CALCULATION OF WEIGHTS IN FINITE DIFFERENCE FORMULAS

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1 Introduction

Derivatives of grid-based functions are often approximated by finite differences. The purpose of this note is to present an elegant algorithm, due to B. Fornberg [1], for finding the optimal weights for equispaced grids for derivatives of any order, approximated to any level of accuracy.

2 The algorithm

A couple of examples would be the best to illustrate both why this algorithm works and how it is used. Consider the following example where we want to find the coefficients which make the following approximation for the first derivative of a function,

$$\frac{\mathrm{d}f}{\mathrm{d}x} \approx a_0 f(x-2h) + a_1 f(x-h) + a_2 f(x) + a_3 f(x+h) + a_4 f(x+2h) \tag{1}$$

as accurate as possible. The weights a_i do not depend on the function which derivative we are taking. We can thus choose a function to our advantage. Substituting

$$f(x) = e^{\omega x} \tag{2}$$

into Eq. (1) gives

$$\omega e^{\omega x} \approx \left[a_0 e^{-2\omega h} + a_1 e^{-\omega h} + a_2 + a_3 e^{\omega h} + a_4 e^{2\omega h}\right] e^{\omega x}. \tag{3}$$

The goal is to make the approximation as accurate as possible, in the limit $h \to 0$. Canceling the common factors $e^{\omega x}$ in both sides of Eq. (3), and introducing the notation

$$u = e^{\omega h}, \tag{4}$$

that is

$$\omega = \frac{\log u}{h}, \tag{5}$$

we get

$$\frac{\log u}{h} \approx \frac{a_0}{u^2} + \frac{a_1}{u} + a_2 + a_3 u + a_4 u^2, \tag{6}$$

or

$$\frac{u^2 \log u}{h} \approx a_0 + a_1 u + a_2 u^2 + a_3 u^3 + a_4 u^4. \tag{7}$$

Note that $u \to 1$ as $h \to 0$. At this point, we want the best possible accuracy when expanded around $u = 1$. Using the Taylor approximation for the left hand side of Eq. (7) around $u = 1$,

$$u^2 \log u = \frac{1}{12} - \frac{2u}{3} + \frac{2u^3}{3} - \frac{u^4}{12} + \dots, \tag{8}$$

and comparing with the right hand side, we obtain:

$$a_0 = \frac{1}{12h}, \quad a_1 = -\frac{2}{3h}, \quad a_2 = 0, \quad a_3 = \frac{2}{3h}, \quad a_4 = -\frac{1}{12h}. \tag{9}$$

Therefore, the approximation Eq. (1) is

$$\frac{\mathrm{d}f}{\mathrm{d}x} \approx \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}. \tag{10}$$

The series expansions of the type we have in Eq. (8) can be done using a computer algebra systems. E.g. in Mathematica the following command can be used:

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CoefficientList[Normal[Series[u^2*Log[u], {u, 1, 4}]], u]
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$\left\{\frac{1}{12}, -\frac{2}{3}, 0, \frac{2}{3}, -\frac{1}{12}\right\}$

As a second example consider the following finite difference approximation for the one-sided second derivative:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \approx b_0 f(x) + b_1 f(x+h) + b_2 f(x+2h) + b_3 f(x+3h) + b_4 f(x+4h). \tag{11}$$

Using the steps similar to the used above, obtain

$$\frac{\log^2 u}{h^2} \approx b_0 + b_1 u + b_2 u^2 + b_3 u^3 + b_4 u^4. \tag{12}$$

Using the Taylor approximation for the left hand side of Eq. (12) around $u = 1$,

$$\log^2 u = \frac{35}{12} - \frac{26u}{3} + \frac{19u^2}{2} - \frac{14u^3}{3} + \frac{11u^4}{12} + \dots \tag{13}$$

Comparing Eq. (13) and Eq. (12) we find the coefficients b_i and finally the following approximation for the second derivative:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \approx \frac{35f(x) - 104f(x+h) + 114f(x+2h) - 56f(x+3h) + 11f(x+4h)}{12h^2}. \tag{14}$$

3 Numerical example

The error of using Eq. (10) to calculate the first derivative and of Eq. (14) to calculate the second derivative, both for $f(x) = \sin(x)$ at $x = 1$, for various values of h is shown in Fig. 1 and 2.

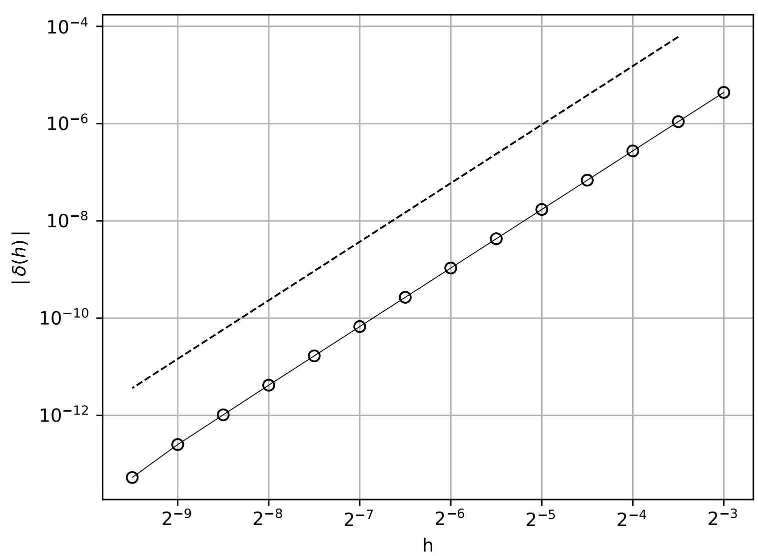

Figure 1: The error of using Eq. (10) to calculate the first derivative for various values of h. The dashed line is the expected error dependence $\delta(h) \sim h^4$.

References

[1] Bengt Fornberg, *Calculation of Weights in Finite Difference Formulas*, SIAM Review, vol. 40, No. 3, pp. 685–691, September 1998

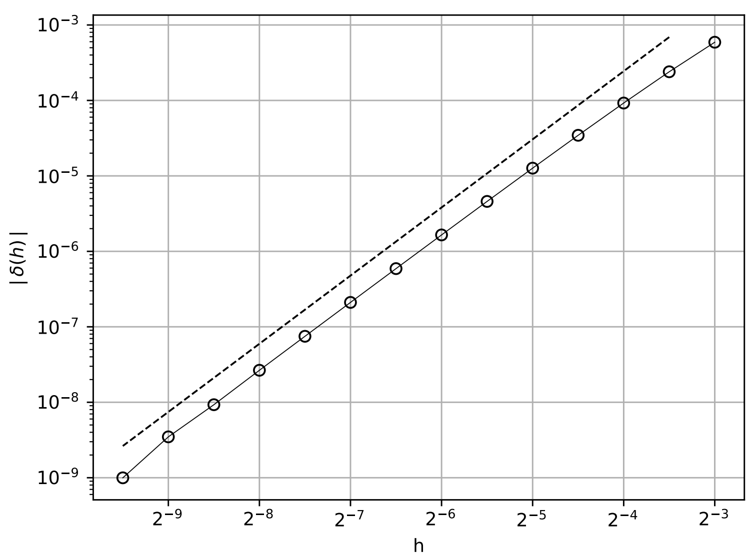

Figure 2: The error of using Eq. (14) to calculate the first derivative for various values of h. The dashed line is the expected error dependence $\delta(h) \sim h^3$.