Suppl. lecture video on eTL watch by Sunday 6pm.

Spline interpolation

$$\begin{pmatrix} \ddots & \ddots & \ddots & & 0 \\ & \frac{\Delta_{i-1}}{6} & \frac{\Delta_{i-1}+\Delta_i}{3} & \frac{\Delta_i}{6} & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} g_1'' \\ g_2'' \\ \vdots \\ g_{n-1}'' \end{pmatrix} = \begin{pmatrix} \cdots + g_0'' \\ \\ \\ \cdots + g_n'' \end{pmatrix}$$

$n+1$ unknowns

$n-1$ eq!.

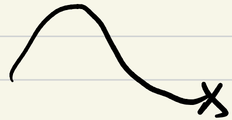
g_0'' & g_n''

End conditions g_0'' and g_n'

① $\begin{cases} g_0'' = g_1'' \\ g_n'' = g_{n-1}'' \end{cases}$ → parabolic runout

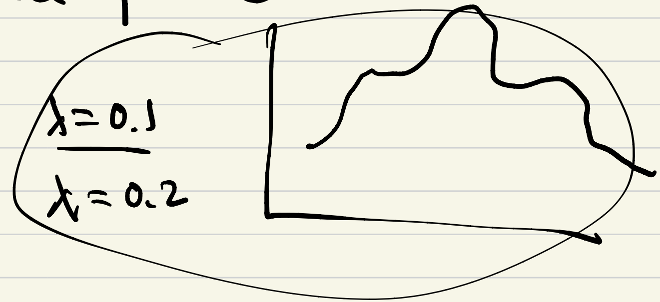
$$\begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ \ddots & \ddots & \ddots & & \\ & & & -1 & 1 \end{pmatrix} \begin{pmatrix} g_0'' \\ g_1'' \\ \vdots \\ g_{n-1}'' \\ g_n'' \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$

② $\begin{cases} g_0'' = 0 \\ g_n'' = 0 \end{cases}$



natural spline

③ $\begin{cases} g_0'' = \lambda g_1'' \\ g_n'' = \lambda g_{n-1}'' \end{cases}$ $\quad 0 \le \lambda \le 1$



④ $\begin{cases} g_0'' = g_n'' \\ g_n'' = g_0'' \end{cases}$ periodic b.c.

$$\begin{pmatrix} 1 & 0 & \cdots & 0 & -1 \\ & \ddots & \ddots & \ddots & \\ -1 & 0 & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} g_0'' \\ g_1'' \\ \vdots \\ g_{n-1}'' \\ g_n'' \end{pmatrix} = \begin{pmatrix} 0 \\ \\ \vdots \\ \\ 0 \end{pmatrix}$$

For equally spaced pts.,
$\Delta_i = \Delta_{i+1} = \Delta$

$$\boxed{\frac{1}{6}\left[g_{i-1}'' + 4 g_i'' + g_{i+1}'' \right] = \frac{1}{\Delta^2}\left(y_{i-1} - 2 y_i + y_{i+1} \right)}$$

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

g_0'' & g_n''

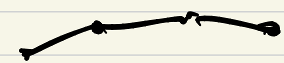
In some cases, you may get wiggles.

→ tension splines → pull on each ends $(y^{(iv)} - \sigma^2 y'' = 0)$

$$\rightarrow \quad g' - \sigma^2 g = (g_i'' - \sigma^2 y_i)\frac{x - x_{i+1}}{x_i - x_{i+1}} + (g_{i+1}' - \sigma^2 y_{i+1})\frac{x - x_i}{x_{i+1} - x_i}$$

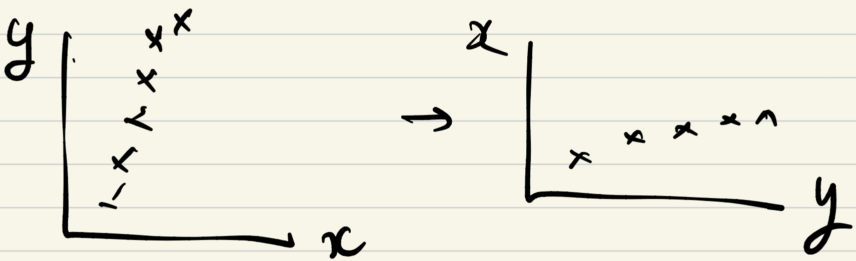
$\sigma \to \infty$: straight line interpolation

