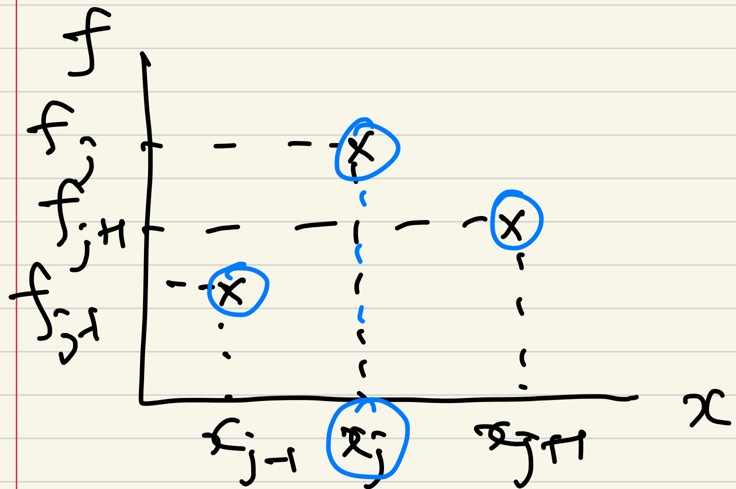
Ch 2. Numerical differentiation – finite difference

2.1 Construction of difference formulae using Taylor series



$(x_i, f_i) \rightarrow f_i'$

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Finite difference using Taylor series expansion

$$f(x_j + \Delta x) = f(x_j) + \Delta x\, f'(x_j) + \frac{1}{2}\Delta x^2 f''(x_j) + \frac{1}{6}\Delta x^3 f'''(x_j) + \cdots$$

$$\rightarrow \boxed{f'(x_j) = \frac{f(x_j+\Delta x) - f(x_j)}{\Delta x}} \underbrace{- \frac{1}{2}\Delta x\, f''(x_j)}_{\text{leading}} - \frac{1}{6}\Delta x^2 f'''(x_j) + \cdots$$

1st-order accurate finite difference (FD)

truncation error $O(\Delta x)$

$$\rightarrow \boxed{f_j' = \frac{f_{j+1} - f_j}{\Delta x}} + O(\Delta x)$$

forward 1st-order FD method

Similarly, $f(x_j - \Delta x) = f(x_j) - \Delta x\, f'(x_j) + \frac{1}{2}\Delta x^2 f''(x_j) - \cdots$

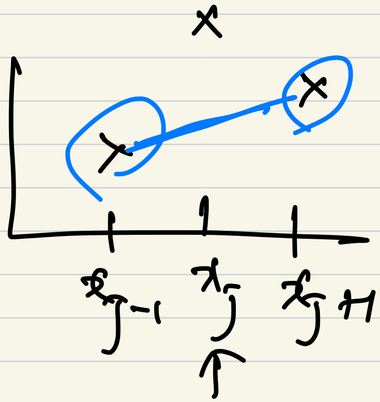
$$\rightarrow \boxed{f_j' = \frac{f_j - f_{j-1}}{\Delta x}} + O(\Delta x) \rightarrow \text{backward 1st-order FD method}$$

$\hookrightarrow + \frac{1}{2}\Delta x\, f''(x_j) - \frac{1}{6}\Delta x^2 f'''(x_j) + \cdots$

$f(x_j + \Delta x) = \cdots$

$+\ f(x_j - \Delta x) = \cdots$

$$\rightarrow \boxed{f_j' = \frac{f_{j+1} - f_{j-1}}{2\Delta x}} \underbrace{- \frac{1}{6}\Delta x^2 f_j''' + \cdots}_{O(\Delta x^2)}$$



