01/13/2026.

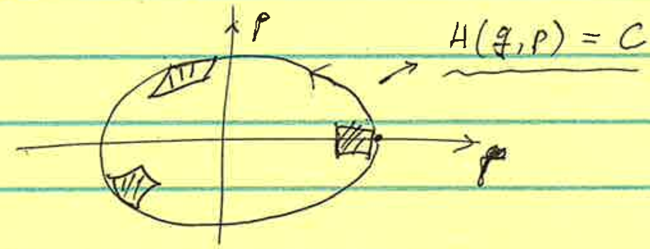
- Reading

- Hamiltonian System. ($q \in \mathbb{R}^n$, $p \in \mathbb{R}^n$)

$$\ddot{x} = -\nabla V(x) \quad \rightarrow \quad \dot{q} = p \qquad (q = x) \rightarrow H(q,p) = \frac{p^2}{2} + V(q)$$

$$\dot{p} = -\nabla U(q)$$

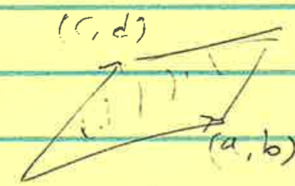
$$\boxed{\begin{cases} \dot{q} = \nabla_p H \\ \dot{p} = -\nabla_q H \end{cases}}$$



① $\frac{d}{dt} H = dH/dt = \nabla_q H \, \dot{q} + \nabla_p H \, \dot{p} = 0$.

$\Rightarrow$ H = constant. ($dH/dt = 0$)

② Infinitesimal square's area is preserved.

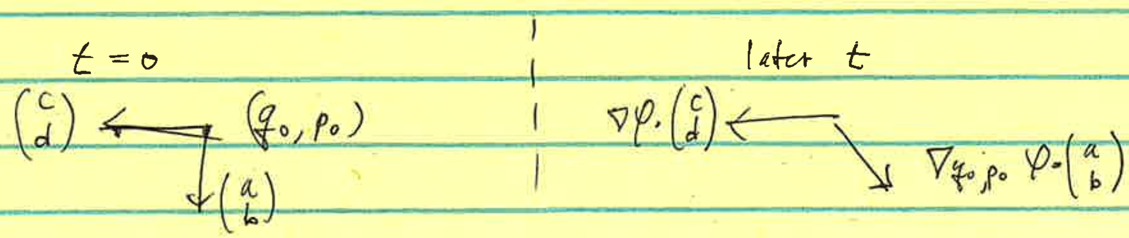


$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \qquad \text{E.g.)} \quad [a, b] \, J \begin{bmatrix} c \\ d \end{bmatrix} = ad - bc = \text{Area.}$$

Define. $\varphi(t) : \begin{bmatrix} q_0 \\ p_0 \end{bmatrix} \rightarrow \begin{bmatrix} q(t) \\ p(t) \end{bmatrix}$

What is $\nabla_{(q_0, p_0)} \varphi(t)$? (Jacobian)

$$= \begin{bmatrix} \partial q / \partial q_0 & \partial q / \partial p_0 \\ \partial p / \partial q_0 & \partial p / \partial p_0 \end{bmatrix}$$



$t = 0$, area $= \begin{pmatrix} a \\ b \end{pmatrix}^T J \begin{pmatrix} c \\ d \end{pmatrix}$

t, area $= \left(\nabla\varphi \cdot \begin{pmatrix} a \\ b \end{pmatrix}\right)^T J \cdot \left(\nabla\varphi \cdot \begin{pmatrix} c \\ d \end{pmatrix}\right)$

$= \begin{pmatrix} a \\ b \end{pmatrix}^T \nabla\varphi^T \cdot J \, \nabla\varphi \cdot \begin{pmatrix} c \\ d \end{pmatrix}$

Shows: $J = \nabla\varphi^T J \nabla\varphi$. (Idea: At $t=0$, $\nabla\varphi = I \to$ True. show that $d/dt\,(\nabla\varphi J \nabla\varphi - J) = 0$)

Define: φ is called symplectic if $J = (\nabla\varphi)^T J (\nabla\varphi)$

Claim: $\varphi(t)$ defined above from $H(q,p)$ is symplectic.

$$d/dt\, \varphi(t, q_0, p_0) = \begin{pmatrix} d/dt\, q(t) \\ d/dt\, p(t) \end{pmatrix} = \begin{pmatrix} H_p \\ -H_q \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} H_q \\ H_p \end{pmatrix} = J \nabla H$$

$\Rightarrow \quad d/dt\, \varphi = J \nabla H$

$\Rightarrow \quad \frac{d}{dt} \nabla_{p_0, q_0} \varphi = J \nabla^2 H(\varphi) \cdot \nabla\varphi$

Recall, $d/dt\,(\nabla\varphi^T J \nabla\varphi - J) = \left(\frac{d}{dt}\nabla\varphi\right)^T J \nabla\varphi + (\nabla\varphi)^T J \cdot \frac{d}{dt}\nabla\varphi$

$$= \nabla\varphi^T \nabla^2 H \underbrace{\overset{J^T}{(-J)}\, J}_{=-I} \nabla\varphi + \nabla\varphi^T \underbrace{J J}_{=I} \nabla^2 H \nabla\varphi$$

$= 0$

- $H(q,p)$ is preserved
- J is preserved + volume form preserved in $\mathbb{R}^{2d}$

$\Rightarrow \quad e^{-\beta H(q,p)}\, dVol$ is preserved. (Boltzmann Distribution).

- Design numerical schemes.

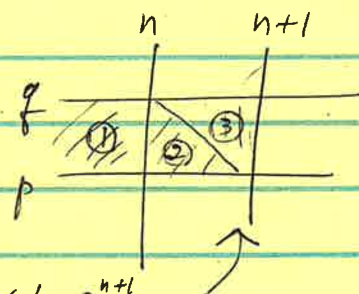
$$\left\{ \begin{array}{l} \dot{q} = H_p \\ \dot{p} = -H_q \end{array} \right\}$$

Euler, RK4 : (1) H not preserved (MD timestep)

(2) $\nabla \varphi^T J \nabla \varphi$ not preserved (MD density)

1) Euler-B

Δt = timestep size $= h$.

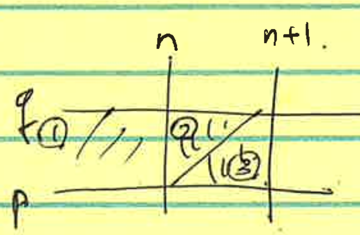


$$q^{n+1} = q^n + \Delta t \, H_p(q^n, p^{n+1})$$
$$p^{n+1} = p^n - \Delta t \, H_q(q^n, p^{n+1})$$

E.g.) $H_p = p$ $\qquad \Rightarrow \qquad q^{n+1} = q_n + \Delta t \, p^{n+1}$

$H_q = \nabla_q V(q)$ $\qquad p^{n+1} = p_n - \Delta t \, \nabla_q V(q^n)$

2) Euler-A



$$q^{n+1} = q^n + \Delta t \, H_p(q^{n+1}, p^n)$$
$$p^{n+1} = p^n + \Delta t(-H_q(q^{n+1}, p^n))$$

Eg) $\Rightarrow \quad q^{n+1} = q_n + \Delta t \, p^n$

$p^{n+1} = p_n - \Delta t \, \nabla_q V(q^{n+1})$

- How Euler preserves (1) and (2).

- Error of Euler - A/B $(O(h))$ $\qquad$ $\dot{x} = Ax \rightarrow e^{hA}x$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\dot{x} = Bx \rightarrow e^{hB}x$

$$H(q,p) = \underbrace{p^2/2}_{A} + \underbrace{V(q)}_{B}$$

$$e^{h(A+B)} \approx e^{hA} \cdot e^{hB} \quad \text{if don't commute } (AB \neq BA)$$
$$\cong \left(I + hA + \frac{h^2}{2}A^2\right)\left(I + hB + \frac{h^2}{2}B^2\right)$$
$$= I + h(A+B) + \frac{h^2}{2}\left(A^2 + B^2 + 2AB\right)$$

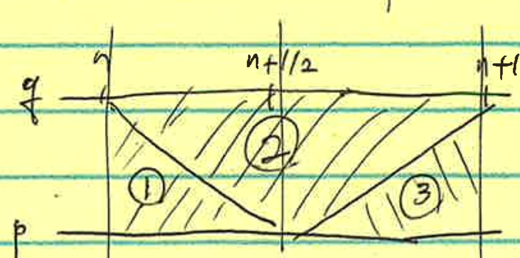
This is caused by having $e^{hA} \cdot e^{hB}$. $e^{hB} \cdot e^{hA}$

$$\Rightarrow \ 1/h \cdot O(h^2) = \underline{O(h)}$$

- Solution to $O(h)$ $\qquad$ 'strong' splitting.
$$e^{h(A+B)} = e^{\frac{h}{2}B} \cdot e^{hA} \cdot e^{\frac{h}{2}B} + O(h^3)$$

$$H(q,p) = \underbrace{p^2/2}_{H^1} + \underbrace{V(q)}_{H^2} \Rightarrow \begin{array}{l} H^2 \text{ for } \Delta t/2 \\ H^1 \text{ for } \Delta t \\ H^2 \text{ for } \Delta t/2 \end{array}$$

