

Formulae for Numerical Derivatives

A. BACKWARD DIFFERENCING

1. First order formulae

$$\begin{aligned} f'_i &= \frac{1}{h}(f_i - f_{i-1}) + O(h) \\ f''_i &= \frac{1}{h^2}(f_i - 2f_{i-1} + f_{i-2}) + O(h) \\ f'''_i &= \frac{1}{h^3}(f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}) + O(h) \\ f^{(4)}_i &= \frac{1}{h^4}(f_i - 4f_{i-1} + 6f_{i-2} - 4f_{i-3} + f_{i-4}) + O(h) \end{aligned}$$

2. Second order formulae

$$\begin{aligned} f'_i &= \frac{1}{2h}(3f_i - 4f_{i-1} + f_{i-2}) + O(h^2) \\ f''_i &= \frac{1}{h^2}(2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}) + O(h^2) \\ f'''_i &= \frac{1}{2h^3}(5f_i - 18f_{i-1} + 24f_{i-2} - 14f_{i-3} + 3f_{i-4}) + O(h^2) \\ f^{(4)}_i &= \frac{1}{h^4}(3f_i - 14f_{i-1} + 26f_{i-2} - 24f_{i-3} + 11f_{i-4} - 2f_{i-5}) + O(h^2) \end{aligned}$$

B. FORWARD DIFFERENCING

1. First order formulae

$$\begin{aligned} f'_i &= \frac{1}{h}(f_{i+1} - f_i) + O(h) \\ f''_i &= \frac{1}{h^2}(f_{i+2} - 2f_{i+1} + f_i) + O(h) \\ f'''_i &= \frac{1}{h^3}(f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i) + O(h) \\ f^{(4)}_i &= \frac{1}{h^4}(f_{i+4} - 4f_{i+3} + 6f_{i+2} - 4f_{i+1} + f_i) + O(h) \end{aligned}$$

2. Second order formulae

$$\begin{aligned} f'_i &= \frac{1}{2h}(-f_{i+2} + 4f_{i+1} - 3f_i) + O(h^2) \\ f''_i &= \frac{1}{h^2}(-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i) + O(h^2) \\ f'''_i &= \frac{1}{2h^3}(-3f_{i+4} + 14f_{i+3} - 24f_{i+2} + 18f_{i+1} - 5f_i) + O(h^2) \\ f^{(4)}_i &= \frac{1}{h^4}(-2f_{i+5} + 11f_{i+4} - 24f_{i+3} + 26f_{i+2} - 14f_{i+1} + 3f_i) + O(h^2) \end{aligned}$$

C. CENTRAL DIFFERENCING

1. Second order formulae

$$\begin{aligned}
 f'_i &= \frac{1}{2h}(f_{i+1} - f_{i-1}) + O(h^2) \\
 f''_i &= \frac{1}{h^2}(f_{i+1} - 2f_i + f_{i-1}) + O(h^2) \\
 f'''_i &= \frac{1}{2h^3}(f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}) + O(h^2) \\
 f^{(4)}_i &= \frac{1}{h^4}(f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}) + O(h^2)
 \end{aligned}$$

2. Fourth order formulae

$$\begin{aligned}
 f'_i &= \frac{1}{12h}(-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}) + O(h^4) \\
 f''_i &= \frac{1}{12h^2}(-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}) + O(h^4) \\
 f'''_i &= \frac{1}{8h^3}(-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3}) + O(h^4) \\
 f^{(4)}_i &= \frac{1}{6h^4}(-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3}) + O(h^4)
 \end{aligned}$$