Review of Finite Difference (FD) Calculus

Objective: approximate derivatives using only discrete points $x_i \Rightarrow$ "grid points"

$u(x_i) \equiv u_i$

Strategy: Expand Talyor Series about point where derivative is desired, evaluate at other grid points ... Use as many as needed to get desired derivative order and accuracy

e.g. Want $\left.\frac{du}{dx}\right|_{x=x_i} = \frac{du_i}{dx} \equiv u_i'$

$$u_{i+1} = u_i + h u_i' + \frac{h^2}{2!} u_i'' + O(h^3)$$

$$\Rightarrow \frac{du_i}{dx} = \frac{u_{i+1} - u_i}{h} \underbrace{- \frac{h}{2!} u_i''}_{} + O(h^2)$$

$$= \frac{\Delta u_i}{h} + \text{Leading error } O(h)$$

"First Forward Difference"

Want $\frac{d^2 u_i}{dx^2}$: write another Taylor Series

$$u_{i+2} = u_i + 2h u_i' + \frac{(2h)^2}{2!} u_i'' + \frac{(2h)^3}{3!} u_i''' + \dots$$

Add with TS for u_{i+1} to make u_i' terms cancel:

$$-2\left[u_{i+1} = u_i + h u_i' + \frac{h^2}{2!} u_i'' + \frac{h^3}{3!} u_i''' + \dots\right]$$
$$u_{i+2} = u_i + 2h u_i' + \frac{(2h)^2}{2!} u_i'' + \frac{(2h)^3}{3!} u_i''' + \dots$$

$$\frac{d^2 u_i}{dx^2} = \frac{u_{i+2} - 2u_{i+1} + u_i}{h^2} - h u_i''' + \dots \equiv \frac{\Delta^2 u_i}{h^2} + O(h)$$

⋮

$$\frac{d^n u_i}{dx^n} = \frac{\Delta^n u_i}{h^n} + O(h)$$ involves points $u_i \to u_{i+n}$

Note: key fact ... $\Delta^n u_i = \Delta(\Delta^{n-1} u_i)$

Check ... $\Delta^2 u_i = \Delta(\Delta u_i) = \Delta(u_{i+1} - u_i)$
$= (u_{i+2} - u_{i+1}) - (u_{i+1} - u_i) = u_{i+2} - 2u_{i+1} + u_i$ ✓

Try $\Delta^3 u_i$: $= \Delta(\Delta^2 u_i) = \Delta(u_{i+2} - 2u_{i+1} + u_i)$

$$= u_{i+3} - u_{i+2} - 2u_{i+2} + 2u_{i+1} + u_{i+1} - u_i$$

$$= u_{i+3} - 3u_{i+2} + 3u_{i+1} - u_i$$

Can do the same thing backwards ⇒ "Backward Differences"

$$\frac{d^n u_i}{dx^n} = \frac{\nabla^n u_i}{h^n} + O(h)$$ involves points $u_{i-n} \rightarrow u_i$

so $\nabla^n u_i = \nabla(\nabla^{n-1} u_i)$

e.g. $\nabla^2 u_i = \nabla(\nabla u_i) = \nabla(u_i - u_{i-1})$

$$= (u_i - u_{i-1}) - (u_{i-1} - u_{i-2})$$

$$= u_i - 2u_{i-1} + u_{i-2}$$

$$\therefore \frac{d^2 u_i}{dx^2} = \frac{u_i - 2u_{i-1} + u_{i-2}}{h^2} + O(h)$$

If desire more accuracy : take more points

e.g. want $\frac{du_i}{dx}$ to $O(h^2)$

① $$u_{i+1} = u_i + h u_i' + \frac{h^2 u_i''}{2!} + \frac{h^3}{3!} u_i''' + \ldots$$