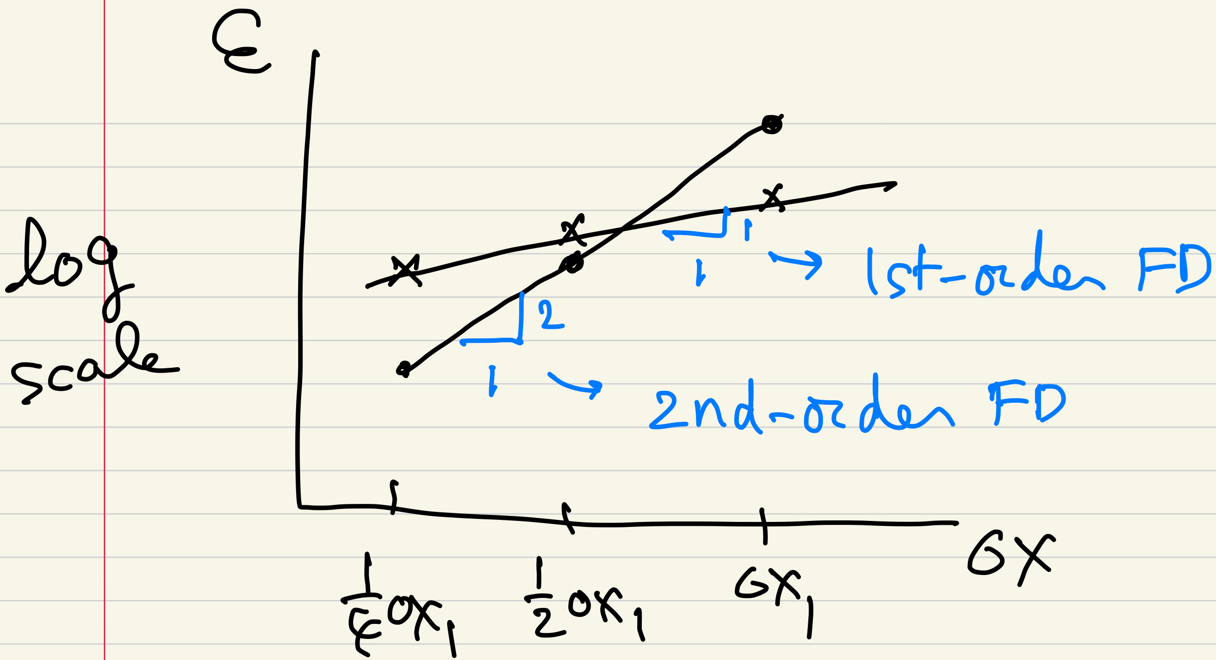
2nd-order central FD method (CD2)

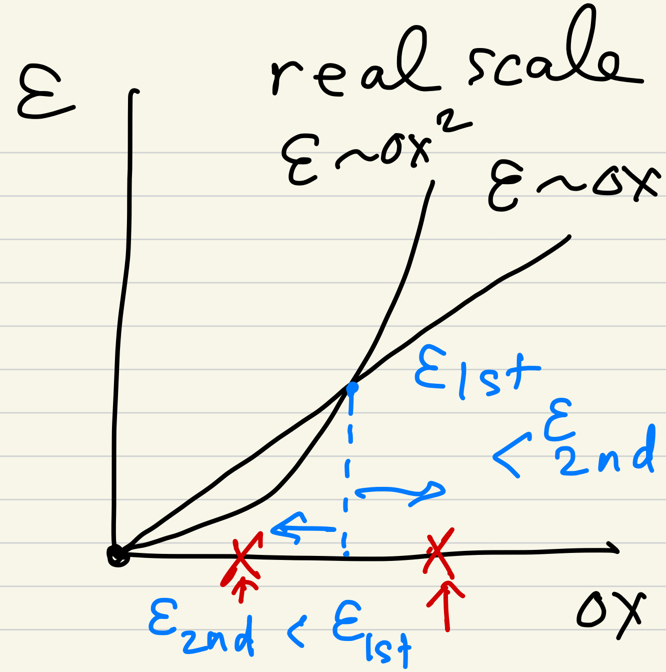
$$\left\{\begin{aligned} f_j' &= \frac{f_{j+1} - f_j}{\Delta x} - \frac{1}{2}\Delta x\, f_j'' + \cdots \\ f_j' &= \frac{f_j - f_{j-1}}{\Delta x} + \frac{1}{2}\Delta x\, f_j'' + \cdots \\ f_j' &= \frac{f_{j+1} - f_{j-1}}{2\Delta x} - \frac{1}{6}\Delta x^2 f_j''' + \cdots \end{aligned}\right.$$

ε

$\varepsilon \sim \Delta x \rightarrow \ln \varepsilon \sim \ln \Delta x$

$\varepsilon \sim \Delta x^2 \rightarrow \ln \varepsilon \sim 2 \ln \Delta x$





$$f_j' = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12\Delta x} + O(\Delta x^4) \qquad \underline{\text{CD4}}$$

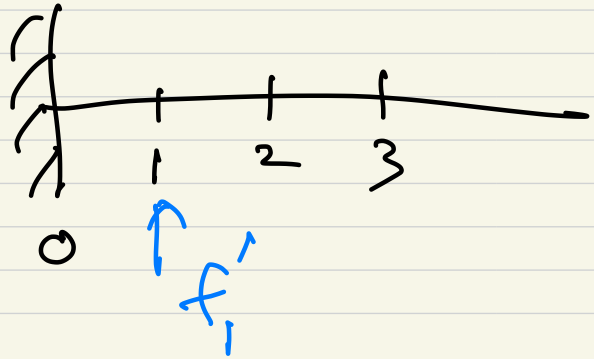
more grid pts. → higher accuracy

problem? → near/on boundary

lower-order accurate formula

@ $j=1$, CD2 → $O(\Delta x^2)$

f_1' using f_0, f_1, f_2, f_3, f_4



2.2 A general technique for construction of FD schemes

- f_j' using function values at $j, j+1, j+2$.

