Recursive Computation of Certain Derivatives—A Study of Error Propagation

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A brief study is made of the propagation of errors in linear first-order difference equations. The recursive computation of successive derivatives of e^x/x and $(\cos x)/x$ is considered as an illustration.

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1. Introduction

In [2] one of us published algorithms for computing successive derivatives of e^x/x, $(\cos x)/x$, and $(\sin x)/x$. It was brought to our attention [5] that the first two of these algorithms are subject to substantial loss of accuracy if x (or $|x|$ in the case of the second algorithm) is large and n, the order of derivative, is larger than $|x|$. In the following we examine the reasons responsible for this difficulty and suggest ways in which it may be overcome. Revised algorithms implementing the results of this article appear as Remark on Algorithm 282 in the Algorithms section of this issue (see footnote).

Although hardly more than an isolated example,[1] the question discussed here well illustrates the pitfalls inherent in the indiscriminate use of recurrence relations. It may also serve to remind us of the computational limitations of analytic formula manipulation systems.

Consider, for example, the derivatives

$$d_n(x) = \frac{d^n}{dx^n}\left(\frac{e^x}{x}\right), \qquad n = 0, 1, 2, \ldots. \tag{1.1}$$

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[1] We note, however, that the function d_n in (1.1) is of some relevance in molecular structure calculations by virtue of $A_n(1,\alpha) = -d_n(-\alpha)$, $A_n(-1,\alpha) = (-1)^n d_n(\alpha)$, where $A_n(\sigma,\alpha) = \int_\sigma^\infty e^{-\alpha t} t^n\, dt$ are auxiliary "molecular integrals" (cf. [4, 6]).

Analytic differentiation yields

$$d_n(x) = (-1)^n \frac{n!}{x^{n+1}} e^x e_n(-x), \tag{1.2}$$

where

$$e_n(z) = \sum_{k=0}^{n} \frac{z^k}{k!}. \tag{1.3}$$

Formula manipulation systems most likely would deal with (1.1) by effectively evaluating the expression in (1.2). Note, however, that for x positive and large, and $n \gg x$, the dominant term in the sum for $e_n(-x)$ has the order of magnitude $e^x/\sqrt{(2\pi x)}$, while the sum itself is close to e^{-x}. For such values of x and n, the evaluation of (1.2) thus involves considerable cancellation of leading digits, the resulting loss of accuracy amounting to about $\log_{10} e^{2x} = (.868\ldots)x$ decimal digits.

Alternatively, one might try to compute the desired derivatives recursively, as in [2], using

$$d_n(x) = -\frac{n}{x} d_{n-1}(x) + \frac{e^x}{x}, \qquad n = 1, 2, 3, \ldots, \qquad d_0(x) = \frac{e^x}{x}. \tag{1.4}$$

While, technically speaking, this recursion is stable, it will be seen that the cancellation problem reappears with the same devastating force.

2. Error Propagation in Linear First-order Difference Equations

The recurrence relation (1.4) is an example of a first-order linear difference equation

$$y_n = a_n y_{n-1} + b_n, \qquad n = 1, 2, 3, \ldots, \qquad a_n \neq 0. \tag{2.1}$$

We consider solutions on the set $\mathfrak{N}$ of nonnegative integers n. Given a particular solution $\{f_n\}$ of (2.1) to be computed, we wish to examine the influence of a single error at $m \in \mathfrak{N}$ upon the value of f_n at any other $n \in \mathfrak{N}$. Since the solution $\{f_n\}$ may vary considerably in magnitude, it is appropriate to consider *relative* errors and restrict attention to the subset $\mathfrak{N}_0 \subset \mathfrak{N}$ on which $f_n \neq 0$. Assuming for simplicity that $f_0 \neq 0$, the question can easily be answered as follows (cf. [1]).

Let $\{\tilde{f}_n\}$ denote the "perturbed" solution of (2.1) corresponding to the starting value $\tilde{f}_m = f_m(1+\epsilon)$, $m \in \mathfrak{N}_0$. Then for any $n \in \mathfrak{N}_0$ we have

$$\tilde{f}_n = f_n\left(1 + \frac{\rho_n}{\rho_m}\epsilon\right), \tag{2.2}$$

where[2]

$$\rho_n = \frac{f_0 h_n}{f_n}, \qquad h_n = a_n a_{n-1} \ldots a_1. \tag{2.3}$$

[2] The factor f_0 in the definition of ρ_n is included only for the purpose of normalization, making $\rho_0 = 1$.

A relative error ϵ introduced at m thus induces a relative error $(\rho_n/\rho_m)\epsilon$ at n. In particular, the error is magnified if $|\rho_n| > |\rho_m|$ and damped if $|\rho_n| < |\rho_m|$. The quantities ρ_n will be referred to as "amplification factors."

