Computation of Successive Derivatives of $f(z)/z$*

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1. Introduction. It is sometimes necessary to calculate derivatives of the form

$$d_n(z) = \frac{d^n}{dz^n}\left(\frac{f(z)}{z}\right) \qquad (n = 0, 1, 2, \cdots), \tag{1.1}$$

where f is a function whose derivatives can be formed readily. Analytic differentiation in (1.1), while elementary, is obviously tedious, and the resulting expressions are of doubtful practical value. In the following we present a simple and effective recursive algorithm to generate these derivatives. As an example, we consider the cases where $f(z) = e^z$, $f(z) = \cos z$, and $f(z) = \sin z$.

Our main observation may be paraphrased in the following surprising way. The calculation of a large number of derivatives (1.1) at a fixed point z is a stable process if the function $g(\zeta) = f(\zeta)/\zeta$ has a pole at $\zeta = 0$, and an unstable process if $g(\zeta)$ is regular at $\zeta = 0$.

2. The Recurrence Relation. Let $z \neq 0$ be arbitrary complex, and let $f(\zeta)$ be analytic in the circle $|\zeta - z| \leqq r$, $r > |z|$, which includes the origin $\zeta = 0$. Our point of departure is the identity

$$\frac{f(z) - f(0)}{z} = \int_0^1 f'(tz)\, dt.$$

Differentiating n times gives

$$d_n(z) - (-1)^n \frac{n!}{z^{n+1}} f(0) = \int_0^1 t^n f^{(n+1)}(tz)\, dt. \tag{2.1}$$

Denoting the integral on the right by I_n, integration by parts yields

$$I_n + \frac{n}{z} I_{n-1} = \frac{f^{(n)}(z)}{z},$$

hence, together with (2.1), the recurrence relation

$$d_n(z) + \frac{n}{z} d_{n-1}(z) = \frac{f^{(n)}(z)}{z} \qquad (n = 1, 2, 3, \cdots). \tag{2.2}$$

We note that (2.2) represents a linear inhomogeneous first-order difference equation for d_n. Computational aspects of such difference equations were discussed at length in [1]. It was noted there, that a naive application of (2.2) in the forward direction is accompanied by an undesirable build-up of rounding errors whenever the quantity

$$\rho_n = \frac{d_0 h_n}{d_n}$$

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becomes large in absolute value for some n. Here, h_n denotes the solution (normalized by $h_0 = 1$) of the homogeneous difference equation that corresponds to (2.2), i.e.

$$h_n = (-1)^n \frac{n!}{z^n}.$$

Numerical instability is particularly prominent if $\lim_{n\to\infty} |\rho_n| = \infty$, or, equivalently, if

$$\lim_{n\to\infty} \frac{d_n}{h_n} = 0. \tag{2.3}$$

By (2.1) we have

$$z \frac{d_n}{h_n} = f(0) + (-1)^n \frac{z^{n+1}}{n!} \int_0^1 t^n f^{(n+1)}(tz)\, dt. \tag{2.4}$$

The second term on the right, disregarding the sign, we recognize as being the nth remainder (in integral form) of the Taylor expansion of $f(0)$ about z. Because of the analyticity assumption made at the beginning of this section, this remainder tends to zero, as $n \to \infty$, and so

$$\lim_{n\to\infty} \frac{d_n}{h_n} = \frac{f(0)}{z}. \tag{2.5}$$

In particular, if $f(0) = 0$, then (2.3) holds, and we have numerical instability. On the other hand, if $f(0) \neq 0$, then

$$\lim_{n\to\infty} \rho_n = \frac{f(z)}{f(0)},$$

and $|\rho_n|$ is bounded for all n, provided $d_n(z)$ does not vanish for some n. Hence, no serious numerical difficulties should attend the use of (2.2), unless $|f(z)/f(0)|$ is very large, or $|\rho_n|$ reaches a large peak prior to converging to the limiting value $|f(z)/f(0)|$.

An alternate proof of (2.5) can be given using Cauchy's formula for the nth derivative of an analytic function,

$$d_n(z) = \frac{n!}{2\pi i} \oint_C \frac{f(\zeta)\, d\zeta}{(\zeta - z)^{n+1}\zeta}.$$

If $f(0) = 0$, we may take for C a circle about z containing the origin and contained in the circle of analyticity of f. If $f(0) \neq 0$, we must add to C a small contour C_0 encircling the origin in the negative direction. Taking for C_0 a small circle, and letting its radius tend to zero, we arrive at

$$d_n(z) = (-1)^n \frac{n!}{z^{n+1}} f(0) + \frac{n!}{2\pi i} \oint_C \frac{f(\zeta)\, d\zeta}{(\zeta - z)^{n+1}\zeta}.$$

Hence,

$$z \frac{d_n}{h_n} = f(0) + \frac{(-1)^n}{2\pi i} \oint_C \left(\frac{z}{\zeta - z}\right)^{n+1} \frac{f(\zeta)}{\zeta}\, d\zeta. \tag{2.6}$$

Since $f(\zeta)/\zeta$ is bounded on C, and

$$\left| \frac{z}{\zeta - z} \right| \leqq q < 1,$$

it is clear that the integral in (2.6) tends to zero, as $n \to \infty$, and so we again obtain (2.5).

