Differentiation Formulas for Analytic Functions*

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Abstract. In a previous paper (Lyness and Moler [1]), several closely related formulas of use for obtaining a derivative of an analytic function numerically are derived.

Each of these formulas consists of a convergent series, each term being a sum of function evaluations in the complex plane.

In this paper we introduce a simple generalization of the previous methods; we investigate the "truncation error" associated with truncating the infinite series. Finally we recommend a particular differentiation rule, not given in the previous paper.

1. Introduction. In a previous publication, Lyness and Moler [1], referred to here as Paper A, the elementary theory of a complex variable was applied to derive several closely related methods for carrying out numerical differentiation. The basis of these methods is Cauchy's theorem which relates the nth derivative $f^{(n)}(0)$ of an analytic function $f(z)$ at $z = 0$ to the value of a closed integral, the contour C enclosing the origin once and remaining within a domain of analyticity of $f(z)$. Cauchy's theorem states

$$a_n = \frac{f^{(n)}(0)}{n!} = \frac{1}{2\pi i}\int_C \frac{f(z)}{z^{n+1}}\,dz \tag{1.1}$$

where a_n is a Taylor coefficient

$$f(z) = \sum_{j=0}^{\infty} a_j z^j\,, \qquad |z| < R_c\,, \tag{1.2}$$

and we have denoted by R_c the radius of convergence of this expansion.

Thus in principle one method for evaluating a high derivative consists of evaluating the integral on the right-hand side of (1.1) numerically.

At first sight it might seem that the evaluation in the complex plane of an integral whose integrand is highly oscillatory would introduce more difficult problems than the one to be solved. However, if we choose for the contour C the circle

$$C_r : |z| = r\,, \qquad r < R_c\,, \tag{1.3}$$

and make a simple change in variable, we find

$$a_n = \frac{1}{r^n}\int_0^1 f(re^{2\pi i t})e^{-2\pi i n t}dt \tag{1.4}$$

and the problem reduces to finding a Fourier coefficient of a periodic function

$$g(t) = f(re^{2\pi i t}) \tag{1.5}$$

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which has continuous derivatives of all orders. As is well known, the trapezoidal quadrature rule

$$R^{[m,1]}g(t) = \frac{1}{m}\sum_{j=1}^{m} g\left(\frac{j}{m}\right) \tag{1.6}$$

may be used to evaluate integrals of this type numerically and is effective and economic. (See for example Lyness [2].)

We define $b_m(r)$ to be the difference between $R^{[m,1]}f(re^{2\pi it})$, and the integral $\int_0^1 f(re^{2\pi it})dt$ to which this rule sum approximates. Thus

$$b_m(r) = R^{[m,1]}f(re^{2\pi it}) - f(0) \tag{1.7}$$

is a quantity which may be calculated at a cost of $m + 1$ function evaluations. The Poisson summation formula, which is in this case the Fourier expansion of $b_m(r)$, leads to the expansion

$$b_m(r) = r^m a_m + r^{2m}a_{2m} + r^{3m}a_{3m} + \cdots, \qquad m = 1, 2, 3, \cdots, \tag{1.8}$$

and this set of equations may be solved to give

$$r^n a_n = \mu_1 b_n(r) + \mu_2 b_{2n}(r) + \mu_3 b_{3n}(r) + \cdots, \qquad n = 1, 2, 3, \cdots, \tag{1.9}$$

where μ_i is the ith Möbius number (either 1, 0, or -1). Since a_n is simply $f^{(n)}(0)/n!$, formula (1.9) expresses an nth derivative in a series each term of which is the very simple sum of function evaluations given in (1.7). It is shown in Paper A that the sum in (1.9) converges rapidly. Thus the suggested method to evaluate $f^{(n)}(0)$ consists in evaluating successively $b_n(r)$, $b_{2n}(r)$, $\cdots$, and using (1.9), terminating the series when it appears to have converged to the required accuracy.

The method described by (1.9) has one major advantage. This is that small errors in function evaluation are *not* amplified in the calculation but tend to be dampened out. The round-off error in the final result is simply what might be expected in any typical numerical calculation, and can be estimated with little difficulty. This feature is discussed in Section 5 of Paper A.