② $$u_{i+2} = u_i + 2h u_i' + \frac{(2h)^2}{2!} u_i'' + \frac{(2h)^3}{3!} u_i''' + \ldots$$

add ① + A*②

$$u_{i+1} + A u_{i+2} = (1+A) u_i + \overbrace{(1+2A) h u_i'}^{\text{Want this}} + \overbrace{(1+4A)\frac{h^2}{2} u_i''}^{\text{Make Vanish}}$$

$$+ \underbrace{(1+8A)\frac{h^3}{3!} u_i'''}_{\text{Leading Error}} + \ldots$$

$$\frac{du_i}{dx} = \frac{1}{(2A+1)h}\left\{\left[A u_{i+2} + u_{i+1} - (1+A) u_i\right] - \overset{0 \to A=-1/4}{\cancel{(4A+1)}}\frac{h^2}{2} u_i'' - \frac{(1+8A)h^3}{3!} u_i''' + \ldots\right\}$$

$$\frac{du_i}{dx} = \frac{-u_{i+2} + 4u_{i+1} - 3u_i}{2h} - \underbrace{\frac{h^2}{3} u_i'''}_{\text{leading error } O(h^2)!} + O(h^3)$$

This approach to generating difference expressions systematic (see handout for general case)

OR ... can use error term to produce higher accuracy differences ⇒ substitute difference expressions for derivatives in leading error terms!

e.g. $$\frac{du_i}{dx} = \frac{\Delta u_i}{h} - \underbrace{\frac{h}{2}\frac{d^2u_i}{dx^2}}_{} + O(h^2)$$

substitute difference formula

$$\frac{d^2u_i}{dx^2} = \frac{\Delta^2 u_i}{h^2} + O(h)$$

$$\therefore \frac{du_i}{dx} = \frac{\Delta u_i}{h} - \frac{h}{2}\left[\frac{\Delta^2 u_i}{h^2} + O(h)\right] + O(h^2)$$

$$= \left(\Delta u_i - \frac{1}{2}(u_{i+2} - 2u_{i+1} + u_i)\right)/h + O(h^2)$$

$$= \frac{-u_{i+2} + 4u_{i+1} - 3u_i}{2h} + O(h^2)$$ ✓ same as before!

Central Differences

- only meaningful on uniform mesh
- forward + backward errors cancel
- get extra $O(h)$ for same # of points

e.g. $$\frac{du_i}{dx} = \frac{\Delta u_i}{h} - \frac{h}{2}\frac{d^2u_i}{dx^2} + O(h^2) \quad \text{Forward}$$

$$\frac{du_i}{dx} = \frac{\nabla u}{h} + \frac{h}{2}\frac{d^2u_i}{dx^2} + O(h^2) \quad \text{Backward}$$

Combine: (add) $$\frac{du_i}{dx} = \frac{\Delta u_i + \nabla u_i}{2h} + \underbrace{O(h^2)}_{\text{doesn't cancel}}$$

$$= \frac{u_{i+1} - u_i + u_i - u_{i-1}}{2h} + O(h^2)$$

$$= \frac{u_{i+1} - u_{i-1}}{2h} + O(h^2)$$

$$= \frac{\delta u_i}{2h} + O(h^2) \qquad \delta u_i \equiv u_{i+1} - u_{i-1}$$

Subtract : $$\frac{d^2 u_i}{dx^2} = \frac{\Delta u_i - \nabla u_i}{h^2} + O(h^2)$$

$$= \frac{\delta^2 u_i}{h^2} + O(h^2)$$

$$\delta^2 u_i = \Delta u_i - \nabla u_i = u_{i+1} - u_i - (u_i - u_{i-1}) = u_{i+1} - 2u_i + u_{i-1}$$

Summary – Equal mesh spacing:

- Forward $\quad \frac{d^n u_i}{dx^n} = \frac{\Delta^n u_i}{h^n} + O(h)$
- Backward $\quad \frac{d^n u_i}{dx^n} = \frac{\nabla^n u_i}{h^n} + O(h)$

Involve $n+1$ pts

- Centered $\quad \frac{d^n u_i}{dx^n} = \frac{\delta^n u_i}{(1 \text{ or } 2) h^n} + O(h^2)$

n odd

More Accuracy: add points

- Uncentered: nth derivative $+ O(h^2) \Rightarrow n+2$ pts
  $+ O(h^3) \Rightarrow n+3$ pts
  $\vdots \qquad \vdots$
- Centered: nth derivative $+ O(h^4) \Rightarrow n+3$ pts
  $+ O(h^6) \Rightarrow n+5$ pts

always add 2pts at a time
always stay 1 order ahead of uncentered

Alternative to Taylor Series: Polynomial fit

$$\underset{i-1}{\bullet} \quad h \quad \underset{\substack{i \\ x=0}}{\bullet} \quad \alpha h \quad \underset{i+1}{\bullet} \qquad \Rightarrow \quad u = ax^2 + bx + c$$

then
$$u_{i-1} = ah^2 + b(-h) + c$$
$$u_i = c$$
$$u_{i+1} = a(\alpha h)^2 + b(\alpha h) + c$$

$$\begin{bmatrix} h^2 & -h & 1 \\ 0 & 0 & 1 \\ \alpha^2 h^2 & \alpha h & 1 \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{Bmatrix} u_{i-1} \\ u_i \\ u_{i+1} \end{Bmatrix}$$

