DIFFERENCE FORMULAS

Centered formulas for unequally spaced meshes

First, expand in a Taylor series' about the point *i*:

$$f_{i+1} = f_i + \left(\frac{\partial f}{\partial x}\right)_i \Delta x_+ + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_+^2 + O(\Delta x_+)^3 \tag{1}$$

$$f_{i-1} = f_i - \left(\frac{\partial f}{\partial x}\right)_i \Delta x_- + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_-^2 + O(\Delta x_-)^3 \tag{2}$$

First derivative

Multiplying equation (1) by Δx_-^2 and equation (2) by Δx_+^2, and subtracting, gives

$$f_{i+1}\Delta x_-^2 - f_{i-1}\Delta x_+^2 = f_i(\Delta x_-^2 - \Delta x_+^2) + \left(\frac{\partial f}{\partial x}\right)_i \Delta x_- \Delta x_+ (\Delta x_- + \Delta x_+) + O(\Delta x_+)^5$$

Therefore,

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i = \frac{f_{i+1}\Delta x_-^2 - f_i(\Delta x_-^2 - \Delta x_+^2) - f_{i-1}\Delta x_+^2}{\Delta x_+ \Delta x_- (\Delta x_+ + \Delta x_-)} + O(\Delta x)^2 \qquad (3)}$$

Second derivative

Multiplying equation (1) by Δx_- and equation (2) by Δx_+, and adding, gives

$$f_{i+1}\Delta x_- + f_{i-1}\Delta x_+ = f_i(\Delta x_- + \Delta x_+) + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_- \Delta x_+ (\Delta x_+ + \Delta x_-) + O(\Delta x_+)^4$$

Therefore,

$$\boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i = 2\,\frac{f_{i+1}\Delta x_- - f_i(\Delta x_- + \Delta x_+) + f_{i-1}\Delta x_+}{\Delta x_+ \Delta x_- (\Delta x_+ + \Delta x_-)} + O(\Delta x) \qquad (4)}$$

The above equation becomes $O(\Delta x)^2$ as Δx_+ approaches Δx_-. To verify this, include third derivatives in equations (1) and (2).

One-sided formulas for equally spaced meshes

First, expand in a Taylor series' about the point *i*:

$$f_{i\pm 1} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i \Delta x + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x^3 + O(\Delta x)^4 \tag{5}$$

$$f_{i\pm 2} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i 2\Delta x + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i 4\Delta x^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i 8\Delta x^3 + O(\Delta x)^4 \tag{6}$$

$$f_{i\pm 3} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i 3\Delta x + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i 9\Delta x^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i 27\Delta x^3 + O(\Delta x)^4 \tag{7}$$

In the above equations, and in those to follow, the top sign is used at a lower boundary, and the bottom sign is used at an upper boundary.

First derivative

Multiplying equation (5) by 4, and subtracting equation (6), gives

$$4f_{i\pm 1} - f_{i\pm 2} = 3f_i \pm \left(\frac{\partial f}{\partial x}\right)_i 2\Delta x + O(\Delta x)^3$$

Therefore,

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i = \pm\frac{-3f_i + 4f_{i\pm 1} - f_{i\pm 2}}{2\Delta x} + O(\Delta x)^2} \tag{8}$$

Second derivative

Multiplying equation (5) by 2, and subtracting equation (6), gives

$$2f_{i\pm 1} - f_{i\pm 2} = f_i - \left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 \mp \left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x^3 + O(\Delta x)^4 \tag{9}$$

Multiplying equation (5) by 3, and subtracting equation (7), gives

$$3f_{i\pm 1} - f_{i\pm 3} = 2f_i - 3\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 \mp 4\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x^3 + O(\Delta x)^4 \tag{10}$$

Multiplying equation (9) by 4, and subtracting equation (10), gives

$$8f_{i\pm 1} - 4f_{i\pm 2} - 3f_{i\pm 1} + f_{i\pm 3} = 2f_i - \left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 + O(\Delta x)^4$$

Therefore,

$$\boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \frac{2f_i - 5f_{i\pm1} + 4f_{i\pm2} - f_{i\pm3}}{\Delta x^2} + O(\Delta x)^2 \qquad (11)}$$

One-sided formulas for unequally spaced meshes

First, expand in a Taylor series' about the point i:

$$f_{i\pm1} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i \Delta x_1 + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_1^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x_1^3 + O(\Delta x_1)^4 \qquad (12)$$

$$f_{i\pm2} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i (\Delta x_1 + \Delta x_2) + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i (\Delta x_1 + \Delta x_2)^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i (\Delta x_1 + \Delta x_2)^3 + O(\Delta x_1 + \Delta x_2)^4 \qquad (13)$$

$$f_{i\pm3} = f_i \pm \left(\frac{\partial f}{\partial x}\right)_i (\Delta x_1 + \Delta x_2 + \Delta x_3) + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i (\Delta x_1 + \Delta x_2 + \Delta x_3)^2 \pm \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i (\Delta x_1 + \Delta x_2 + \Delta x_3)^3$$
$$+ O(\Delta x_1 + \Delta x_2 + \Delta x_3)^4 \qquad (14)$$

where,

$$\Delta x_1 = |x_i - x_{i\pm1}|$$
$$\Delta x_2 = |x_{i\pm1} - x_{i\pm2}|$$
$$\Delta x_3 = |x_{i\pm2} - x_{i\pm3}|$$

