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ON THE CHOICE OF STEP IN COMPUTING DERIVATIVES

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Abstract

Full Text

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MATHEMATICS

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ON THE CHOICE OF STEP IN COMPUTING DERIVATIVES

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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 $L_{\Delta, x_0}^k[f]$ is defined by the equality

$$L_{\Delta, x_0}^k[f] = \frac{(-1)^k}{\Delta^k} \sum_{s=0}^k (-1)^s C_k^s f(x_k). \quad (1)$$

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

Theorem.

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

Proof. It is verified directly that

$$L_{\Delta, x_0}^k[f] = \frac{1}{\Delta} \{L_{\Delta, x_1}^{k-1}[f] - L_{\Delta, x_0}^{k-1}[f]\}. \quad (3)$$

Observe that the operator L_{Δ, x_0}^k 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_{Δ, x_0}^k , applied to $f(x)$ on the grid $x_0, x_1, \dots, x_k$, where $x_0 = -x_k$, by $L_{\Delta}^k[f(x)]$.

In this notation (3) is written as follows:

$$L_{\Delta}^k[f(x)] = \frac{1}{\Delta} \left\{ L_{\Delta}^{k-1} \left[f \left(x + \frac{\Delta}{2} \right) \right] - L_{\Delta}^{k-1} \left[f \left(x - \frac{\Delta}{2} \right) \right] \right\}. \quad (4)$$

We shall prove by induction that:

A. $L_{\Delta}^s(x^m) = 0$ for $m < s$.

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

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

For $k = 1$ we have:

A⁰. $L_{\Delta}^1(x^0) = 0$.

B⁰. $L_{\Delta}^1(x) = \frac{1}{\Delta} \left(\frac{\Delta}{2} + \frac{\Delta}{2} \right) = 1!$ and $L_{\Delta}^1(x^2) = \left[\frac{1}{\Delta} \left(\frac{\Delta^2}{2^2} - \frac{\Delta^2}{2^2} \right) \right] = 0$.

C⁰. $L_{\Delta}^1(x^3) = \frac{1}{\Delta} \left(\frac{\Delta^3}{2^3} + \frac{\Delta^3}{2^3} \right) = \frac{\Delta^2}{4} = \frac{1 \cdot \Delta^2}{24} \cdot 3!$

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

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

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

From (5) we obtain:

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

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

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

$$\begin{aligned}
 C^1. \quad \text{For } m = k + 3 \quad L_{\Delta}^{k+1}(x^{k+3}) &= C_{k+3}^1 L_{\Delta}^k(x^{k+2}) + C_{k+3}^3 \left(\frac{\Delta}{2}\right)^2 L_{\Delta}^k(x^k) = \\
 &= (k+3) \frac{k\Delta^2}{24} (k+2)! + \frac{(k+3)(k+2)(k+1)}{6} \frac{\Delta^2}{4} k! = \frac{k\Delta^2}{24} (k+3)! + \\
 &\quad + \frac{\Delta^2}{24} (k+3)! = \frac{(k+1)\Delta^2}{24} (k+3)!
 \end{aligned}$$

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

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

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,

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

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

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

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 $f^{(k)}(x)$:

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

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

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

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

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

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

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

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

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

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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