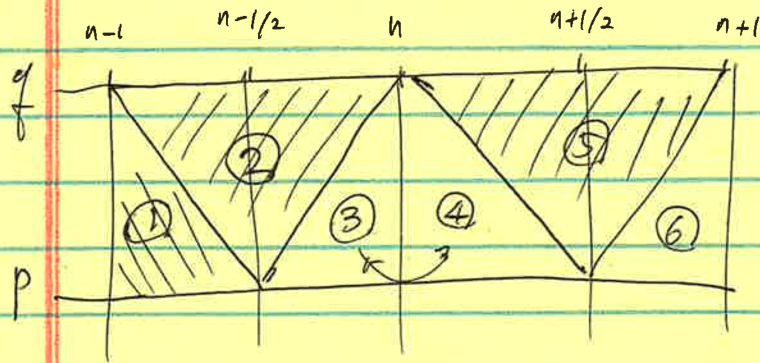
$H^2(q,p) = V(q)$	$H^1(q,p) = p^2/2$
$q \leftarrow q^n + \frac{\Delta t}{2} \cdot 0$	$q \leftarrow q^n + hp^n$
$p \leftarrow p^n - \frac{\Delta t}{2} \cdot V(q^n)$	$p \leftarrow p^n + \frac{\Delta t}{2} \cdot 0$



① : $p^n - \frac{\Delta t}{2} V(q^n) = p^{n+1/2}$

② $q^n + h\, p^{n+1/2} = q^{n+1}$

③ $p^{n+1/2} - h\, V(q^{n+1}) = p^n$



③ + ④ merged.

$$\Rightarrow \begin{cases} p^{n+1/2} = p^{n-1/2} - \Delta t \; \nabla_q V(q^n) \\ q^{n+1} = q^n + h \, p^{n+1/2} \end{cases}$$ Velocity - verlet.

staggered!

- Energy conservation. and J preservation.

1) J conservation.

Euler-β) $q^{n+1} = q^n + \Delta t \, p^n$

$p^{n+1} = p^n - \Delta t \, V_q(q^n)$

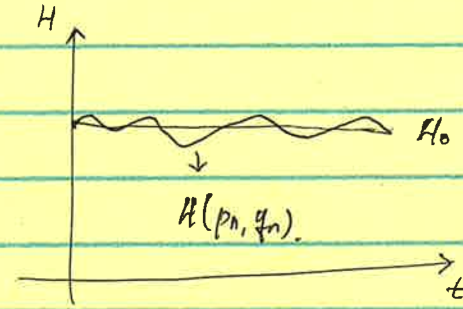
Infinitesimal map, $\varphi_n : \begin{pmatrix} q \\ p \end{pmatrix} \rightarrow \begin{pmatrix} \tilde{q} \\ \tilde{p} \end{pmatrix}$ where $\begin{pmatrix} \tilde{q} = q + \Delta t \, p \\ \tilde{p} = p - \Delta t \cdot V_q(\tilde{q}) \end{pmatrix}$

$$\nabla_h \varphi = \begin{array}{c c} & \begin{array}{cc} q & p \end{array} \\ \begin{array}{c} \tilde{q} \\ \tilde{p} \end{array} & \begin{pmatrix} 1 & \Delta t \\ -\Delta t V_{qq} & 1 - \Delta t^2 V_{qq} \end{pmatrix} \end{array}$$

$$(\nabla_h \varphi)^T J (\nabla_h \varphi) = J \quad \#$$

01/15/2026.

- Symplectic Integrators



	preserve J	preserve H	order
Euler A	o	o	$O(h^1)$
Euler B	o	o	$O(h^1)$
Verlet	o	o	$O(h^2)$

Preserves $\tilde{H}_n$ which is close enough to H

- Consider $H(q, p) = \frac{1}{2} p^2 + \frac{1}{2} q^2$, $V(q) = \frac{1}{2} q^2$

  〃 Verlet, $p_{n+1/2} = p_{n-1/2} - \Delta t\, q_n$

$$q_{n+1} = q_n + \Delta t\, p_{n+1/2}$$

Define, $\tilde{H}_n = \frac{1}{2}\left(p_{n-1/2}^2 + q_n^2 - \Delta t\, p_{n-1/2} q_n \right)$

Then, $\tilde{H_n} = \tilde{H_{n+1}}$

(pf) $2\tilde{H_n} = p_{n-1/2}^2 + q_n^2 - \Delta t\, p_{n-1/2} q_n = p_{n+1/2}^2 + q_n q_{n+1}$

$2\tilde{H_{n+1}} = p_{n+1/2}^2 + q_{n+1}^2 - \Delta t\, p_{n+1/2} q_{n+1} =$ 〃 #

Define. $H_n = \frac{1}{2}\left(q_n^2 + p_{n-1/2}^2 \right)$

$H_n \longrightarrow H_m$
$\tilde{H_n} \longrightarrow \tilde{H_m}$ } show; $|H_n - H_m|$ is bounded

$$|H_n - H_m| \leq |H_n - \tilde{H_n}| + |\tilde{H_m} - H_m| + \underbrace{|(\tilde{H_n} - \tilde{H_m})|}_{= 0 \text{ by (pf)}}$$

$$p_{n-1/2}^2 + q_n^2 - \Delta t\, p_{n-1/2}\, q_n \geq (2-\Delta t)\, p_{n-1/2} \cdot q_n \quad \text{(cauchy-schwartz)}$$

$$\Rightarrow \quad \Delta t\, p_{n-1/2}\, q_n \leq \frac{\Delta t\, \tilde{H_n}}{2-\Delta t} \quad (1) \quad = \frac{\Delta t\, \tilde{H_0}}{2-\Delta t}$$

Similarly,

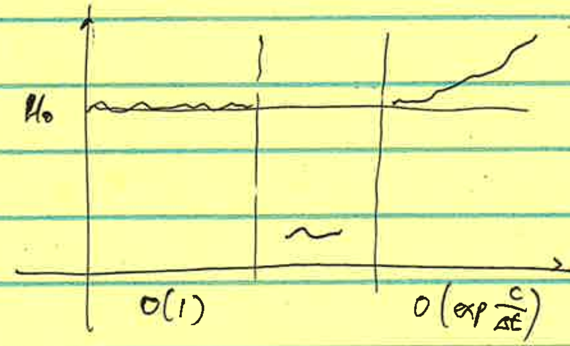
$$\Delta t\, p_{m-1/2}\, q_m \leq \frac{\Delta t\, \tilde{H_m}}{2-\Delta t} \quad (2) \quad = \frac{\Delta t\, \tilde{H_0}}{2-\Delta t}$$

$$\therefore \underline{\left| H_n - H_m \right| \leq \frac{\Delta t}{2-\Delta t} \tilde{H_0}} \quad \text{always bounded.}$$

- For $H(q,p) = \frac{p^2}{2} + V(q)$

$$\left| H(q^n, p^{n-1/2}) - H_0 \right| \leq O(\Delta t)$$

for a long time, $\equiv \exp\left(\frac{c}{\Delta t}\right)$



- PDE (elliptic)

$$\begin{cases} -u'' = f & (x \in \Omega) \\ u(0) = u_0 & \\ u(1) = u_1 & \end{cases} \longleftrightarrow \quad \begin{aligned} -u'' &= f & \underset{\approx}{x} \in \Omega \\ u(\underset{\approx}{x}) &= b(\underset{\approx}{x}) & \underset{\approx}{x} \in \partial\Omega \end{aligned}$$

- Maximum principle $(f=0)$

  " The $\frac{\text{max}}{\text{min}}$ value has to be on the bdry "

$f < 0$

The max is on bdry

$f \geq 0$

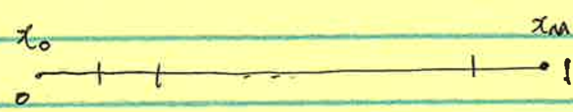
The min is on bdry.

• Elliptic

$$u = e^{i(\xi x + \eta y)} \to \left.\begin{aligned} u_{xx} &= -\xi^2 u \\ u_{yy} &= -\eta^2 u \end{aligned}\right\} \to -u'' = \underbrace{(\xi^2+\eta^2)}_{①} u$$

$$①:\ \left.\begin{aligned} &\xi^2+\eta^2 \to \text{elliptic} \\ &\xi^2-\eta^2 \to \text{hyperbolic} \\ &\xi-\eta^2 \to \text{parabolic.} \end{aligned}\right\}$$

• Numerical methods



$x_i = i \cdot h,$

$h = 1/M$

Find $U_j = u(x_j)$, $^{(1)}\ u_0 = u_L$ and $^{(2)}\ u_M = u_R$ (B.C.s).

(3) $$-\frac{U_{j+1} + U_{j-1} - 2U_j}{h^2} = f_j \quad \text{(finite difference)}$$

(4) Taylor expansion

How accurate? (sampling $U_j = u(x_j)$)

$$\left.\begin{aligned} &\text{FD} \quad \partial U_j \sim u'(x_j) \\ &\text{BD} \quad \bar{\partial} U_j \sim u'(x_j) \\ &\text{CD} \quad \hat{\partial} U_j \sim u'(x_j) \\ &\text{CD 2nd} \quad \partial\bar{\partial} U_j \sim u''(x_j) \end{aligned}\right\}$$

Thm. $|\bar{\partial} u_j - u'(x_j)| \leq C h^2 |u|_{C^3}$

$|\partial\bar{\partial} u_j - u''(x_j)| \leq C h^2 |u|_{C^4}$

$|u|_{C^4} = \max |u''''(x)|$.