Q : what is the most accurate formula?

$$f_j' + a_0 f_j + a_1 f_{j+1} + a_2 f_{j+2} = O(h^?) \quad (h = \Delta x)$$

Taylor table

	f_j	f_j'	f_j''	f_j'''	$\cdots$
f_j'	0	1	0	0	$\cdots$
$a_0 f_j$	a_0	0	0	0	$\cdots$
$a_1 f_{j+1}$	$a_1 \cdot 1$	$a_1 \cdot h$	$a_1 \cdot \frac{1}{2} h^2$	$a_1 \cdot \frac{1}{6} h^3$	$\cdots$
$+$ $a_2 f_{j+2}$	$a_2 \cdot 1$	$a_2 \cdot (2h)$	$a_2 \cdot \frac{1}{2}(2h)^2$	$a_2 \cdot \frac{1}{6}(2h)^3$	$\cdots$

$$\rightarrow f_j' + a_0 f_j + a_1 f_{j+1} + a_2 f_{j+2} = (a_0 + a_1 + a_2) f_j$$
$$+ (1 + a_1 h + 2 a_2 h) f_j' + \left(\frac{1}{2} a_1 h^2 + 2 a_2 h^2\right) f_j'' + \left(\frac{1}{6} a_1 h^3 + \frac{4}{3} a_2 h^3\right) f_j'''$$
$$+ \cdots$$

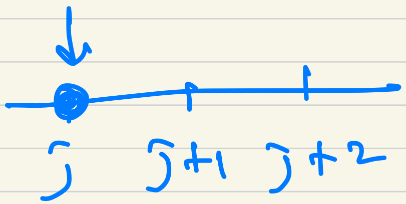
Set as many lower-order coeffs to zero as possible.

$$\rightarrow \left.\begin{aligned} a_0 + a_1 + a_2 &= 0 \\ 1 + a_1 h + 2a_2 h &= 0 \\ \tfrac{1}{2} a_1 h^2 + 2a_2 h^2 &= 0 \end{aligned}\right) \rightarrow a_0 = \frac{3}{2h}, \quad a_1 = -\frac{2}{h}, \quad a_2 = \frac{1}{2h}$$

$$\rightarrow f_j' + \frac{3}{2h} f_j - \frac{2}{h} f_{j+1} + \frac{1}{2h} f_{j+2} = \frac{1}{3} h^2 f_j''' + \cdots$$

$$\rightarrow \boxed{f_j' = \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}} + \frac{1}{3} h^2 f_j''' + \cdots$$

2nd-order FD



← one-side difference

2.3 An alternative measure for the accuracy of FD,

* modified wavenumber approach for measuring accuracy.

$f(x) = e^{ikx} = \cos kx + i \sin kx$: pure harmonic ft. of period L.

k : wave number

$\Delta x = h = L/N$: grid spacing

uniform mesh

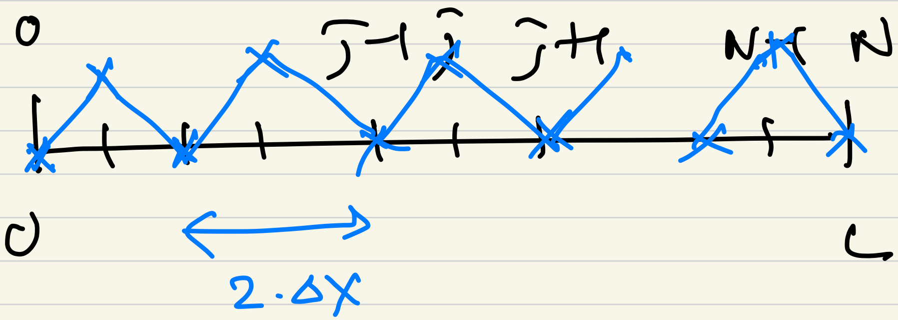
largest wavelength $e^{i\Delta k L} = 2\pi$

$\Delta k \cdot L = 2\pi$

$\rightarrow \boxed{\Delta k = \frac{2\pi}{L}}$: smallest wavenumber

largest wavenumber?