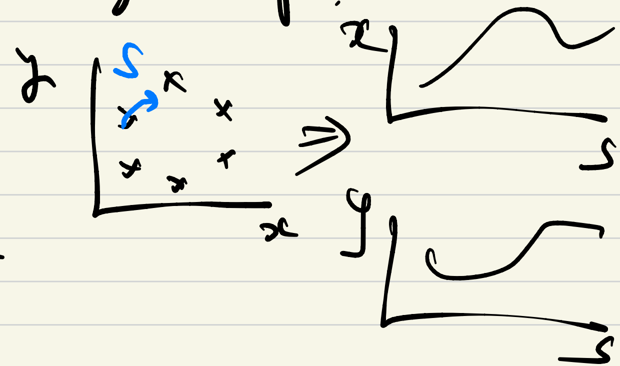
$\sigma = 0$: usual spline



$\sigma = 0 \Rightarrow$ wiggles in sol. → increase σ.

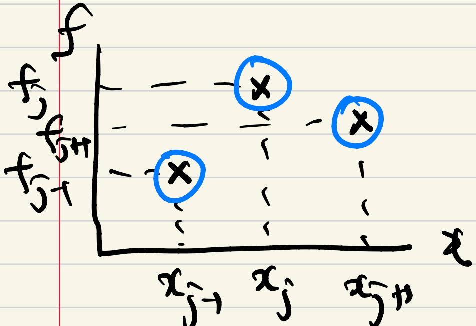
* spline has difficulties with large slops.





Ch. 2. Numerical differentiation – finite difference

2.1 Construction of difference formulae using Taylor series.



$(x_i, f_i) \to f_i'$

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

Finite difference using Taylor series expansion

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

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

1st-order accurate finite difference (FD) method

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

forward 1st-order FD method.

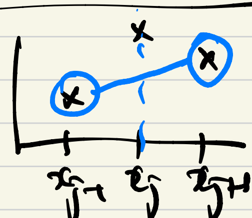
Similarly, $f(x_j - \Delta x) = f(x_j) - \Delta x f'(x_j) + \frac{1}{2}\Delta x^2 f''(x_j) - \frac{1}{6}\Delta x^3 f'''(x_j) + \cdots$

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

backward 1st-order FD method

$$\left.\begin{aligned} f(x_j+\Delta x) &= \cdots \\ f(x_j-\Delta x) &= \cdots \end{aligned}\right] \Rightarrow \boxed{f_j' = \frac{f_{j+1}-f_{j-1}}{2\Delta x}} \underbrace{-\frac{1}{6}\Delta x^2 f_j''' + \cdots}_{O(\Delta x^2)}$$

2nd-order central FD method (CD2)

