

# Numerical PDE

Step 1: Numerical app. of  $u_{xx}$

$$u_t = c \cdot u_{xx} \quad \left. \begin{array}{l} u(x+\Delta x, t) - 2u(x, t) + u(x-\Delta x, t) \\ c \cdot \frac{(u(x+\Delta x, t) - 2u(x, t) + u(x-\Delta x, t))}{(\Delta x)^2} \end{array} \right\}$$

$$c \cdot u_{xx}(x, t) = u_t$$

Step 2: Solve ODEs for each fixed  $x_j$

$$\frac{d u(x_j, t)}{dt} = c \cdot \frac{u(x_m, t) - 2u(x_j, t) + u(x_l, t)}{(\Delta x)^2}$$

$$x_{j+1} \triangleq x_j + \Delta x$$

↑  
Backward Euler for stiff ODEs.

$$\dot{U} = \frac{c}{(\Delta x)^2} \cdot A U.$$

key: Numerical dif. | Comes from the definition

$$f'(x) \triangleq \lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \quad (*)$$

② Two choices

$$\left. \begin{array}{l} \Delta x > 0, \text{ write } \Delta x = h \\ \Delta x < 0, \text{ write } \Delta x = -h \end{array} \right\} \quad (*) \Rightarrow f'(x) \simeq \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{Forward difference}}$$

Best one =  $\frac{F+B}{2}$ .

$$f'(x) \simeq \frac{\frac{f(x+h) - f(x)}{h} + \frac{f(x) - f(x-h)}{h}}{2} \quad \xrightarrow{\text{L}} \text{Backward diff.}$$

$$\frac{f(x+h) - f(x-h)}{2h} : \text{Central diff.}$$

key: to understand the origin of

$$f'(x) \simeq \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \quad (*)$$

Example:  $f(x) = \sin x$ ,  $h = 0.1$ ,  $x = \frac{\pi}{4}$ . (Example: central diff is better!)

③ Explain why central diff is better?

$$\frac{u(x+ah) - u(x+bh)}{(a-b) \cdot h} \approx u'(x)$$

how to choose  $a, b$ ?

$$+ \frac{u'''(\xi)}{3!} h^3$$

$$u(x+\Delta x) = u(x) + u'(x) \cdot \Delta x + \frac{u''(\xi)}{2!} \Delta x^2 \quad \xi \in [x, x+\Delta x]$$

$$u(x+ah) = u(x) + u'(x) \cdot ah + \frac{u''(x)}{2!} (ah)^2 + \frac{u'''(x)}{3!} (ah)^3$$

$$u(x+bh) = u(x) + u'(x) \cdot bh + \frac{u''(x)}{2!} (bh)^2 + \frac{u'''(x)}{3!} (bh)^3$$

⇓

$$\frac{u(x+ah) - u(x+bh)}{(a-b)h} = u'(x) + \frac{u''(x)}{2} \frac{h^2 (atb) (atb)}{(atb)h} + \frac{O(h^3)}{(a-b) \cdot h}$$

|| when  $atb=0$

Only when  $a=-b$  (central diff),  
this term vanishes.

# Newton interpolation to explain formulas for $f^{(k)}(x)$

$$k=2$$

$$\begin{array}{c} x_0 \quad x_1 \quad x_2 \\ + \qquad + \\ x-h \quad x \quad x+h \end{array}$$

$$P_2(y) = \frac{f[x_0, x_1, x_2](y-x_0)(y-x_1)}{+ f[x_0, x_1](y-x_0)}$$

$$P_2(y) \sim f(y)$$

$$P_2''(y) \sim f''(y) \Rightarrow \left\{ \begin{array}{l} \text{Let } y=x \\ P_2''(x) \sim f''(x) \end{array} \right.$$

$$2 \underbrace{f[x_0, x_1, x_2]}_{!!}$$

$x_0$	$f(x_0)$
$x_1$	$\frac{f(x_1) - f(x_0)}{h}$
$x_2$	$f(x_2) - \frac{f(x_1) - f(x_0)}{h}$

$$\frac{\frac{f(x_2) - f(x_1)}{h} - \frac{f(x_1) - f(x_0)}{h}}{2h} = \frac{f(x_2) - 2f(x) + f(x_0)}{2h^2} //$$

Example ( $k=3$ )

$f'''(x)$  (4 points)

