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

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

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

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

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

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

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

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

The aim is to construct a numerical approximation of the form

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

such that

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

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

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

The Lagrange interpolant of $f(x)$ is given by

$$l(z) = f(x)L_0(z) + f(x+h)L_1(z) + f(x+2h)L_2(z) \tag{13}$$

Differentiating l with respect to z gives

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

This leads to the finite-difference approximation

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

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.