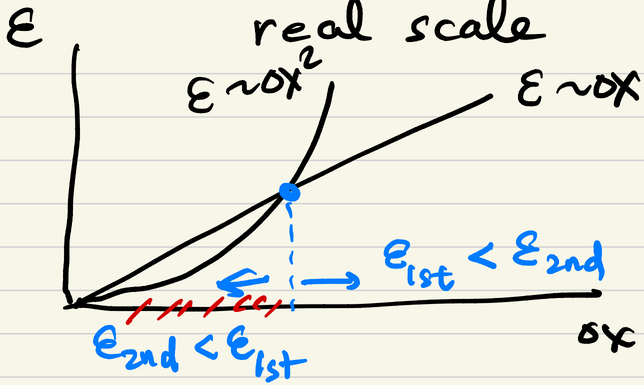


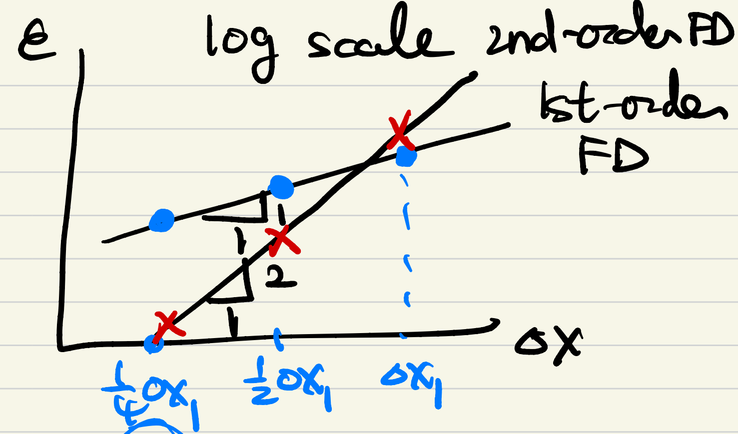
$$\begin{cases} f_j' = \dfrac{f_{j+1}-f_j}{\Delta x} - \dfrac{1}{2}\Delta x f_j'' + \cdots \\ f_j' = \dfrac{f_j - f_{j-1}}{\Delta x} + \dfrac{1}{2}\Delta x f_j'' + \cdots \\ f_j' = \dfrac{f_{j+1}-f_{j-1}}{2\Delta x} - \dfrac{1}{6}\Delta x^2 f_j''' + \cdots \end{cases}$$

ε

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

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



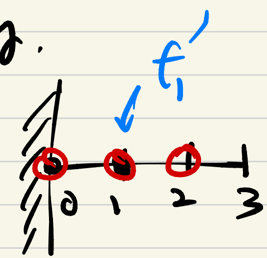


$$f_j' = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12\,\Delta x} + O(\Delta x^4)$$

CD4

more grid pts. → higher accuracy.

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

$$\to f_j' + a_0 f_j + a_1 f_{j+1} + a_2 f_{j+2} = \underline{(a_0 + a_1 + a_2)} f_j$$
$$+ (\underline{1 + a_1 h + 2a_2 h}) f_j' + (\underline{\tfrac{1}{2}a_1 h^2 + 2a_2 h^2}) f_j''$$
$$+ (\tfrac{1}{6}a_1 h^3 + \tfrac{4}{3}a_2 h^3) f_j''' + \cdots\cdots$$

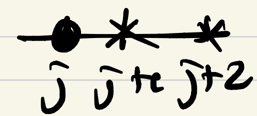
3 unknowns.

set as many lower-order coeffs to zero as possible

$$\rightarrow \left.\begin{aligned} a_0+a_1+a_2&=0 \\ 1+a_1h+2a_2h&=0 \\ \tfrac{1}{2}a_1h^2+2a_2h^2&=0 \end{aligned}\right\} \Rightarrow a_0=\frac{3}{2h},\ a_1=-\frac{2}{h},\ a_2=\frac{1}{2h}$$