Invert:
$$\begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{Bmatrix} \left[\alpha(u_{i-1} - u_i) + (u_{i+1} - u_i)\right] / (\alpha^2 + \alpha)h^2 \\ \left[-\alpha^2(u_{i-1} - u_i) + (u_{i+1} - u_i)\right] / (\alpha^2 + \alpha)h \\ u_i \end{Bmatrix}$$

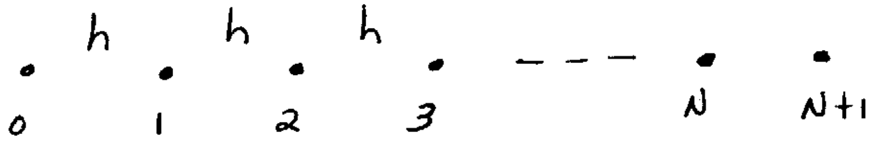
then
$$\frac{du}{dx} = 2ax + b$$

$$\frac{d^2u}{dx^2} = 2a = 2\left[\frac{u_{i+1} - u_i(1+\alpha) + \alpha u_{i-1}}{\alpha(\alpha+1)h^2}\right]$$

Same as Taylor!

Example: $K(x)\dfrac{d^2u}{dx^2} = r$ $\qquad K(x) = x$

BC's: $\left.\begin{array}{l} u(0) = u_0 \\ u(L) = u_L \end{array}\right\}$ given