Pf) $$\partial\bar{\partial} u_j = \frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2} \Rightarrow u(x_{j+1}) = u(x_j) + \cdots + u''''(x_j) \cdot h^4 \frac{1}{4!} + \cdots$$

$$u(x_{j+1}) = u(x_j) + h u'(x_j) + \cdots + \frac{h^4}{4!} \cdot u''''(\xi_+)$$
$$u(x_{j-1}) = u(x_j) - h u'(x_j) + \cdots + \frac{h^4}{4!} u''''(\xi_-)$$
$$\partial\bar{\partial} u_j = \frac{h^2 u'' + \frac{h^4}{12}\left[u''''(\xi_+) + u''''(\xi_-)\right]}{h^2} \qquad \text{(Taylor)}$$

$$\Rightarrow \quad |\partial\bar{\partial} u_j - u''(x_j)| \leq O(h^2)\, |u|_{C^4} \qquad \#$$

- Accuracy of finite difference.

$$\| U_j - u_j \| \leq O(h^2)$$

Discrete maximum principle. → " Our discretization preserves the continuous max principle "

Cont → $-u'' \leq 0$ (max is on bdry)

Disc →
$$\begin{bmatrix} -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & & \ddots & & \\ & & & -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} u_0 \\ \vdots \\ u_M \end{bmatrix} \leq 0$$

Show, $\max_j u_j = \max(V_0, V_M)$

Pf) $-u_{j-1} + 2u_j - u_{j+1} \leq 0$ for $\forall_j \quad 1 \leq j \leq M$

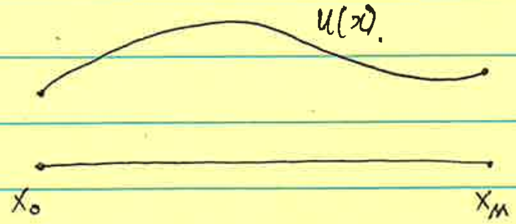
$$u_j \leq \frac{1}{2}\left(u_{j-1} + u_{j+1}\right) \quad \text{— (1)}$$

Suppose $j^* = \arg\max_j u_j$ → By (1), $u_j = \text{const}$.

∴ max has to be boundary.

01/20/2026.

- PDEs



Solve : $-u'' = f \qquad x \in (0,1)$

$u(0) = u_1, \quad u(1) = u_2$

$-\partial\bar{\partial}\, u(x_j) = f(x_j)$: Approx eqn. for exact sol.

$-\partial\bar{\partial}\, U_j = f_j$: Approx eqn. for approx sol.

$\downarrow$ Linear system. $AU = \tilde{F}$ $\qquad A = \begin{pmatrix} -1\ 2\ -1 & & \\ -1 & 2\ -1 & \\ & \ddots & \\ & & -1\ 2\ -1 \end{pmatrix}$

- Bound of $U_j - u_j$

Lemma 1 : Max. principle (discrete)

$\Omega = (0,1)$

$\bar{\Omega} = [0,1]$

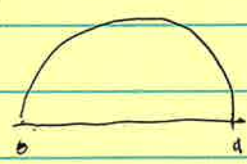
$|V|_\Omega = \max_{j,\, x_j \in \Omega} |V_j|$ (Def)

If $AV \le 0$, then $\max_j V_j = \max(V_0, V_M)$

$\Rightarrow |V|_{\bar{\Omega}} = \max_{j \in \bar{\Omega}} |V_j|$

Lemma 2 : $Az = g$, then $|z|_{\bar{\Omega}} \le \max(|z_0|, |z_M|) + 1/8 \cdot |g|_\Omega$

pf) $w(x) =$



$= \frac{1}{4} - (x - 1/2)^2, \quad (0 \le w(x) \le 1/4)$

$(W(x_j) = W_j, \quad W_0 = W_M = 0)$

Using $\| -\partial\bar{\partial} w - (\underbrace{-w''}_{=2}) \| \le C \cdot h^2 \max \overbrace{\|w''''\|}^{=0}$

$\therefore -\partial\bar{\partial} w = 2.$

Define $V^+ = z - \frac{1}{2} \overset{\overset{g}{\|}}{|Az|_\Omega} W$

Then, $AV^+ = Az - \frac{1}{2}|Az|_\Omega \cdot \underbrace{Aw}_{=2}$

$$= Az - |Az|_\Omega \le 0 \qquad (\because f - \max(f) \le 0).$$

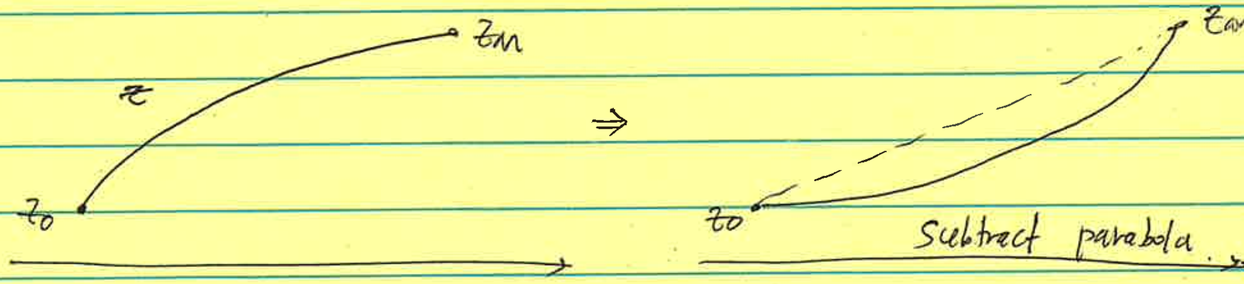
Now, use lemma 1 for $AV^+ \le 0 \Rightarrow V^+$ max on bdry.

$\Rightarrow V_j^+ \le \max(\underset{\overset{\|}{z_0}}{V_0^+}, \underset{\overset{\|}{z_M}}{V_M^+})$

$\Rightarrow z_j - \frac{1}{2}|Az|_\Omega w_j \le \max(z_0, z_M)$

$\Rightarrow z_j \le \max(z_0, z_M) + \frac{1}{2}|Az|_\Omega \underbrace{w_j}_{\le 1/4}$

$\therefore z_j \le \max(z_0, z_M) + 1/8 \cdot |Az|_\Omega$



Try : $V^- = -z - \frac{1}{2}|Az|_\Omega w$ for concave function.

$\Rightarrow -z_j \le \max(|z_0|, |z_M|) + \frac{1}{8} \cdot |Az|_\Omega$

$\therefore |z_j| \le \max(|z_0|, |z_M|) + \frac{1}{8}|Az|_\Omega$

Thm.

$$|U - u|_\Omega \le h^2 |u|_{C^4}$$

$$\shortparallel$$

$$\max_{x_j \in \Omega} |U_j - u(x_j)|$$

pf) $z_j = U_j - u(x_j)$ $\quad z_0 = 0, \; z_M = 0.$

$$Az = \underbrace{AU}_{\text{num.}} - \underbrace{Au}_{\text{exact.}} = f_j - \left(\frac{1}{h^2}\left(u_{j+1} + u_{j-1} - 2u_j\right)\right)$$

$$= f_j - \partial\bar{\partial} u_j$$

$$\left(\begin{aligned} &\text{Recall, } \|\partial\bar{\partial}u_j - u''(x_j)\| \le C \cdot h^2 |u|_{C^4} \\ &\Rightarrow Au_j = -u''(x_j) \pm Ch^2 |u|_{C^4} \\ &\qquad = +f_j \pm Ch^2 |u|_{C^4} \end{aligned}\right)$$

$$\Rightarrow Az_j = \cancel{f_j} - \cancel{f_j} + Ch^2 |u|_{C^4}$$

$$\Rightarrow |Az|_\Omega \le h^2 |u|_{C^4}$$

Using lemma 2,

$$|z|_{\bar{\Omega}} \le \underbrace{\max(|z_0|, |z_M|)}_{=0} + Ch^2 |u|_{C^4}$$

$$\therefore |z|_{\bar{\Omega}} \le Ch^2 |u|_{C^4}$$

- 2D problem.

$$-\Delta u = f \quad \text{in } (0,1)^2 = \Omega$$

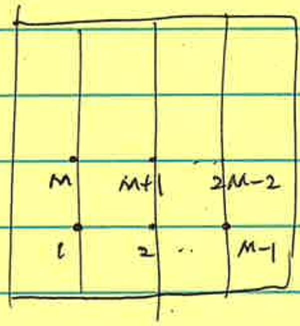
$$u = 0 \quad \text{for } x \in \partial\Omega$$

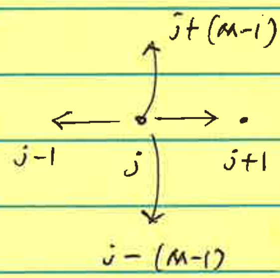
* Cont. max principle.

