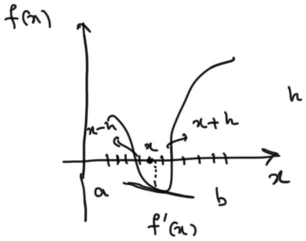
Numerical differentiation and integration :

Approximation of function derivatives using finite differences :

$f : [a,b] \longrightarrow \mathbb{R}$



$h = x_n - x_{n-1}$

$\xrightarrow{\text{recall}}$ Taylor series

• Forward finite difference :

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h}$$

$$f(x+h) = f(x) + \frac{f'(x)}{1!}h + \overbrace{\frac{f''(\xi)}{2!}h^2}^{\Theta(h^2)} \quad , \ (1)$$

where ξ is some point between $[x, x+h]$

$$\Rightarrow \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{f.d approx.}} - \underbrace{f'(x)}_{\text{exact}} = \underbrace{\frac{h}{2} f''(\xi)}_{\text{error}}$$

1^{st}-order approxima

• Backward finite difference ;

$$(2) \quad f(x-h) = f(x) - h f'(x) + \underbrace{\frac{h^2}{2} f''(\xi)} \longrightarrow \frac{df}{dx} \approx \frac{f(x) - f(x-h)}{h}$$

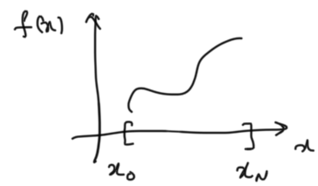
$$f(x+h) - f(x-h) = 2h f'(x) + 2\frac{h^3}{3!} f'''(\xi)$$

$$\Rightarrow \frac{f(x+h) - f(x-h)}{2h} - f'(x) = \frac{h^2}{3!} f'''(\xi)$$

• Centered difference approximation : $\boxed{\frac{df}{dx} \approx \frac{f(x+h) - f(x-h)}{2h}}$

2^{nd}-order accurate approximati

(*) What happens at the endpoints of the domain ?



$$\begin{cases} \left.\frac{df}{dx}\right|_{x=x_0} \approx \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] \\ \left.\frac{df}{dx}\right|_{x=x_n} \approx \frac{1}{2h}\left[3f(x_N) - 4f(x_{N-1}) + f(x_{N-2})\right] \end{cases}$$

(*) Adding more neighbors results in higher-order accurate schemes! Using all neighbors results in so-called "spectral methods" that have exponential convergence rates.

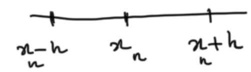
• Second order-derivatives :

Central difference approximation : $\frac{d^2f}{dx^2} \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$

n $\qquad \mathcal{O}(h^2)/2^{n\ldots}$ accurate

- Stencil rules for implementation :

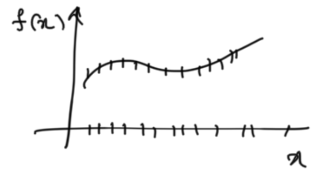
  - centered diff. approx. for $\frac{df}{dx}$:



$$\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & & 0 \\ -1 & 0 & 1 & \cdots & & 0 \\ 0 & -1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & -1 & 0 & 1 \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & & -1 & 0 & 1 \\ 0 & \cdots & & -1 & -4 & 3 \end{bmatrix}\begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N-1}) \\ f(x_N) \end{bmatrix} = \begin{bmatrix} \left.\frac{df}{dx}\right|_{x_0} \\ \vdots \\ \left.\frac{df}{dx}\right|_{x_N} \end{bmatrix}$$