In this paper, a deeper investigation is made into differentiation methods based on Cauchy's theorem. It is shown that there exists a family of simple rules which includes rules based on the method described above. The truncation error arising from terminating the series such as that in (1.9) is investigated and a simple bound is given. It is shown that members of this family have very similar properties in terms of the maximum degree of the polynomial which is differentiated exactly.

Finally, a single member of the family (which is not the member described in Paper A) is chosen as being likely to give the most economic results. This choice turns out to be almost independent of which of several standard criteria is used.

2. Generalization of Method of Paper A. A generalization of this method follows from the simple observation that the nth derivative of $f(z)$ at $z = 0$ is a constant multiple of the $(n + p)$th derivative of $\bar{f}(z) = z^p f(z)$ at $z = 0$. Thus we may apply the same formula to evaluate a different derivative of a different function, and finally represent the result in terms of the original function and derivative.

We define

$$\bar{f}(z) = z^p f(z)\,, \qquad p > 0\,, \tag{2.1}$$

and define quantities $\bar{a}_s$ and $\bar{b}_s(r)$ as in (1.1) and (1.7), but with respect to the function $\bar{f}(z)$ instead of $f(z)$. Thus

$$\bar{b}_m(r) = R^{[m,1]}(\bar{f}(re^{2\pi i t})) = \frac{1}{m}\sum_{q=1}^{m} r^p e^{2\pi i p q/m} f(re^{2\pi i q/m}) \tag{2.2}$$

and applying (1.9) to the function $\bar{f}(z)$

$$r^{n+p}\bar{a}_{n+p} = \sum_{k=1}^{\infty} \mu_k \bar{b}_{(n+p)k}(r)\,. \tag{2.3}$$

However, since $\bar{a}_{n+p} = a_n$, we may set $N = p + n$ and substituting expression (2.2) into (2.3) we find

$$r^n a_n = \sum_{k=1}^{\infty} \mu_k \frac{1}{Nk} \sum_{q=1}^{Nk} e^{2\pi i(N-n)q/Nk} f(re^{2\pi i q/Nk})\,, \qquad N > n\,. \tag{2.4}$$

Expression (1.9) is of this form with $N = n$ but includes a minor modification which occurs because $\bar{f}(0) = 0$ if $p > 0$, but $\bar{f}(0) = f(0)$ if $p = 0$. (See (2.5) below.)

Expansion (2.4), together with (1.9) constitute a set of exact formulas which express a_n in terms of an infinite series, each of whose terms is a sum of function evaluations. A numerical rule to determine a_n is completely specified once r and N, the parameters in the expansion, are specified together with Q, the number of terms of the infinite expansion, which are retained. In general the rule does not produce an exact result for a_n because of the omitted terms in the expansion. We refer to this error as the truncation error $\mathcal{E}_{n,Q}^{(N)}(r)$.

N, Q, r family of rules to calculate a_n. One such rule is obtained from

$$\begin{aligned} r^n a_n = &\sum_{k=1}^{Q} \mu_k \left[\frac{1}{Nk}\sum_{q=1}^{Nk} e^{2\pi i(N-n)q/Nk} f(re^{2\pi i q/Nk}) - \delta_{N,n} f(0)\right] \\ &+ \mathcal{E}_{n,Q}^{(N)}(r)\,, \qquad N \geqq n;\, Q \geqq 1\,, \end{aligned} \tag{2.5}$$

by specifying N, Q, and r and setting $\mathcal{E}_{n,Q}^{(N)}(r)$ to be zero. The method of Paper A specified $N = n$.

In the rest of this section we derive properties of this family of rules. We investigate first the number of function evaluations required by a rule. This is clearly independent of r, the radius of the circle on which function evaluations are made. We note also that n occurs on the right-hand side only as a parameter in the weighting coefficients. Thus the number of function evaluations depends on n only insofar as a particular value of n can make a weighting coefficient become zero. Except for the coefficient of $f(0)$, the modulus of the weighting coefficients is independent of n. Thus the number of function evaluations is almost independent of n. For $N > n$, this number is independent of n. For $N = n$, one additional function evaluation is required. Thus it is convenient to make the following definition.

