Chapter 4

Difference and average operators

4.1 Derivation

Recall the Taylor series expansion about a point a:

$$y(x) = y(a) + \sum_{1}^{\infty} \frac{1}{n!} \left.\frac{\mathrm{d}^n y}{\mathrm{d}x^n}\right|_{x=a} (x-a)^n \tag{4.1}$$

Suppose we have a regular grid, $x_i = i\Delta x$. It is useful to think of a set of points exactly half way between the grid points, i.e. $x_{i+\frac{1}{2}} = \left(i + \frac{1}{2}\right)\Delta x$. We can Taylor expand about a midpoint to arrive at function values at adjacent grid points. At x_{i+1}, $x_{i+1} - x_{i+\frac{1}{2}} = \Delta x/2$ so

$$\begin{aligned} y(x_{i+1}) =& y\left(x_{i+\frac{1}{2}}\right) + \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \frac{\Delta x}{2} + \frac{1}{2!} \left.\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^2 \\ &+ \frac{1}{3!} \left.\frac{\mathrm{d}^3 y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^3 + \frac{1}{4!} \left.\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^4 + \ldots \end{aligned} \tag{4.2}$$

At x_i, $x_i - x_{i+\frac{1}{2}} = -\Delta x/2$ so

$$\begin{aligned} y(x_{i}) =& y\left(x_{i+\frac{1}{2}}\right) - \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \frac{\Delta x}{2} + \frac{1}{2!} \left.\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^2 \\ &- \frac{1}{3!} \left.\frac{\mathrm{d}^3 y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^3 + \frac{1}{4!} \left.\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^4 - \ldots \end{aligned} \tag{4.3}$$

If we subtract eq. (4.3) from eq. (4.2), we obtain

$$y(x_{i+1}) - y(x_i) = \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \Delta x + \frac{2}{3!} \left.\frac{\mathrm{d}^3 y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \left(\frac{\Delta x}{2}\right)^3 + \ldots \tag{4.4}$$

Rearranging, we obtain the centred difference estimate of the gradient:

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} = \frac{y\left(x_{i+1}\right) - y\left(x_i\right)}{\Delta x} + O\left(\Delta x^2\right) \tag{4.5}$$

Likewise, if we add eq. (4.3) to eq. (4.2), we obtain the centred average estimate of y:

$$y\left(x_i\right) + y\left(x_{i+1}\right) = 2y\left(x_{i+\frac{1}{2}}\right) + \frac{2}{2!}\left.\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}}\left(\frac{\Delta x}{2}\right)^2 + \frac{2}{4!}\left.\frac{\mathrm{d}^4y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}}\left(\frac{\Delta x}{2}\right)^4 + ... \tag{4.6}$$

Thus

$$y\left(x_{i+\frac{1}{2}}\right) = \frac{y\left(x_i\right) + y\left(x_{i+1}\right)}{2} + O\left(\Delta x^2\right) \tag{4.7}$$

Thus, eq. (4.5) provides a *second order accurate* estimate of the gradient at $x_{i+\frac{1}{2}}$. In other words, the error is $O\left(\Delta x^2\right)$, so if we half Δx we quarter the error. At no other point can we construct an estimate with this order of accuracy using just two points - at any other point we obtain first order accuracy, and to gain higher order accuracy we need to employ more points.

Likewise, eq. (4.7) provides a *second order accurate* estimate of the value of y at $x_{i+\frac{1}{2}}$. At no other point can we construct an estimate with this order of accuracy using just two points - at any other point we obtain first order accuracy, and to gain higher order accuracy we need to employ more points.

We therefore define the following two operators:

$$\delta\left(\ \right)_{i+\frac{1}{2}} = \frac{\left(\ \right)_{i+1} - \left(\ \right)_i}{\Delta x} \tag{4.8}$$

$$\overline{\left(\ \right)}_{i+\frac{1}{2}} = \frac{\left(\ \right)_i + \left(\ \right)_{i+1}}{2} \tag{4.9}$$

So

$$\delta y_{i+\frac{1}{2}} = \frac{y_{i+1} - y_i}{\Delta x} \tag{4.10}$$

$$\overline{y}_{i+\frac{1}{2}} = \frac{y_i + y_{i+1}}{2} \tag{4.11}$$

4.2 Some applications

With these operators, we can construct more complex finite difference operators which retain the second order accuracy of the operators.