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

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



2nd-order FD

one-side difference

2.3 An alternative measure for the accuracy of FD.

HW 1

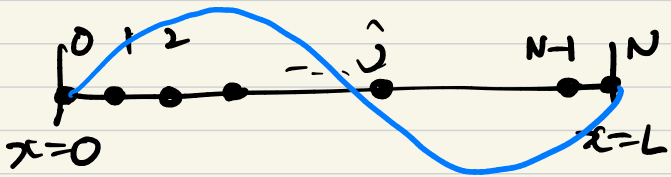
$O(h^2)$ $O(h^3)$

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 : wavenumber

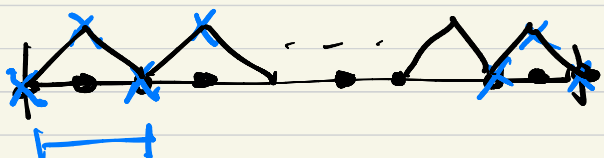


uniform mesh

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

smallest wavenumber Δk

$\Delta k \cdot L = 2\pi \rightarrow \boxed{\Delta k = \frac{2\pi}{L}}$



largest wavenumber K

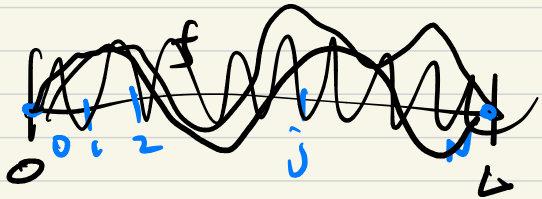
$K \cdot (2\Delta x) = 2\pi$

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

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

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

$O(h^2)$



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

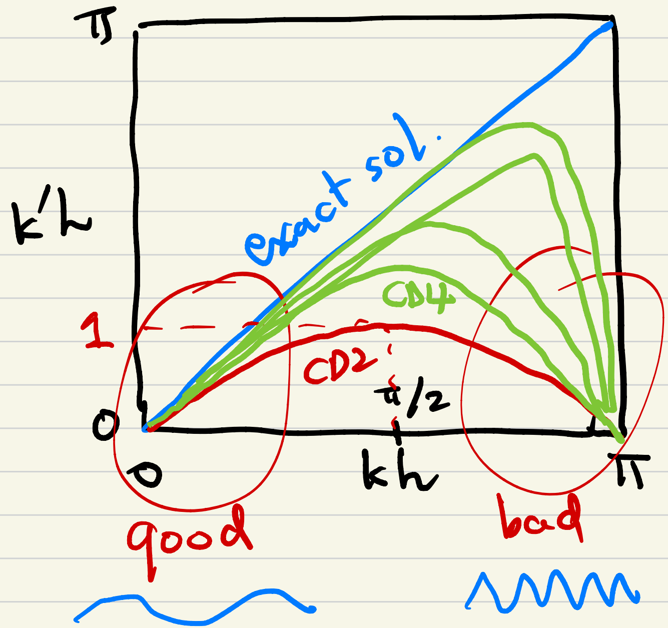
On this grid, e^{ikx} ranges from a constant for $k=0$ to a highly oscillatory ft. of period equal to mesh width ($2\Delta x$) for $k = \pi N / L$.

CD2: $f_j' = \frac{f_{j+1} - f_{j-1}}{2h} = \frac{1}{2h}\left(e^{ikx_{j+1}} - e^{ikx_{j-1}}\right)$

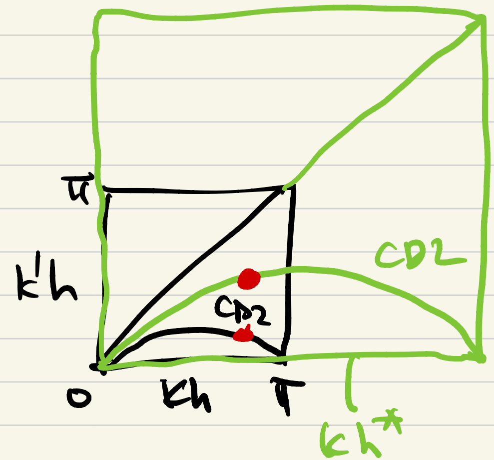
$$= \frac{1}{2h} e^{ikx_j}\big(\underbrace{e^{ikh} - e^{-ikh}}_{= i \cdot 2\sin kh}\big) = i\frac{\sin kh}{h} e^{ikx_j} = i\frac{\sin kh}{h} f_j$$

k' : modified wavenumber

$\rightarrow \; k'h = \sin kh \quad (CD2)$



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



• 1st order FD $\quad f_j' = \frac{f_{j+1} - f_j}{h} + O(h)$ $\qquad f = e^{ikx}$

$f' = ikf$

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

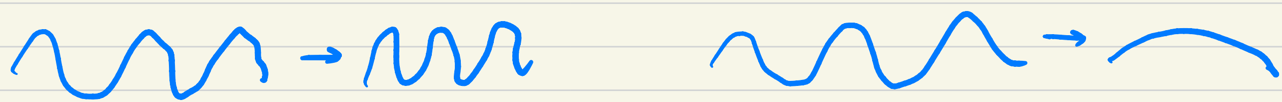
$$= \frac{1}{h} e^{ikx_j}\left(\cos kh + i\sin kh - 1\right)$$