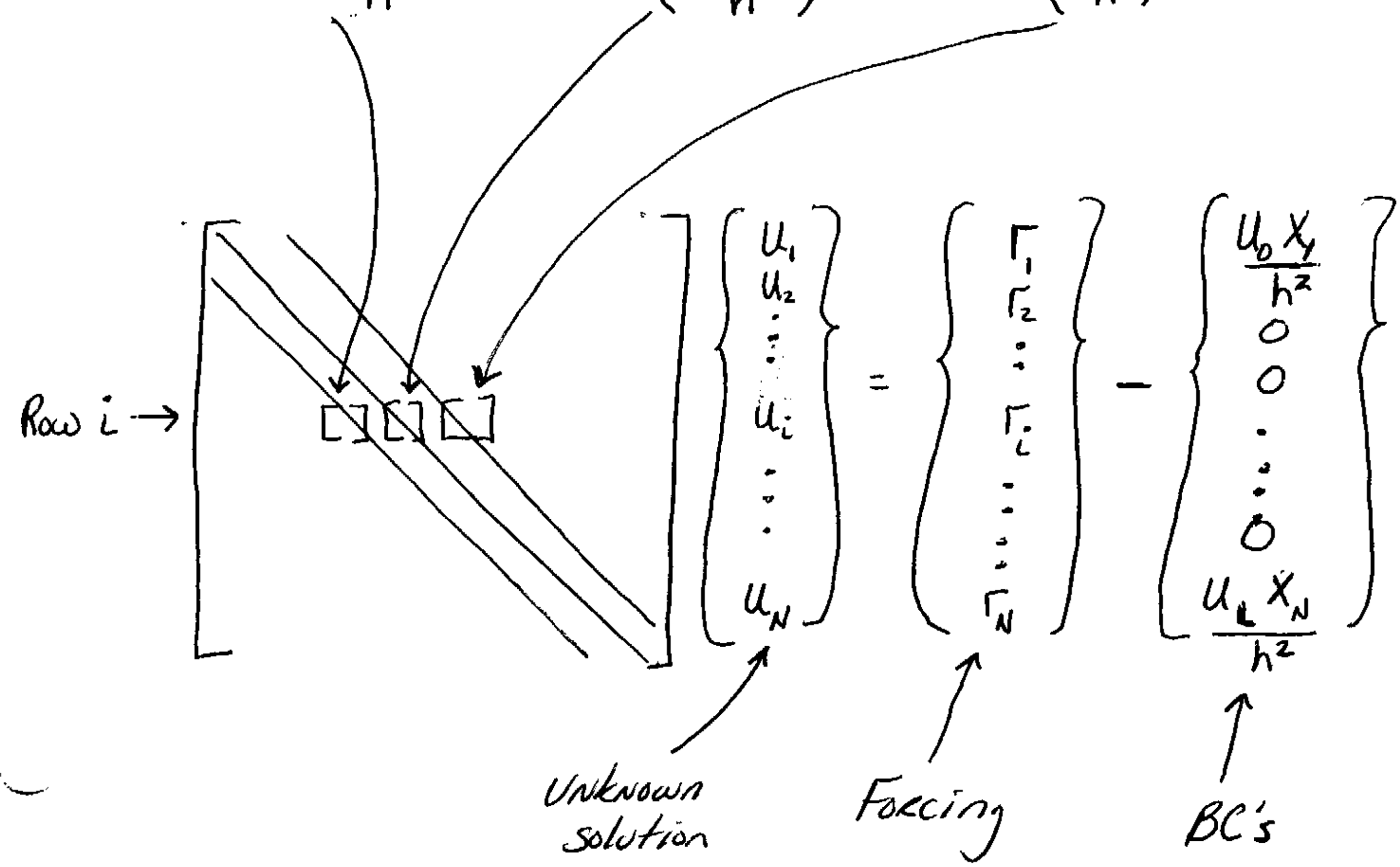


Uniform Mesh

Use 2nd order FD expression for PDE:

$$x_i \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = r_i + O(h^2)$$

$$\Rightarrow \quad u_{i-1}\left(\frac{x_i}{h^2}\right) + u_i\left(\frac{-2x_i}{h^2}\right) + u_{i+1}\left(\frac{x_i}{h^2}\right) = r_i$$



	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}
$hf'(x_i) =$	-1	1			
$h^2f''(x_i) =$	1	-2	1		
$h^3f'''(x_i) =$	-1	3	-3	1	
$h^4f''''(x_i) =$	1	-4	6	-4	1

$+ \quad O(h)$

(*a*) **Forward difference representations**

	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$hf'(x_i) =$				-1	1
$h^2f''(x_i) =$			1	-2	1
$h^3f'''(x_i) =$		-1	3	-3	1
$h^4f''''(x_i) =$	1	-4	6	-4	1

$+ \quad O(h)$

(*b*) **Backward difference representations**

Fig. 3.2 Forward and backward difference representations of $O(h)$.

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}	f_{i+5}
$2hf'(x_i) =$	-3	4	-1			
$h^2f''(x_i) =$	2	-5	4	-1		
$2h^3f'''(x_i) =$	-5	18	-24	14	-3	
$h^4f''''(x_i) =$	3	-14	26	-24	11	-2

$+ \quad O(h)^2$

(*a*) **Forward difference representations**

	f_{i-5}	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$2hf'(x_i) =$				1	-4	3
$h^2f''(x_i) =$			-1	4	-5	2
$2h^3f'''(x_i) =$		3	-14	24	-18	5
$h^4f''''(x_i) =$	-2	11	-24	26	-14	3

$+ \quad O(h)^2$

(*b*) **Backward difference representations**

Fig. 3.3 Forward and backward difference representations of $O(h)^2$.

	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}
$2hf'(x_i) =$		-1	0	1	
$h^2f''(x_i) =$		1	-2	1	
$2h^3f'''(x_i) =$	-1	2	0	-2	1
$h^4f''''(x_i) =$	1	-4	6	-4	1

$+ \quad O(h)^2$

(*a*) Representations of $O(h)^2$

	f_{i-3}	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	f_{i+3}
$12hf'(x_i) =$		1	-8	0	8	-1	
$12h^2f''(x_i) =$		-1	16	-30	16	-1	
$8h^3f'''(x_i) =$	1	-8	13	0	-13	8	-1
$6h^4f''''(x_i) =$	-1	12	-39	56	-39	12	-1

$+ \quad O(h)^4$

(*b*) Representations of $O(h)^4$

Fig. 3.4 Central difference representations.