On Accuracy of Derivatives on Uniform Grids (Revised)

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1 Finite-Difference Derivatives for Function Values

Consider a one-dimensional grid of uniform spacing h with nodal coordinates given by

$$x_j = (j-1)h, \quad j = 1, 2, \cdots, N, \tag{1}$$

where N denotes the number of nodes. At each node, we assume that function values are given: $f_j = f(x_j)$, and consider numerically computing its derivatives at nodes. In particular, we consider the finite-difference formula:

$$f'(x_j) \approx \frac{f_{j+1} - f_{j-1}}{2h}. \tag{2}$$

This is known as the central-difference formula. It is known to be second-order accurate:

$$\frac{f_{j+1} - f_{j-1}}{2h} = f'(x_j) + O(h^2). \tag{3}$$

One may ask: Can we apply it once again to obtain the second derivative? The answer is, of course, yes:

$$f''(x_j) \approx \frac{f'_{j+1} - f'_{j-1}}{2h}, \tag{4}$$

where

$$f'_{j+1} = \frac{f_{j+2} - f_j}{2h}, \quad f'_{j-1} = \frac{f_j - f_{j-2}}{2h}. \tag{5}$$

An interesting question is: How accurate is it? To find the answer, expand them in Taylor series around the node j:

$$f'_{j+1} = f'(x_j) + \frac{1}{2h}\left(\frac{1}{2}f''(x_j)\,(2h)^2 + \frac{1}{6}f'''(x_j)\,(2h)^3 + \frac{1}{24}f''''(x_j)\,(2h)^4\right) + O(h^4), \tag{6}$$

$$f'_{j-1} = f'(x_j) - \frac{1}{2h}\left(\frac{1}{2}f''(x_j)\,(-2h)^2 + \frac{1}{6}f'''(x_j)\,(-2h)^3 + \frac{1}{24}f''''(x_j)\,(-2h)^4\right) + O(h^4), \tag{7}$$

and substitute them into Equation (4) to get

$$\frac{f'_{j+1} - f'_{j-1}}{2h} = f''(x_j) + \frac{1}{3}f''''(x_j)h^2 + O(h^3) = f''(x_j) + O(h^2). \tag{8}$$

Observe that the first-order errors in f'_{j-1} and f'_{j+1} have been canceled because of the uniform spacing. Therefore, quite remarkably, the second derivative is obtained also with second-order accuracy. It seems like derivatives of arbitrary order can be obtained with second-order accuracy by successively applying the central difference formula. For example, given the second-order derivatives computed by the central formula, f''_{j-1} and f''_{j+1}, the third-order derivative can be obtained by

$$f'''(x_j) \approx \frac{f''_{j+1} - f''_{j-1}}{2h}. \tag{9}$$

It is straightforward to show (by Taylor expansion) that this is, indeed, second-order accurate:

$$\frac{f''_{j+1} - f''_{j-1}}{2h} = f'''(x_j) + \frac{h^2}{2}f'''''(x_j) + O(h^3). \tag{10}$$

It may appear that the same holds for any higher-order derivative: derivatives of arbitrary order can be obtained with second-order accuracy. However, there are two potential reasons that it cannot be true. First, the successive application of the central-difference formula will not be possible in a bounded domain. Near the boundaries, a non-central formula needs to be introduced to maintain second-order accuracy, but then nearby stencils are no longer symmetric, thus losing the error cancellation property. For example, successively applying the second-order one-sided difference formula at the left boundary $j = 1$:

$$\frac{3f_1 - 4f_2 + f_3}{2h}, \tag{11}$$

we find

$$f'_1 = \frac{3f_1 - 4f_2 + f_3}{2h} = f'(0) - \frac{h^2}{3}f'''(0) + O(h^3), \tag{12}$$

$$f''_1 = \frac{3f'_1 - 4f'_2 + f'_3}{2h} = f''(0) + \frac{3h}{4}f'''(0) + O(h^2), \tag{13}$$

$$f'''_1 = \frac{3f''_1 - 4f''_2 + f''_3}{2h} = \frac{3}{8}f'''(0) + O(h), \tag{14}$$

$$f''''_1 = \frac{3f'''_1 - 4f'''_2 + f'''_3}{2h} = \frac{1}{4h}f''''(0) + O(1), \tag{15}$$

$$f'''''_1 = \frac{3f''''_1 - 4f''''_2 + f''''_3}{2h} = \frac{1}{32h^2}f'''''(0) + O\left(\frac{1}{h}\right), \tag{16}$$

and so on. Interestingly, the errors in high-order derivatives grow on finer grids. See Figures 1 and 2 for numerical results. The other reason for not getting accuracy is that accuracy of high-order derivatives will be quickly lost by the effect of the so-called round-off error as h gets smaller (See Figure 3).