Definition. $\nu_Q^{(N)}$ is the number of function evaluations *on the circle* $|z| = r$ required by the rule (2.5).

This is the same as the total number of function evaluations except in the case $N = n$, when the total number is $\nu_Q^{(N)} + 1$. In the following discussion we disregard this special case. It is easy to verify that it does not affect any of the conclusions here.

The actual determination of $\nu_Q^{(N)}$ is a problem in Number Theory. It may be noted that it is equal to the number of distinct fractions q/Nk where $0 < q/Nk \leqq 1$, where q is any integer and k is any integer for which $\mu_K \neq 0$ and for which $1 \leqq k \leqq Q$.

For the purposes of this paper only a simple bound on $\nu_Q^{(N)}$ is required. If $\mu_Q \neq 0$, the final term in (2.5), that with $k = Q$, requires NQ distinct function evaluations. Thus

$$\nu_Q^{(N)} \geqq NQ\,, \qquad \mu_Q \neq 0\,. \tag{2.6}$$

This inequality is still valid even if $\mu_Q = 0$, but the proof is rather cumbersome and is not given here. Moreover, the equality in (2.6) is valid only in the cases $Q = 1, 2, 4$. For other values of Q the value of $\nu_Q^{(N)}$ exceeds NQ by a comfortable margin which increases in general (but not monotonically), with increasing Q. We state this inequality as a theorem.

THEOREM.

$$\begin{aligned} \nu_Q^{(N)} &= NQ\,, \qquad Q = 1, 2, 4\,, \\ \nu_Q^{(N)} &> NQ\,, \qquad Q = 3, 5, 6, 7, \cdots\,. \end{aligned} \tag{2.7}$$

The rules described in (2.5) give exact results in some cases. This may happen if $f(z)$ is a polynomial of degree d. In this case

$$f(z) = \sum_{j=0}^{d} a_j z^j \tag{2.8}$$

and

$$a_j = 0\,, \qquad j \geqq d + 1\,. \tag{2.9}$$

If we refer to the expansion given by (1.8), we see that

$$b_i(r) = 0\,, \qquad i \geqq d + 1\,. \tag{2.10}$$

Applying this reasoning to the function $\bar{f}(z) = z^p f(z)$, we find that

$$\bar{a}_i = 0\,, \qquad i \geqq p + d + 1\,, \tag{2.11}$$

and

$$\bar{b}_i(r) = 0\,, \qquad i \geqq p + d + 1\,. \tag{2.12}$$

So the terms in the expansion (2.4) for which $Nk \geqq p + d + 1$ are zero. Since in the rule the final included term is that for which $k = Q$, it follows that all the nonzero terms are included if $N(Q + 1) \geqq p + d + 1$. Since $p = N - n$, we have the following theorem.

THEOREM. *The rule* (2.5) *is exact, i.e.* $\mathcal{E}_{n,Q}^{(N)}(r) = 0$, *if* $f(z)$ *is a polynomial of degree* d *where*

$$d \leqq NQ + n - 1\,. \tag{2.13}$$

This is not necessarily the strongest possible inequality. If $\mu_{Q+1} = \mu_{Q+2} = \cdots$

$= \mu_{Q+s} = 0$ but $\mu_{Q+s+1} \neq 0$, this inequality may be replaced by

$$d \leqq N(Q+s) + n - 1 . \tag{2.14}$$

This is strict in the sense that if d does not satisfy this inequality there exists a polynomial of degree d for which $\mathcal{E}_{n,Q}^{(N)}(r) \neq 0$.

We complete this section by combining the results of the two previous theorems. We note that

$$\nu_Q^{(N)} = \nu_{Q+s}^{(N)} \geqq N(Q+s) . \tag{2.15}$$

Thus if a rule (2.5) differentiates a polynomial of degree d exactly, it follows from (2.14) and (2.15) that

$$\nu_{Q+s}^{(N)} \geqq d + 1 - n . \tag{2.16}$$

However,

$$\nu_1^{(d+1-n)} = d + 1 - n \tag{2.17}$$

and so an optimum choice is $Q = 1$ and $N = d + 1 - n$.