If $-\vec{\nabla} V \le 0$, $\Delta V \ge 0$, (on average, V bends up)

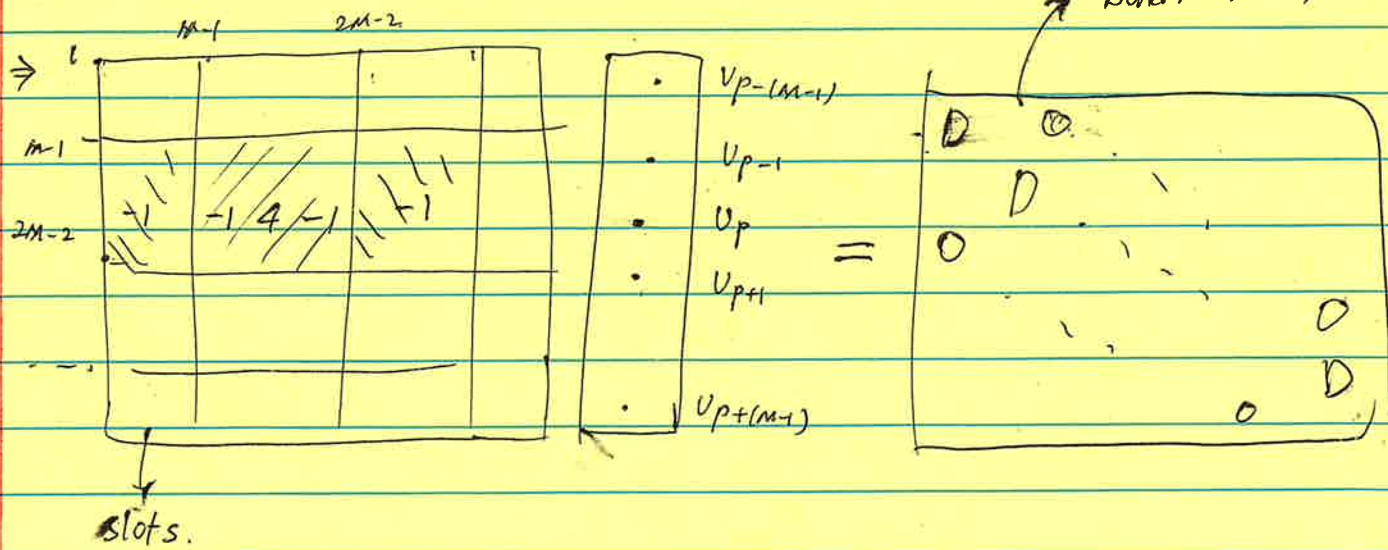
Then, $\max\limits_{x,y\in\Omega} (V(x,y)) = \max\limits_{x,y\in\partial\Omega} V(x,y)$

$$\partial\bar{\partial} U = \frac{U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} - 4U_{i,j}}{h^2} = -f_j$$





Sparse
sym
Band ~ 2M



$\Rightarrow$ Diagonal slots (D)

$$\begin{bmatrix} 4 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{bmatrix}$$

off diagonal slots (O)

$$\begin{bmatrix} -1 & & \\ & \ddots & \\ & & -1 \end{bmatrix}$$

Cost to solve matrix eq.

$$\text{Cost} \sim O(M^2 \cdot B^2) = O(\underbrace{M^4}_{(\# DOF)^2}) \quad (2D) \rightarrow \text{Comp. burden}$$

$$\text{cost} \sim O(M \cdot 2^2) = O(\underbrace{M}_{(\# DOF)^1}) \quad (1D)$$

Algorithms :

① Multi-frontal : reorder and LU $\sim O((\# DOF)^{3/2})$

② Iterative methods : Conjugate gradient + preconditioner
$\sim O(DOF)$

③ Fourier transform : $\sim O(DOF \cdot \log(DOF))$

- Discrete maximum principle.

If $(AV)_j \le 0$, then $|V|_{\bar{\Omega}} = |V|_{\partial\Omega}$

Pf). $\frac{1}{h^2}\left(4V_j + (-1)\cdot\{V_{j-e_1} \cdots V_{j+e_2}\}\right) \le 0$

$\Rightarrow V_j \le \frac{1}{4}\{V_{j-e_1} + \cdots + V_{j+e_2}\}$.

Let j_x be pt achieves max V_j value.

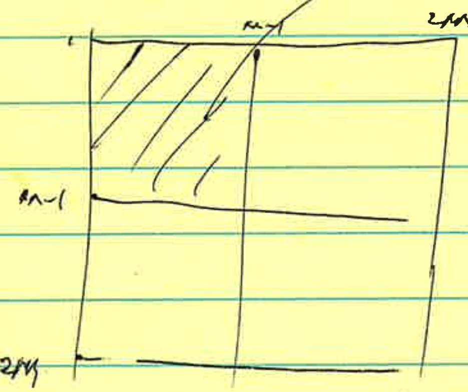
Then, $V_j = V$ all same $\rightarrow$ reach bdry.

- Finite Difference in 1D   01/22/2026.

$$AU = f \to U = A^{-1}f = Q\Lambda^{-1}\overset{O(M^2)}{Q^{-1}}f$$
$$= Q\Lambda^{-1}Q\,f$$

Note $\quad q_{jk} = C\cdot\sin\left(\pi jk/M\right) = C\cdot\sin\left(\frac{2\pi(jk)}{(2M)}\right)$
$$= C\,\mathrm{Im}\left\{e^{\frac{2\pi jk}{2M}}\right\}$$

Since $1 \le j,k \le M-1$



$\boxed{FFT}$: $O(M^2) \to O(M\cdot\log M)$

→ block padding ~ quantum algorithm's ?

Note : 1D is $O(M)$ but 2D ... $O(M^2)$
FFT is $\underline{O(M\log M)}$ regardless of dimension

- Finite Element methods (using functional analysis) ~ linear algebra.

$$V = \begin{pmatrix} V_{-\infty} \\ \vdots \\ V_{-1} \\ V_0 \\ V_1 \\ \vdots \\ V_{\infty} \end{pmatrix} \qquad f = \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix}$$

Linear functional :
$p : \mathbb{R}^n \to \mathbb{R}$ $(p^T x)$
$L : \mathbb{R}^n \to \mathbb{R}^n$ (Mx)

Linear algebra :
$p : V \to \mathbb{R}$
$L : V \to V$

Bilinear form :
$\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$
$B(x,y) \to$ scalar
$(x^T B y)$

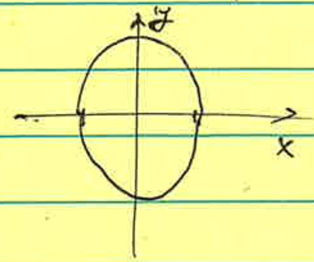
→ Sym. pos. Def.
$x^T B x > 0$

- Functional analysis (continued)

For any B S.P.D., $\|x\|_B = (x^T B x)^{1/2}$ is a norm.

E.g.)

$$B = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix},$$



$f(x)$ on Ω, $B = I$, $\mathbb{I}(f, g) = \int_\Omega f(x) \cdot 1 \cdot g(x) \cdot dx$.

$$= \begin{pmatrix} & f(x) & \end{pmatrix} \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & \ddots \; 1 \end{pmatrix} \begin{pmatrix} g(x) \end{pmatrix} \quad \#$$

$$I(x) = \left\{ \int f(x)^2 \, dx \right\}^{1/2}$$

- B is a "kernal"

$$\|f\|_B = \left\{ \iint_\Omega f(x) \; k(x,y) \, g(y) \; dx \, dy \right\}^{1/2}$$

- Hilbert space $\underline{(V, B)}$ pair s/t
  1. V is abstract vector space
  2. B is SPD in V
  3. V complete w.r.t B

     $(f_1, \dots f^n)$

     If f^n is cauchy sequence,

     the limit is in V.

$\|x\|_A = \sqrt{x^T A x}$ can find $C_{AB} > 0$, $D_{AB} > 0$ s.t

$\|x\|_B = \sqrt{x^T B x}$

$$C \|x\|_B \le \|x\|_A \le D \|x\|_B$$

↘ Wrap ellipse.

Hilbert $\mathbb{R}^{\mathbb{Z}}$ $x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \infty \end{pmatrix}$

$$A = \begin{pmatrix} 1 & & & \\ & 2 & & \\ & & 3 & \\ & & & \ddots \end{pmatrix}, \quad B = \begin{pmatrix} 1 & & & \\ & 1/2 & & \\ & & 1/3 & \\ & & & \ddots \end{pmatrix}$$

In this case we can't find $C\,\|x\|_B \le \|x\|_A \le D\,\|x\|_B$

$\because$ $M \cdot x$ and $1/M\, x$ infinitely bounded ...

01/27/2026.

Hilbert Space. (∞ - dimensional)

- V : vector space
- $\|v\|_B = \{B(v,v)\}^{1/2}$
  sym. pos. def.

Lin. Alg (fin-dimensional)

$\|v\|_B = (v^T B v)^{1/2}$

Equivalent norms $\frac{1}{c}\|v\|_A \leq \|v\|_B \leq c\|v\|_A$
(only in finite) c exists.

- Bounded linear map.

$L : V \to W$ L is bounded iff $\|Lu\|_W \leq C\|u\|_V$

$\| \|_V$ $\| \|_W$

$$\|L\| = \max_{u \in V} \frac{\|Lu\|_W}{\|u\|_V}$$

* In finite space, always bounded!