(5)



$$P_3(y) = f[x-2h, x-h, x+h, x+2h] y^3$$

$$\underline{f'''(x) - P_3'''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}$$

$$\underline{\text{Error estimate } f'''(x) - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}$$

$$\underline{e_2(x) = -\frac{f^{(4)}(\sigma)}{12} h^2, \quad \sigma \in [x-h, x+h]}$$

Proof: Taylor expansion

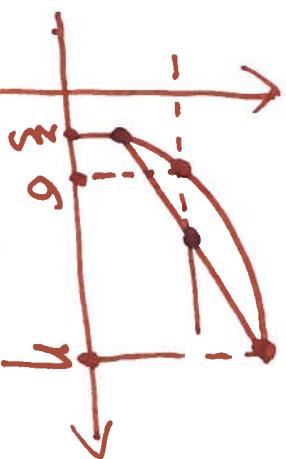
$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{3!} + \frac{f^{(4)}(\xi)}{24}h^4 \\ f(x-h) &= f(x) - f'(x)h + f''(x)\frac{h^2}{2} + \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(n)}{24}h^4 \end{aligned}$$

$$\begin{aligned} \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} &= f''(x) + \left( \frac{f^{(4)}(\xi)}{24} + \frac{f^{(4)}(\eta)}{24} \right) h^2 \\ &= f''(x) + \frac{f^{(4)}(\sigma)}{12} \cdot h^2 \quad \# \end{aligned}$$

Rolle theorem.

Write  $g(y) = f^{(4)}(y)$

$$\frac{g(\xi) + g(\eta)}{2} = g(\sigma) \quad \sigma \in [\xi, \eta]$$



Remark :  $|f^{(4)}(\sigma)| \leq 1$ , for all  $\sigma \in [x-h, x+h]$ .



$$|c_2| \leq \frac{h^2}{12}$$

Application : Boundary value problem for ODEs

(7)

$$\frac{u'' + p(x)u' + q(x)u}{u(b)} = r(x), \quad x \in [a, b]$$

$$u(a) = u_a, \quad u(b) = u_b$$

$$x_0 \leftarrow h \rightarrow x_1 \leftarrow h \rightarrow x_2$$

$$h = \frac{b-a}{2}$$

$$\frac{a+b}{2} \quad b$$

Numerical value for  $u(\frac{a+b}{2})$ : aim

Idea: Equation at  $x = \frac{a+b}{2}$  gives

$$u''(x_1) + \frac{p(x_1)u'(x_1)}{h} + q(x_1)u(x_1) = r(x_1)$$

Central diff.

$$\frac{u(x_0) - 2u(x_1) + u(x_2)}{h^2} - p(x_1) \cdot \frac{u(x_2) - u(x_0)}{2h} = p(x_1) \frac{u_b - u_a}{2h}$$

|| Solve  $u(x_1)$ :

$$\frac{u_a - 2u(x_1) + u_b}{h^2} + p(x_1) \frac{u_b - u_a}{2h} + q(x_1)u(x_1) = r(x_1)$$

(8)

$$\left( \frac{-2}{h^2} + g(x_1) \right) u(x_1) = \left( \text{known terms} = r(x_1) - \frac{u_a + u_b}{h^2} - \frac{p(x_1) u_b - u_a}{2h} \right)$$

when  $h$  is small  $g(x_1) < \frac{2}{h^2} \Rightarrow \frac{-2}{h^2} + g(x_1) \neq 0$

~~so it's OK~~  $\Downarrow$

Summary : We can get the value at  $x_1$

$$u(x_1) = \frac{\text{known terms}}{\frac{-2}{h^2} + g(x_1)}$$

Recall:

$$\left\{ \begin{array}{l} u'' + p(x)u' + q(x)u = r(x) \quad x \in [a, b] \\ u(a) = u_a, \quad u(b) = u_b. \end{array} \right. \quad \textcircled{1}$$

Idea:

$$\left\{ \begin{array}{l} u'(x) = \frac{u(x+h) - u(x-h)}{2h} - \frac{h^2}{6} f'''(\xi), \exists \xi \in [x-h, x+h] \\ (*) \quad u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi), \exists \xi \in [x-h, x+h]. \end{array} \right.$$

$x_0 \quad x_1 \quad x_2 \dots \quad x_{N-1} \quad x_N$   $\rightarrow O(h^2)$

Step 1:

$a \xleftarrow[h=\frac{b-a}{N}]{} x_j = a + jh \xrightarrow[0 \leq j \leq N]{} b$