THEOREM. *The rule* (2.5) *with* $Q = 1$ *and* $N = d + 1 - n$ *gives an exact result for* $f^{(n)}(0)$ *when* $f(z)$ *is a polynomial of degree* d. *This rule requires* $d + 1 - n$ *function evaluations. No other choice of* N *and* Q *having this property gives a rule requiring fewer function evaluations.*

These results indicate that, in the absence of further information about the truncation error, the most economical use of function evaluations may result from using only one term of (2.5) and choosing N to be correspondingly large. An investigation of the truncation error, whose results are given in Section 4, tends to confirm this conclusion. We write down this preferred rule explicitly. Setting $Q = 1$ in (2.5), we obtain

$$\begin{aligned} r^n a_n \approx r^n a_n^{(N)} &= \frac{1}{N} \sum_{q=1}^{N} e^{-2\pi i n q/N} f(re^{2\pi i q/N}) \\ &= R^{[N,1]}(e^{-2\pi i n t} f(re^{2\pi i t})) . \end{aligned} \tag{2.18}$$

This is exactly the result obtained by approximating the contour integral in (1.1) by a trapezoidal rule using N function evaluations. We refer to this rule as the *t rapezoidal rule.*

3. The Truncation Error $\mathcal{E}_{n,Q}^{(N)}(r)$. In this section we obtain an integral representation for, and a bound on the magnitude of the truncation error. We restrict our attention to an analytic function $f(z)$ regular within the circle C_{R_c}: $|z| = R_c$. We define an intermediate circle C_R: $|z| = R$ where

$$0 < r < R < R_c . \tag{3.1}$$

The case $N = n$ is considered in detail and after carrying out the calculation, the technique of Section 2 is used to generalize the results to other values of N. We recall that the truncation error is defined by

$$\mathcal{E}_{n,Q}^{(n)}(r) = r^n a_n - \sum_{k=1}^{Q} \mu_k b_{kn}(r) . \tag{3.2}$$

In the special case $Q = 0$, there is a well-known integral representation for this term, namely Cauchy's theorem (1.1)

$$\mathcal{E}_{n,0}^{(n)}(r) = r^n a_n = \frac{1}{2\pi i}\int_{C_r} f(z)\left(\frac{r}{z}\right)^n \frac{dz}{z}\,; \tag{3.3}$$

also a bound is given by Cauchy's inequality for the nth derivative

$$|\mathcal{E}_{n,0}^{(n)}(r)|^2 = |r^n a_n|^2 \leqq I(R)(r/R)^{2n} \tag{3.4}$$

where $I(r)$ is defined by

$$I(R) = \frac{1}{2\pi i}\int_{C_R} |f(z)|^2 \frac{dz}{z} = \int_0^1 |f(Re^{2\pi i t})|^2 dt\,. \tag{3.5}$$

In this section we obtain the appropriate generalizations of (3.3) and (3.4). These are (3.14) and (3.21) below and differ from (3.3) and (3.4) merely insofar as the terms $(r/z)^n$ and $(r/R)^{2n}$ are replaced by functions $g_Q((r/z)^n)$ and $G_Q((r/R)^{2n})$ respectively, these functions being defined below. Finally the complicated function $G_Q(\rho)$ is bounded by a simpler function $\tilde{G}_Q(\rho)$. The results of this section are summarized in Theorem (3.37). The remainder of this section consists of a proof of this theorem.

We require two elementary results before we proceed. The first is the familiar Schwarz's inequality

$$|(F, G)|^2 \leqq (F, F)(G, G) \tag{3.6}$$

applied to the closed contour integral round C_R. This is

Schwarz's inequality.

$$\left|\frac{1}{2\pi i}\int_{C_R} f(z)g(z)\,\frac{dz}{z}\right|^2 \leqq \frac{1}{2\pi i}\int_{C_R} |f(z)|^2 \frac{dz}{z}\cdot\frac{1}{2\pi i}\int_{C_R} |g(z)|^2 \frac{dz}{z}\,. \tag{3.7}$$

