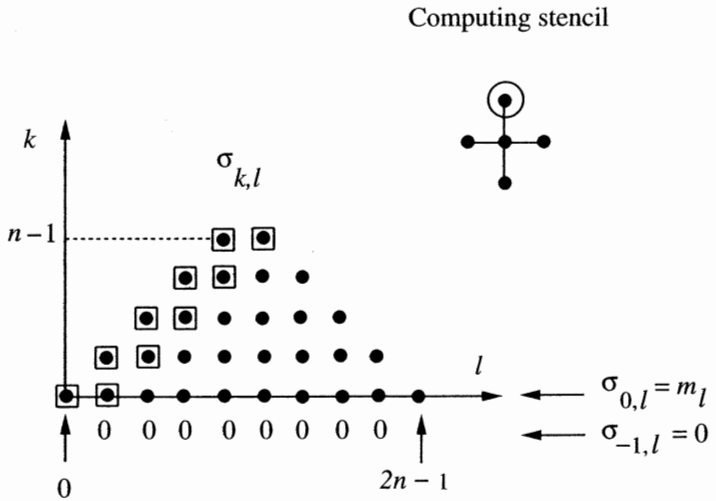

Fig. 3. The modified Chebyshev algorithm, schematically

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,

$$\mu_k(d\lambda_\sigma) = \frac{1}{\sigma + 1 + k}, \qquad k = 0, 1, 2, \ldots, \tag{5.36}$$

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

$$\gamma_1 = \beta > -1; \qquad \gamma_i > -1, \qquad i = 2,\ldots,m; \qquad \gamma_{m+1} = \alpha > -1. \tag{6.16}$$

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 $\mathrm{d}\lambda$ 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 $\mathrm{supp}(\mathrm{d}\lambda)$); he represented the polynomial $u(t)\pi_n(t; u\,\mathrm{d}\lambda)$ in determinantal form as a linear combination of $\pi_n(t; \mathrm{d}\lambda), \ldots, \pi_{n+\ell}(t; \mathrm{d}\lambda)$. 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 $u(t)\pi_n(t; (u/v)\,\mathrm{d}\lambda)$ again in determinantal form as a linear combination of $\pi_{n-m}(t; \mathrm{d}\lambda), \ldots, \pi_{n+\ell}(t; \mathrm{d}\lambda)$ if $m \leq n$, and of $\pi_0(t; \mathrm{d}\lambda), \ldots, \pi_{n+\ell}(t; \mathrm{d}\lambda)$ 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 $\alpha_k(\mathrm{d}\hat{\lambda})$, $\beta_k(\mathrm{d}\hat{\lambda})$ for the modified measure $\mathrm{d}\hat{\lambda} = (u/v)\,\mathrm{d}\lambda$ in terms of those for $\mathrm{d}\lambda$, 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 $\alpha_k(\mathrm{d}\lambda)$, $\beta_k(\mathrm{d}\lambda)$ for the measure $\mathrm{d}\lambda$, compute the recursion coefficients $\alpha_k(\mathrm{d}\hat{\lambda})$, $\beta_k\,\mathrm{d}(\hat{\lambda})$ for the measures $\mathrm{d}\hat{\lambda} = u\,\mathrm{d}\lambda$ and $\mathrm{d}\hat{\lambda} = \mathrm{d}\lambda/v$, 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 $\hat{\pi}_k(\cdot) = \hat{\pi}_k(\cdot\,; z)$,

$$\begin{gathered}\hat{\pi}_{k+1}(t) = (t-\hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k\hat{\pi}_{k-1}(t), \qquad k = 0, 1, 2, \ldots, \\ \hat{\pi}_{-1}(t) = 0, \qquad \hat{\pi}_0(t) = 1,\end{gathered} \tag{7.6}$$

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 $\mathrm{d}\lambda$ is a positive measure. The support of $\mathrm{d}\lambda$ may extend to infinity at one end, when dealing with linear factors, but will be arbitrary otherwise.

Consider first modification by a linear factor,

$$\mathrm{d}\hat{\lambda}(t) = (t-x)\,\mathrm{d}\lambda(t), \qquad x \in \mathbb{R}\backslash I_{\mathrm{supp}}(\mathrm{d}\lambda),$$

where, as indicated, x is any real number outside the 'support interval' $I_{\mathrm{supp}}(\mathrm{d}\lambda)$ of $\mathrm{d}\lambda$, that is, outside the smallest interval containing the support of $\mathrm{d}\lambda$. Then $\mathrm{d}\hat{\lambda}$ is positive definite if x is to the left of this interval, and negative definite otherwise. In either case, $\pi_n(x; \mathrm{d}\lambda) \neq 0$ 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,

$$\mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{t-x}, \qquad x \in \mathbb{R}\backslash I_{\mathrm{supp}}(\mathrm{d}\lambda), \tag{7.16}$$

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

$$p_\nu = \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{m/2} \frac{(\xi_\nu + \mathrm{i}\eta_\nu)^2}{(\xi_\nu - \xi_\mu)^2 - (\eta_\nu^2 - \eta_\mu^2) + 2\,\mathrm{i}\eta_\nu(\xi_\nu - \xi_\mu)},$$

with $p_1 = 1$ if $m = 2$. One can proceed as before, except that the modification of the measure $\mathrm{d}\lambda$ 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 $\mathrm{d}\lambda$ 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 $k = 1, 2, \ldots, n-1$,

$$\begin{aligned} \beta_0^k &= \frac{\sigma_{k,k+1}}{\sigma_{k,k}} + a_k - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \\ \beta_{k-j}^k &= \frac{\sigma_{j,k+1}}{\sigma_{j,j}} + a_k\frac{\sigma_{j,k}}{\sigma_{j,j}} + b_k\frac{\sigma_{j,k-1}}{\sigma_{j,j}} - \frac{\sigma_{j-1,k}}{\sigma_{j-1,j-1}} - \sum_{\ell=j}^{k-1}\beta_{\ell-j}^\ell\frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}, \\ &\qquad\qquad j = k-1, k-2, \ldots, 1 (\text{ if } k \geq 2), \\ \beta_k^k &= \frac{\sigma_{0,k+1}}{\sigma_{0,0}} + a_k\frac{\sigma_{0,k}}{\sigma_{0,0}} + b_k\frac{\sigma_{0,k-1}}{\sigma_{0,0}} - \sum_{\ell=0}^{k-1}\beta_\ell^\ell\frac{\sigma_{\ell,k}}{\sigma_{\ell,\ell}}, \end{aligned}$$

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).

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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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).