Numerische Mathematik 5, 439—442 (1963)

An Error Formula for Numerical Differentiation

By

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1. Introduction

Suppose the function $f(x)$ is approximated by the Lagrange interpolating polynomial $P_n(x)$ of degree n relative to the tabular points $x_0, x_1, \ldots, x_n$ (arranged in increasing order). Assuming that $f(x)$ is $n+1$ times continuously differentiable, it is well known that the error

$$e(x) = f(x) - P_n(x) \tag{1.1}$$

may be written in the form

$$e(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\, w(x), \tag{1.2}$$

where ξ is some point (varying with x) which belongs to the smallest interval I containing x and all the tabular points x_i, while

$$w(x) = \prod_{i=0}^{n} (x - x_i) \tag{1.3}$$

is a polynomial of degree $n+1$ with roots at the tabular points. Since $P_n^{(k)}(x)$ is often used as an approximation to the k-th derivative $(1 \leqq k \leqq n)$ of f, it would be useful to have an equally simple formula for the corresponding error $e^{(k)}(x)$.

The earliest, and perhaps the closest, approach to this goal is found in STEFFENSEN [1], who shows that

$$e^{(k)}(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\, w^{(k)}(x) \tag{1.4}$$

provided x lies outside the open interval (x_0, x_n). For x in (x_0, x_n), HILDEBRAND [2] gives an expression for $e^{(k)}(x)$ involving derivatives of f up to the order $n+1+k$. An alternative derivation of this expression was recently indicated by RALSTON [3].

BRODSKIĬ [4] produced a formula containing only $(n+1)$-th derivatives and from it obtained sharp bounds on $|e^{(k)}|$ in terms of the maximum value M of $|f^{(n+1)}(x)|$ in I. However, his formula is far from simple. It involves a sum of $n+1$ integrals whose integrands and intervals of integration all vary with x. BRODSKIĬ also showed that Steffensen's formula (1.4) cannot hold for arbitrary x and f, and, more generally, that no formula can exist of the type

$$e^{(k)}(x) = f^{(n+1)}(\xi)\, \varphi(x), \tag{1.5}$$

where $\varphi(x)$ is for fixed $x_0, \ldots, x_n$ a well-determined function of x.

It is the purpose of this paper to present a simple formula for $e^{(k)}(x)$ which is "almost" of the forbidden type (1.5). The formula (Equation (2.1)) is stated and proved in section 2, while section 3 contains a discussion of some possible applications. In most cases, our formula leads to upper estimates on $|e^{(k)}|$ which are somewhat weaker, but far easier to obtain, than those derivable from BRODSKIĬ's paper [4]. On the other hand, it provides better insight into the functional dependence of $e^{(k)}$ on x, and can in certain special situations produce smaller upper bounds than [4].

2. The Error Formula

Theorem. There exist $n+1-k$ constants $y_k, y_{k+1}, \ldots, y_n$ depending on the function f but not on x such that

$$e^{(k)}(x) = \frac{f^{(n+1)}(\xi)}{(n+1-k)!}\, Q(x), \tag{2.1}$$

where $\xi = \xi(x)$ belongs to I and $Q(x)$ denotes the polynomial

$$Q(x) = \prod_{i=k}^{n} (x - y_i). \tag{2.2}$$

The constants y_i satisfy the inequalities

$$x_{i-k} < y_i < x_i. \tag{2.3}$$

Proof. From (1.1) and the definition of the Lagrange interpolation polynomial, we have $e(x)=0$ at the $n+1$ points $x_0, \ldots, x_n$. Applying Rolle's theorem k times, we find that $e^{(k)}(x)$ must have at least $n+1-k$ roots in (x_0, x_n), and specifically one root y_i in each subinterval (x_{i-k}, x_i), $i=k, \ldots, n$, with the y_i all distinct. Defining $Q(x)$ by (2.2), we now set

$$g(x) = e^{(k)}(x) - \lambda Q(x), \tag{2.4}$$

with λ a constant to be determined. For $x = y_i$, (2.1) is trivially satisfied: both sides are zero. Suppose $x = \bar{x}$ is not equal to any of the y_i; we wish to establish (2.1) for $\bar{x}$. Since $Q(\bar{x}) \neq 0$, we can find a λ such that $g(\bar{x}) = 0$. But also $g(y_i) = 0$ for $i = k, \ldots, n$. Hence $g(x)$ has $n+2-k$ distinct zeros in the interval I. Again by Rolle's theorem, $g^{(n+1-k)}(x)$ has a zero in I, say at ξ. But from (2.4) and (1.1),

$$0 = g^{(n+1-k)}(\xi) = f^{(n+1)}(\xi) - (n+1-k)!\,\lambda.$$

Solving for λ and substituting its value in the relation $g(\bar{x}) = 0$, we find $e^{(k)}(\bar{x}) = f^{(n+1)}(\xi)\, Q(\bar{x})/(n+1-k)!$, which is relation (2.1) for $\bar{x}$. Since $\bar{x}$ is arbitrary, this concludes the proof.

3. Remarks and Applications

At first sight, formula (2.1) seems to belong to the class (1.5) with $\varphi(x) = Q(x)/(n+1-k)!$. This does not contradict Brodskiĭ's conclusion that (1.5) is impossible, since the function $Q(x)$ depends on the partially undetermined constants y_i. Despite this indeterminacy, the bounds (2.3) on the y_i permit the convenient use of (2.1) in obtaining upper bounds on the absolute error $|e^{(k)}|$.