circulant matrix $(N+1)(N+1)$ $\qquad (N+1)\times 1$ $\qquad (N+1)\times 1$

$$\left.\frac{df}{dx}\right|_{x=x_1} \approx \frac{f(x_2) - f(x_0)}{2h}$$

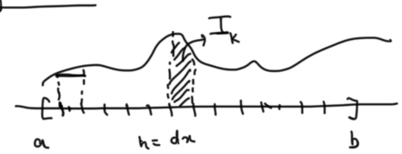


  - Centered f.d. approx. for $\frac{d^2f}{dx^2}$

$$\begin{bmatrix} 1 & -2 & 1 & \cdots & & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & 0 \\ 0 & & & 1 & -2 & 1 \end{bmatrix}\begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-1}) \\ f(x_N) \end{bmatrix} = \begin{bmatrix} \left.\frac{d^2f}{dx^2}\right|_{x_1} \\ \vdots \\ \left.\frac{d^2f}{dx^2}\right|_{x_{n-1}} \end{bmatrix}$$

Numerical Integration :

$$I(f) = \int_a^b f(x)\,dx, \quad x \in [a,b]$$



M : # of int

- Midpoint rule : $I(f) \approx \sum_{k=1}^{M} \underbrace{\int_{I_k} f(x)\,dx}$

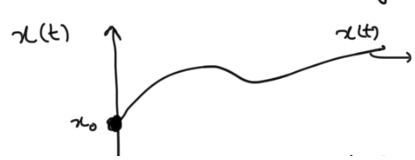
goal : discretize/evaluate

Constant polynomial approximation of $f(x)$ at the midpoint :

$$\bar{x}_k = \frac{x_{k-1} - x_k}{2}, \quad I^c_{mp}(f) = h\sum_{k=1}^{M} f(\bar{x}_k)$$

Solving ordinary differential equations via numerical integration

$$\frac{dx}{dt} = \underbrace{f(x,t)}, \quad \underbrace{x(t_0) = x_0}_{\text{initial}}$$



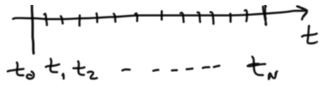
goal : com

$x(t)$

IVP

known forcing function / dynamics

condition



Solution :

$$x(t) = x(t_0) + \underbrace{\int_{t_0}^{t_N} f(x(\tau),\tau)\,d\tau}_{\text{goal : approximate this integral.}}$$

1.) Euler method :

$$\underline{\underline{x(t_1)}} = \underbrace{x(t_0)}_{x_0} + \int_{t_0}^{t_1} f(x(\tau),\tau)\,d\tau \approx \underline{\underline{x_0}} + \underbrace{(t_1 - t_0)}_{\Delta t} f(x_0, t_0)$$

$$\xrightarrow[\text{general}]{\text{in}} \quad x_{n+1} = x_n + \Delta t\, f(x_n, t_n)$$

2.) Trapezoidal rule :

$$x_{n+1} = x_n + \frac{\Delta t}{2}\left[f(x_n, t_n) + f(x_{n+1}, t_{n+1}) \right]$$

- Notice how x_{n+1} appears in both sides of the equation (possibly in a non-li fashion

$\Rightarrow$ In order to calculate x_{n+1} we need to solve a linear / non-linear systei

3.) Runge-Kutta method (4th-order) :

$$x_{n+1} = x_n + \underbrace{\int_{t_n}^{t_{n+1}} f(x(\tau),\tau)\,d\tau}$$

Update rule :

$$K_1 = f(x_n, t_n)$$

$$K_2 = f\left(x_n + K_1 \frac{\Delta t}{2},\ t_n + \frac{\Delta t}{2}\right)$$

$$K_3 = f\left(x_n + K_2 \frac{\Delta t}{2},\ t_n + \frac{\Delta t}{2}\right)$$

$$K_4 = f(x_n + K_3 \Delta t,\ t_n + \Delta t)$$

$$x_{n+1} = x_n + \Delta t\left(\frac{1}{6}K_1 + \frac{1}{3}K_2 + \frac{1}{3}K_3 + \frac{1}{6}K_4\right)$$

SS

$$\int_{t_n}^{t_{n+1}} \underline{\underline{f}}(x(\tau),\tau)\,d\tau$$