Chapter 4

Numerical Differentiation

We would like to calculate the derivative of a smooth function defined on a discrete set of grid points $x_0, x_1, \ldots, x_N$. Assume that the data are the exact values of the function at the data points, and we need the derivative only at the data points. We will look into the construction of numerical approximations of the derivative called finite differences. There are two approaches to such constructions: using interpolation formulas, or Taylor series approximations.

4.1 Finite Differences from Interpolation

From linear piecewise Lagrange interpolation we have

$$f(x) = \frac{x_{i+1} - x}{x_{i+1} - x_i} f(x_i) + \frac{x - x_i}{x_{i+1} - x_i} f(x_{i+1}).$$

Differentiating, we find that the derivative is a constant and the same at the two ends of the interval

$$f'(x_i) = \frac{f_{i+1} - f_i}{h_i} \equiv \frac{1}{h_i} \Delta f_i, \qquad f'(x_{i+1}) = \frac{f_{i+1} - f_i}{h_i} \equiv \frac{1}{h_i} \nabla f_{i+1},$$

where Δ and ∇ are forward and backward difference operators. Note that the derivative is discontinuous at the end points.

From quadratic piecewise Lagrange interpolation we have

$$\begin{aligned} f(x) \quad = \quad & \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f(x_{i-1}) + \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} f(x_i) + \\ & \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f(x_{i+1}). \end{aligned}$$

Differentiating and evaluating the result at the midpoint of the interval we obtain

$$f'(x_i) = -\frac{h_i}{h_{i-1}\left(h_{i-1} + h_i\right)} f_{i-1} + \left(\frac{1}{h_{i-1}} - \frac{1}{h_i}\right) f_i + \frac{h_{i-1}}{h_i\left(h_{i-1} + h_i\right)} f_{i+1}.$$

For equally spaced intervals $h_{i-1} = h_i = h$, so

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} = \frac{1}{2h}\left(\Delta + \nabla\right) f_i.$$

This is the central difference formula, and is the average of the forward and backward formulas.

If we differentiate $f(x)$ twice and evaluate the result at x_i we obtain a constant in the interval $x_{i-1} \leq x \leq x_{i+1}$

$$f''(x_i) = \frac{2}{h_{i-1}\left(h_{i-1} + h_i\right)} f_{i-1} - \frac{2}{h_{i-1} h_i} f_i + \frac{2}{h_i\left(h_{i-1} + h_i\right)} f_{i+1},$$

which for equally spaced intervals reduces to

$$f''(x_i) = \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2} = \frac{1}{h^2}\Delta\nabla f_i = \frac{1}{h^2}\nabla\Delta f_i.$$

Since f'' is constant, it is called a forward, central, or backward formula depending whether it is evaluated at x_{i-1}, x_i, or x_{i+1}, respectively.

The use of cubic splines to derive finite difference approximations has received little attention. It requires the solution of the tridiagonal system

$$\frac{h_{i-1}}{6}f''(x_{i-1}) + \frac{(h_{i-1}+h_i)}{3}f''(x_i) + \frac{h_i}{6}f''(x_{i+1}) = \frac{f(x_{i+1}) - f(x_i)}{h_i} - \frac{f(x_i) - f(x_{i-1})}{h_{i-1}}.$$

For uniform intervals we obtain

$$\frac{1}{6}f''_{i-1} + \frac{2}{3}f''_i + \frac{1}{6}f''_{i+1} = \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}.$$

Note that the solution of this system gives us the approximation for the second derivative, and the effect of the spline is to distribute the previous result over the central point and its neighbors with weights 1/6, 2/3, and 1/6. Once this tridiagonal system is solved, the appropriate f''_i can be used in the first derivative approximation obtained by differentiating the spline approximation for $f(x)$ and evaluating the result at x_i.

