0.1 Numerical grid

The numerical grid is the basic tool of most numerical models. In this approach a function is tabulated on an equally spaced lattice in the domain $x = [x_{min}, x_{max}]$ with a fixed lattice spacing h. The grid points are characterized by an index $i = [0, N_{grid} - 1]$ (C language convention).

$$x_i = x_{min} + ih \tag{1}$$

$$h = \frac{(x_{max} - x_{min})}{N_{grid} - 1} \tag{2}$$

The function f(x) is then tabulated on the lattice

$$f_i = f(x_i) \tag{3}$$

0.2 Differentiation - Finite Difference

First write Taylor series expansions centered at x_i on the lattice:

$$f(x_i + h) = f(x_i) + h\frac{df}{dx} + \frac{h^2}{2}\frac{d^2f}{dx^2}$$
(4)

$$f(x_i) = f(x_i) \tag{5}$$

$$f(x_i - h) = f(x_i) - h\frac{df}{dx} + \frac{h^2}{2}\frac{d^2f}{dx^2}$$
(6)

From these, one derives the forward and backward first derivative formula of order O(h) (terms in h^2 neglected)

$$\frac{df}{dx} = \frac{f(x_i + h) - f(x_i)}{h} = \frac{f_{i+1} - f_i}{h}$$
(7)

$$\frac{df}{dx} = \frac{f(x_i) - f(x_i - h)}{h} = \frac{f_i - f_{i-1}}{h}$$
(8)

and the symmetric formula of order $O(h^2)$

$$\frac{df}{dx} = \frac{f(x_i + h) - f(x_i - h)}{2h} = \frac{f_{i+1} - f_{i-1}}{2h} \tag{9}$$

The second derivative formula of order $O(h^2)$ is similarly derived by combining the Taylor series expansions:

$$\frac{d^2f}{dx^2} = \frac{f(x_i+h) - 2f(x_i) + f(x_i-h)}{h^2} = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \tag{10}$$