To begin with the crudest estimation procedure, note that x and all the y_i belong to the interval I. Hence $|Q(x)| \leqq L^{n+1-k}$, where L denotes the length of I. [In the usual situation $x \in (a_0, a_n)$, we have $L = a_n - a_0$.] Denoting by M the maximum value of $|f^{(n+1)}(x)|$ in I, we obtain from (2.1) the uniform estimate

$$(3.1) \qquad |e^{(k)}(x)| \leqq M L^{n+1-k}/(n+1-k)!.$$

This is exactly the same estimate that would be obtained by a similarly crude treatment of the Steffensen formula (1.4) if the latter were valid for $x \in (a_0, a_n)$. The derivation of (3.1) is the shortest means known to the author of proving that $e^{(k)} = O(M L^{n+1-k})$; its crudity lies only in the unnecessarily large constant factor.

We can considerably improve this constant by making more explicit use of inequality (2.3). We find

$$|x - y_i| \leqq \max(|x - x_{i-k}|, |x - x_i|)$$

and therefore $|Q(x)| \leqq R(x)$, where

$$(3.2) \qquad R(x) = \left| \frac{w(x)}{(x-z_1)\dots(x-z_k)} \right|.$$

Here $w(x)$ is defined by (1.3), while $z_1, \dots, z_k$ denote those k among the $n+1$ tabular points $x_0, \dots, x_n$ which are nearest to x. (Note that $R(x)$ is "piecewise" a polynomial.) Hence

$$(3.3) \qquad |e^{(k)}(x)| \leqq \frac{M R(x)}{(n+1-k)!}.$$

We illustrate this formula by two examples involving the first derivative ($k=1$). For example A, we take $n=1$, $x_0 = -L/2$, and $x_1 = +L/2$. Then $R(x) = L/2 + |x| \leqq L$ for $x \in (x_0, x_1)$ and we find the uniform estimate $|e'| \leqq ML$, coinciding with (3.1), and the particular estimates $|e'(0)| \leqq (1/2) ML$ and $|e'(\pm L/4)| \leqq (3/4) ML$. For example B, we choose $n=2$, $x_0 = -L/2$, $x_1 = 0$, and $x_2 = L/2$. Then

$$R(x) = \begin{cases} L^2/4 - x^2 & \text{for} \quad |x| \leqq L/4 \\ L|x|/2 + x^2 & \text{for} \quad L/4 \leqq |x| \leqq L/2 \end{cases}$$

leading to the uniform estimate $|e'| \leqq (1/4) ML^2$, half the size of (3.1), and the particular estimate $|e'(\pm L/4)| \leqq (3/32) ML^2$. Though these estimates are not sharp, they are surprisingly close to the sharp bounds of Brodskiĭ [4], who gives the bound $|e'(x)| \leqq M(L/4 + x^2/L)$ in example A and whose estimate leads in example B to the uniform bound $|e'| \leqq (1/4) ML^2$ and the point estimate $|e'(\pm L/4)| \leqq (1/96) ML^2$.

In addition to upper estimates, formula (2.1) yields useful information on the form of $e^{(k)}(x)$ as a function of x. For example, the error must be precisely zero at some $n+1-k$ points of I, and, if $f^{(n+1)}$ does not change sign, the error will have exactly $n+1-k$ changes of sign. If somehow, perhaps by a previous calculation or a fortuitous special circumstance, the points of zero error can be determined, (2.1) becomes almost an exact formula for $e^{(k)}$. Even if just one point x of small error (small compared to mL^{n+1-k}, where m is the minimum of $|f^{(n+1)}|$) is known, (2.1) can be used to pinpoint more closely the position of a neighboring y_i. Several separated points of small error will, of course, result in close fixes on several y_i, which in turn will allow a more accurate determination of $e^{(k)}(x)$ throughout $x_0 \leqq x \leqq x_n$.

Finally, (2.1) yields bounds sharper than any previously known on the minimum of $|e^{(k)}(x)|$ over two or more suitably chosen points x. We give two illustrations.

In example A, described above, consider $x = \pm L/4$. For each of these two points x separately, we can only conclude $|Q(x)| = |\pm L/4 - y_1| \leqq 3L/4$ and therefore, as above, $|e'| \leqq (3/4) ML$. But $|Q(x)|$ cannot be as great as $3L/4$ at both points, since y_1, being a definite point for a fixed f, cannot be simultaneously both positive and negative. In particular, we must have $|Q(x)| < L/4$ for at least one of the points, whence (2.1) yields $|e'(x)| \leqq (1/4) ML$ at that point. This is smaller than Brodskiĭ's bound for $|e'(\pm L/4)|$, which is $(5/16) ML$.

A similar procedure can be used in example B for the points $x = 1/4$, $3/4$ (where we have fixed $L = 2$ for simplicity of notation). Here a division is made into the cases $0 < y_2 \leqq 1/2$ and $1/2 \leqq y_2 < 1$. In the first case, we find $|e'(1/4)| \leqq (5/32) M$, while in the second case $|e'(3/4)| \leqq (7/32) M$. The corresponding Brodskiĭ bounds are $69/256$ at $x = 1/4$ and $143/256$ at $x = 3/4$. Naturally, an even smaller error value can be obtained by including the points $-1/4$ and $-3/4$ and distinguishing in addition the cases $y_1 \gtrless -1/2$.

References

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(Received August 6, 1963)