Scientific Computing

Finite-difference formulae: derivation and error analysis

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A number of formulae for numerically approximating derivatives using finite differences are presented in the videos for Week 19. These formulae can be derived through the use of Taylor expansions. Recall that the Taylor expansion of a function $u(x)$ about the point $x = a$ is given by

$$u(x) = u(a) + (x-a)u'(a) + \frac{1}{2}(x-a)^2 u''(a) + O((x-a)^3), \tag{1}$$

where

$$u'(a) = \left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=a}, \qquad u''(a) = \left.\frac{\mathrm{d}^2u}{\mathrm{d}x^2}\right|_{x=a}. \tag{2}$$

Now, evaluating the Taylor expansion in (1) at $x = a \pm \Delta x$ leads to

$$u(a+\Delta x) = u(a) + \Delta x\, u'(a) + \frac{1}{2}(\Delta x)^2 u''(a) + O((\Delta x)^3), \tag{3a}$$

$$u(a-\Delta x) = u(a) - \Delta x\, u'(a) + \frac{1}{2}(\Delta x)^2 u''(a) + O((\Delta x)^3). \tag{3b}$$

We could also evaluate the Taylor expansion in (1) at $x = a \pm 2\Delta x$ to find

$$u(a+2\Delta x) = u(a) + 2\Delta x\, u'(a) + 2(\Delta x)^2 u''(a) + O((\Delta x)^3), \tag{4a}$$

$$u(a-2\Delta x) = u(a) - 2\Delta x\, u'(a) + 2(\Delta x)^2 u''(a) + O((\Delta x)^3). \tag{4b}$$

In fact, we could continue the process to find Taylor expansions for $u(a \pm 3\Delta x)$, $u(a \pm 4\Delta x)$, or even $u(a \pm (1/2)\Delta x)$. By taking linear combinations of these Taylor expansions, it is possible to obtain finite-difference formulae for any derivative.

For example, the forwards difference formula for the first derivative can be obtained by considering the combination $u(a+\Delta x) - u(a)$. Using the Taylor expansion in (3a) shows that

$$\begin{aligned} u(a+\Delta x) - u(a) &= u(a) + \Delta x u'(a) + \frac{1}{2}(\Delta x)^2 u''(a) + O((\Delta x)^3) - u(a) \\ &= \Delta x u'(a) + \frac{1}{2}(\Delta x)^2 u''(a) + O((\Delta x)^3. \end{aligned} \tag{5}$$

Thus, solving for $u'(a)$ leads to:

$$u'(a) = \frac{u(a+\Delta x) - u(a)}{\Delta x} - \frac{1}{2}\Delta x\, u''(a) + O((\Delta x)^2). \tag{6}$$

The forwards difference formula is obtained by neglecting terms of $O(\Delta x)$ and higher in (6). We say that the forwards difference formula is accurate to first order in Δx because the largest terms that have been neglected are $O(\Delta x)$ in size.

The same approach can be used to derive the backwards difference formula for the first derivative and to show that it accurate to $O(\Delta x)$. The central difference formula is obtained by considering the combination $u(a+\Delta x) - u(a-\Delta x)$. Using the Taylor expansions in (3) shows that

$$u(a+\Delta x) - u(a-\Delta x) = 2\Delta x\, u'(a) + O((\Delta x)^3). \tag{7}$$

Importantly, the terms that are proportional to $\Delta x\, u''(a)$ have cancelled out. This leads to the central difference formula for the first derivative being second-order accurate in Δx, which can be seen by rearranging for $u'(a)$ to find

$$u'(a) = \frac{u(a+\Delta x) - u(a-\Delta x)}{2\Delta x} + O((\Delta x)^2). \tag{8}$$

In general, using N points to create a finite-difference approximation of the first derivative will lead to a formula that is accurate to order $(\Delta x)^{N-1}$. For instance, we can combine $u(a)$, $u(a+\Delta x)$, and $u(a+2\Delta x)$ to obtain a forwards difference formula for $u'(a)$ that is second-order accurate. Although at this stage we do not know what linear combination of $u(a)$, $u(a+\Delta x)$, and $u(a+2\Delta x)$ to take, we can determine this algebraically. The idea is to introduce finite-difference coefficients c_1, c_2, and c_3 such that

$$\frac{c_1 u(a+2\Delta x) + c_2 u(a+\Delta x) + c_3 u(a)}{\Delta x} = u'(a) + O((\Delta x)^2). \tag{9}$$

Using the Taylor expansions in (3a) and (4a) and collecting powers of Δx leads to a system of equations for the coefficients:

$$O((\Delta x)^{-1}): \quad c_1 + c_2 + c_3 = 0, \tag{10a}$$
$$O((\Delta x)^{0}): \quad 2c_1 + c_2 = 1, \tag{10b}$$
$$O((\Delta x)^{1}): \quad 2c_1 + c_2/2 = 0. \tag{10c}$$

Solving this system leads to $c_1 = -1/2$, $c_2 = 2$, and $c_3 = -3/2$. Hence, the second-order forwards difference formula for the first derivative is given by

$$u'(a) = \frac{-u(a+2\Delta x) + 4u(a+\Delta x) - 3u(a)}{2\Delta x} + O((\Delta x)^2). \tag{11}$$

These approaches can be used to obtain formulae for higher-order derivatives as well. For example, to obtain a central difference formula for the second derivative, we seek coefficients such that

$$\frac{c_1 u(a+\Delta x) + c_2 u(a) + c_3 u(a-\Delta x)}{(\Delta x)^2} = u''(a) + O((\Delta x)^2). \tag{12}$$

Using the Taylor expansions in (3) and collecting powers of Δx lead to the following equations:

$$O((\Delta x)^{-2}): \quad c_1 + c_2 + c_3 = 0, \tag{13a}$$
$$O((\Delta x)^{-1}): \quad c_1 - c_3 = 0, \tag{13b}$$
$$O((\Delta x)^{0}): \quad c_1 + c_3 = 2. \tag{13c}$$

This solution gives $c_1 = c_3 = 1$ and $c_2 = -2$ and hence

$$u''(a) = \frac{u(a+\Delta x) - 2u(a) + u(a-\Delta x)}{(\Delta x)^2} + O((\Delta x)^2). \tag{14}$$

Note that in writing (12) we assumed that the error is $O((\Delta x)^2)$ in size. However, the algebraic system in (13) only eliminates the $O((\Delta x)^{-2})$, $O((\Delta x)^{-1})$, and $O((\Delta x)^{0})$ terms from (12), which means that there could be $O(\Delta x)$ terms that remain. These $O((\Delta x))$ terms would lead to a first-order accurate central difference formula. However, the same type of serendipitous cancellation of the $O(\Delta x)$ terms that we saw when deriving the central difference formula for the first derivative also occurs here. So, indeed, the central difference formula for the second derivative is also accurate to second order in Δx.