2 Finite-Difference Formula for Numerical Solutions

What if the function values are numerical solutions to differential equations? This is relevant to *a posteriori* derivative estimates for numerical solutions. Given numerical solutions $\{u_j\}$ obtained by a second-order numerical scheme on the one-dimensional grid, we apply the central-difference formula to compute the first-order derivative:

$$u'(x_j) \approx \frac{u_{j+1} - u_{j-1}}{2h}, \tag{17}$$

where u_{j-1} and u_{j+1} denote the numerical solutions at nodes $j-1$ and $j+1$. These values involve second-order errors:

$$u_{j-1} = u(x_{j-1}) + C_{j-1}h^2 + O(h^3), \tag{18}$$

$$u_{j+1} = u(x_{j+1}) + C_{j+1}h^2 + O(h^3), \tag{19}$$

where the error constants C_{j-1} and C_{j+1} depend on the local solution derivatives and thus they are generally different, $C_{j+1} \neq C_{j-1}$. Then, the central-difference approximation seems only first-order accurate:

$$\frac{u_{j+1} - u_{j-1}}{2h} = \frac{u(x_{j+1}) + C_{j+1}h^2 - (u(x_{j-1}) + C_{j-1}h^2) + O(h^3)}{2h} \tag{20}$$

$$= \frac{u(x_{j+1}) - u(x_{j-1})}{2h} + (C_{j+1} - C_{j-1})h + O(h^2) \tag{21}$$

$$= u'(x_j) + O(h). \tag{22}$$

But we can expand the error constants around the node j,

$$C_{j+1} = C_j + hC'_j + \frac{h^2}{2}C''_j + (h^3), \tag{23}$$

$$C_{j-1} = C_j - hC'_j + \frac{h^2}{2}C''_j + (h^3), \tag{24}$$

and therefore

$$\frac{u_{j+1} - u_{j-1}}{2h} = \frac{u(x_{j+1}) - u(x_{j-1})}{2h} + (C_{j+1} - C_{j-1})h + O(h^2) \tag{25}$$

$$= \frac{u(x_{j+1}) - u(x_{j-1})}{2h} + 2C'_j h^2 + O(h^2) \tag{26}$$

$$= u'(x_j) + O(h^2). \tag{27}$$

Note that again the first-order errors have been canceled due to the uniform spacing. How about the second-derivative? That is a good question. Given the first derivatives obtained by the central-difference formulas,

$$u'_{j+1} = \frac{u_{j+2} - u_j}{2h}, \quad u'_{j-1} = \frac{u_j - u_{j-2}}{2h}, \tag{28}$$

the second-derivative may be computed by

$$u''(x_j) \approx \frac{u'_{j+1} - u'_{j-1}}{2h}. \tag{29}$$

The story goes the same as that in the previous section: (1)With no boundary effects, the errors in successively computed derivatives maintain second-order accuracy but they are prone to round-off errors; (2)With boundary effects, second-order accuracy is lost in second- and higher-order derivatives. See Figures 4, 5, and 6.

3 Remark

In a practical situation, where we have second-order numerical solutions on a uniform grid, the first-order derivatives can be obtained with accuracy $O(h^2)$, but higher-order derivatives will lose accuracy: second-derivatives are $O(h)$, third-derivatives are $O(1)$, fourth-derivatives are $O(1/h)$, and so on.

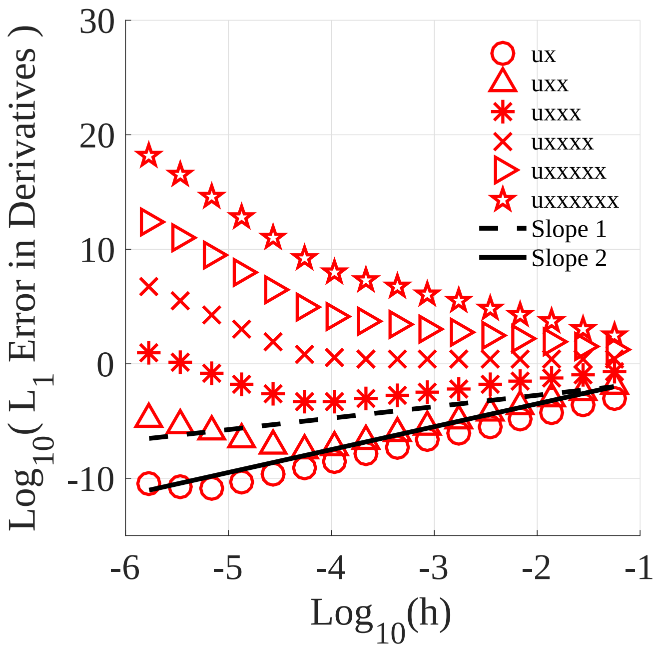

Figure 1: L_1 error convergence of derivatives computed for $f(x) = e^x$ by successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots, 15$. *The errors have been computed at all points, including boundary points.* The error increase is caused by both round-off errors and truncation errors. It is interesting that the second derivatives maintain second-order accuracy through the boundary.

