Project 1 Theory
Deriving Finite Difference Formulas

If you have taken a Calculus 1, you are probably already familiar with one finite difference formula:

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

In applied mathematics this is called a forward-difference first-derivative, i.e. a first derivative determined by displacing the function argument by $+h$. An example of a central-difference first-derivative formula is

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x-h)}{2h}$$

which involves both forward and backward displacements.

A straightforward method of deriving these formulas starts from a Taylor expansion.

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{\partial^n f}{\partial x^n}\right|_{x=0} x^n \tag{1}$$

Which, for our purposes, is more conveniently expressed as

$$f(x) = f_0 + f_0^{(1)} x + \frac{1}{2!} f_0^{(2)} x^2 + \frac{1}{3!} f_0^{(3)} x^3 + \mathcal{O}(x^4) \tag{2}$$

where $f_0^{(n)}$ denotes the value of the n^{th} derivative of f at $x = 0$. The last term, $\mathcal{O}(x^4)$, describes the magnitude of the error incurred by truncating the Taylor expansion at a particular point.

The basic strategy used to derive expressions for the derivatives is to plug in a grid of x-values $\{x_k\}$, yielding a series of equations, and then solve for the derivatives in terms of the function values at these points $\{f(x_k)\}$. Here we will take the "uniform grid" approach, in which we use x values with a fixed interval h between them $\{\ldots, -2h, -h, 0, +h, +2h, \ldots\}$.

Derivatives of one variable

To get a first approximation of the first and second derivatives in one variable, we only need three points from our grid $\{-h, 0, +h\}$. Let $f_{\pm k}$ represent $f(\pm kh)$ to keep things a little bit neater.

$$\begin{aligned} f_{+1} &= f_0 + f_0^{(1)} h + \frac{1}{2!} f_0^{(2)} h^2 + \mathcal{O}(h^3) \\ f_{-1} &= f_0 - f_0^{(1)} h + \frac{1}{2!} f_0^{(2)} h^2 - \mathcal{O}(h^3) \end{aligned}$$

When we subtract the two equations, the even powers of h cancel and we can solve for the first derivative.

$$f_0^{(1)} = \frac{f_{+1} - f_{-1}}{2h} + \mathcal{O}(h^2) \qquad \Longleftrightarrow \qquad \left(\frac{\partial f}{\partial x}\right)_{x=x_0} = \frac{f(x_0+h) - f(x_0-h)}{2h} + \mathcal{O}(h^2)$$

Adding the two equations cancels even powers, allowing us to solve for the second derivative.

$$f_0^{(2)} = \frac{f_{+1} + f_{-1} - 2f_0}{h^2} + \mathcal{O}(h^2) \qquad \Longleftrightarrow \qquad \left(\frac{\partial^2 f}{\partial x^2}\right)_{x=x_0} = \frac{f(x_0+h) + f(x_0-h) - 2f(x_0)}{h^2} + \mathcal{O}(h^2)$$

Mixed partials

The Taylor expansion for a multivariate function is

$$f(x_1,\ldots,x_n) = f_0 + \sum_{i=1}^{n}\left(\frac{\partial f}{\partial x_i}\right)_0 x_i + \frac{1}{2!}\sum_{i,j=1}^{n}\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_0 x_i x_j + \frac{1}{3!}\sum_{i,j,k=1}^{n}\left(\frac{\partial^3 f}{\partial x_i \partial x_j \partial x_k}\right)_0 x_i x_j x_k + \ldots$$

In order to determine the elements of f's second-derivative (Hessian) matrix $H_{ij} = \dfrac{\partial^2 f}{\partial x_i \partial x_j}$ we need mixed partial derivatives of the form $\dfrac{\partial^2 f}{\partial x \partial y}$ in addition to the one-variable formulas above, which give us the diagonal elements. These can be derived from a bivariate Taylor expansion.

$$f(x,y) = f_{0,0} + f_{0,0}^{(1,0)}x + f_{0,0}^{(0,1)}y + \frac{1}{2!}f_{0,0}^{(2,0)}x^2 + f_{0,0}^{(1,1)}xy + \frac{1}{2!}f_{0,0}^{(0,2)}y^2 + \ldots$$

The equations for double-forward and double-backward displacement are then

$$\begin{aligned} f_{+1,+1} &= f_{0,0} + f_{0,0}^{(1,0)}h + f_{0,0}^{(0,1)}h + \frac{1}{2!}f_{0,0}^{(2,0)}h^2 + f_{0,0}^{(1,1)}h^2 + \frac{1}{2!}f_{0,0}^{(0,2)}h^2 + \mathcal{O}(h^3) \\ f_{-1,-1} &= f_{0,0} - f_{0,0}^{(1,0)}h - f_{0,0}^{(0,1)}h + \frac{1}{2!}f_{0,0}^{(2,0)}h^2 + f_{0,0}^{(1,1)}h^2 + \frac{1}{2!}f_{0,0}^{(0,2)}h^2 - \mathcal{O}(h^3)\ . \end{aligned}$$

Adding these equations and rearranging, we obtain

$$f_{0,0}^{(1,1)} = \frac{f_{+1,+1} + f_{-1,-1} - 2f_{0,0}}{2h^2} - \frac{f_{0,0}^{(2,0)} + f_{0,0}^{(0,2)}}{2} + \mathcal{O}(h^2)\ .$$

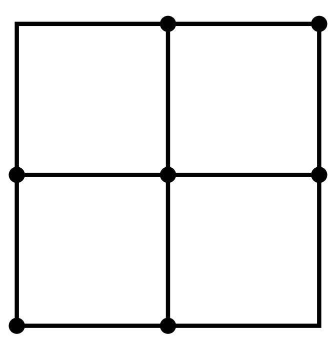
Since $f_{0,0}^{(2,0)}, f_{0,0}^{(0,2)}$ are partials with respect to a single variable, we can plug in the expressions derived above

$$f_{0,0}^{(1,1)} = \frac{f_{+1,+1} + f_{-1,-1} - f_{+1,0} - f_{-1,0} - f_{0,+1} - f_{0,-1} + 2f_{0,0}}{2h^2} + \mathcal{O}(h^2)$$

giving the following central-difference formula for mixed second derivatives.

$$\left(\frac{\partial^2 f}{\partial x \partial y}\right)_{\substack{x=x_0\\y=y_0}} = \frac{f(x_0+h,y_0+h) + f(x_0-h,y_0-h) - f(x_0+h,y_0) - f(x_0-h,y_0) - f(x_0,y_0+h) - f(x_0,y_0-h) + 2f(x_0,y_0)}{2h^2} + \mathcal{O}(h^2)$$

These expressions are sometimes described by to the grid of points used in them. In this case, the grid is



where the middle point is the origin and all line segments have length h.