Step 2: Use (\*) to each  $1 \leq j \leq N-1$

$$\frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2} + p(x_j) \frac{u(x_{j+1}) - u(x_{j-1})}{2h} + q(x_j) u(x_j) + O(h^2) = r(x_j), \quad 1 \leq j \leq N-1$$

Step 3: Ignore  $O(h^2)$ , write  $u(x_j)$  as  $U_j$

$$\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + p(x_j) \frac{U_{j+1} - U_{j-1}}{2h} + q(x_j) U_j = r(x_j) \quad (**)$$

$1 \leq j \leq N-1$

$$\left. \begin{array}{l} U_0 = u_a \\ U_N = u_b \end{array} \right\} : \text{boundary conditions.}$$

$(**)$   $\Leftrightarrow$  our equation ① up to an  $O(h^2)$  error

$$\text{so } U_j \sim u(x_j)$$

Remark

$$(**) \Leftrightarrow \boxed{\left(1 + \frac{h}{2} p(x_j)\right) U_{j+1} + \underbrace{\left(g(x_j)h^2 - 2\right) U_j}_{d_i} + \underbrace{\left(1 - \frac{h}{2} p(x_j)\right) U_{j-1}}_{V_j} = h^2 r(x_j).}$$

Step 4. Solve

$$\left[ \begin{array}{ccc|c} 1 & 0 & & 0 \\ v_1 & d_1 & w_1 & \\ v_2 & d_2 & w_2 & \\ \vdots & \vdots & \vdots & \vdots \\ 0 & v_{N+1} & d_{N+1} & w_{N+1} \\ 0 & 0 & 1 & 1 \end{array} \right] \left[ \begin{array}{c} u_0 \\ \vdots \\ u_N \\ \end{array} \right] = \left[ \begin{array}{c} u_a \\ h^2 r(x_1) \\ \vdots \\ h^2 r(x_{N+1}) \\ u_b \end{array} \right].$$

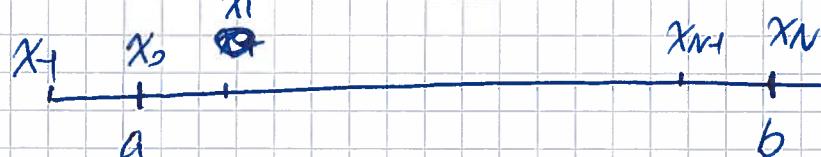
$A \cdot U = b$

$(N+1)$ -equations

Other boundary conditions

$$\left. \begin{array}{l} u'' + p(x)u' + q(x)u = r(x) \\ u'(a) = u_a, \quad u(b) = u_b \end{array} \right\}$$

Idea: Add  $u(x_1)$



Get  $N+2$  equations

$$\left. \begin{array}{l} \frac{U_1 - U_1}{2h} = u_a' \\ \frac{U_1 - 2U_0 + U_1}{h^2} + p(x_0) \frac{U_1 - U_1}{2h} + q(x_0) U_0 = r(x_0) \\ \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + p(x_j) \frac{U_{j+1} - U_{j-1}}{2h} + q(x_j) U_j = r(x_j) \\ U_N = u_b \end{array} \right\} \quad 1 \leq j \leq N-1$$

See the example 2 (page 6) in the Jupyter notes.

## Heat equation:

$$\left. \begin{array}{l} u_t = \frac{1}{2} u_{xx} \quad (1) \quad 0 \leq x \leq \pi \\ u(0, t) = g_0(t), \quad u(\pi, t) = g_1(t) \quad \text{Boundary conditions} \\ u(x, 0) = f(x) \quad \text{initial condition} \end{array} \right\}$$

Solve the equation from  $t=0$  to  $t=t_{\text{end}}$

Step 1:  $\Delta x := \frac{\pi}{M}, \quad x_j := j \cdot \Delta x \quad 0 \leq j \leq M.$

Step 2: (1)  $\Leftrightarrow \frac{\partial u(x_j, t)}{\partial t} = \frac{1}{2} \cdot \frac{u(x_{j+1}, t) - 2u(x_j, t) + u(x_{j-1}, t)}{(\Delta x)^2} + O(\Delta x^2)$

Step 3: Ignore  $O(\Delta x^2)$  ~~then~~ gives  
replace  $u(x_j, t)$  by  $U_j(t)$

$$\Rightarrow U_j'(t) = \frac{1}{2} \frac{U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)}{(\Delta x)^2} \quad \left. \begin{array}{c} 1 \leq j \leq M-1 \\ U_0(t) = g_0(t) \\ U_M(t) = g_1(t) \end{array} \right\}$$

input

Get  $M-1$  ODEs on  $U_1, \dots, U_{M-1}$ .