The behavior of the function $\{|\rho_n|\}$ clearly determines the error propagation pattern associated with the particular solution $\{f_n\}$ of (2.1). If there is any choice of direction in which the recursion (2.1) can be employed, then the direction in which $|\rho_n|$ decreases (or has a tendency to decrease) is generally the one to be preferred. Following this direction, errors introduced at each step of the recursion (due to rounding, for example) have a tendency to be consistently damped out. Proceeding in direction of increasing $|\rho_n|$ is tolerable only if the maximum error amplification remains within acceptable limits.

3. Successive derivatives of e^x/x

From (1.2) and (2.3) we find that the amplification factors ρ_n associated with the solution (1.1) of the difference equation (1.4) are given by

$$\rho_n(x) = \frac{1}{e_n(-x)}. \qquad (3.1)$$

If $x < 0$, then $|\rho_n|$ decreases monotonically from 1 to $e^{-|x|}$. In this case the recursion (1.4) is properly applied in the forward direction for all $n > 0$. If $x > 0$, the behavior of $|\rho_n|$ is as shown in Figure 1. Disregarding relatively small values of x (for which $|\rho_n|$ remains within acceptable limits for all $n \geq 0$), it is seen that $|\rho_n|$ initially decreases until it reaches a minimum value near $n_0 = [x]$, and from then on increases, reaching the limit $|\rho_\infty| = e^x$ rather abruptly. The recursion (1.4) is now properly applied in the forward direction on the interval $0 < n \leq n_0$, and in the backward direction on $n_0 < n < \infty$, unless an error amplification of $|\rho_\infty/\rho_{n_0}|$ is tolerable, in which case forward recursion may be used on the whole interval $0 < n < \infty$.

We note that $|e_n(-n)| \sim e^n/2\sqrt{(2\pi n)}$ as $n \to \infty$, from which it follows that the maximum error amplification is approximately $e^{2x}/2\sqrt{(2\pi x)}$, when x is large.

The graphs in Figure 1 may be interpreted as follows. Writing $d_n(x)$ in the form

$$d_n(x) = (-1)^n \frac{n!}{x^{n+1}} + \int_0^1 t^n e^{xt}\, dt \qquad (3.2)$$

[by using the remainder term of the exponential series in (1.2)] and assuming $x > 0$ large, one observes that the integral on the right of (3.2) initially dominates, until n is large enough to make the first term of comparable magnitude. From this point on, the first term quickly becomes the dominant term. As long as the integral dominates, $d_n(x)$ varies relatively slowly with n, so that by (2.3) $|\rho_n|$ is approximately proportional to $|h_n| = n!\,x^{-n}$. Once the first term takes over, $|\rho_n|$ becomes constant, equal to e^x. Therefore, the curves in Figure 1, up to a scale factor, are essentially those for $n!\,x^{-n}$, levelled off at the value of n for which the integral in (3.2) becomes negligible.

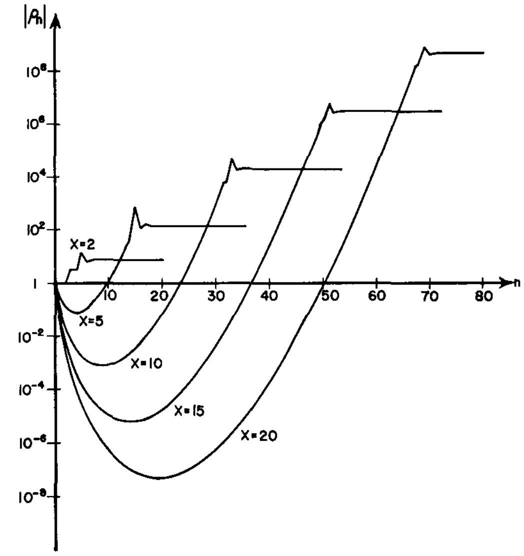

FIG. 1. Amplification factors $|\rho_n(x)|$ of (3.1), for $0 \leq n \leq 80$, $x = 2, 5, 10, 15, 20$

It remains to consider the question of computing an appropriate starting value in cases where backward recurrence is called for. From the remarks just made, it is clear that $d_n(x)$ can be approximated by

$$q_n(x) = (-1)^n \frac{n!}{x^{n+1}} \qquad (3.3)$$

to any degree of accuracy, if n is taken sufficiently large. To analyze this more carefully, observe that the integral in (3.2) is bounded by $e^x/(n+1)$, and that $n! > (n/e)^n$ for every integer $n \geq 1$. Therefore,

$$\left|\frac{d_n - q_n}{q_n}\right| = \frac{x^{n+1}}{n!}\int_0^1 t^n e^{xt}\, dt < \frac{x^{n+1}}{(n+1)!} e^x < \left(\frac{ex}{n+1}\right)^{n+1} e^x,$$

from which it follows that $|(d_n - q_n)/q_n| \leq \delta$ $(0 < \delta < 1)$, and consequently $|(d_n - q_n)/d_n| \leq \delta/(1-\delta)$, as soon as n is large enough to satisfy

$$\left(\frac{ex}{n+1}\right)^{n+1} e^x \leq \delta. \qquad (3.4)$$

In particular, q_n approximates d_n to s significant digits if (3.4) holds with $\delta = \frac{1}{2}10^{-s}$. Taking logarithms, this condition amounts to

