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ON THE CHOICE OF STEP IN COMPUTING DERIVATIVES

MATHEMATICS

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Abstract

Full Text

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MATHEMATICS

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ON THE CHOICE OF STEP IN COMPUTING DERIVATIVES

(Presented by Academician I. G. Petrovskii on 24 III 1970)

1°. Let $f(x)$ be a function differentiable up to order $k+2$ inclusive. Let $x_0, x_1, \dots, x_k$ be points forming a grid with equal step Δ: $x_{p+1} = x_p + \Delta$. Suppose, further, that the operator $L^k_{\Delta,x_0}[f]$ is defined by the equality

$$L^k_{\Delta,x_0}[f] = \frac{(-1)^k}{\Delta^k}\sum_{s=0}^{k}(-1)^s C^s_k f(x_k). \tag{1}$$

Finally, let $x = \frac{1}{2}(x_0 + x_k)$. Then the following holds.

Theorem.

$$L^k_{\Delta,x_0}[f] = f^{(k)}(x) + \frac{k\Delta^2}{24} f^{(k+2)}(x) + o(\Delta^2). \tag{2}$$

Proof. It is verified directly that

$$L^k_{\Delta,x_0}[f] = \frac{1}{\Delta}\{L^{k-1}_{\Delta,x_1}[f] - L^{k-1}_{\Delta,x_0}[f]\}. \tag{3}$$

Observe that the operator L^k_{Δ,x_0} is linear and invariant with respect to the change of variable $z = x - \frac{1}{2}(x_0 + x_k)$. Therefore in what follows we shall denote the operator L^k_{Δ,x_0}, applied to $f(x)$ on the grid $x_0, x_1, \dots, x_k$, where $x_0 = -x_k$, by $L^k_\Delta[f(x)]$.

In this notation (3) is written as follows:

$$L^k_\Delta[f(x)] = \frac{1}{\Delta}\left\{L^{k-1}_\Delta\left[f\left(x + \frac{\Delta}{2}\right)\right] - L^{k-1}_\Delta\left[f\left(x - \frac{\Delta}{2}\right)\right]\right\}. \tag{4}$$

We shall prove by induction that:

A. $L^s_\Delta(x^m) = 0$ for $m < s$.

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B. $L_\Delta^s(x^s) = s!$ and $L_\Delta^s(x^{s+1}) = 0$.

C. $L_\Delta^s(x^{s+2}) = \dfrac{s\Delta^2}{24}(s+2)!$

For $k = 1$ we have:

A^0. $L_\Delta^1(x^0) = 0$.

B^0. $L_\Delta^1(x) = \dfrac{1}{\Delta}\left(\dfrac{\Delta}{2} + \dfrac{\Delta}{2}\right) = 1!$ and $L_\Delta^1(x^2) = \left[\dfrac{1}{\Delta}\left(\dfrac{\Delta^2}{2^2} - \dfrac{\Delta^2}{2^2}\right)\right] = 0$.

C^0. $L_\Delta^1(x^3) = \dfrac{1}{\Delta}\left(\dfrac{\Delta^3}{2^3} + \dfrac{\Delta^3}{2^3}\right) = \dfrac{\Delta^2}{4} = \dfrac{1\cdot\Delta^2}{24}\cdot 3!$

Let A, B, and C be true for all $s \le k$. Then

$$L_\Delta^{k+1}(x^m) = \frac{1}{\Delta}\left\{L_\Delta^k\left[\left(x+\frac{\Delta}{2}\right)^m\right] - L_\Delta^k\left[\left(x-\frac{\Delta}{2}\right)^m\right]\right\} =$$

$$= \frac{1}{\Delta}\left\{L_\Delta^k(x^m) + C_m^1\frac{\Delta}{2}L_\Delta^k(x^{m-1}) + C_m^2\left(\frac{\Delta}{2}\right)^2 L_\Delta^k(x^{m-2}) + C_m^3\left(\frac{\Delta}{2}\right)^3 L_\Delta^k(x^{m-3}) +\right.$$

$$+ L_\Delta^k[P_{m-4}(x)] - L_\Delta^k(x^m) + C_m^1\frac{\Delta}{2}L_\Delta^k(x^{m-1}) - C_m^2\left(\frac{\Delta}{2}\right)^2 L_\Delta^k(x^{m-2}) +$$
$$+ C_m^3\left(\frac{\Delta}{2}\right)^3 L_\Delta^k(x^{m-3}) - L_\Delta^k[Q_{m-4}(x)] = \frac{2}{\Delta}\left\{C_m^1\frac{\Delta}{2}L_\Delta^k(x^{m-1}) + C_m^3\left(\frac{\Delta}{2}\right)^3 L_\Delta^k(x^{m-3}) +\right.$$
$$\left. + \frac{1}{2}L_\Delta^k[P_{m-4}(x)] - \frac{1}{2}L_\Delta^k[Q_{m-4}(x)]\right\}. \tag{5}$$

Here $P_{m-4}(x)$ and $Q_{m-4}(x)$ are polynomials of degree $m-4$.