smallest wave length



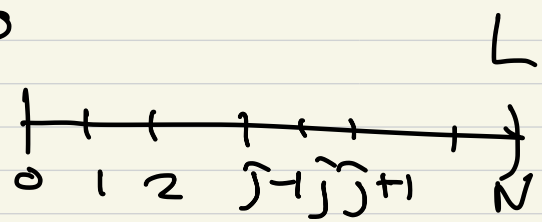
$k \cdot (2\Delta x) = 2\pi$

$\rightarrow \boxed{k = \frac{\pi}{\Delta x} = \frac{\pi}{h} = \frac{\pi N}{L}}$

largest wavenumber

$$f(x) = e^{ikx} \longrightarrow f' = ike^{ikx} = ikf \quad : \text{exact sol.}$$

Q: how accurately CD2 computes the derivatives of f for different values of k?



$$x_j = h \cdot j = \frac{L}{N} j, \quad j = 0, 1, 2, \dots, N$$

On this grid, e^{ikx} ranges from a constant for $k=0$ to a highly oscillatory ft. of period equal to mesh width ($2\Delta x$) for $k = \pi N/L$ $(=\pi/h)$.

$$f_j' = \frac{f_{j+1} - f_{j-1}}{2h} \quad (\text{CD2})$$

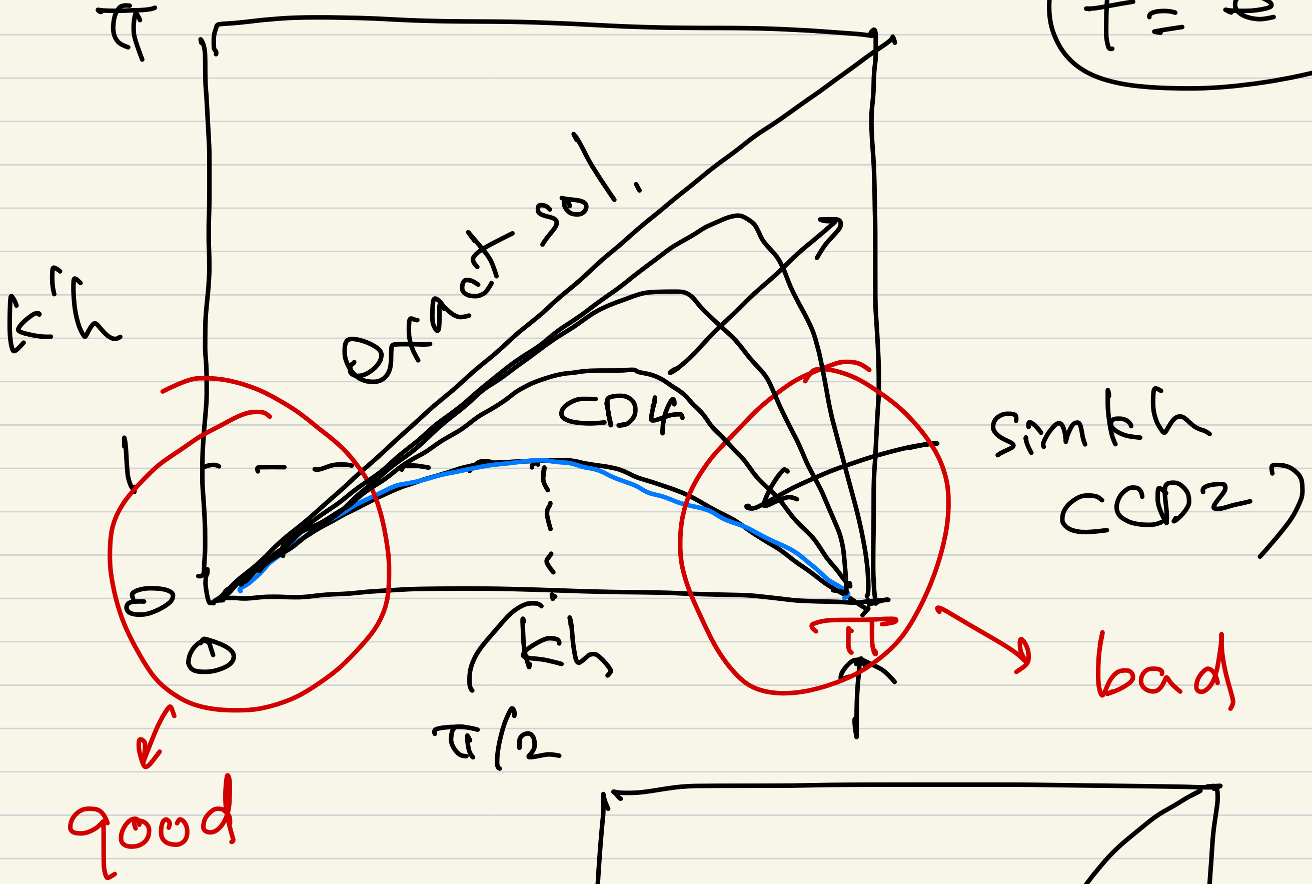
$$= \frac{1}{2h}\left(e^{ikx_{j+1}} - e^{ikx_{j-1}}\right) = \frac{1}{2h} e^{ikx_j} \Big(\underbrace{e^{ikh} - e^{-ikh}}_{i \cdot 2\sin kh}\Big)$$