We may summarize as follows: *Let f be analytic in a circle about z which includes the origin in its interior. Then the generation of a large number of derivatives* (1.1), *using forward recursion by* (2.2), *is in general numerically stable if* $f(0) \neq 0$, *but highly unstable if* $f(0) = 0$.

We observe, however, that forward recursion by (2.2), even in the case $f(0) = 0$, may still be adequate, if only a relatively small number of derivatives are required. In fact, the recursion should be adequate as long as $n \leqq |z|$.

3. Recursive Algorithm in the Case $f(0) = 0$. We take advantage of a remark made on p. 25 of [1]. Since $|\rho_n| \to \infty$, we may apply the recursion (2.2) in the backward direction, starting with $n = \nu$ sufficiently large, and using zero initial value,

$$(3.1) \quad d_{n-1}^{[\nu]} = (f^{(n)}(z) - z d_n^{[\nu]})/n \qquad (n = \nu, \nu - 1, \cdots, 1), \qquad d_\nu^{[\nu]} = 0.$$

Then, for $n \geqq 0$ in any bounded set, we will have

$$d_n^{[\nu]} \to d_n \quad \text{as} \quad \nu \to \infty.$$

Moreover, the relative error of $d_n^{[\nu]}$ is given by

$$(3.2) \qquad \frac{d_n^{[\nu]} - d_n}{d_n} = \frac{\rho_n}{\rho_\nu}.$$

It remains to estimate a reasonable starting value ν for n, given, say, that the results for $n = 0, 1, 2, \cdots, N$ are to be accurate to S significant digits. According to (3.2), we must require that $|\rho_n/\rho_\nu| \leqq \epsilon$ for all $0 \leqq n \leqq N$, where

$$\epsilon = \tfrac{1}{2} 10^{-S},$$

that is,

$$(3.3) \qquad \frac{n!}{\nu!} |z|^{\nu-n} \left| \frac{d_\nu}{d_n} \right| \leqq \epsilon \qquad (n = 0, 1, 2, \cdots, N).$$

In addition to the analyticity assumption introduced earlier, we now *assume that $f^{(n)}$ is uniformly bounded, and bounded away from zero on the segment from* 0 *to z as* $n \to \infty$. Then it is clear from (2.1), where now $f(0) = 0$, that $|d_\nu/d_n| < 1$ for ν sufficiently large. Hence, it appears reasonable to replace $|d_\nu/d_n|$ in (3.3) by 1, and to require

$$(3.4) \qquad \frac{n!}{\nu!} |z|^{\nu-n} \leqq \epsilon \qquad (n = 0, 1, 2, \cdots, N).$$

Denote the expression on the left by p_n. Clearly, $\{p_n\}$ is a sequence of positive numbers which initially decrease, until n is near $|z|$, and from then on increase rapidly to ∞. (The case $|z| < 1$, in which p_n increases from the beginning, is of

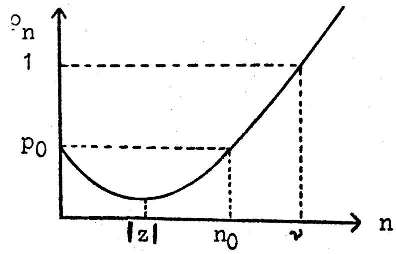

FIGURE 1. Behavior of $p_n = n! \mid z \mid^{\nu-n}/\nu!$

little consequence for the following.) Denote by n_0 the integer $n > 0$ for which p_n is near to p_0 "for the second time" (see Figure 1), hence $| z |^n/n!$ near 1. Then, (3.4) is implied by $p_0 \leqq \epsilon$, if $N \leqq n_0$, and by $p_N \leqq \epsilon$ if $N > n_0$. We may replace (3.4) therefore by

$$\frac{| z |^\nu}{\nu!} \leqq \epsilon \qquad (N \leqq n_0), \qquad \frac{N!}{\nu!} | z |^{\nu-N} \leqq \epsilon \qquad (N > n_0).$$

Using Stirling's formula, these conditions are adequately approximated by

$$\left(\frac{e | z |}{\nu}\right)^\nu \leqq \epsilon \qquad (N \leqq n_0), \qquad \left(\frac{e | z |}{\nu}\right)^\nu \left(\frac{N}{e | z |}\right)^N \leqq \epsilon \qquad (N > n_0).$$