From (5) we obtain:

$$\text{A}^1. \quad \text{For } m < k+1 \quad L_\Delta^{k+1}(x^m) = 0.$$

$$\text{B}^1. \quad \text{For } m = k+1 \quad L_\Delta^{k+1}(x^{k+1}) = \frac{2}{\Delta}C_{k+1}^1\frac{\Delta}{2}L_\Delta^k(x^k) =$$

$$= (k+1)k! = (k+1)! \quad \text{and for } m = k+2 \quad L_\Delta^{k+1}(x^{k+2}) = \frac{2}{\Delta}C_{k+2}^1\frac{\Delta}{2}L_\Delta^k(x^{k+1}) = 0.$$

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C^1. For $m = k+3$ $\quad L_\Delta^{k+1}(x^{k+3}) = C_{k+3}^1 L_\Delta^k(x^{k+2}) + C_{k+3}^3 \left(\frac{\Delta}{2}\right)^2 L_\Delta^k(x^k) =$

$$= (k+3)\frac{k\Delta^2}{24}(k+2)! + \frac{(k+3)(k+2)(k+1)}{6}\frac{\Delta^2}{4}k! = \frac{k\Delta^2}{24}(k+3)! +$$

$$+\frac{\Delta^2}{24}(k+3)! = \frac{(k+1)\Delta^2}{24}(k+3)!$$

From A^0, B^0, C^0 and A^1, B^1, C^1 there follow A, B, and C.

Since the function $f(x)$ is assumed differentiable up to order $(k+2)$, the assertion of the theorem is easily obtained from A, B, and C.

2°. Let the computations be performed on a machine with an n-digit binary mantissa. Suppose that we compute the k-th derivative of f at the point x by the formula

$$f^{(k)}(x) = L_{\Delta,x_0}^k[f], \tag{6}$$

using the scheme of successive differences, i.e., applying formula (3) $k(k+1)/2$ times. Then the absolute error in the right-hand side of (6) as a result of the inaccuracy of machine computation is, on average,

$$\mathrm{err}_M \simeq \frac{k \cdot 2^{-n}|f(x)|}{\sqrt{2}\,\Delta^k}. \tag{7}$$

On the other hand, it follows from (2) that, when computing by formula (6), we incur an absolute error

$$\mathrm{err}_B \simeq \frac{k\Delta^2}{24}\,|f^{(k+2)}(x)|. \tag{8}$$

Minimizing with respect to Δ the sum of (7) and (8), we obtain an expression for the optimal step Δ_k in the machine computation of $f^{(k)}(x)$:

$$\Delta_k = \sqrt[k+2]{\frac{2^{-n}\cdot 12\,k\,|f(x)|}{\sqrt{2}\,|f^{(k+2)}(x)|}}. \tag{9}$$

3°. When computing a one-sided derivative (at the points $x_0, x_1, \dots, \dots, x_k$), we obtain an absolute error in $f^{(k)}(x_0)$ of order

$$f^{(k)}\left(\frac{x_0+x_k}{2}\right) - f^{(k)}(x_0) \simeq \frac{k\Delta}{2} f^{(k+1)}(x). \tag{8'}$$

Hence the expression for the optimal step in computing a one-sided derivative is

$$\Delta_k^{\text{one-sided}} = \sqrt[k+1]{\frac{2^{-n}\cdot 2k\,|f(x)|}{\sqrt{2}\,|f^{(k+1)}(x)|}}. \tag{9'}$$

4°. **Numerical example.** For $n = 40$, for $f(x) = \exp(x)$ at $x = 1$, the quantities obtained for Δ_k are

$$\Delta_1 = 0.000198, \qquad \Delta_2 = 0.00198, \qquad \Delta_3 = 0.00746.$$

Under the same assumptions, for the step in the case of one-sided derivatives the quantities Δ_k^{one} are substantially smaller, namely:

$$\Delta_1^{\text{one}} = 0.00000113, \qquad \Delta_2^{\text{one}} = 0.000137, \qquad \Delta_3^{\text{one}} = 0.00140.$$

To compute the $(k+2)$-nd derivative one may use, for example, the same $L_{\Delta,x_0}^{k+2}[f]$. It is only necessary to ensure that, for the given step, not all correct digits disappear. If this nevertheless happens, one should increase Δ when computing $L_{\Delta,x_0}^{k+2}[f]$.

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Note: Figure translations are in progress. See original paper for figures.

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