Lecture 35

- Approximation of derivatives

(1) Taylor's series to build higher order derivatives (assuming uniform discretization)

Table 21.3 $\quad (x_i, x_{i+1}, \dots)$

$x_i \quad x_{i+1}$

- $$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$
- $$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$
- $$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$
- $$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) - f(x_i)}{h^2} + O(h^2)$$

→ forward difference

Table 21.4

- $$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$
- $$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2)$$
- $$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + O(h)$$
- $$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) + f(x_{i-3})}{h^2} + O(h^2)$$

backward difference

(2) Richardson's Extrapolation

$D[h] \rightarrow f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$

$x_{i+1} - x_i = h = x_{i+2} - x_{i+1}$

$D[h/2] \rightarrow$ same formula but

$x_{i+1} - x_i = h/2 = x_{i+2} - x_{i+1}$

$I[h_1], \quad I[h_2]$

$I \approx I[h_2] + \dfrac{I[h_2] - I[h_1]}{\frac{h_1^2}{h_2^2} - 1}$

$I = I[h_1] + E[h_1]$

$= I[h_2] + E[h_2]$

$E[h_1] = C\, h_1^2$

$E[h_2] = C\, h_2^2$

$D \approx \frac{4}{3} D[h/2] - \frac{1}{3} D[h] \longrightarrow O(h^4)$

(3) Using interpolation

- Not restricted to uniform discretization
- Provides derivative function that can be evaluated at any point in the interval

Example : (A) Linear interpolation

$(x_i, f_i = f(x_i)), \quad (x_{i+1}, f_{i+1} = f(x_{i+1}))$

model $\quad \hat{f}(x) = Z(x)\, a$

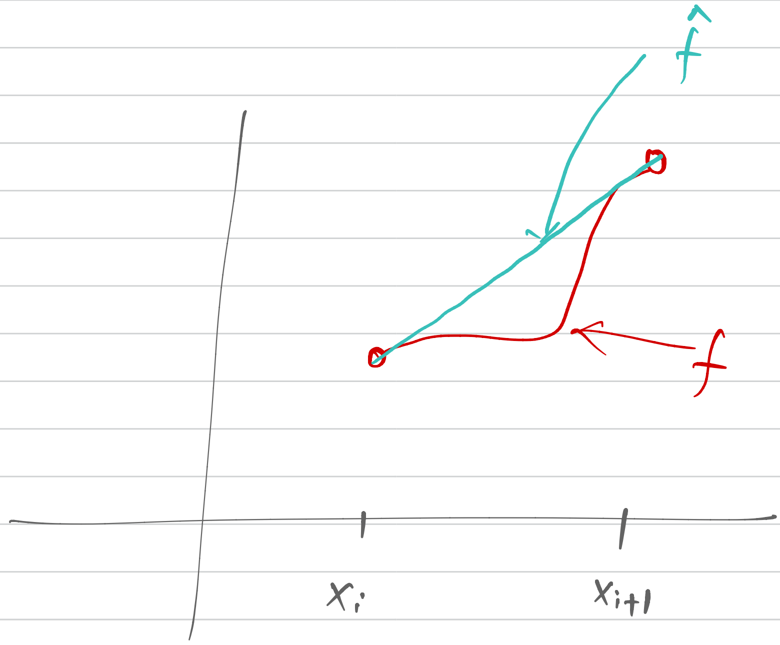
$$a = \begin{bmatrix} f_i \\ f_{i+1} \end{bmatrix}, \qquad z = [L_1(x), \quad L_2(x)]$$

$$L_1(x) = \frac{(x - x_{i+1})}{(x_i - x_{i+1})}, \quad L_2(x) = \frac{(x - x_i)}{(x_{i+1} - x_i)}$$

Compute

$f'(x_i)$, $f'(x_{i+1})$

$$\approx \frac{d\hat{f}}{dx}(x_i), \quad \approx \frac{d\hat{f}}{dx}(x_{i+1})$$



$$f'(x) \approx \frac{d\hat{f}}{dx}(x)$$

at any $x \in [x_i, x_{i+1}]$

$$\frac{d\hat{f}}{dx}(x) = \left[\frac{dL_1}{dx}(x), \quad \frac{dL_2}{dx}(x)\right] a$$

$$\hat{f}(x) = [L_1(x), L_2(x)]\, a$$

$$\Rightarrow \boxed{\frac{d\hat{f}}{dx}(x) = \left[\frac{-1}{x_{i+1} - x_i}, \quad \frac{1}{x_{i+1} - x_i}\right] a}$$

(B) Quadratic interpolation

$(x_i, f_i = f(x_i))$, (x_{i+1}, f_{i+1}), (x_{i+2}, f_{i+2})

model

$$\hat{f}(x) = z(x)\, a$$

$$a = \begin{bmatrix} f_i \\ f_{i+1} \\ f_{i+2} \end{bmatrix}, \quad Z(x) = [L_1(x), L_2(x), L_3(x)]$$

$$L_1(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})}$$

$$L_2(x) = \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}$$

$$L_3(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}$$

$$\frac{df}{dx}(x) \approx \frac{d\hat{f}}{dx}(x) = \frac{dZ}{dx}(x)\, a$$

$$= \left[\frac{dL_1}{dx}(x), \frac{dL_2}{dx}(x), \frac{dL_3}{dx}(x)\right] a$$

$$\frac{d^2 f}{dx^2}(x) \approx \frac{d^2\hat{f}}{dx^2}(x) = \left[\frac{d^2L_1}{dx^2}(x), \frac{d^2L_2}{dx^2}(x), \frac{d^2L_3}{dx^2}(x)\right] a$$

Numerically solving ordinary differential equations

- **Order of ODE**

$$\frac{dy}{dt} = f(t, y(t)) \quad 1^{st} \text{ order ODE}$$

$$\frac{d^2y}{dt^2} = f\left(t, y(t), \frac{dy}{dt}\right) \quad 2^{nd} \text{ order ODE}$$

- **Linear / Nonlinear ODE**

$$a\frac{d^2y}{dt^2} + b\frac{dy}{dt} + cy = d$$

$$\underbrace{\text{if } a, b, c, d \text{ do not depend on } y, \frac{dy}{dt}, \frac{d^2y}{dt^2}}_{\downarrow}$$

Linear ODE

$$\underbrace{\text{if any of } a, b, c, d \text{ depend on } \left(y, \frac{dy}{dt}, \frac{d^2y}{dt^2}\right)}_{\downarrow}$$

nonlinear ODE

- **Conditions**

(i) IVP (Initial value problem)

Examples

- $\frac{dy}{dt} = f(t, y(t)) \Rightarrow y(0) = y_0$

- $$\frac{d^2y}{dt^2} = f\left(t, y(t), \frac{dy}{dt}(t)\right) \Rightarrow \begin{array}{l} y(0) = y_0 \\ \frac{dy}{dt}(0) = \dot{y}_0 \end{array}$$

(ii) BVP (Boundary value Problem)

Examples :

$$\frac{d^2y}{dt^2} = f\left(t, y, \frac{dy}{dt}\right) \Rightarrow \begin{array}{l} y(t=0) = y_0 \\ y(t=L) = y_L \end{array}$$