First derivative

Multiplying equation (12) by $(\Delta x_1 + \Delta x_2)^2$ and equation (13) by Δx_1^2, and subtracting, gives

$$f_{i\pm1}(\Delta x_1 + \Delta x_2)^2 - f_{i\pm2}\Delta x_1^2 = f_i(2\Delta x_1 + \Delta x_2)\Delta x_2 \pm \left(\frac{\partial f}{\partial x}\right)_i \Delta x_1 \Delta x_2 (\Delta x_1 + \Delta x_2) + O(\Delta x)^5$$

Therefore,

$$\boxed{\left(\frac{\partial f}{\partial x}\right)_i = \frac{\mp f_i(2\Delta x_1 + \Delta x_2)\Delta x_2 \pm f_{i\pm1}(\Delta x_1 + \Delta x_2)^2 \mp f_{i\pm2}\Delta x_1^2}{\Delta x_1 \Delta x_2 (\Delta x_1 + \Delta x_2)} + O(\Delta x)^2 \qquad (15)}$$

Second derivative

Multiplying equation (12) by $(\Delta x_1 + \Delta x_2)$ and equation (13) by Δx_1, and subtracting, gives

$$f_{i\pm1}(\Delta x_1+\Delta x_2)-f_{i\pm2}\Delta x_1 = f_i\Delta x_2 - \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_1\Delta x_2(\Delta x_1+\Delta x_2)$$
$$\mp\frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x_1\Delta x_2(\Delta x_1+\Delta x_2)(2\Delta x_1+\Delta x_2)+O(\Delta x)^5 \tag{16}$$

Multiplying equation (12) by $(\Delta x_1+\Delta x_2+\Delta x_3)$ and equation (14) by Δx_1, and subtracting, gives

$$f_{i\pm1}(\Delta x_1+\Delta x_2+\Delta x_3)-f_{i\pm3}\Delta x_1 = f_i(\Delta x_2+\Delta x_3) - \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x_1(\Delta x_2+\Delta x_3)(\Delta x_1+\Delta x_2+\Delta x_3)$$
$$\mp\frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x_1(\Delta x_2+\Delta x_3)(\Delta x_1+\Delta x_2+\Delta x_3)(2\Delta x_1+\Delta x_2+\Delta x_3)$$
$$+O(\Delta x)^5 \tag{17}$$

Now, let $\Delta x_2 = a\Delta x_1$ and $\Delta x_3 = b\Delta x_1$. We can then rewrite equations (16) and (17) as

$$f_{i\pm1}(1+a)\Delta x_1 - f_{i\pm2}\Delta x_1 = f_i a\Delta x_1 - \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i a(1+a)\Delta x_1^3$$
$$\mp\frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i a(1+a)(2+a)\Delta x_1^4+O(\Delta x)^5 \tag{18}$$

$$f_{i\pm1}(1+a+b)\Delta x_1 - f_{i\pm3}\Delta x_1 = f_i(a+b)\Delta x_1 - \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i (a+b)(1+a+b)\Delta x_1^3$$
$$\mp\frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i (a+b)(1+a+b)(2+a+b)\Delta x_1^4+O(\Delta x)^5 \tag{19}$$

Multiplying equation (18) by $(a+b)(1+a+b)(2+a+b)$ and equation (19) by $a(1+a)(2+a)$, and subtracting, gives

$$f_{i\pm1}b(1+a)(1+a+b)(2+2a+b)\Delta x_1 - f_{i\pm2}(a+b)(1+a+b)(2+a+b)\Delta x_1 + f_{i\pm3}a(1+a)(2+a)\Delta x_1 =$$
$$f_i ab(a+b)(3+2a+b)\Delta x_1 - \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i ab(1+a)(a+b)(1+a+b)\Delta x_1^3 + O(\Delta x)^5$$

Therefore,

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \Big[f_i ab(a+b)(3+2a+b) - f_{i\pm1} b(1+a)(1+a+b)(2+2a+b) + f_{i\pm2}(a+b)(1+a+b)(2+a+b)$$

$$- f_{i\pm3} a(1+a)(2+a)\Big]\left[\frac{1}{2} ab(1+a)(a+b)(1+a+b)\Delta x_1^2\right]^{-1} + O(\Delta x)^2 \quad (20)$$