The second is an elementary property of the Mobius numbers, proved in Pólya and Szegö [4] (problem 69). The set of equations

$$\frac{x^m}{1-x^m} = x^m + x^{2m} + x^{3m} + \cdots\,, \qquad m = 1, 2, 3, \cdots; |x| < 1\,, \tag{3.8}$$

may be inverted to give

$$x^n = \mu_1 \frac{x^n}{1-x^n} + \mu_2 \frac{x^{2n}}{1-x^{2n}} + \mu_3 \frac{x^{3n}}{1-x^{3n}} + \cdots\,, \qquad n = 1, 2, 3, \cdots; |x| < 1\,. \tag{3.9}$$

This identity is used in Eq. (3.13) and subsequently.

We now obtain an integral representation for $b_m(r)$. Since

$$r^s a_s = \frac{1}{2\pi i}\int_{C_R} f(z)\left(\frac{r}{z}\right)^s \frac{dz}{z}\,, \tag{3.10}$$

and by (1.8)

$$b_m(r) = \sum_{s=1}^{\infty} r^{sm} a_{sm} \tag{3.11}$$

we find

$$b_m(r) = \frac{1}{2\pi i}\int_{C_R} f(z)\sum_{s=1}^{\infty}\left(\frac{r}{z}\right)^{sm}\frac{dz}{z} = \frac{1}{2\pi i}\int_{C_R} f(z)\,\frac{(r/z)^m}{1-(r/z)^m}\,\frac{dz}{z},$$

this interchange of the integration and summation operators being allowed because as $|r/z| < 1$ on C_R, the resulting series is absolutely convergent. We now use this integral representation for $b_m(r)$ to obtain an integral representation for $\mathcal{E}^{(n)}_{n,Q}(r)$ by means of

$$\mathcal{E}^{(n)}_{n,Q}(r) = r^n a_n - \sum_{k=1}^{Q}\mu_k b_{kn}(r) = \sum_{k=Q+1}^{\infty}\mu_k b_{kn}(r)\,, \tag{3.12}$$

the second expression following from the first through (1.9).

We define a function $g_Q(\sigma)$

$$g_Q(\sigma) = \sigma - \sum_{k=1}^{Q}\mu_k\sigma^k/(1-\sigma^k) = \sum_{k=Q+1}^{\infty}\mu_k\sigma^k/(1-\sigma^k)\,, \tag{3.13}$$

the second equality being a consequence of identity (3.9) and, substituting (3.11) into (3.12), it follows that:

Integral representation for truncation error.

$$\mathcal{E}^{(n)}_{n,Q}(r) = \frac{1}{2\pi i}\int_{C_R} f(z)g_Q((z/r)^n)\,\frac{dz}{z}\,. \tag{3.14}$$

The first form of $g_Q(\sigma)$ is convenient for the calculation of individual expressions. For example

$$\begin{aligned} g_0(\sigma) &= \sigma\,, \\ g_1(\sigma) &= -\sigma^2/(1-\sigma)\,, \\ g_2(\sigma) &= -\sigma^3/(1-\sigma^2)\,, \\ g_3(\sigma) &= g_4(\sigma) = -\sigma^5/[(1+\sigma)(1-\sigma^3)]\,. \end{aligned} \tag{3.15}$$

The result (3.14) with $Q = 0$ is identical with (3.3).

We now apply Schwarz's inequality (3.7) to expression (3.14) for the truncation error. We find

$$|\mathcal{E}^{(n)}_{n,Q}(r)|^2 \leqq I(R)\left[\frac{1}{2\pi i}\int_{C_R}|g_Q((r/z)^n)|^2\frac{dz}{z}\right]. \tag{3.16}$$

We show now that the expression in square brackets depends on R and r only in the combination r/R.