Suppose, for example, we actually want the gradient at x_i. We can obtain a second order accurate formula by averaging the gradients at $x_{i-\frac{1}{2}}$ and $x_{i+\frac{1}{2}}$, viz:

$$\begin{aligned}\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_i} &= \overline{(\delta y)}_i \\ &= \frac{\delta y_{i-\frac{1}{2}} + \delta y_{i+\frac{1}{2}}}{2} \\ &= \frac{\frac{y_i - y_{i-1}}{\Delta x} + \frac{y_{i+1} - y_i}{\Delta x}}{2} \\ &= \frac{y_{i+1} - y_{i-1}}{2\Delta x} \end{aligned} \tag{4.12}$$

This is just the centred difference estimate of the gradient on a grid with spacing $2\Delta x$.

We can construct higher order derivatives. The second derivative at x_i is particularly easy, because we need a the derivatives at half points:

$$\begin{aligned}\left.\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right|_{x_i} &= \delta\left(\delta y\right)_i \\ &= \frac{\delta y_{i+\frac{1}{2}} - \delta y_{i-\frac{1}{2}}}{\Delta x} \\ &= \frac{\frac{y_{i+1} - y_i}{\Delta x} - \frac{y_i - y_{i-1}}{\Delta x}}{\Delta x} \\ &= \frac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} \end{aligned} \tag{4.13}$$

Likewise

$$\begin{aligned}\left.\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} &= \delta\left(\delta\left(\delta y\right)\right)_{i+\frac{1}{2}} \\ &= \frac{\delta\left(\delta y\right)_{i+1} - \delta\left(\delta y\right)_i}{\Delta x} \\ &= \frac{\frac{y_i - 2y_{i+1} + y_{i+2}}{\Delta x^2} - \frac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2}}{\Delta x} \\ &= \frac{y_{i+2} - 3y_{i+1} + 3y_i - y_{i-1}}{\Delta x^3} \end{aligned} \tag{4.14}$$

$(i+n)^3 = (i+n)(i+n)(i+n) = (i^2+2in+n^2)(i+n) = i^3+2ni^2+n^2i+i^2n+2in^2+n^3 = i^3+3ni^2+3n^2i+n^3$

Example - $y = x^3$, $\frac{\mathrm{d}^3y}{\mathrm{d}x^3} = 6$. $(i+2)^3 - 3(i+1)^3 + 3(i)^3 - (i-1)^3 = i^3+6i^2+12i+8-3(i^3+3i^2+3i+1)+3i^3-(i^3-3i^2+3i-1) = (1-3+3-1)i^3+(6-9+3)i^2+(12-9-3)i+(8-3+1) = 6$

Note the emergence of Pascal's triangle in the difference formulae for derivatives, plus the alternating signs which ensure the gradients are zero for a uniform field (all ys equal).

We can extend the averaging operator to derive uncentred difference formulae. Suppose we want a second order accurate estimate of the first derivative at i using points i, $i+1$, $i+2$. We can construct a linear fit to values at $i+\frac{1}{2}$ and $i+\frac{3}{2}$,

$$()_x = [(x - x_{i+\frac{1}{2}})()_{i+\frac{3}{2}} + (x_{i+\frac{3}{2}} - x)()_{i+\frac{1}{2}}]/(x_{i+\frac{3}{2}} - x_{i+\frac{1}{2}}) \tag{4.15}$$

Thus

$$\begin{aligned}
\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_i} &= \frac{-\frac{\Delta x}{2}\delta y_{i+\frac{3}{2}} + \frac{3\Delta x}{2}\delta y_{i+\frac{3}{2}}}{\Delta x} \\
&= -\frac{1}{2}\frac{y_{i+2} - y_{i+1}}{\Delta x} + \frac{3}{2}\frac{y_{i+1} - y_i}{\Delta x} \\
&= \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2\Delta x}
\end{aligned} \tag{4.16}$$

4.3 Higher Order Estmates

We can introduce more points to the 'stencil'.

$$\begin{aligned}
y\left(x_{i+2}\right) =& y\left(x_{i+\frac{1}{2}}\right) + \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \frac{3\Delta x}{2} + \frac{1}{2!}\left.\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^2 \\
&+ \frac{1}{3!}\left.\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^3 + \frac{1}{4!}\left.\frac{\mathrm{d}^4y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^4 + ...
\end{aligned} \tag{4.17}$$

$$\begin{aligned}
y\left(x_{i-1}\right) =& y\left(x_{i+\frac{1}{2}}\right) - \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \frac{3\Delta x}{2} + \frac{1}{2!}\left.\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^2 \\
&- \frac{1}{3!}\left.\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^3 + \frac{1}{4!}\left.\frac{\mathrm{d}^4y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}} \left(\frac{3\Delta x}{2}\right)^4 - ...
\end{aligned} \tag{4.18}$$