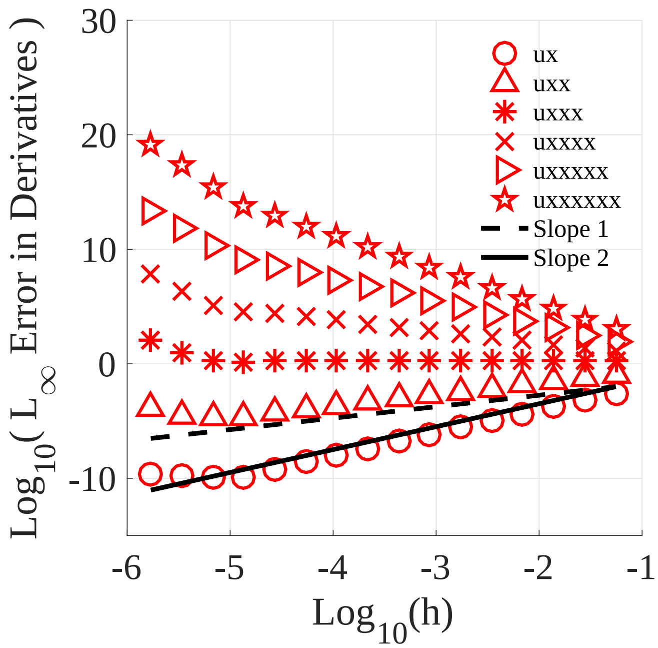

Figure 2: L_∞ error convergence of derivatives computed for $f(x) = e^x$ by successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots , 15$. *The errors have been computed at all points, including boundary points.* The error increase is caused by both round-off errors and truncation errors. The L_∞ errors show clearly the effect of the irregular boundary stencils.

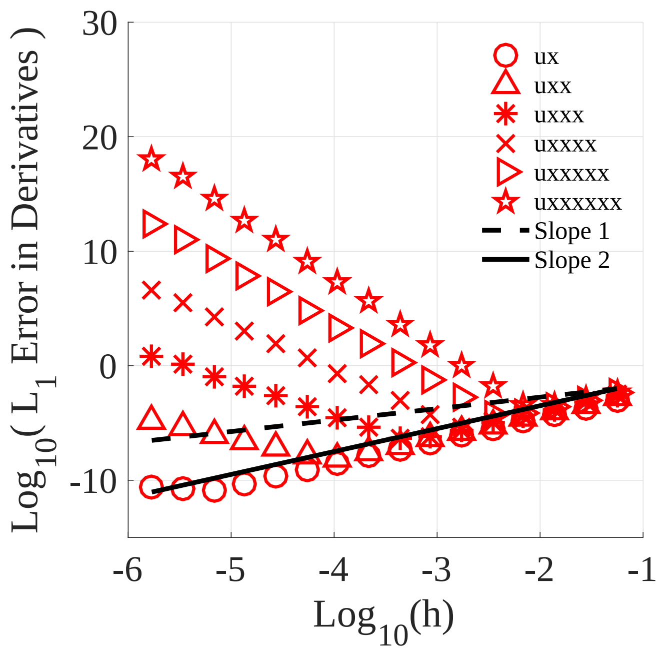

Figure 3: Error convergence of derivatives computed for $f(x) = e^x$ by successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots, 15$. *The errors have been computed only in the region* $x \in (0.45, 0.55)$ *to exclude boundary effects.* The error increase for finer grids is caused by round-off errors.