We define

$$G_Q(\rho) = \int_0^1 |g_Q(\rho e^{-2\pi i t})|^2 dt\,. \tag{3.17}$$

Since the integrand is a periodic function of t with period 1, it follows that

$$G_Q(\rho^n) = \int_0^1 |g_Q(\rho^n e^{-2\pi i t})|^2 dt = \int_0^1 |g_Q(\rho^n e^{-2\pi i n t})|^2 dt\,. \tag{3.18}$$

If we set

$$\rho = r/R\,, \tag{3.19}$$

we find

$$G_Q(\rho^n) = \frac{1}{2\pi i}\int_{C_R} |g_Q((r/z)^n)|^2 \frac{dz}{z}\,. \tag{3.20}$$

THEOREM. *The truncation error* $\mathcal{E}^{(n)}_{n,Q}(r)$ *defined in* (3.2) *satisfies the following inequality*:

$$|\mathcal{E}^{(n)}_{n,Q}(r)|^2 \leqq E^{(n)}_{n,Q}(r, R) = I(R)G_Q((r/R)^n)\,, \tag{3.21}$$

where $I(R)$ *is given by* (3.5) *and* $G_Q(\rho)$ *by* (3.17).

It is possible to evaluate $G_Q(\rho)$ directly by substituting expression (3.13) for $g_Q(\sigma)$ into (3.20). This may be expanded to give

$$\begin{aligned} G_Q(\rho) = \frac{1}{2\pi i}\int_{C_R} \Bigg\{ \left(\frac{r}{z}\right)\left(\frac{r}{\bar z}\right) &- \sum_{k=1}^{Q} \mu_k \frac{(r/\bar z)(r/z)^k}{1-(r/z)^k} - \sum_{k=1}^{Q} \mu_k \frac{(r/z)(r/\bar z)^k}{1-(r/\bar z)^k} \\ &+ \sum_{s=1}^{Q}\sum_{w=1}^{Q} \mu_s\mu_w \frac{(r/z)^s (r/\bar z)^w}{(1-(r/z)^s)(1-(r/\bar z)^w)} \Bigg\} \frac{dz}{z}\,. \end{aligned} \tag{3.22}$$

On the contour $|z| = R$ we may replace $\bar z$ by R^2/z. Thus each of the $(Q+1)^2$ independent integrals in (3.22) may be written as the integral of an analytic function, having known poles within the contour C_R, and each may be evaluated separately using the calculus of residues. For example

$$\begin{aligned} H_{s,w}(\rho) = \frac{1}{2\pi i}\int_{C_R} \frac{(r/z)^s (r/\bar z)^w}{(1-(r/z)^s)(1-(r/\bar z)^w)} \frac{dz}{z} = \frac{\rho^{2h}}{1-\rho^{2h}}\,, \\ R > r;\, w, s \geqq 1\,, \end{aligned} \tag{3.23}$$

where

$$h = \text{lowest common multiple of } s \text{ and } w\,.$$

The terms in the summations over k in (3.22) are zero, with the exception of the $k = 1$ terms. Consequently we are led to an expression for $G_Q(\rho)$ as a rational algebraic function, namely

$$G_Q(\rho) = -\rho^2 + \sum_{s=1}^{Q}\sum_{w=1}^{Q} \mu_s\mu_w H_{s,w}(\rho)\,, \qquad Q \geqq 1\,. \tag{3.24}$$

The first few of these expressions are:

$$\begin{aligned} G_0(\rho) &= \rho^2\,, \\ G_1(\rho) &= \rho^4/(1-\rho^2)\,, \\ G_2(\rho) &= \rho^6/(1-\rho^4)\,, \\ G_3(\rho) &= G_4(\rho) = \rho^{10}/[(1-\rho^2)(1+\rho^6)]\,. \end{aligned} \tag{3.25}$$

It is elementary, but tedious, to calculate more of these. For our purposes a bound $\tilde G_Q(\rho)$ which we calculate below is sufficiently accurate and is easier to use. This bound is derived as follows. The modulus of $g_Q(\sigma)$ may be bounded by replacing each term in the summation

$$g_Q(\sigma) = \sum_{k=Q+1}^{\infty} \mu_k \sigma^k/(1 - \sigma^k) \tag{3.26}$$

by its modulus and replacing μ_k by 1. Thus

$$|g_Q(\rho e^{-2\pi i t})| \leqq \sum_{k=Q+1}^{\infty} \rho^k/|1 - \rho^k e^{-2\pi i k t}| . \tag{3.27}$$