Consider an arbitrary combination of eqs. (4.18), (4.3), (4.2) and (4.17) with multipliers a, b, c and d respectively:

$$\begin{aligned} ay_{i-1} + by_i + cy_{i+1} + dy_{i+2} =& \left(a+b+c+d\right) y_{i+\frac{1}{2}} \\ &+ \left(-\frac{3}{2}a - \frac{1}{2}b + \frac{1}{2}c + \frac{3}{2}d\right) \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} \Delta x \\ &+ \left[\left(\frac{3}{2}\right)^2 a + \left(\frac{1}{2}\right)^2 b + \left(\frac{1}{2}\right)^2 c + \left(\frac{3}{2}\right)^2 d\right] \frac{1}{2!} \left.\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right|_{x_{i+\frac{1}{2}}} \Delta x^2 \\ &+ \left[\left(-\frac{3}{2}\right)^3 a - \left(\frac{1}{2}\right)^3 b + \left(\frac{1}{2}\right)^3 c + \left(\frac{3}{2}\right)^3 d\right] \frac{1}{3!} \left.\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}} \Delta x^3 \\ &+ \left[\left(\frac{3}{2}\right)^4 a + \left(\frac{1}{2}\right)^4 b + \left(\frac{1}{2}\right)^4 c + \left(\frac{3}{2}\right)^4 d\right] \frac{1}{4!} \left.\frac{\mathrm{d}^4y}{\mathrm{d}x^4}\right|_{x_{i+\frac{1}{2}}} \Delta x^4 \\ &+ O\left(\Delta x^5\right) + ... \end{aligned} \tag{4.19}$$

We can derive a fourth order accurate estimate of the first derivative by requiring:

$$-\frac{3}{2}a - \frac{1}{2}b + \frac{1}{2}c + \frac{3}{2}d = 1 \tag{4.20}$$

$$\left(\frac{3}{2}\right)^2 a + \left(\frac{1}{2}\right)^2 b + \left(\frac{1}{2}\right)^2 c + \left(\frac{3}{2}\right)^2 d = 0 \tag{4.21}$$

$$\left(-\frac{3}{2}\right)^3 a - \left(\frac{1}{2}\right)^3 b + \left(\frac{1}{2}\right)^3 c + \left(\frac{3}{2}\right)^3 d = 0 \tag{4.22}$$

$$\left(\frac{3}{2}\right)^4 a + \left(\frac{1}{2}\right)^4 b + \left(\frac{1}{2}\right)^4 c + \left(\frac{3}{2}\right)^4 d = 0 \tag{4.23}$$

$$\frac{1}{2}\left(c-b\right) + \frac{3}{2}\left(d-a\right) = 1 \tag{4.24}$$

$$\left(\frac{1}{2}\right)^2 \left(c+b\right) + \left(\frac{3}{2}\right)^2 \left(d+a\right) = 0 \tag{4.25}$$

$$\left(\frac{1}{2}\right)^3 \left(c-b\right) + \left(\frac{3}{2}\right)^3 \left(d-a\right) = 0 \tag{4.26}$$

$$\left(\frac{1}{2}\right)^4 \left(c+b\right) + \left(\frac{3}{2}\right)^4 \left(d+a\right) = 0 \tag{4.27}$$

By symmetry, $a = -d$ and $b = -c$. Thus

$$c + 3d = 1 \tag{4.28}$$

$$\left(\frac{1}{2}\right)^3 2c + \left(\frac{3}{2}\right)^3 2d = 0 \tag{4.29}$$

Thus$c = 1 - 3d$ and $c = -27d$, so $d = -1/24$, $c = 27/24$. Hence

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} = \frac{y_{i-1} - 27y_i + 27y_{i+1} + y_{i+2}}{24\Delta x} + O\left(\Delta x^4\right) \tag{4.30}$$

We can even use the δ operator arrive at the same result, when combined with Taylor's theorem. From eq. (4.4) we can write (4.5) more completely:

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} = \frac{y\left(x_{i+1}\right) - y\left(x_i\right)}{\Delta x} - \frac{1}{3!}\left.\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right|_{x_{i+\frac{1}{2}}}\left(\frac{\Delta x}{2}\right)^2 + O\left(\Delta x^4\right) \tag{4.31}$$

We can then apply eq. (4.14) to estimate the third derivative:

$$\begin{aligned}
\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_{i+\frac{1}{2}}} &= \frac{y_{i+1} - y_i}{\Delta x} - \frac{\Delta x^2}{24}\frac{y_{i+2} - 3y_{i+1} + 3y_i - y_{i-1}}{\Delta x^3} + O\left(\Delta x^4\right) \\
&= \frac{24y_{i+1} - 24y_i - y_{i+2} + 3y_{i+1} - 3y_i + y_{i-1}}{24\Delta x} \\
&= \frac{y_{i-1} - 27y_i + 27y_{i+1} - y_{i+2}}{24\Delta x} + O\left(\Delta x^4\right)
\end{aligned} \tag{4.32}$$