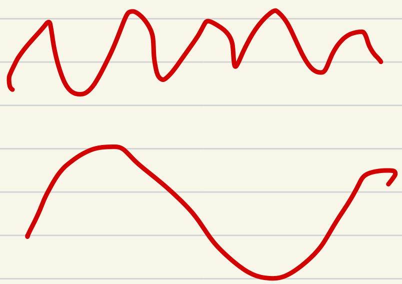
$$= i \cdot \frac{\sin kh}{h} e^{ikx_j} = i \frac{\sin kh}{h} f_j$$

k' : modified wavenumber

$\rightarrow k'h = \sin kh \; (\text{CD2})$

$f = e^{ikx} \rightarrow f' = ike^{ikx}$





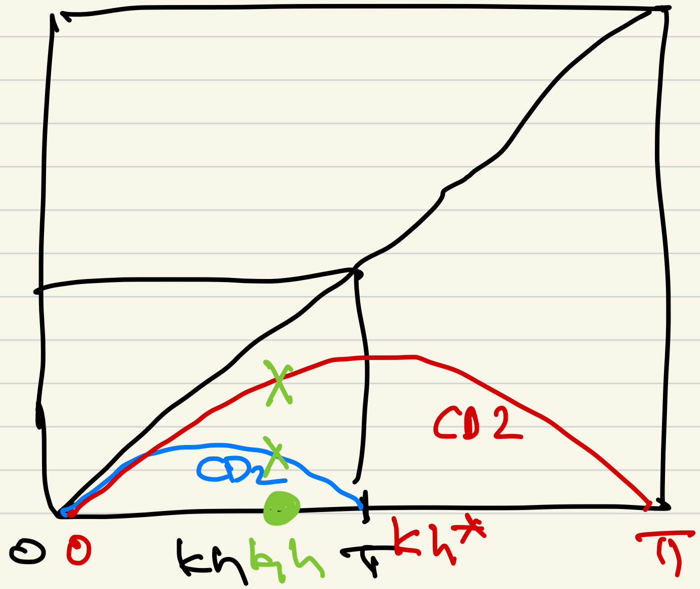
$f = e^{ikx}$

k_1

h

$N \rightarrow 2N$

$h \rightarrow \frac{h}{2} = h^*$



$f' = i k f$
exact sol.

• 1st-order FD : $f_j' = \dfrac{f_{j+1} - f_j}{h} + O(h)$

$$= \frac{1}{h}\left(e^{ikx_{j+1}} - e^{ikx_j} \right)$$

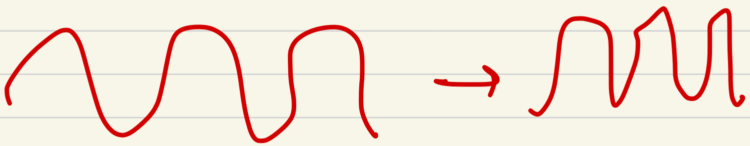
$$= \frac{1}{h} e^{ikx_j}\left(e^{ikh} - 1 \right) = \frac{1}{h}\left(-1 + \cos kh + i \sin kh \right) \times e^{ikx_j}$$

$$\rightarrow \quad f_j' = i \boxed{\left[\frac{\sin kh}{h} + i\, \frac{1 - \cos kh}{h} \right]} f_j$$

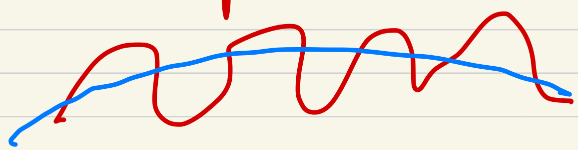
$= k'$: modified wavenumber
complex number

$\dfrac{\sin kh}{h} = k'_{CD2}$

dispersive error



dissipative error



each FD method has its own modified wavenumber.