We use this in expression (3.17) for $G_Q(\rho)$. Applying Minkowski's inequality we find

$$\begin{aligned} G_Q(\rho) &\leqq \int_0^1 \left(\sum_{k=Q+1}^{\infty} \left| \frac{\rho^k}{1 - \rho^k e^{-2\pi i k t}} \right| \right)^2 dt \\ &\leqq \left[\sum_{k=Q+1}^{\infty} \left\{ \int_0^1 \left| \frac{\rho^k}{1 - \rho^k e^{-2\pi i k t}} \right|^2 dt \right\}^{1/2} \right]^2 . \end{aligned} \tag{3.28}$$

Since

$$\int_0^1 \frac{dt}{|1 - \rho^k e^{-2\pi i k t}|^2} = \frac{1}{1 - \rho^{2k}} , \tag{3.29}$$

we find

$$G_Q(\rho) \leqq \left[\sum_{k=Q+1}^{\infty} \frac{\rho^k}{(1 - \rho^{2k})^{1/2}} \right]^2 \leqq \tilde{G}_Q(\rho) , \tag{3.30}$$

where

$$\tilde{G}_Q(\rho) = \frac{\rho^{2(Q+1)}}{(1 - \rho)^2 (1 - \rho^{2(Q+1)})} . \tag{3.31}$$

As a direct consequence of (3.30) and Theorem (3.21) we find

COROLLARY.

$$|\mathcal{E}_{n,Q}^{(n)}(r)|^2 \leqq E_{n,Q}^{(n)}(r, R) \leqq \tilde{E}_{n,Q}^{(n)}(r, R) = I(R)\tilde{G}_Q(\rho^n) \tag{3.32}$$

where $\rho = r/R$ *and* $\tilde{G}_Q(\rho)$ *is given by* (3.31).

Up to this point in this section we have treated the truncation error $\mathcal{E}_{n,Q}^{(N)}(r)$ only in the special case $N = n$. We now generalize the principle results to the general case $N \geqq n$ following the technique of Section 2. We recall that the rule (2.5) in the case $N = n + p$ is derived by applying the rule with $N = n$ to the function

$$\bar{f}(z) = z^p f(z) . \tag{3.33}$$

Consequently the truncation error in the calculation of $r^{n+p} a_{n+p}$ using a rule with $N = n + p$ is the same as the truncation error in the calculation of $r^n a_n$ using this rule, except for a multiplicative factor of r^p, the same value of Q being used in either calculation. This gives

$$\mathcal{E}_{n,Q}^{(N)}(r) = r^{-p} \bar{\mathcal{E}}_{N,Q}^{(N)}(r) , \tag{3.34}$$

the bar indicating, as usual, that the function $f(z)$ is replaced by $\bar{f}(z)$. Substitution of (3.14) into (3.34) yields

Integral representation for truncation error.

$$\mathcal{E}_{n,Q}^{(N)}(r) = \frac{1}{2\pi i} \int_{C_R} (z/r)^{N-n} f(z) g_Q((z/r)^N) \frac{dz}{z}. \tag{3.35}$$

The inequalities of Theorem (3.21) and Corollary (3.32) are easy to generalize as the function $f(z)$ occurs in $I(R)$ and

$$\overline{I(R)} = R^{2p} I(R). \tag{3.36}$$

Thus we find

THEOREM.

$$|\mathcal{E}_{n,Q}^{(N)}(r)|^2 \leqq E_{n,Q}^{(N)}(r, R) \leqq \tilde{E}_{n,Q}^{(N)}(r, R) \tag{3.37}$$

where

$$E_{n,Q}^{(N)}(r, R) = I(R) G_Q(\rho^N)/\rho^{2(N-n)} \tag{3.38}$$

and

$$\tilde{E}_{n,Q}^{(N)}(r, R) = I(R) \tilde{G}_Q(\rho^N)/\rho^{2(N-n)}. \tag{3.39}$$

Here $\rho = r/R$ *and* G_Q *and* $\tilde{G}_Q$ *are given by* (3.24) *and* (3.31) *respectively.*

An important case, that with $Q = 1$, is

$$|\mathcal{E}_{n,1}^{(N)}(r)|^2 \leqq E_{n,1}^{(N)}(r, R) = I(R) \rho^{2(N+n)}/(1 - \rho^{2N}). \tag{3.40}$$