- Linear functional (Hilbert)

$l : V \to \mathbb{R}$, if this is bounded,

l is bdd lin. func. , $\exists v > 0$, $|l(v)| \leq C\|u\|_V$

E.g.) $l(v) = \sum_{k \geq 0} k^2 v_k$, suppose $v = \begin{pmatrix} 1 \\ 1/2 \\ \vdots \\ 1/\infty \end{pmatrix}$ $B = \begin{pmatrix} 1 & & \\ & 2 & \\ & & \ddots \\ & & & \infty \end{pmatrix}$

$l(v) = \sum_{k \geq 0} k^2 \cdot 1/k \to \infty$ $\|v\| = (1^2 + 1/2^2 + \cdots)^{1/2} < \infty$

finite (not Hilbert)

- Claim : $\exists$. $x \in \mathbb{R}^n$ s.t $l^T u = B(x_l, u)$

pf)

$l^T u = x_l^T B u \Rightarrow l^T = x_l^T B \Rightarrow B x_l = l \Rightarrow \underline{x_l = B^{-1} l}$

($\because$ B is SPD).

- Rietz Representation Thm.

  Hilbert space V, $\|\cdot\|_B$

  Given any bdd lin. func. $\ell(\cdot): V \to \mathbb{R}$

  $\exists\, x_\ell \in V$ s.t. for any $u \in V$

  $\to \ell(u) = B(x_\ell, u)$

- In Lin. Alg, $\|x_\ell\|^2 = x_\ell^T B x_\ell = \ell^T B^{-1} \cancel{B} \cancel{B^{-1}} \ell = \ell^T B^{-1} \ell$

  $= \|\ell\|_{B^{-1}}$

  $\to \|\ell\|_{B^*}$ is called dual norm.

- In Hilbert Space,

  $\ell \to x_\ell$ (by Rietz)

  Define $\|\ell\|_{B^*} = \|x_\ell\|_B = \{B(x_\ell, x_\ell)\}^{1/2}$ (dual norm)

Ex) $L^2 = \{ f \mid f: \mathbb{R} \to \mathbb{R}, \int f^2 < \infty \}$

$$\hat{f}(\xi) = \int e^{-2\pi j \xi x} f(x)\, dx$$

① $\widehat{f'}(\xi) = -\int e^{-2\pi j x \xi} (-2\pi j \xi) f(x)\, dx = 2\pi j \xi\, \hat{f}$

② $\|f\|_{L^2} = \|\hat{f}\|_{L^2(\xi)}$ ~ rotation.

$$\begin{pmatrix} \cdots & f(\xi) & \cdots \end{pmatrix} \underbrace{\begin{pmatrix} \ddots & & \\ & 1+4\pi\xi^2 & \\ & & \ddots \end{pmatrix}}_{=B} \begin{pmatrix} \vdots \\ f(\xi) \\ \vdots \end{pmatrix} \quad \xi \in \mathbb{R}$$

Define $H^1 = \{ f \mid f \text{ s.t. } \int |f|^2 + |f'|^2\, dx < \infty \}$,

$$\|f\|_{H^1} = \left\{ \int |f|^2 + |f'|^2\, dx \right\}^{1/2}$$

$$= \left\{ \int |\hat{f}|^2 + |\widehat{f'}|^2\, d\xi \right\}^{1/2} = \left\{ \int (1+4\pi\xi^2) \|\hat{f}\|^2\, d\xi \right\}^{1/2}$$

- The set of all bdd lin. func. on $H^1 \equiv H^{-1}$!

$$B = \begin{pmatrix} \ddots & & \\ & 1+4\pi k^2 & \\ & & \ddots \end{pmatrix}, \quad B^{-1} = \begin{pmatrix} \ddots & & \\ & 1 & \\ & & \ddots \end{pmatrix}$$

- Elliptic Problems $\longrightarrow AU = F$.

  $A(\cdot,\cdot)$ sym. mat.

  1) A to be bdd $\quad \|A(u,v)\| \leq C \|u\|_B \|v\|_B$

  2) A is coercive w.r.t $\|\|\|_B \quad A(u,u) \geq \alpha \|u\|_B^2$

     $\alpha > 0$ $\rightarrow$ eigenvalue (smallest) > 0 for symm invertible

- Claim : $\|v\|_A = \{A(v,v)\}^{1/2}$

  thm $(V, \|\cdot\|_B) \leftrightarrow (V, \|\cdot\|_A)$

  If 1.) and 2), $\|\ \|_A$ and $\|\ \|_B$ is <u>equivalent</u>.

- Lin. Alg. : $Au = \ell \rightarrow u^T A = \ell^T$

  $\Rightarrow \underline{u^T A u = \ell^T u}$

Hilb. Spc : Fin u, $\forall \varphi \in (V, \|\cdot\|_B)$

$\underline{A(u,\varphi) = \ell(\varphi)}$

Suppose, A is bdd $\|\cdot\|_B$, A is coercive $\|\cdot\|_B$ $\Big\} \Rightarrow \|A\|_A \equiv \|\cdot\|_B$

$\rightarrow$ Swap to $(V, \|\cdot\|_A) \rightarrow$ By Reitz RT, $\exists u_\ell \in (V, \|\cdot\|_A)$ $\boxed{A(u_\ell, \varphi) = \ell(\varphi)}\ \forall \varphi$

Since $A(u_\ell, \varphi) = \ell(\varphi)$,

$$\underset{\text{coercivity}}{\alpha \|u_\ell\|_B^2 \leq} A(u_\ell, u_\ell) = \ell(u_\ell) \underset{\text{bdd}}{\leq} C_{B,\ell} \|u_\ell\|_B$$

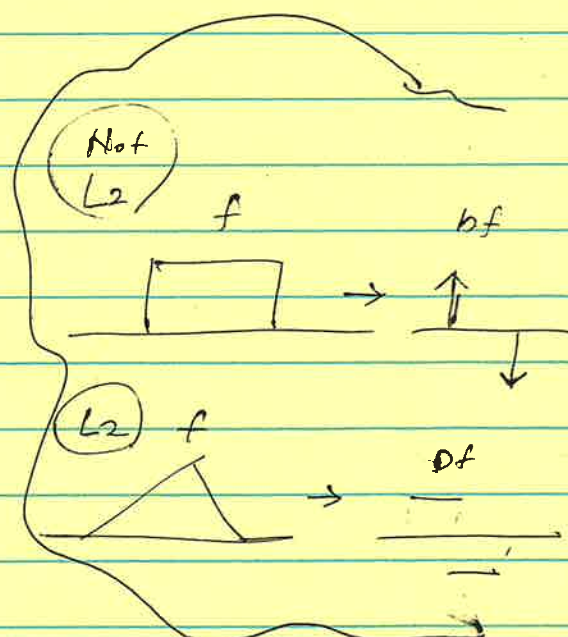
$$\Rightarrow \underline{\|u_\ell\|_B \leq \frac{C_{B\ell}}{\alpha}} \rightarrow \text{solution is bounded.}$$

- Weak derivative. (when f not smooth).

$$\int f' \underset{\text{smooth}}{\varphi} = \int f(-\varphi')$$

$$\boxed{(Df)(\varphi) = -\int f \varphi'}$$

↳ called "functional / distribution"



- $H^1(\mathbb{R}) = \left\{ f : \left\{ \int |f|^2 + |f'|^2 \, dx \right\}^{1/2} < \infty \right\}$.

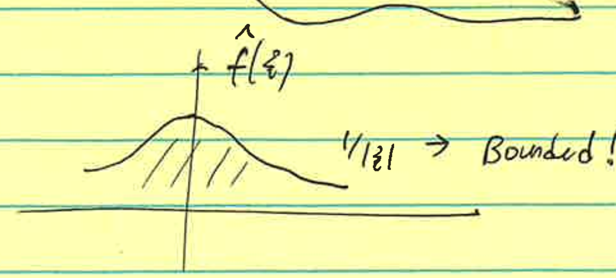
↳ Sobolev

$f \in L^2$, $Df \rightarrow$ if this is function in L_2

$$H' = \{ f, f \in L^2, Df \in L^2 \}$$

$$\|f\|_{H_1} = \left\{ \int |f|^2 + |Df|^2 \right\}^{1/2}$$

$$\equiv \left\{ \int |\hat{f}|^2 + 4\pi^2 \xi^2 |\hat{f}|^2 \, d\xi \right\}^{1/2}$$



- Extend to $D^2 f$

$$\|f\|_{H_2} = \left\{ \int |f|^2 + |Df|^2 + |D^2 f|^2 \, dx \right\}^{1/2}$$

$$\equiv \left\{ \int |\hat{f}|^2 + (2\pi\xi)^2 |\hat{f}|^2 + (2\pi\xi)^4 |\hat{f}|^2 \right\}^{1/2}$$

$\sim 1/\xi^{2.5} \rightarrow$ Bounded.