2.4 Padé approximations

$$f_j' + a f_j + b f_{j-1} + c f_{j+1} + d f_{j+2} = O(h^?)$$

Include derivatives too in the formula.

ex) Find the most accurate formula of f_j' that involves

$$f_{j+1},\ f_{j-1},\ f_j,\ f_{j+1}',\ f_{j-1}'$$

$$\rightarrow f_j' + a_0 \underline{f_{j+1}'} + a_1 \underline{f_{j-1}'} + b_0 f_j + b_1 f_{j-1} + b_2 f_{j+1} = O(h^?)$$

Taylor table

	f_j	f_j'	f_j''	f_j'''	$f_j^{(iv)}$	$f_j^{(v)}$ ...
f_j'	0	1	0	0	0	0 ...
$a_0 f_{j+1}'$	$a_0 \cdot 0$	$a_0 \cdot 1$	$a_0 \cdot h$	$a_0 \cdot \frac{1}{2}h^2$	$a_0 \cdot \frac{1}{6}h^3$	$a_0 \cdot \frac{1}{24}h^4$ ...
$a_1 f_{j-1}'$	0	$a_1 \cdot (-1)$	$a_1 \cdot h$	$a_1 \cdot \frac{1}{2}h^2$	$a_1 \cdot \frac{1}{6}(-h)^3$	$a_1 \cdot \frac{1}{24}h^4$ ...
$b_0 f_j$	b_0	0	0	0	0	0
$b_1 f_{j-1}$	$b_1 \cdot 1$	$b_1 \cdot (-h)$	$b_1 \cdot \frac{1}{2}h^2$	$b_1 \cdot \frac{1}{6}h^3$	$b_1 \cdot \frac{1}{24}h^4$	---
+ $b_2 f_{j+1}$	$b_2 \cdot 1$	$b_2 \cdot h$	$b_2 \cdot \frac{1}{2}h^2$	$b_2 \cdot \frac{1}{6}(-h)^3$	$b_2 \cdot \frac{1}{24}h^4$	...

$$f_j' + a_0 f_{j+1}' + a_1 f_{j-1}' + b_0 f_j + b_1 f_{j-1} + b_2 f_{j+1}$$

$$= \underbrace{(b_0+b_1+b_2)}_{=0} f_j + \underbrace{(1+a_0-a_1-b_1h+b_2h)}_{=0} f_j'$$

$$+ \underbrace{(a_0h + a_1h + \tfrac{1}{2} b_1 h^2 + \tfrac{1}{2} b_2 h^2)}_{=0} f_j'' + \underbrace{(\cdots)}_{=0} f_j''' + \underbrace{(\cdots)}_{=0} f_j^{(iv)} + \cdots$$

5 unknowns

↳ $a_0 = \cdots,\ a_1 = \cdots,\ b_0 = \cdots,\ b_1 = \cdots,\ b_2 = \cdots$

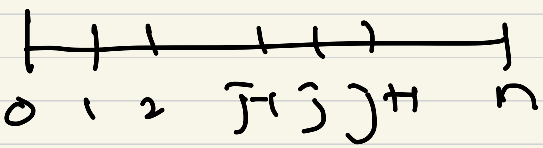
$$\rightarrow f_j' + \frac{1}{4} f_{j+1}' + \frac{1}{4} f_{j-1}' - \frac{3}{4h} f_{j+1} + \frac{3}{4h} f_{j-1} = \frac{h^4}{120} f_j^{(v)} + \cdots$$

$$\rightarrow \boxed{f_{j-1}' + 4 f_j' + f_{j+1}' = \frac{3}{h}(f_{j+1} - f_{j-1})} + \underbrace{\frac{1}{30} h^4 f_j^{(v)}}_{O(h^4)} + \cdots,$$

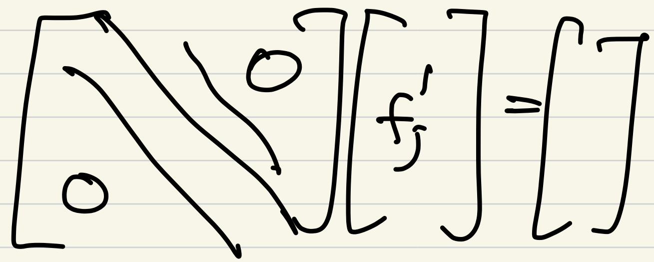
3 grid pts. → 4th order accuracy

$O(h^4)$ → 4th order accuracy

⇒ "compact" scheme



$j = 1, 2, \cdots, n-1$



tri-diagonal matrix system → easy to solve

$n-1$ eqs. for $n+1$ unknowns. $(f_0', f_1', \cdots, f_n')$

① $j=0$: $f_0' = \frac{1}{2h}(-3f_0 + 4f_1 - f_2) + O(h^2)$

② ⓐ $j=1$: $f_2' + 4f_1' = \frac{1}{2h}(7f_2 - 3f_0 - 4f_1) + O(h^?)$ $O(h^{②③})$

$$\begin{pmatrix} 4 & 1 & 0 & \cdots & 0 \\ 1 & 4 & 1 & 0 \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ & & & 1 & 4 \end{pmatrix} \begin{pmatrix} f_1' \\ f_2' \\ \vdots \\ \vdots \\ f_{n-1}' \end{pmatrix} = \begin{pmatrix} \frac{1}{2h}(7f_2 - 3f_0 - 4f_1) \\ \frac{3}{h}(f_3 - f_1) \\ \vdots \\ \vdots \\ \boxed{} \end{pmatrix}$$