$$\frac{n+1}{ex} \ln \frac{n+1}{ex} \geq \frac{x + s\ln 10 + \ln 2}{ex},$$

which in turn is equivalent to

$$n + 1 \geq ex\, t\left(\frac{x + s\ln 10 + \ln 2}{ex}\right), \qquad (3.5)$$

where $t(y)$ denotes the inverse function of $y = t \ln t$. (Low-accuracy approximations to $t(y)$ are obtained in another context in [3, p. 51].) Thus, if n^0 is the smallest integer n satisfying (3.5), then $q_n(x)$ in (3.3) may be used to approximate $d_n(x)$ (to s significant digits) for $n \geq n^0$, while backward recursion in (1.4) may be used to obtain $d_n(x)$ for $n_0 \leq n < n^0$.

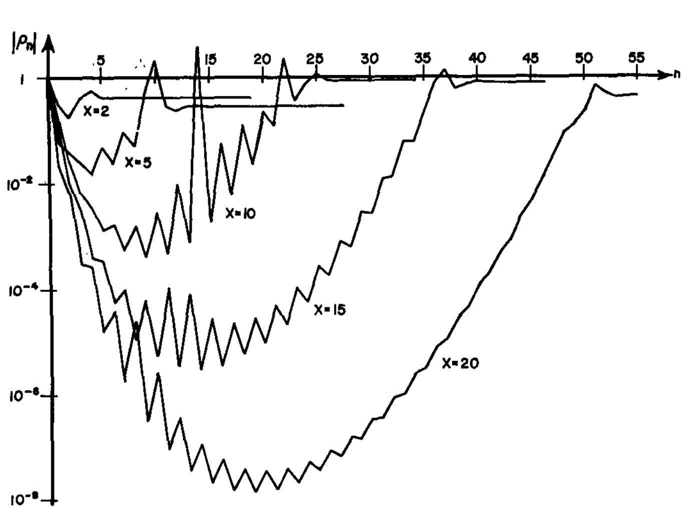

FIG. 2. Amplification factors $|\rho_n(x)|$ of (4.3), for $0 \leq n \leq 55$, $x = 2, 5, 10, 15, 20$

4. Successive Derivatives of (cos x)/x and (sin x)/x

The derivatives

$$c_n(x) = \frac{d^n}{dx^n}\left(\frac{\cos x}{x}\right) \qquad (4.1)$$

satisfy the difference equation

$$c_n(x) = -\frac{n}{x}c_{n-1}(x) + \frac{1}{x}\operatorname{Re}(i^n e^{ix}), \qquad n = 1, 2, 3, \cdots, \qquad (4.2)$$

and the associated amplification factors ρ_n are now

$$\rho_n(x) = \frac{\cos x}{\operatorname{Re}[e^{ix}e_n(-ix)]}. \qquad (4.3)$$

Clearly, $\rho_n(-x) = \rho_n(x)$. The behavior of $|\rho_n|$ is shown in Figure 2. The graphs are basically the same as those in Figure 1, except that they are leveled off at an earlier stage (due to the limiting value now being $\rho_\infty = \cos x$) and are not nearly as smooth.

The recurrence (4.2) is again properly applied in the forward direction for $0 < n \leq n_0$ ($n_0 = [|x|]$), and should be used in this backward direction for $n_0 < n < \infty$, unless the maximum error amplification $|1/\rho_{n_0}|$ (now approximately half as large as in the case of $d_n(x)$) is within tolerable limits. Due to the fluctuations in $|\rho_n|$, occasional losses of significant digits must be expected, even if the recursion is used in the proper direction. Loss of significance is apt to occur for those values of n for which $|c_n(x)|$ is exceptionally small.

The identity

$$c_n(x) = \frac{(-1)^n n!}{x^{n+1}} + \int_0^1 t^n \operatorname{Re}[i^{n+1}e^{ixt}]\,dt \qquad (4.4)$$

permits us to interpret the graphs of Figure 2 in a similar manner as we did previously for the graphs of Figure 1. It also follows from (4.4) that $q_n(x)$ in (3.3) can be used to approximate $c_n(x)$ to s significant digits for all n satisfying

$$n + 1 \geq e|x|\,t\left(\frac{s \ln 10 + \ln 2}{e|x|}\right).$$

Replacing "Re" by "Im" in (4.2) and (4.3), and "cos x" by "sin x" in (4.3), one obtains the difference equation and associated amplification factors for the derivatives $s_n(x) = (d^n/dx^n)(\sin x/x)$. The graphs of $|\rho_n|$ in this case resemble those of Figure 2, except that no leveling-off occurs, since $\operatorname{Im}[e^{ix}e_n(-ix)] \to 0$ as $n \to \infty$.

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is in preparation, and more research is required in that area. An important topic for future investigation is a comparison of performance improvement and cost of segmentation for Boolean and probabilistic methods. Such an investigation could well include empirical testing.

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