L.F. Dual

$$H_0 \supset H_1 \supset H_2 \cdots \supset H_k \quad (\text{constrained})$$

$H_0 = L^2$

B matrix
$$\begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \begin{pmatrix} 1+\xi^2 & & \\ & 1 & \\ & & \ddots & \\ & & & 1+\xi^2 \end{pmatrix} \begin{pmatrix} 1+\xi^2+\xi^4 & & \\ & 1 & \\ & & \ddots & \\ & & & 1+\xi^2+\xi^4 \end{pmatrix} \cdots$$

β^{-1}
$$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{1+\xi^2} & & \\ & 1 & \\ & & \frac{1}{1+\xi^2} \end{pmatrix} \cdots$$

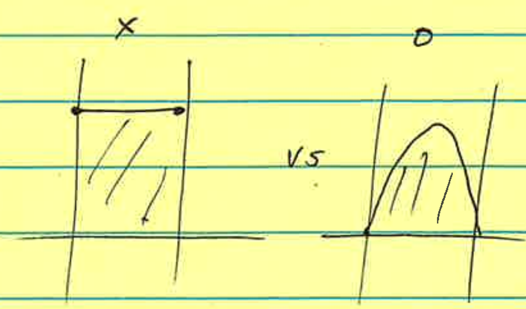
$$H^0 \subset H^{-1} \subset H^{-2} \cdots \subset H^{-k} \quad (\text{relaxed})$$

- Poincare Inequality

Ω

$$H_1(\Omega) = \{ f \in L^2, Df \in L^2, \text{in } \Omega \}$$

$$H_0^1(\Omega) = \{ \quad '' \quad f|_{\partial\Omega} = 0 \}$$



$$\rightarrow \|f\|_{L_2} \leq \|Df\|_{L_2} \quad \text{for } f \in H_0^1(\Omega)$$

- Proof of Poincare inequality.

$$\left|f(x)\right| = \left|\int_0^x f(y)\,dy\right| \le \left\{\left(\int_0^x 1^2\,dy\right)\left(\int_0^x |f'(y)|^2\,dy\right)\right\}^{1/2} \le \|Df\|_{L_2}$$

$$\|f\|_{L^2} = \sqrt{\left|\int_0^1 f^2\,dx\right|} \le \sqrt{\int_0^1 |Df|^2} = \|Df\|_{L_2}$$

→ For $f \in H_0^1(\Omega)$

$$\|Df\|_{L_2}^2 \le \|f\|_{H_0^1(\Omega)} = \left\{\int f^2 + (Df)^2\right\}^{1/2} = \left\{\|f\|_{L_2}^2 + \|Df\|_{L_2}^2\right\}^{1/2}$$

$$\le \sqrt{2}\,\|Df\|_{L_2}^2$$

$\therefore$ $\|f\|_{H_0^1(\Omega)}$ is equ to $\|Df\|_{L_2}$

01/29/2026

① MCMC (primary) (Rare event) — 100%.
② Hye Tensor + stress. (Dislocation) — 80%.
③ MLIP. + CGMD (MD) — 20%.

- Finite element method

$$\left.\begin{aligned} -(a\cdot u')' &= f \\ u(0) = u(1) &= 0 \end{aligned}\right\}$$

Choose $\varphi(x)$ s.t. $\varphi(0) = \varphi(1) = 0$.
$(\underline{A} \le a(x) \le \bar{A} < \infty)$

$$\Rightarrow \int_0^1 -(au')'\varphi = \underbrace{\int_0^1 a u'\varphi'}_{\text{Bilinear Form}} = \underbrace{\int_0^1 f\varphi}_{\text{Linear Form}}$$

$= A(u, \varphi)$ $\quad = (f, \varphi)$

$\Rightarrow$ Find u, $A(u,\varphi) = (f,\varphi)$ //

- $H_0^1(\Omega)$, $\|v\|_{H_0^1} = \left\{\int_0^1 v^2 + v'^2 \, dx\right\}^{1/2}$

Is A – SPD in $H_0^1(\Omega)$

① $\|A(u,\varphi)\| = \left|\int a u'v'\right| \le \bar{A}\int \|u'\| \, \|\varphi'\| \le A\left\{\int |u'|^2\right\}^{1/2} \cdot \left\{\int |\varphi'|^2\right\}^{1/2}$
$\le A\|u\|_{H_0^1}\|\varphi\|_{H_0^1}$ $\rightarrow$ Bddness

② $|A(u,u)| = \int a u'u' \ge \underline{A}\int |u'|^2 \ge \underline{A}\cdot C\|u\|^2_{H_0^1}$ $\rightarrow$ Coercive.

By Poincaré

$\therefore$ A is SPD in H_0^1.

Given. $f \in H^{-1}$, Find $u \in H_0^1(\Omega)$ s.t

$\forall \varphi \in H_0^1(\Omega)$, $A(u, \varphi) = (f, \varphi)$ → Weak form.

∴ By Rietz Representation Thm, in $(H_0^1(\Omega), \|\cdot\|_a)$

$\exists u$ s.t. $A(u, \varphi) = (f, \varphi)$ for $\forall \varphi \in H_0^1(\Omega)$

Note : $A(u_f, u_f) = (f, u_f)$

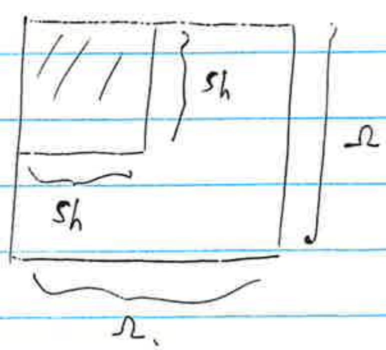
$\geq C \cdot \|u_f\|_{H_0^1}^2$ $\qquad \leq \|f\|_{H^{-1}} \cdot \|u_f\|_{H_0^1}$

$\Rightarrow \|u_f\|_{H_0^1} \leq \|f\|_{H^{-1}}$ (bounded by)

• Numerics of FEM (from weak form).

Find $u \in H_0^1(\Omega)$ s.t. $A(u, \varphi) = (f, \varphi)$ $\forall \varphi \in H_0^1(\Omega)$

Fin $u_h \in S_h$ s.t $A(u_h, \varphi_h) = (f, \varphi_h)$ $\forall \varphi \in S_h$.



→ Restrict(truncate) the matrix.

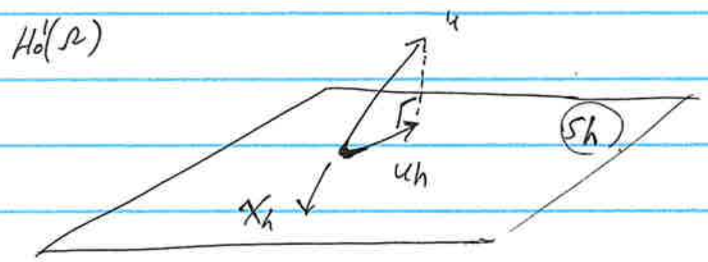
· Error

u : (weak) $A(u, \chi_h) = (f, \chi_h) \quad \chi \in S_h \subseteq H_0^1(\Omega)$

u_h ( ) $A(u_h, \chi_h) = (f, \chi_h) \quad \chi \in S_h$

$\Rightarrow A(u-u_h, \chi_h) = 0 \quad \forall \chi_h$ — A-orthogonal

Recall $(H_0^1(\Omega), \|u\|_a = \{A(u,u)\}^{1/2})$ is Hilbert space



($u - u_h$ is A-orthogonal to S_h.)

$\therefore$

$\Rightarrow \|u-u_h\|_a = \quad \|u-\chi_h\|_a \quad \forall \chi_h$

$\geq C_1 \|u-u_h\|_{H_0^1(\Omega)} \quad \leq C_2 \|u-\chi_h\|_{H_0^1(\Omega)}$

$\Rightarrow \|u-u_h\|_{H_0^1(\Omega)} \leq \frac{C_2}{C_1} \cdot \|u-\chi_h\|_{H_0^1(\Omega)} \quad (\forall \chi_h \in S_h)$

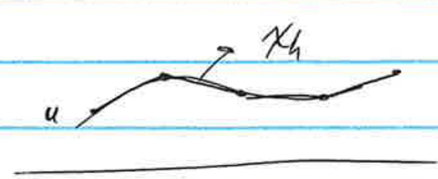
$\rightarrow$ Find χ_h s.t. RHS small.

* If a is smooth, $f \in L^2(\Omega)$, then sol u of $-(au')' = f$ in $H^2(\Omega)$

$\Rightarrow$ Under smooth $f \in L^2$, we have $u \in H^2(\Omega)$.

$\Rightarrow$ Use $u \in H^2(\Omega)$ to find good χ_h.

$\chi_h \leftarrow$ p.w. linear interpolation of u.

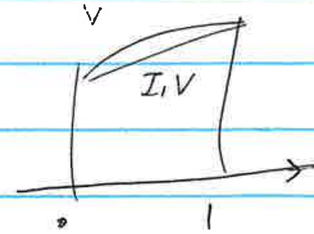


$\chi_h = \underset{\sim}{I_h} u \rightarrow \chi_h \in S_h$.

$\quad \searrow$ linear intep.

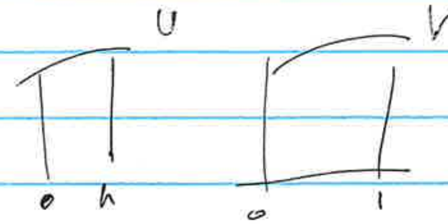
Goal : $u - I_h u$ is small in $H_0^1(\Omega)$.