$O(h^4)$

$\rightarrow$ ③ $O(h^{②} \sim h^4)$

③ ⓐ $j=0$: $f_0' + a_0 f_1' + b_0 f_0 + b_1 f_1 + b_2 f_2 = O(h^?)$

$\longrightarrow f_0' + 2f_1' = \frac{1}{h}\left(-\frac{5}{2} f_0 + 2f_1 + \frac{1}{2} f_2\right) + O(h^3)$

$$\begin{pmatrix} 1 & 2 & 0 \\ 1 & 4 & 1 \\ & & \end{pmatrix} \begin{pmatrix} \\ \\ \end{pmatrix} = \begin{pmatrix} \cdots \\ \cdot \\ \ddots \end{pmatrix}$$

Padé approximations can be easily extended to higher derivatives.

ex) $$\frac{1}{12} f''_{j-1} + \frac{10}{12} f''_j + \frac{1}{12} f''_{j+1} = \frac{1}{h^2}\left(f_{j+1} - 2f_j + f_{j-1}\right) + O(h^4)$$

3pts $\rightarrow$ $O(h^4)$ 4th-order accurate compact scheme

S. Lele (JCP, 1992) – compact schemes → #6246 citations

↓

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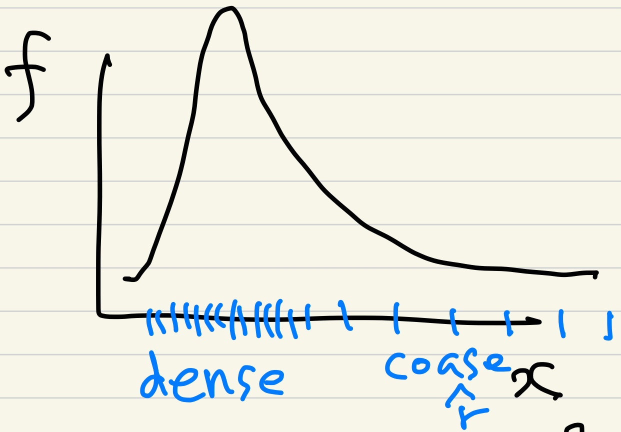
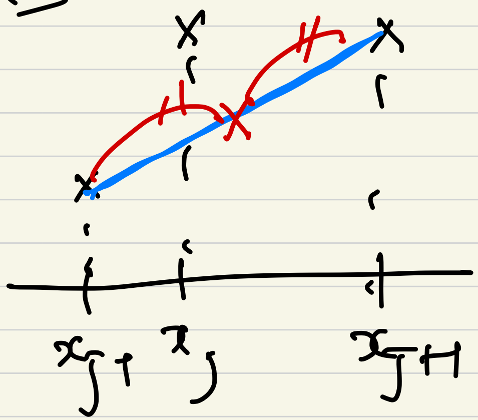
2.5 Non-uniform grids





$$f'_j = \frac{f_{j+1} - f_{j-1}}{x_{j+1} - x_{j-1}} + \cancel{O(h^2)}$$

strictly 1st-order accurate

$$h_j = x_{j+1} - x_j$$

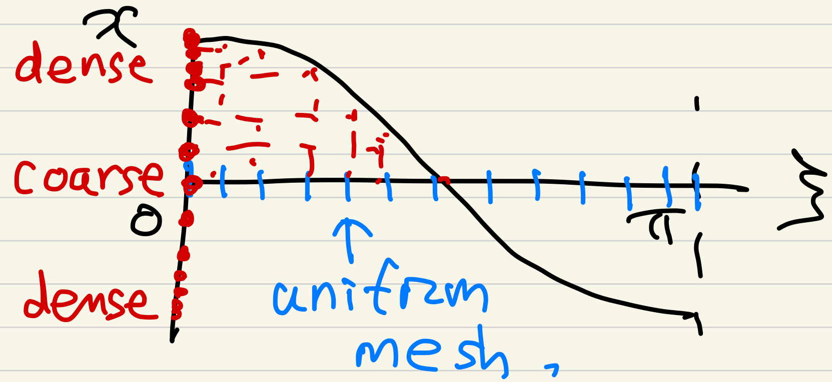
$$f''_j = 2\left[\frac{f_{j-1}}{h_j(h_j + h_{j+1})} - \frac{f_j}{h_j h_{j+1}} + \frac{f_{j+1}}{h_{j+1}(h_j + h_{j+1})}\right] + \cancel{O(h^2)}$$

FD formula for non-uniform mesh generally has a lower order of accuracy than their counterpart with the same stencil for uniform mesh.

