Week 2 : Finite-Difference Method

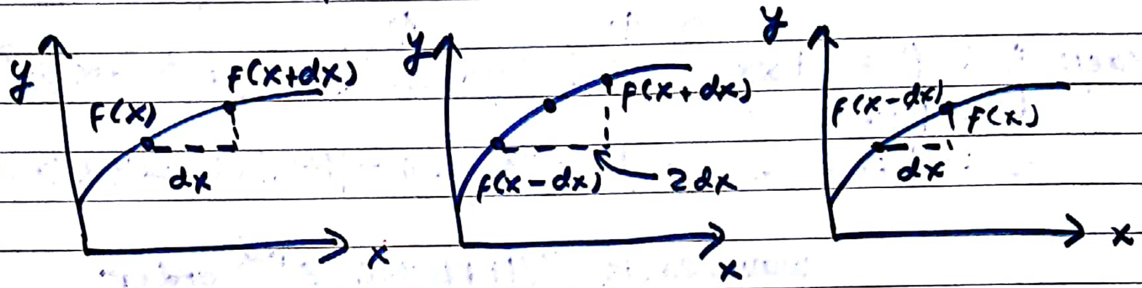
Date

Definitions of a derivative :

① $\frac{df}{dx} = \lim_{dx\to 0} \frac{f(x+dx)-f(x)}{dx} \rightarrow \frac{df}{dx} \overset{\text{forward}}{\approx} \frac{f(x+dx)-f(x)}{dx}$

② $\frac{df}{dx} = \lim_{dx\to 0} \frac{f(x+dx)-f(x-dx)}{2dx} \rightarrow \frac{df}{dx} \overset{\text{centered}}{\approx} \frac{f(x+dx)-f(x-dx)}{2dx}$

③ $\frac{df}{dx} = \lim_{dx\to 0} \frac{f(x)-f(x-dx)}{dx} \rightarrow \frac{df}{dx} \overset{\text{backward}}{\approx} \frac{f(x)-f(x-dx)}{dx}$



Forward FD Centred FD Backward FD

these three definitions (techniques) of FD gives DIFFERENT RESULTS

★ Taylor series

$$f(x+dx) = f(x) + \partial_x f\, dx + \frac{1}{2!}\partial_x^2 f\, dx^2 + \frac{1}{3!}\partial_x^3 f\, dx^3 + \dots$$

$$= \boxed{\sum_{n=0}^{\infty} \frac{1}{n!}\partial_x^n f\, dx^n}$$

Example: $f(x) = \cos x \approx 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} + \dots$

$$f(x) = e^x \approx \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$\frac{f(x+dx)-f(x)}{dx} = \partial_x f + \frac{1}{2!}\partial_x^2 f\, dx + \frac{1}{3!}\partial_x^3 f\, dx^2 + \dots$$

$$= f' + \frac{1}{2!}f''\, dx + \frac{1}{3!}f'''\, dx^2 + \dots$$

$O(dx)$ First order term

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$$\frac{f(x+dx)-f(x)}{dx} = f' + \frac{1}{2!} f''\,dx + \frac{1}{3!} f'''\,dx^2 + \cdots$$

$$\frac{f(x+dx)-f(x)}{dx} = f' + O(dx)$$

Example: $\dfrac{f(x+dx)-f(x-dx)}{2dx} = f'(x) + O(?) \nearrow$ determine with Taylor series

$$f(x+dx) = f(x) + f'\,dx + \frac{1}{2!} f''\,dx^2 + \frac{1}{3!} f'''\,dx^3 + \cdots$$

$$f(x+(-dx)) = f(x) + f'(-dx) + \frac{1}{2!} f''(-dx)^2 + \frac{1}{3!} f'''(-dx)^3 + \cdots$$