4.2 Finite Differences from Taylor Series

Finite difference formulas can be easily derived from Taylor series expansions. For example, to obtain an approximation for the derivative of $f(x)$ at the point x_i, we use

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)f'(x_i) + \frac{(x_{i+1} - x_i)^2}{2}f''(x_i) + \cdots.$$

Rearrangement leads to:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h_i} - \frac{h_i}{2}f''(x_i) + \cdots.$$

When the grid points are uniformly spaced, the above formula can be recast in the following form

$$f'_i = \frac{f_{i+1} - f_i}{h} + O(h).$$

This formula is referred to as the first order forward difference. The exponent of h in $O(h)$ is the order of accuracy of the method. With a first order scheme, if we refine the mesh size by a factor of 2, the error (called the truncation error) is reduced by approximately a factor of 2. Similarly,

$$f'_i = \frac{f_i - f_{i-1}}{h} + O(h)$$

is called the first order backward difference formula. Higher order (more accurate) schemes can be derived by Taylor series of the function f at different points about the point x_i. For example, the widely used central difference formula can be obtained from subtraction of the two Taylor series expansions:

$$f_{i+1} = f_i + hf'_i + \frac{h^2}{2}f''_i + \frac{h^3}{6}f'''_i + \cdots \tag{4.1}$$

$$f_{i-1} = f_i - hf'_i + \frac{h^2}{2}f''_i - \frac{h^3}{6}f'''_i + \cdots. \tag{4.2}$$

This leads to:

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{6} f_i''' + \cdots . \tag{4.3}$$

This is, of course, a second order formula. In general, we can obtain higher accuracy if we include more points. Here is a fourth order formula:

$$f_i' = \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{12h} + O(h^4).$$

The main difficulty with higher order formulas occurs near the boundaries of the domain. They require the functional values at points outside the domain which are not available. Near the boundaries one usually resorts to lower order formulas.

Similar formulas can be derived for second or higher order derivatives. For example, the second order central difference formula for the second derivative is

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2),$$

and is obtained by adding formulas (4.1) and (4.2).

4.3 Difference Operators

In order to develop approximations to differential equations, we will occasionally be using the following operators:

$Ef(x) = f(x+h)$	The shift operator
$\Delta f(x) = f(x+h) - f(x)$	The forward difference operator
$\nabla f(x) = f(x) - f(x-h)$	The backward difference operator
$\delta f(x) = f(x+\frac{h}{2}) - f(x-\frac{h}{2})$	The central difference operator
$\mu f(x) = \frac{1}{2}\left[f(x+\frac{h}{2}) + f(x-\frac{h}{2})\right]$	The average operator
$Df(x) = f'(x)$	Differential operator

where h is the difference interval. For linking the difference operators with the differential operator we consider Taylor's formula

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2!}h^2 f''(x) + \cdots .$$

In operator notations we can write

$$Ef(x) = \left[1 + hD + \frac{1}{2!}(hD)^2 + \cdots\right] f(x).$$

The series in brackets is the expression for the exponential and hence we have (formally)

$$E = e^{hD}.$$

This relation is very important, since it can be used by symbolic programs such as Maple or Mathematica to analyze the accuracy of finite difference schemes. For example, consider the finite difference operator defined by Eq. (4.3). Applying the shift operator to f_i we can write $f_{i+1} = Ef_i = e^{hD} f_i$ and $f_{i-1} = E^{-1} f_i = e^{-hD} f_i$. Now, substituting these expressions into central difference approximation for the derivative we obtain:

$$\frac{f_{i+1} - f_{i-1}}{2h} = \frac{e^{hD} f_i + e^{-hD} f_i}{2h} = \frac{e^{hD} + e^{-hD}}{2h} f_i. \tag{4.4}$$

Now using the Taylor series expansion for e^{hD} and e^{-hD} for small values of h we obtain:

$$\begin{aligned} e^{hD} &= 1 + hD + \frac{1}{2}h^2D^2 + \frac{1}{6}h^3D^3 + \ldots + \frac{1}{n!}h^nD^n + \ldots, \\ e^{-hD} &= 1 - hD + \frac{1}{2}h^2D^2 - \frac{1}{6}h^3D^3 + \ldots + \frac{(-1)^n}{n!}h^nD^n + \ldots. \end{aligned}$$

Substituting these expressions to Eq. (4.4) we obtain:

$$\frac{f_{i+1} - f_{i-1}}{2h} = \left(D + \frac{1}{6}h^2D^3 + \ldots\right) f_i. \tag{4.5}$$

Reorganizing left and right hand sides of this equation would result in Eq. (4.3).