AM205: Examples of calculating a finite difference stencil

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

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

(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

$$f(x) = f(x) + 0f'(x) + 0f''(x),$$
$$f(x + h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x),$$
$$f(x + 2h) = f(x) + 2hf'(x) + \frac{4h^2}{2} f''(x).$$

(3) (4) (5)

The aim is to construct a numerical approximation of the form

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

(6)

such that

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

(7)

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

$$0 = \alpha + \beta + \gamma,$$
$$1 = h\beta + 2h\gamma,$$
$$0 = \frac{\beta}{2} + 2\gamma.$$ (8) (9) (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

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

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

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