$$\left. \begin{array}{l} U_1' = \frac{1}{2} \frac{U_2 - 2U_1 + g_0(t)}{(\Delta x)^2} \\ U_j' = \frac{1}{2} \frac{U_{j+1} - 2U_j + U_{j-1}}{(\Delta x)^2} \quad 2 \leq j \leq M-2 \\ U_{M-1}' = \frac{1}{2} \frac{g_1(t) - 2U_{M-1} + U_{M-2}}{(\Delta x)^2} \end{array} \right\}$$

Step 4: Solve (\*) using backward Euler

$$(*) \Leftrightarrow \vec{U}' = \vec{f}(t, \vec{U}) \cdot \frac{1}{2(\Delta x)^2}$$

$$\vec{U}(0) = (f(x_1), \dots, f(x_{M-1}))^T \quad \text{initial condition}$$

$$\vec{U}^n = \vec{U}^0 + \Delta t \cdot \frac{\vec{f}(t, \vec{U}^n)}{2(\Delta x)^2}$$

Example:  $g_0(t) = g_1(t) = 0$

$$u(x, 0) = f(x) = \begin{cases} x & 0 \leq x \leq \frac{\pi}{2} \\ \pi - x & \frac{\pi}{2} < x \leq \pi \end{cases}$$

sine

The exact solution is given by the Fourier series of  $f$ , but not precise!

$$M=4, t_{\text{end}}=1, \Delta x = \frac{\pi}{4}, \Delta t = \frac{1}{20}, N=20$$

$$\left. \begin{array}{l} U_1' = \frac{1}{2} \frac{U_2 - 2U_1}{(\Delta x)^2} \\ U_2' = \frac{1}{2} \frac{U_3 - 2U_2 + U_1}{(\Delta x)^2} \\ U_3' = \frac{1}{2} \frac{-2U_3 + U_2}{(\Delta x)^2} \end{array} \right\}$$

$$\left( \begin{array}{l} U_1 \\ U_2 \\ U_3 \end{array} \right)' = \frac{1}{2(\Delta x)^2} \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix} \left( \begin{array}{l} U_1 \\ U_2 \\ U_3 \end{array} \right)$$

$$\left( \begin{array}{l} U_1 \\ U_2 \\ U_3 \end{array} \right)(0) = \left( \begin{array}{l} f\left(\frac{\pi}{4}\right) \\ f\left(\frac{2\pi}{4}\right) \\ f\left(\frac{3\pi}{4}\right) \end{array} \right) = \left( \begin{array}{l} \frac{\pi}{4} \\ \frac{\pi}{2} \\ \frac{3\pi}{4} \end{array} \right) \stackrel{\text{def}}{=} \vec{U}^0$$

$$\vec{U}' = \vec{U}^0 + \Delta t \cdot \frac{1}{2(\Delta x)^2} A \cdot \vec{U}^0 : \text{backward Euler} \quad (A \text{ not stable})$$

$$\vec{U}' = \vec{U}^0 + \Delta t \cdot \frac{1}{2(\Delta x)^2} A \cdot \vec{U}^0 : \text{Euler (NOT A-stable)}$$

$$\text{Crank-Nicolson: } \vec{U}' = \vec{U}^0 + \frac{\Delta t}{2(\Delta x)^2} \frac{1}{2} (A\vec{U}' + A\vec{U}^0) : (A\text{-stable})$$

## Stability analysis for Euler.

Euler of stability function  $R_E = 1 + \lambda$

stability interval  $|1 + \lambda| \leq 1$



$$-2 \leq \lambda \leq 0$$

Need eigenvalue of  $\frac{\Delta t}{2(\Delta x)^2} A$  lies in  $[-2, 0]$

$$A - \lambda I_3 = \begin{pmatrix} -2-\lambda & 1 & 0 \\ 1 & -2-\lambda & 1 \\ 0 & 1 & -2-\lambda \end{pmatrix}$$

$$\det(A - \lambda I_3) = (-2-\lambda)((-2-\lambda)^2 - 1)$$

$$= (-2-\lambda)(\lambda^2 + 4\lambda + 3 - 1)$$

$$= -(\lambda+2)(\lambda^2 + 4\lambda + 2)$$

$$\lambda = -2$$

$$\lambda = \frac{-4 \pm \sqrt{16-8}}{2} = -2 \pm \sqrt{2}$$



Need

$$\lambda \frac{\Delta t}{2(\Delta x)^2} \in [-2, 0)$$



Need

$$(2+\sqrt{2}) \frac{\Delta t}{2(\Delta x)^2} < 2 \quad (**)$$

Example:  $\Delta t = \frac{1}{20}$ ,  $\Delta x = \frac{1}{4}$  satisfies (\*\*)

(optional) (The remaining part is not related to exam!)

