AM205: Examples of calculating a finite difference stencil

In the lectures, we discussed several typical methods of numerically calculating the derivative of a function $f: \mathbb{R} \to \mathbb{R}$ using finite differences. Two of the simplest methods are the forward and backward differences, defined as

$$f'_{\text{fwd}}(x) = \frac{f(x+h) - f(x)}{h}, \qquad f'_{\text{bck}}(x) = \frac{f(x) - f(x-h)}{h},$$
 (1)

respectively, where h is a small step size. Another common method is the centered-difference formula,

$$f'_{\text{cen}}(x) = \frac{f(x+h) - f(x-h)}{2h}.$$
 (2)

By analyzing the Taylor series expansion of f at x, one can verify that the forward and backward finite differences have errors of size O(h), making them first-order accurate approximations. Due to some additional cancellations because of symmetry, the centered difference has errors of size $O(h^2)$, and is therefore a second-order approximation.

Given any set of n points, it is possible to construct an approximation to f'. Usually, the order of accuracy is n-1, although in some cases like the centered-difference formula additional cancellations may lead to a higher order of accuracy. In this document, two methods to construct finite difference operators are presented, using the example set of points x, x + h, and x + 2h.

The Taylor series approach

The Taylor series of f at the points are x, x + h, and x + 2h are

$$f(x) = f(x) + 0f'(x) + 0f''(x), \tag{3}$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x), \tag{4}$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x).$$
 (5)

The aim is to construct a numerical approximation of the form

$$f'_{\text{tav}}(x) = \alpha f(x) + \beta f(x+h) + \gamma f(x+2h) \tag{6}$$

such that

$$f'_{\text{tav}}(x) = f'(x) + O(h^2).$$
 (7)

Equating the Taylor series terms in f(x), f'(x), and f''(x) gives three equations,

$$0 = \alpha + \beta + \gamma, \tag{8}$$

$$1 = h\beta + 2h\gamma,\tag{9}$$

$$0 = \frac{\beta}{2} + 2\gamma. \tag{10}$$

Equation 10 states that $\beta = -4\gamma$, and substituting this into Eq. 9 gives $\beta = 2/h$. Hence $\gamma = -1/2h$, and by using Eq. 8, $\alpha = -3/2h$. Hence

$$f'_{\text{tay}}(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \tag{11}$$

is a second-order accurate expression for f'(x).

The Lagrange interpolant approach

An alternative approach is to construct the Lagrange interpolant through the function at x, x + h, and x + 2h. To accomplish this, it is useful to introduce a shifted dummy variable z such that z = 0 at x. Then the three Lagrange basis functions through z = 0, h, 2h are

$$L_0(z) = \frac{(z-h)(z-2h)}{2h^2}, \qquad L_1(z) = \frac{-z(z-2h)}{h^2}, \qquad L_2(z) = \frac{z(z-h)}{2h^2}.$$
 (12)

The Lagrange interpolant of f(x) is given by

$$l(z) = f(x)L_0(z) + f(x+h)L_1(z) + f(x+2h)L_2(z)$$
(13)

Differentiating *l* with respect to *z* gives

$$l'(z) = f(x)\frac{2z - 3h}{2h^2} + f(x+h)\frac{-2z + 2h}{h^2} + f(x+2h)\frac{2z - h}{2h^2}.$$
 (14)

This leads to the finite-difference approximation

$$f'_{lgr}(x) = l'(0) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h},$$
(15)

which exactly matches the Taylor series stencil found in Eq. 11. A benefit of the Lagrange interpolant approach is that even for a large number of points, it is an explicit, direct procedure, whereas the Taylor series approach requires solving a linear system.