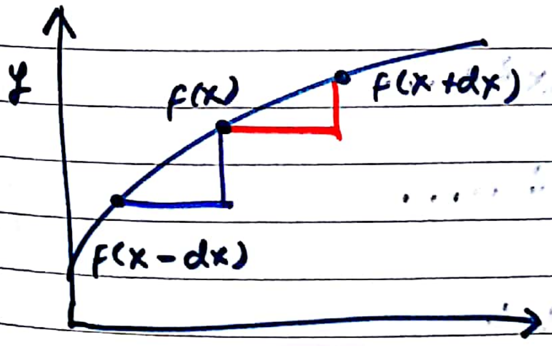
$$f(x-dx) = f(x) - f'\,dx + \frac{1}{2!} f''\,dx^2 - \frac{1}{3!} f'''\,dx^3 + \cdots$$

$$f(x+dx) - f(x-dx) = 2f'\,dx + \frac{2}{3!} f'''\,dx^3 + \cdots$$

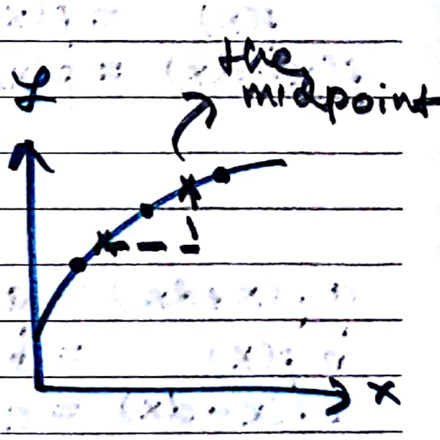
$$\frac{f(x+dx)-f(x-dx)}{2dx} = f' + \frac{1}{3!} f'''\,dx^2$$

$$\frac{f(x+dx)-f(x-dx)}{2dx} = f' + \underline{\underline{O(dx^2)}}$$

Second order derivative



$$\frac{\frac{df}{dx} - \frac{df}{dx}}{dx} = \frac{d^2 f}{dx^2}$$



$$f'' \approx \frac{\dfrac{f(x+dx)-f(x)}{dx} - \dfrac{f(x)-f(x-dx)}{dx}}{dx}$$

$$\boxed{f'' \approx \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}}$$

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Calculate the order of the error of the 2^{nd} derivative :

$$\frac{d^2f}{dx^2} \approx \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}$$

$$f(x+dx) = \cancel{f(x)} + \cancel{f'dx} + \frac{1}{2!} f'' dx^2 + \cancel{\frac{1}{3!} f''' dx^3} + \dots$$

$$f(x-dx) = \cancel{f(x)} - \cancel{f'dx} + \frac{1}{2!} f'' dx^2 - \cancel{\frac{1}{3!} f''' dx^3} + \dots$$

$$\cancel{-2f(x)}$$

$$= \frac{1}{2!} f'' dx^2 + \frac{1}{4!} f^{(4)} dx^4 + \dots$$

$$\frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2} = \frac{1/2\, f'' dx^2 + 1/4!\, f^{(4)} dx^4 + \dots}{dx^2}$$

$$\frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2} \approx \frac{1}{2!} f'' + \underbrace{\frac{1}{4!} f^{(4)} dx^2}_{O(dx^2)}$$

second order

* Operators

Taylor series :

$$f(x+dx) = f(x) + f'(x)\, dx + \frac{1}{2!} f''(x)\, dx^2 + \dots$$

$$f(x) = f(x)$$

$$f(x-dx) = f(x) - f'(x) dx + \frac{1}{2!} f''(x)\, dx^2 - \dots$$

$\downarrow$ multiplied by a, b, c

$$a f(x+dx) = a\left[f(x) + f'(x)\, dx + \frac{1}{2!} f''(x) dx^2 + \dots\right]$$

$$b f(x) = b\left[f(x)\right]$$

$$c f(x-dx) = c\left[f(x) - f'(x)\, dx + \frac{1}{2!} f''(x) dx^2 + \dots\right]$$

$$a f(x+dx) + b f(x) + c f(x-dx) \approx f(x)[a+b+c] + dx\, f'(x)\,[a-c] + \frac{1}{2!} dx^2 f''(x)\,[a+c]$$

$$a f(x+dx) + b f(x) + c\, f(x-dx) = f(x)[a+b+c] + dx\, f'(x)[a-c] + \frac{1}{2!} dx^2 f''(x)[a+c]$$

if $\boxed{\begin{aligned} a+b+c &= 0 \\ a+c &= 0\ ;\ a-c = 1/dx \end{aligned}}$

then $a f(x+dx) + b f(x) + c f(x-dx) \approx dx\, f'(x)[a-c]$

$$\left.\begin{aligned} a+b+c &= 0 \\ a \quad -c &= 1/dx \\ a \quad +c &= 0 \end{aligned}\right\} \text{into matrix}$$

$$\downarrow$$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 1/dx \\ 0 \end{pmatrix}$$

$$A \quad w = s$$

$$\downarrow$$

$$w = A^{-1} s$$

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 & 0.5 & 0.5 \\ 1 & 0 & -1 \\ 0 & -0.5 & 0.5 \end{pmatrix} \begin{pmatrix} 0 \\ 1/dx \\ 0 \end{pmatrix}$$

$$\downarrow$$

$$\boxed{a = 1/2dx}\ ;\ \boxed{b = 0}\ ;\ \boxed{c = -1/2dx}$$

for the 1st derivative

$$f'(x) \approx \frac{f(x+dx) - f(x-dx)}{2dx}.$$

central finite-difference approximation.