4. Choice of N and Q for a Rule Based on $\tilde{E}$. The final theorem of the last section enables us to make an optimum choice of N and Q based on the bound $\tilde{E}_{n,Q}^{(N)}(r, R)$ and the number of function evaluations $\nu_Q^{(N)}$. We find from (3.39) that

$$\frac{\tilde{E}_{N\,Q}^{(N)}(r, R)}{\tilde{E}_{N,Q'}^{(N')}(r, R)} = \frac{\rho^{2QN}}{\rho^{2Q'N'}} \left\{ \frac{1 - \rho^{N'}}{1 - \rho^N} \right\}^2 \frac{1 - \rho^{2N'(Q'+1)}}{1 - \rho^{2N(Q+1)}}. \tag{4.1}$$

This may be used to compare the choice N, Q with the choice N', Q'. Remembering that $\rho < 1$, elementary inequalities applied to (4.1) give:

THEOREM. *If* $Q'N' \geqq QN$ *and* $N' \geqq N$, *then*

$$\tilde{E}_{n,Q}^{(N)}(r, R) \geqq \tilde{E}_{n,Q'}^{(N')}(r, R), \tag{4.2}$$

the equality being valid only in the case $N = N'$, $Q = Q'$.

In particular we may set $N' = NQ$ and $Q' = 1$ to find

COROLLARY.

$$\tilde{E}_{n,Q}^{(N)}(r, R) > \tilde{E}_{n,1}^{(NQ)}(r, R), \qquad Q \neq 1. \tag{4.3}$$

We recall from Section 2 that $\nu_Q{}^{(N)}$, the number of function evaluations, satisfies

$$\nu_Q{}^{(N)} \geqq NQ = \nu_1{}^{(NQ)}. \tag{4.4}$$

Thus we may compare the rule specified by $N = N'$, $Q = Q'$, with the rule specified by $N = N'Q'$, $Q = 1$. The second of these has a smaller error bound $\tilde{E}_{n,Q}^{(N)}(r, R)$ than the first and involves either the same number of, or fewer, function evaluations. We state this result as a theorem and a corollary.

THEOREM. *If* n, r *and* R *are specified, and* N *and* Q *may take all values for which* $\nu_Q{}^{(N)} \leqq \nu$ (*where* $\nu \geqq n$) *then*

$$\min_{N,Q} \tilde{E}^{(N)}_{n,Q}(r, R) = \tilde{E}^{(\nu)}_{n,1}(r, R) . \tag{4.5}$$

In terms of the rules (2.5) this may be written

COROLLARY. *Given n, r and R, the rule specified by $N = \nu$ and $Q = 1$ gives a smaller error bound $\tilde{E}^{(N)}_{n,Q}(r, R)$ than any other rule of set* (2.5) *requiring ν or fewer function evaluations.*

5. Conclusion. In this paper we have considered a particular family of rules for differentiation which arises naturally from Cauchy's theorem. This family is a generalization of the rules previously considered in Paper A. We have derived a truncation error bound and have compared different members of this family of rules using two specific criteria. These are both standard in Numerical Analysis; one relates the degree of the polynomials differentiated exactly to the number of function evaluations required. The other compares a bound on the truncation error to this number.

Both these criteria indicate that the "best" rule is the one which uses the simplest discretization of the contour integral. We have referred to this rule as the trapezoidal rule, and it is given explicitly by (2.5) with $Q = 1$,

$$r^n \frac{f^{(n)}(0)}{n!} = r^n a_n \approx r^n a_n{}^{(N)} = \frac{1}{N} \sum_{q=1}^{N} e^{-2\pi inq/N} f(re^{2\pi iq/N}) , \qquad N > n .$$

This rule is not the one considered in Paper A.

In a sequel [3] the author considers the implementation of this rule, in particular the specification of parameters r and N. It appears that this rule is more convenient than other members of the family for the additional reason that it is the easiest to implement in the form of an algorithm. In the sequel the round-off error is discussed, and is shown to be the same character for any rule of the family. In the author's opinion this is the most important practical feature of this method of differentiation.

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