- Use a coordinate transformation

$x \rightarrow \xi$

ex) $x = \cos\xi$



$$\xi = g(x)$$

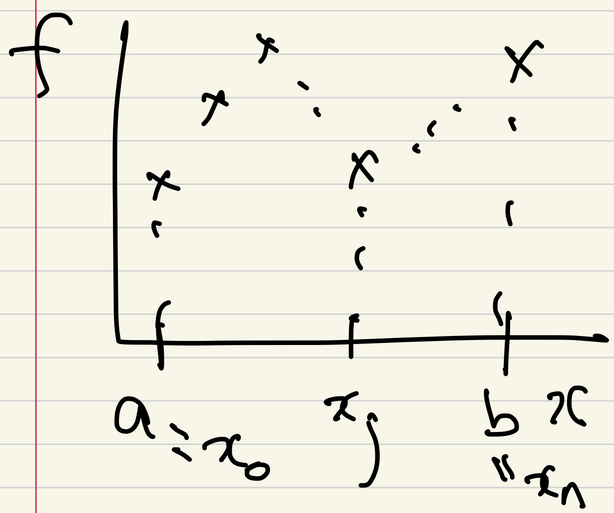
$$\frac{df}{dx} = \frac{df}{d\xi}\frac{d\xi}{dx} = g' \boxed{\frac{df}{d\xi}}$$

FD on uniform mesh in ξ.

$$\frac{d^2f}{dx^2} = \frac{d}{dx}\left(\frac{df}{dx}\right) = \frac{d}{dx}\left(g'\frac{df}{d\xi}\right) = g''\frac{df}{d\xi} + g'\frac{d^2f}{d\xi^2}\frac{d\xi}{dx}$$

$$= g''\boxed{\frac{df}{d\xi}} + g'^2\boxed{\frac{d^2f}{d\xi^2}}$$

Ch.3 Numerical integration (quadrature)



$$I = \int_a^b f(x)\,dx = \sum_{j=0}^{n} f_j w_j$$

weight

3.1 Trapezoidal and Simpson's rule

Lagrange polynomial $P(x) = \sum_{j=0}^{n} f_j L_j(x)$

$$I = \int_a^b f(x)\,dx = \int_a^b P(x)\,dx = \int_a^b \sum_{j=0}^{n} f_j L_j\,dx = \sum_{j=0}^{n} f_j \overbrace{\boxed{\int_a^b L_j(x)\,dx}}^{w_j}$$

$$= \boxed{(b-a)\sum_{j=0}^{n} C_j^n f_j} \quad \text{where } C_j^n = \frac{1}{b-a}\int_a^b L_j(x)\,dx$$

Newton–Cotes formula

Cotes number

For $n=1$, $x_0 = a$, $x_1 = b$

$$L_0(x) = \frac{x-b}{a-b}, \quad L_1(x) = \frac{x-a}{b-a}$$

$$C_0^1 = \frac{1}{b-a}\int_a^b L_0(x)\,dx = \frac{1}{2}, \quad C_1^1 = \frac{1}{b-a}\int_a^b L_1(x)\,dx = \frac{1}{2}$$

$$I = (b-a)\left(\frac{1}{2}f_0 + \frac{1}{2}f_1\right) = \boxed{(b-a)\left[\frac{1}{2}f(a) + \frac{1}{2}f(b)\right]}$$

trapezoidal rule

For $n=2$, $x_0 = a$, $x_1 = \frac{1}{2}(a+b)$, $x_2 = b$ $\rightarrow$ C_0^2, C_1^2, C_2^2

$$\rightarrow \quad I = \boxed{\frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]} \qquad L_0, L_1, L_2$$

Simpson's rule

n	N	NC_0^n	NC_1^n	NC_2^n	NC_3^n	NC_4^n	NC_5^n	NC_6^n	error
1	2	1	1						$8.3\times10^{-2}\Delta^3 f''$
2	6	1	4	1					$3.5\times10^{-4}\Delta^5 f^{iv}$
3	8	1	3	3	1				$1.6\times10^{-4}\Delta^5 f^{iv}$
4	90	7	32	12	32	7			$5.2\times10^{-7}\Delta^7 f^{vi}$
5	288	19	25	50	50	25	19		$3.6\times10^{-7}\Delta^7 f^{vi}$
6	840	41	216	27	272	27	216	41	$6.4\times10^{-10}\Delta^9 f^{viii}$
$\vdots$			$\vdots$						