For 2nd Derivative:

$$\left.\begin{aligned} a+b+c &= 0 \\ a \quad -c &= 0 \\ a \quad +c &= \frac{2!}{dx^2} \end{aligned}\right\} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2/dx^2 \end{pmatrix}$$

$$\downarrow$$

$$\boxed{\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \frac{1}{dx^2} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}}$$

$$\Downarrow$$

$$f''(x) = \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}$$

Practice : known 2 equations

$f(x) = f(x) \quad \dots ①$

$f(x+dx) = f(x) + f'dx + O(dx^2) \quad \dots ②$

multiply ① by a : $af(x) = af(x)$

multiply ② by b : $bf(x+dx) = [f(x) + f'dx + O(dx^2)]\, b$

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$af(x) + bf(x+dx) = af(x) + bf(x) + bf'dx + bO(dx^2)$

$af(x) + bf(x+dx) = f(x)[a+b] + f'dx[b] + \underbrace{O(dx^2)[b]}_{\text{neglected}}$

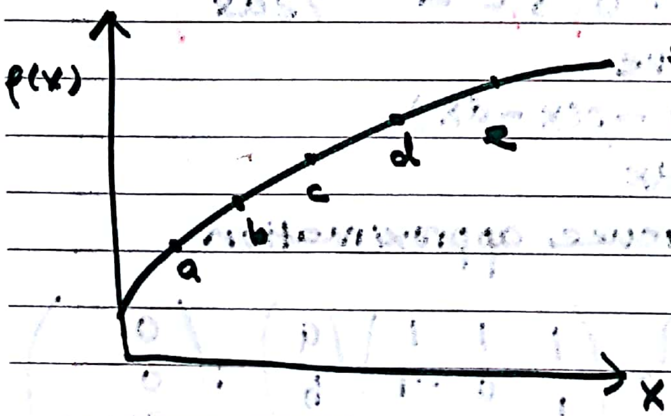
$$\left.\begin{array}{r} a+b=0 \\ b = 1/dx \end{array}\right\} \boxed{\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ dx \end{bmatrix}} \text{ matrix result}$$

$a = -\frac{1}{dx} \; ; \; b = \frac{1}{dx}$

* **High-order Operators**

2nd derivative

5-point operator



$a = f(x-2dx)$

$b = f(x-dx)$

$c = f(x)$

$d = f(x+dx)$

$e = f(x+2dx)$

$$* f(x+2dx) = f(x) + \overbrace{f'(x)(2dx)}^{2f'(x)\,dx} + \frac{1}{2!}f''(x)(2dx)^2 + \frac{1}{3!}f'''(x)(2dx)^3 + \frac{1}{4!}f^{(4)}(x)(2dx)^4 + \dots$$

$$* f(x+dx) = f(x) + f'(x)(dx) + \frac{1}{2!}f''(x)(dx)^2 + \frac{1}{3!}f'''(x)(dx)^3 + \frac{1}{4!}f^{(4)}(x)(dx)^4 + \dots$$

* $f(x) = f(x)$

* $f(x-dx) = f(x) - f'(x)\,dx + \frac{1}{2!} f''(x)\,dx^2 - \frac{1}{3!} f'''(x)\,dx^3 + \frac{1}{4!} f^{(4)}(x)\,dx^4 + \dots$

* $f(x-2dx) = f(x) - f'(x)2dx + \frac{1}{2!} f''(x)(2dx)^2 - \frac{1}{3!} f'''(x)(2dx)^3 + \frac{1}{4!} f^{(4)}(x)(2dx)^4 + \dots$

multiply each equation by a, b, c, d, e, then sum them up. (neglecting high-order term) Up To 4th order.

$$\Rightarrow f''(x) \approx a\,f(x+2dx) + b\,f(x+dx) + c\,f(x) + d\,f(x-dx) + e\,f(x-2dx)$$

