

Finite Difference Approximation of Higher Derivatives

One can also use the Taylor series to approximate a higher order derivative. For example, to approximate $f''(x)$, the Taylor series is

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2\Delta x) + \frac{f''(x_i)}{2!}(2\Delta x)^2 + \frac{f'''(x_i)}{3!}(2\Delta x)^3 + \dots (3)$$

where

$$x_{i+2} = x_i + 2\Delta x,$$

and

$$f(x_{i+1}) = f(x_i) + f'(x_i)(\Delta x) + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 \dots (4)$$

where

$$x_{i+1} = x_i + \Delta x.$$

Subtracting 2 times Equation (4) from Equation (3) gives

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)(\Delta x)^3 \dots$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} - f'''(x_i)(\Delta x) + \dots$$

$$f''(x_i) \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} + O(\Delta x) \quad (5)$$