$e^{ik'x}$

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

k'_{CD2} $\qquad k'$: modified wavenumber, complex number

dispersive error $\qquad$ dissipative error



Each FD scheme 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

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

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

Taylor table

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

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

5 unknowns

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

$$+ \underbrace{(a_0 h + a_1 h + \tfrac{1}{2} b_1 h^2 + \tfrac{1}{2} b_2 h^2)}_{=0} f_j'' + \underbrace{(\cdots)}_{=0} f_j''' + \underbrace{(\cdots)}_{=0} f_j^{(iv)} + \cdots$$

$\rightarrow a_0 = \cdots, \; a_1 = \cdots, \; b_0 = \; , \; b_1 = \; , \; b_2 = \; \cdots$

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

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

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

4th order accurate FD

3 grid pts! → compact scheme

$$\begin{bmatrix} \ddots & \ddots & \ddots \\ 1 & 4 & 1 \\ \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \; \end{bmatrix} = \begin{bmatrix} \; \end{bmatrix}$$

tri-diagonal matrix sys.

→ easy to solve.

$n-1$ eqs. for $n+1$ unknowns $\quad f_0', f_1', \cdots, f_{n-1}', f_n'$

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

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

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

overall accuracy $O(h^2 \sim h^4)$

③ @ $j=0$: $\quad f_0' + 2f_1' = \frac{1}{h}\left(-\frac{5}{2}f_0 + 2f_1 + \frac{1}{2}f_2\right) + O(h^3)$

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

Pade approx. can be easily extended to higher derivatives.

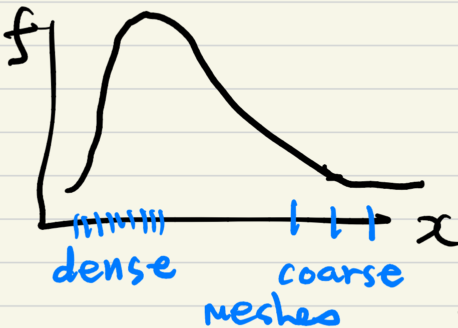
ex) $\frac{1}{12} f''_{j-1} + \frac{10}{12} f''_j + \frac{1}{12} f''_{j+1} = \frac{1}{h^2}\left(f_{j+1} - 2f_j + f_{j-1}\right) + O(h^6)$

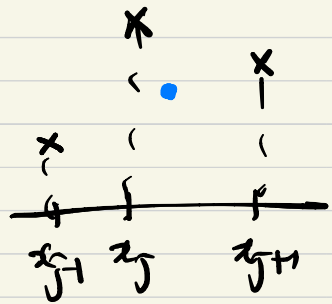
3pts. $\rightarrow O(h^4)$ 4th order accurate compact scheme

S. Lele (J. Comput. Phys, 1992) – compact schemes

7267 citations

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 formula

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

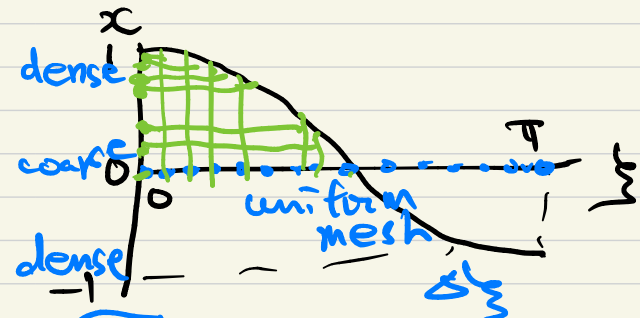
$$f''_j = 2\left[\frac{f_{j-1}}{h_j(h_j + h_{j+1})} - \frac{f_j}{h_j h_{j+1}} + \frac{f_{j+1}}{h_{j+1}(h_j + h_{j+1})}\right] + \cancel{O(h^2)}$$

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

- Use a coordinate transformation

$x \to \xi$

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.

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

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