$\| v - I_1 v \|_{L^2} \lesssim \| (v - I_1 v)' \|_{L^2}$ (Poincaré)



$\| (v - I_1 v)' \|_{L^2} \lesssim \| (v - \underbrace{I_1 v)''}_{= 0} \|_{L^2}$ (")

$= \| v'' \|_{L_2}$



For spacing h, $\cancel{u(x \geq x_k) = v(x/h)}$

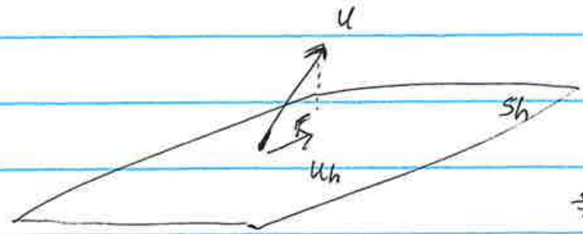
$$u(x) = v\left(\frac{x - x_k}{h} \right)$$

$\Rightarrow u'' = v'' \frac{1}{h^2}$

$\therefore$ $\| u - I_h u \| \lesssim h^2 \| u'' \|_{L^2}$ //

- Error analysis. 2026/02/05

$\varphi_h \in S_h, \quad A(\varphi_h,\ u - u_h) = 0$



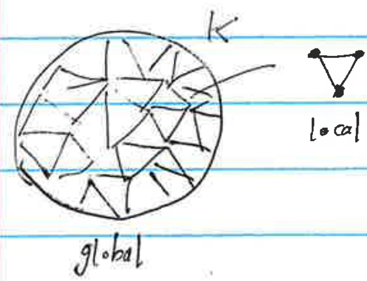
$\|u - u_h\|_A \leq \|u - \chi_h\|_A \quad (\chi_h \in S_h)$

A-norm equ. to H_0^1

$\Rightarrow \|u - u_h\|_{H_0^1} \leq \|u - \chi_h\|_{H_0^1} \quad (\chi_h \in S_h)$

We generally interpolate $I_h u \rightarrow \|u - I_h u\| = ?$

(($\Rightarrow$ If v vanishes at $\partial\Omega$, $\|v\|_{L_2} \leq \|\nabla v\|_{L_2}$ (by Poincare)))



Iv vanishes at node points.

$\|v - Iv\|_{L_2} \leq \|\nabla(v - Iv)\|_{L_2}$

Gradient is 0 between (on edge)

$\|\nabla(v - Iv)\|_{L_2} \leq \|\nabla^2(v - \underset{\text{linear!}}{Iv})\|_{L_2} = \|\nabla^2 v\|_{L_2}$

$\Rightarrow \|v - Iv\|_{L_2} \leq \|v - Iv\|_{H^1} \leq \|v - Iv\|_{H^2}$

$$\left\{\begin{array}{lll} u(x) & v(Fx) & F \text{ is a map } (\approx 1/h) \\ \text{global} & \text{local} & \\ & & \underline{F^T v'} \\ u'(x) & v'(Fx)\,\cancel{d}(F) & \rightarrow \nabla v \sim \cancel{d}(F^{-1})\,\nabla u \\ u''(x) & v''(Fx)\,(\cancel{d}(F))^2 & \rightarrow \nabla^2 v \sim (\cancel{d}(F^{-1}))^2\,\nabla^2 u \\ & \underline{F^T v'' F} & \end{array}\right.$$

$\Rightarrow \|u - Iu\|_{L_2} \leq \det(F^{-1})\|\cancel{\nabla}(u - Iu)\|_{L_2} \leq (\det(F^{-1}))^2 \cdot \|\nabla^2(u - Iu)\|_{L_2}$

By Poincare, $\|u - I_h u\|_{H_0^1} \leq h\|u\|_{H^2} \leq h\|f\|_{L^2} \sim O(h^1)$ (1D)

$\|u - I_h u\|$ (2D)

• In 2D, $\|e\|_{L_2}^2 = A(\varphi, e) = A(\varphi - I_h\varphi, e)$

$$\le \|\varphi - I_h\varphi\|_A \cdot \|e\|_A$$

$$\le \|\varphi - I_h\varphi\|_{H_0^1} \, \|u - u_h\|_{H_0^1}$$

$$\le h \cdot \|\varphi\|_{L_2} \cdot h\|f\|_{L_2} = h^2 \|f\|_{L^2} \sim o(h^2).$$

$\therefore$ $(u - u_h)$ bounded!

★ Parabolic PDEs. $\quad (\alpha_1 - \alpha_2)/(\alpha_1 + \alpha_2)$

$$\begin{cases} u_t = u_{xx} & x \in \mathbb{R},\ t > 0 \\ u(x,0) = v(x) \end{cases}$$

Fourier $\to$ $\hat{u}$ $\to$ easy!

$$\left.\begin{aligned} &\partial_t \hat{u} = -\xi^2 \hat{u} \\ &\Rightarrow \partial_t \hat{u} + \xi^2 \hat{u} = 0 \\ &\hat{u}(t=0) = \hat{v}(\xi) \end{aligned}\right]$$

$$\hat{u} = e^{-\xi^2 t} \cdot \hat{v}(\xi)$$

$$\downarrow$$

$$u = \mathcal{F}\{\hat{u}\}$$

$$\frac{d}{dt}\begin{pmatrix} \hat{u}(\xi) \end{pmatrix} = \begin{pmatrix} -\xi^2 & & \\ & \underbrace{0}_{\text{no decay}} & \\ & & -\xi^2 \end{pmatrix} \begin{pmatrix} \hat{u}(\xi) \end{pmatrix}$$

Stiff!

• Fourier Transform.

$f(x) \in L^2(\mathbb{R}) \longleftrightarrow \hat{f}(\xi) \in L_\xi(\mathbb{R})$

$$\hat{f}(\xi) = \int_{\mathbb{R}} e^{-j\xi x} f(x)\, dx$$

$$\xi \to \overset{\downarrow x}{\begin{bmatrix} e^{-j\xi x} \end{bmatrix}} \begin{bmatrix} f \end{bmatrix} = \begin{bmatrix} \hat{f} \end{bmatrix}$$

$$f(x) = \frac{1}{2\pi}\int e^{j\xi x} \hat{f}(\xi)\, d\xi$$

$$= \int e^{j\xi x} f(\xi) \frac{d\xi}{2\pi}$$

shrinked measure.

$*$ EE

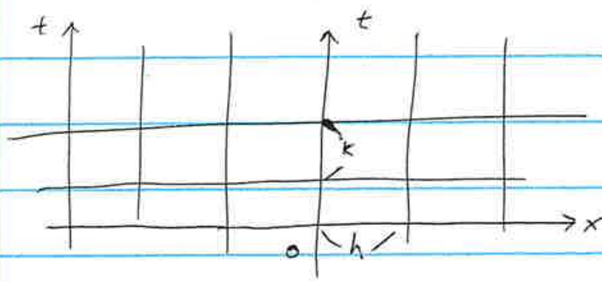
$$\left.\begin{aligned} \hat{f} &= \int e^{-2\pi \xi x} f(x)\, dx \\ \check{f} &= \int e^{2\pi \xi x} \hat{f}(\xi)\, d\xi \end{aligned}\right] \quad \text{Symmetric}$$

$$\|f\|_{L_2(dx)} = \|\hat{f}\|_{L_2(d\xi)}$$

- $u_t = u_{xx}$

  $u(x,0) = v(x)$

- Discretize



$x_j = j\cdot h \quad , \quad t_n = nk$

$$\Rightarrow \quad \frac{U_j^{n+1} - U_j^n}{k} = \frac{U_{j+1}^n + U_{j-1}^n - 2U_j^n}{h^2} \qquad \text{(central diff)}$$

$$\Rightarrow \quad U_j^{n+1} = \lambda U_{j+1}^n + (1-2\lambda) U_j^n + \lambda U_{j-1}^n \quad (\lambda = k/h^2) \quad \rightarrow \quad \text{Explicit}$$

(Time marching)

$$\begin{bmatrix} U_j^{n+1} \end{bmatrix} = \underbrace{\begin{bmatrix} \ddots & \ddots & \lambda & \\ \ddots & 1-2\lambda & \ddots & \ddots \\ & \lambda & \ddots & \ddots \end{bmatrix}}_{=E_{k,h}} \begin{bmatrix} U \end{bmatrix}$$

$= E_{k,h}$: $\sim$ convolution.

Symplectic ??

Search. KDV

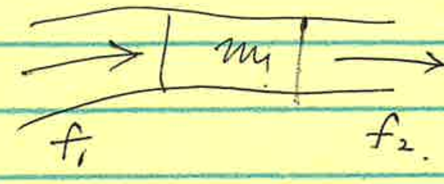
- Error analysis

$U_j^n \approx u(x_j, t_n)$

density   flux   02/24/2026.

Conservation Law.

$$\begin{cases} u_t + [f(u)]_x = 0 & x \in \mathbb{R},\ t \geq 0 \\ u(x,0) = u_0(x) \end{cases}$$



* In regions $[a,b]$.

$$\int_a^b u_t + [f(u)]_x \, dx = 0 \Rightarrow \underbrace{\frac{d}{dt}\int_a^b u \, dx}_{\text{Mass} = m_1} = \underbrace{f(u(t,a)) - f(u(t,b))}_{\text{flux difference}} \quad \text{— ①}$$

Eqn. ① does not require smoothness in x (advantage).