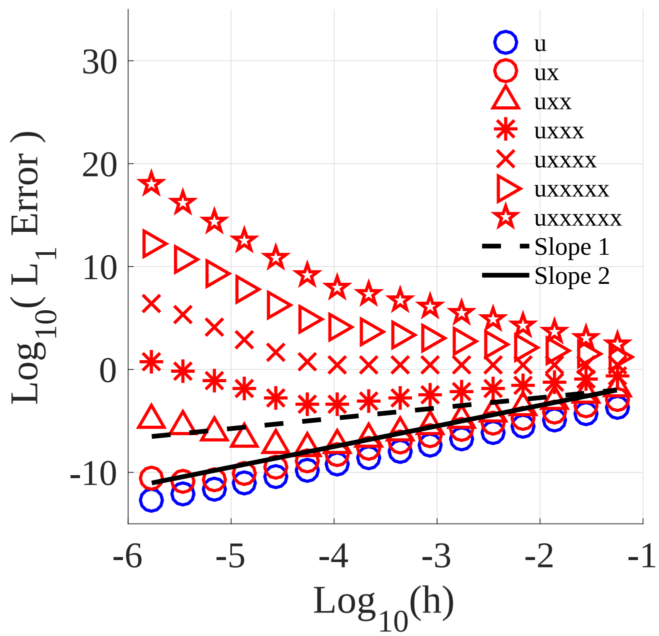

Figure 4: L_1 error convergence of derivatives computed for second-order numerical solutions to $\partial_x u = \exp(x)$, successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The exact solution is $u(x) = \exp(x)$. Numerical solutions have been computed by a second-order scheme: $u_i = u_{i-1} + \frac{1}{2}(f(x_i) + f(x_{i-1}))h$, $i = 2, 3, ..., N$. The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots, 15$. *The errors have been computed at all points, including boundary points.*

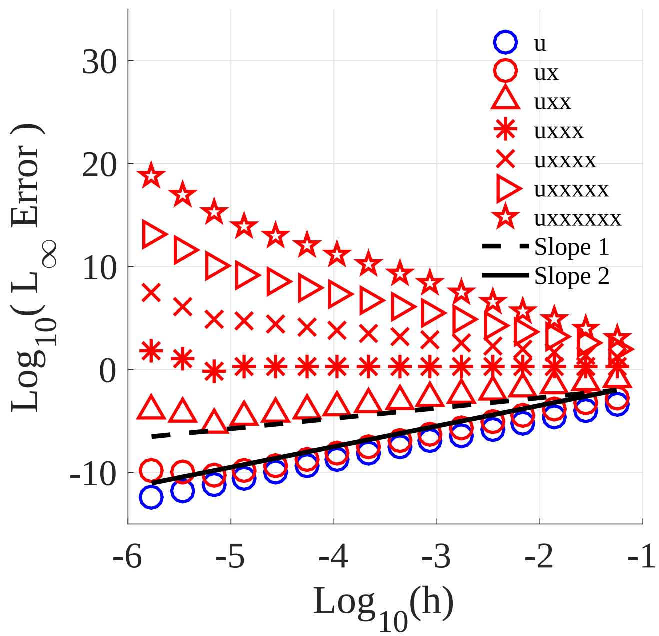

Figure 5: L_∞ error convergence of derivatives computed for second-order numerical solutions to $\partial_x u = \exp(x)$, successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The exact solution is $u(x) = \exp(x)$. Numerical solutions have been computed by a second-order scheme: $u_i = u_{i-1} + \frac{1}{2}(f(x_i) + f(x_{i-1}))h$, $i = 2, 3, ..., N$. The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots, 15$. *The errors have been computed at all points, including boundary points.*

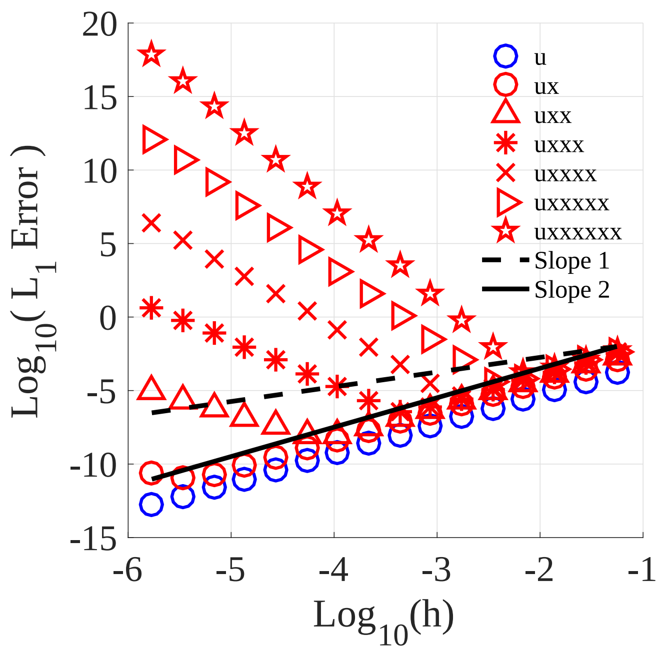

Figure 6: L_1 error convergence of derivatives computed for second-order numerical solutions to $\partial_x u = \exp(x)$, successively applying the central-difference formula on uniform grids (the second-order one-sided formula at boundary points). The exact solution is $u(x) = \exp(x)$. Numerical solutions have been computed by a second-order scheme: $u_i = u_{i-1} + \frac{1}{2}(f(x_i) + f(x_{i-1}))h$, $i = 2, 3, ..., N$. The mesh spacing h is given by $h = 1/n$, where $n = 18 \times 2^m$ with $m = 0, 1, 2, , \cdots, 15$. *The errors have been computed only in the region* $x \in (0.45, 0.55)$ *to exclude boundary effects.*