We note, incidentally, that again by Stirling's formula,

$$n_0 \approx [e | z |], \qquad e = 2.71828 \cdots .$$

The first inequality, upon taking logarithms, can be written in the form

$$\frac{\nu}{e | z |} \ln \left(\frac{\nu}{e | z |}\right) \geqq \frac{s}{e | z |}, \tag{3.5}$$

where

$$s = S \ln 10 + \ln 2.$$

Similarly, the second inequality amounts to

$$\nu \ln \left(\frac{\nu}{e | z |}\right) - N \ln \left(\frac{N}{e | z |}\right) \geqq s,$$

which can be written in the form

$$\left(\frac{\nu}{N} - 1\right) \ln \left(\frac{N}{e | z |}\right) + \frac{\nu}{N} \ln \frac{\nu}{N} \geqq \frac{s}{N}. \tag{3.6}$$

Since certainly $\nu > N$, and moreover $N \geqq e | z |$ (N now being larger than n_0, and $n_0 \approx e | z |$), the first term on the left is $\geqq 0$. Hence, (3.6) will be satisfied if we require

$$\frac{\nu}{N} \ln \frac{\nu}{N} \geqq \frac{s}{N}. \tag{3.7}$$

Both conditions (3.5), (3.7) now have the form $t \ln t \geqq c$. Denoting by $t(y)$ the inverse function of $y = t \ln t$ $(t \geqq 1)$, we obtain our final estimate of ν in the form

$$(3.8) \quad \nu \geqq e\,|\,z\,|\,t\left(\frac{s}{e\,|\,z\,|}\right) \qquad (N \leqq n_0), \qquad \nu \geqq Nt\left(\frac{s}{N}\right) \qquad (N > n_0).$$

We note that in (3.8) the function $t(y)$ need only be available to low accuracy. Formulas giving 1% accuracy, or better, may be found in [2].

The algorithm just described may still be unsatisfactory, numerically, if $|\,z\,|$ is relatively large. The recursion (3.1) then is likely to suffer from loss of accuracy, due to cancellation of digits, particularly for n near 1. For such n, indeed, z/n in (3.1) will have large absolute value, yet $d_{n-1}^{[\nu]}$ has normally the same order of magnitude as $d_n^{[\nu]}$. The difficulty may be resolved by *applying* (2.2) *in forward direction as long as* $n \leqq |\,z\,|$, *and using the backward recurrence algorithm described above for the remaining* n *with* $|\,z\,| < n \leqq N$.

4. Examples. Consider first $f(z) = e^z$, and let

$$d_n(z) = \frac{d^n}{dz^n}\left(\frac{e^z}{z}\right).$$

Then (2.2) gives immediately

$$(4.1) \qquad d_n(z) + \frac{n}{z}\,d_{n-1}(z) = \frac{e^z}{z} \qquad (n = 1, 2, 3, \cdots).$$

Our theory of Sections 2 and 3 clearly applies. Since $f(0) = 1$, it follows that (4.1) is numerically stable in the forward direction. We note, incidentally, that

$$(4.2) \qquad d_n(z) = (-1)^n \frac{n!}{z^{n+1}}\,e^z e_n(-z),$$

where

$$(4.3) \qquad e_n(z) = \sum_{k=0}^{n} \frac{z^k}{k!}$$

is the nth partial sum of the exponential series.

Likewise, if $f(z) = \cos z$, and

$$c_n(z) = \frac{d^n}{dz^n}\left(\frac{\cos z}{z}\right),$$

we obtain

$$(4.4) \qquad c_n(z) + \frac{n}{z}\,c_{n-1}(z) = \tau_n(z) \qquad (n = 1, 2, 3, \cdots),$$

where $\{\tau_n(z)\}_{n=1}^{\infty} = \{-\sin z, -\cos z, \sin z, \cos z, \cdots\}$. Like the previous recursion, (4.4) is numerically stable. On the other hand, if $f(z) = \sin z$, and

$$s_n(z) = \frac{d^n}{dz^n}\left(\frac{\sin z}{z}\right),$$

then

$$s_n(z) + \frac{n}{z} s_{n-1}(z) = \sigma_n(z) \qquad (n = 1, 2, 3, \cdots), \tag{4.5}$$

$\{\sigma_n(z)\}_{n=1}^{\infty} = \{\cos z, -\sin z, -\cos z, \sin z, \cdots\}$, is numerically unstable, and the algorithm of Section 3 should be applied, including the device mentioned at the end of Section 3.

In terms of (4.3), we may also write

$$c_n(z) = \frac{(-1)^n n!}{2z^{n+1}} [e^{iz} e_n(-iz) + e^{-iz} e_n(iz)],$$

$$s_n(z) = \frac{(-1)^n n!}{2iz^{n+1}} [e^{iz} e_n(-iz) - e^{-iz} e_n(iz)],$$

as follows readily from (4.2) and Euler's formula.

The functions $s_n(x)$ have found wide applications in diffraction theory, and are extensively tabulated (see [4]). The generation of d_n, c_n, and s_n, may also be useful for the analytic continuation of the exponential-, cosine-, and sine-integrals, respectively. ALGOL procedures generating $d_n(x)$, $c_n(x)$, and $s_n(x)$ for real x may be found in [3].

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