## Eigentheory for

$$\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & 0 \\ & 1 & -2 & 1 \\ 0 & & 1 & -2 \end{pmatrix} = \begin{pmatrix} -2 & & 0 & \\ & 0 & & \\ & & 2 & \\ & & & 2 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Denote by  $A_n$  an  $(n \times n)$  matrix of the following form

$$\begin{pmatrix} 0 & 1 & & 0 \\ 1 & 0 & 1 & 0 \\ & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix} \quad A_1 = (0), \quad A_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\lambda \cdot \text{id} - A_n = \begin{pmatrix} \lambda & -1 & & \\ -1 & \lambda & -1 & \\ & -1 & \lambda & -1 \\ & & -1 & \lambda \end{pmatrix}$$

Def:  $f_n(\lambda) := \det(\lambda \cdot \text{id} - A_n)$ ,  $f_0(\lambda) \equiv 1$

$$\left. \begin{array}{l} f_1(\lambda) = \lambda \\ f_2(\lambda) = \lambda^2 - 1 \\ f_n(\lambda) = \lambda f_{n-1}(\lambda) - f_{n-2} \end{array} \right\} \Rightarrow \begin{array}{l} f_3(\lambda) \\ = \lambda^3 - \lambda - \lambda \\ = \lambda^3 - 2\lambda \end{array}$$

Theorem:  $f_n(2 \cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta}$

Proof:  $n=0, 1, \dots, k+1 \checkmark$   $\sin 2\theta = \sin \theta \cdot 2 \cos \theta$

Assume  $n=0, \dots, k+1 \checkmark$ .

$$\begin{aligned} f_k(2 \cos \theta) &= 2 \cos \theta \frac{\sin k \theta}{\sin \theta} - \frac{\sin(k+1)\theta}{\sin \theta} && \left| \begin{array}{l} \sin(k-1)\theta \\ \vdots \\ \sin(k+1)\theta \\ - (k+1)\theta \sin \theta \end{array} \right. \\ &= \frac{2 \cos \theta \sin k \theta + (k+1) \sin \theta}{\sin \theta} \\ &= \frac{\sin(k+1)\theta}{\sin \theta}. \quad \times \end{aligned}$$

Def.: chebyshew polynomial of the second kind

$U_n$ : degree  $n$  polynomial s.t.

$$U_n(x) = f_n(2x).$$

Remark. Iteration formula for  $f_n$  gives

$$\left. \begin{array}{l} U_0(x) \equiv 1, \quad U_1(x) \equiv 2x \\ U_n(x) = 2x U_{n-1}(x) - U_{n-2} \end{array} \right\}$$

$$U_n(1 \circ \sin \theta) = \frac{\sin((n+1)\theta)}{\sin \theta}$$

Zeros of  $f_n(\lambda)$ :

$$f_n(1 \circ \sin \theta) = \frac{\sin((n+1)\theta)}{\sin \theta} = 0$$

$$\Leftrightarrow \begin{cases} (n+1)\theta = k\pi & k=1, 2, \dots \\ \sin \theta \neq 0 & n \end{cases}$$



$$\Leftrightarrow \theta = \frac{k\pi}{n+1} \quad k=1, 2, \dots, n$$

$$\boxed{| f_n(\lambda) = 0 \text{ for } \lambda = 1 \circ \sin \frac{k\pi}{n+1}, \quad (1 \leq k \leq n)}$$

Remark, These are all ~~roots~~ roots of  $f_n$  (since  $\deg(f_n) = n$ )

Summary: Eigenvalues for  $A_n$  are  $1 \circ \sin \frac{k\pi}{n+1}$ , ( $1 \leq k \leq n$ )

for  $-2 + A_n$  are

$$2 \left( 1 \circ \sin \frac{k\pi}{n+1} - 1 \right)$$

$$-4 \sin \frac{k\pi}{2(n+1)}$$

$$(1 \leq k \leq n).$$

End of the course!