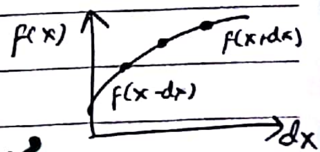
into matrix :

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & -1 & -2 \\ 4 & 1 & 0 & 1 & 4 \\ 8 & 1 & 0 & -1 & -8 \\ 16 & 1 & 0 & 1 & 16 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a \\ b \\ c \\ d \\ e \end{pmatrix}}_{W} = \underbrace{\begin{pmatrix} 0 \\ 0 \\ 2/dx^2 \\ 0 \\ 0 \end{pmatrix}}_{S} \begin{array}{l} \to f(x) \\ \to f'(x) \\ \to f''(x) \\ \to f'''(x) \\ \to f^{(4)}(x) \end{array}$$

Inversion

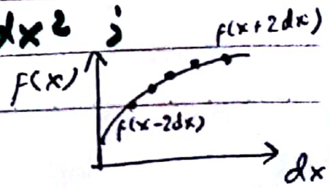
$\boxed{a = -\frac{1}{12dx^2}}$; $\boxed{b = \frac{4}{3dx^2}}$; $\boxed{c = -\frac{5}{2dx^2}}$; $\boxed{d = \frac{4}{3dx^2}}$; $\boxed{e = -\frac{1}{12dx^2}}$

SUMMARY : We have derived operators for 3-point and 5-point for 2nd derivative



3-point $\to$ $a = 1/dx^2$; $b = -2/dx^2$; $c = 1/dx^2$

5-point $\to$ $a = -1/12dx^2$; $b = 4/3dx^2$; $c = -5/dx^2$; $d = 4/3dx^2$; $e = -1/12dx^2$



① $a = 1/2$, $b = -1/2$

QUIZ ② $a = 1$, $b = -2$, $c = 1$

Date

③ Calculate FD operator for the 1st derivative using the values $f(x + dx/2)$ and $f(x - dx/2)$, thus

$$\frac{d}{dx} f(x) \approx a f(x + dx/2) + b f(x - dx/2)$$

Write down the Taylor series for the two points, omitting order ≥ 2. Multiply the first eq. with a and the second eq. with b, then sum up. Find a and b!

$$a \quad f(x + \tfrac{1}{2}dx) = \left[f(x) + f'(\tfrac{1}{2}dx) + \tfrac{1}{2!}f''(\tfrac{1}{2}dx)^2 + \dots\right] a$$

$$b \quad f(x - \tfrac{1}{2}dx) = \left[f(x) + f'(-\tfrac{1}{2}dx) + \tfrac{1}{2!}f''(-\tfrac{1}{2}dx)^2 + \dots\right] b$$

$$\Downarrow$$

$$a \quad f(x + \tfrac{1}{2}dx) = \left[f(x) + \tfrac{1}{2}f' dx + \tfrac{1}{8}f'' dx^2 + \dots\right] a$$

$$b \quad f(x - \tfrac{1}{2}dx) = \left[f(x) - \tfrac{1}{2}f' dx + \tfrac{1}{8}f'' dx^2 + \dots\right] b$$

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$$a f(x + \tfrac{1}{2}dx) + b f(x - \tfrac{1}{2}dx) = f(x)[a+b] + \tfrac{1}{2}f' dx[a-b] + \dots$$

$$\left.\begin{matrix} a + b = 0 \\ a - b = \frac{2}{dx} \end{matrix}\right\} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 2/dx \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}^{-1}\begin{bmatrix} 0 \\ 2/dx \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & -0.5 \end{bmatrix}\begin{bmatrix} 0 \\ 2/dx \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1/dx \\ -1/dx \end{bmatrix} \qquad \frac{1}{dx} \quad -\frac{1}{dx}$$

$\dots 1 = 0$

$-1 + -1 = -2$

$b = -a$

$a - (-a) = \frac{2}{dx}$

$2a = \frac{2}{dx}$

$a = 1$

$\Rightarrow \frac{1}{2} \cdot \frac{1}{4}$

$+ \dots \frac{1}{16}$

$2 + \dots$

$\dots (x a)$

$(x b)$

$' dx[a-b] + \frac{1}{8} f'' dx [a$

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 2/dx \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}^{-1}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & -0.5 \end{bmatrix}$$

$a = \frac{1}{dx}$

$b = -\frac{1}{dx}$