- $\boxed{\text{Characteristics Method}}$

$$\dot{x} = f'(u(x,t)) \rightarrow \text{line}$$

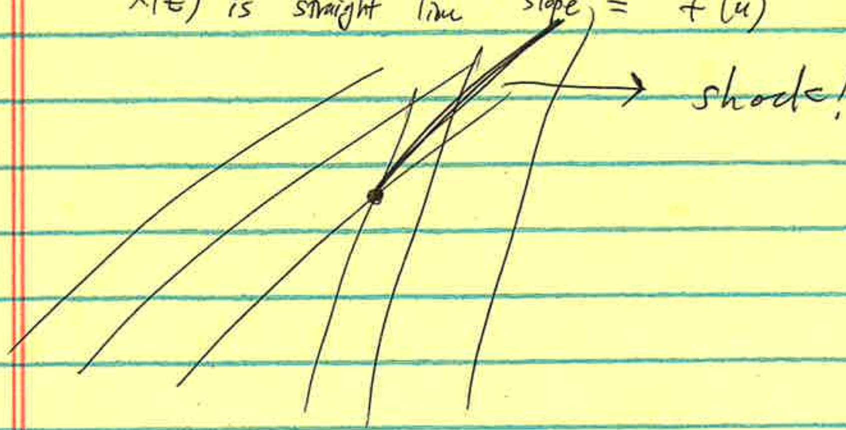
$$d/dt\, u = u_t + u_x \dot{x} = u_t + f'(u)\, u_x = 0$$

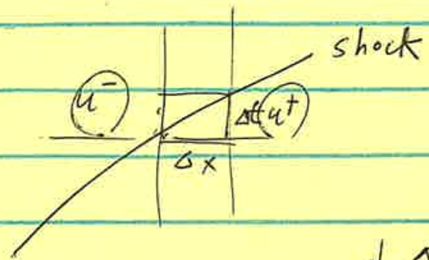
But if u remains same on / $(\dot{x} = a)$

$f'(u)$ "

$\dot{x}$ "

$x(t)$ is straight line slope $\equiv f'(u)$ (e.g) $f'(u) = u$ (burger's)



• 

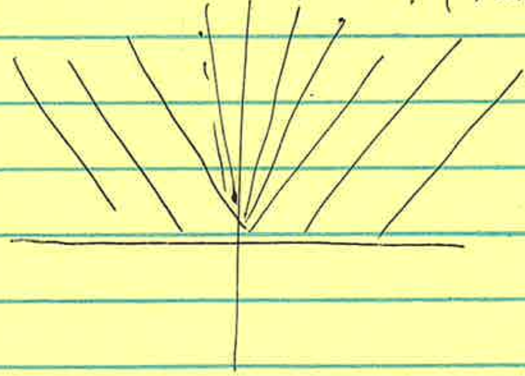
$s \cdot \Delta t = \Delta x$ (slope of shock)

$$\frac{d}{dt}\Delta mass = \frac{\Delta x\,(u_- - u_+)}{\Delta t} = f(u^-) - f(u^+)$$

$$\Rightarrow s = \frac{f(u^-) - f(u^+)}{u^- - u^+}$$ (Rankine – Hugoniot) jump condition.

$$= \frac{[[f(u)]]}{[[u]]}$$ $[[\cdot]] \rightarrow$ "jump!" operator.

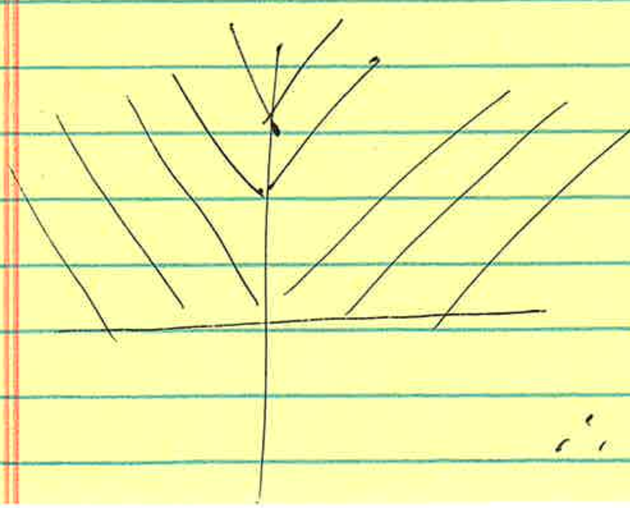
• expansion. (rarefaction wave)

sol 1) 

$u_t + u \cdot u_x = 0$

$$u = \begin{cases} -1 & x < -t \\ x/t & \text{otherwise} \\ 1 & x > t \end{cases}$$

$\rightarrow$ satisfies weak sol

sol 2) 

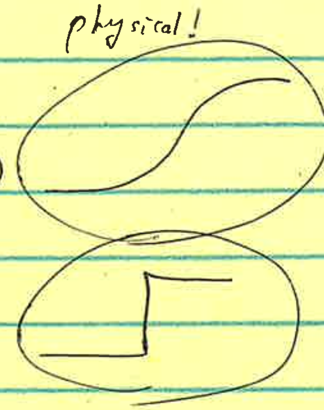
$\rightarrow$ also satisfies weak sol.

$$s = \frac{u_L + u_R}{2} = 0$$

$\therefore$ Weak sol is too weak //

- Viscosity Solution.

$$u_t^\varepsilon + [f(u^\varepsilon)]_x = \varepsilon u_{xx}^\varepsilon \quad \text{(smoothed version)}$$



$\varepsilon \to 0$, $\to$ Burger's Eqn.

- Assume $f(x)$ convex

Prop. ① $u(x,0)$, $v(x,0)$ 2 diff.

$$u(x,0) > v(x,0) \to u(x,t) > v(x,t)$$

prop ② $\| u(t,x) - v(t,x) \|_{L^1} \leq \| u(0,x) - v(0,x) \|_{L^1}$

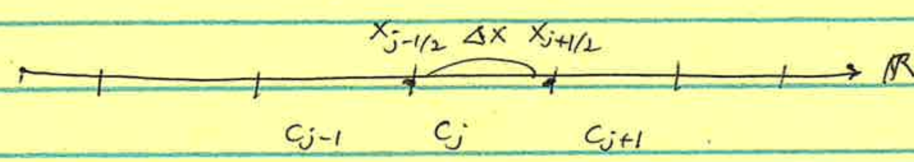
- Numerics

$$u_t + [f(u)]_x = 0$$

$\to$ weak form. $\displaystyle \frac{d}{dt}\int_a^b u(x,t)\,dt = f(u(a,t)) - f(u(b,t))$

< Discretize! >

$$U_{j-1} \quad U_j \quad U_{j+1}.$$



[Finite Volume]

numerical flux.

$[a,b] \equiv C_j$

$$\Delta x \frac{d}{dt}\int_{C_j} u(x,t)\,dx = f(u(x_{j-1/2},t)) - f(u_{j+1/2},t))$$

$$\Delta x \frac{U_j^{n+1} - U_j^n}{\Delta t} = \hat{f}(U_{j-1}^n, U_j^n) - \hat{f}(U_j^n, U_{j+1}^n)$$

//

03/03/2026

Finite Volume Method

1) Godonov
2) Lax - Frederich (L-F)
3) Local L-F

Maintain "monotonicity" of FVM level

(L-F)

$U_j^{n+1} = G(\cdot, \cdot, \cdot)$ is monotonic $\overset{\text{iff.}}{\Longleftrightarrow}$ $-\partial_1 f(u_L, u_R) \geq 0$

$-\partial_2 f(\;''\;) \leq 0$

$-1 + \frac{\Delta t}{\Delta x}[\partial_2 f - \partial_1 f] \geq 0$

L-F is monotone if $\Delta t \leq \frac{\Delta x}{\max|f'|}$

(Godonov)

-

- Thm 1

$G(\uparrow, \uparrow, \cdot)$ monotone $\longrightarrow$ $\|U^n - V^n\|_{L_1} \leq \|U^0 - V^0\|_{L_1}$ (contraction)

$\rightarrow$ "stability"

- Thm 2

If G monotone, $\Delta t, \Delta x \to 0$, $\Delta t \leq \frac{\Delta x}{\|\max f'\|}$, $\hat{f}(u, u) = f(u)$ and $\hat{f}$ is Lipschitz.

then, U converges to entropic solution.

$\rightarrow$ "convergence"

- Thm 3

Any monotone scheme has $O(h)$ accuracy in $L1$ norm.

$\because$ Lack of regularity

> Apply high-order / D.G.

- Monte Carlo / Stochastic D.E.

Integration,

$$I[f] = \int f(x)\, p(x)\, dx$$

$$\hat{I}[f] = \frac{1}{N} \sum_i f(X_i) \qquad X_i \sim p$$

$$\Rightarrow \operatorname{Var} \hat{I}_n(f) = \frac{1}{N^2} \cdot \operatorname{Var}(f(X)) \cdot N = \frac{1}{N} \operatorname{Var}(f(x))$$

$$\Rightarrow \sigma(\hat{I}_n(f)) = \frac{1}{\sqrt{N}} \cdot \sigma(f(x)) \qquad \left(\text{convergence speed} : 1/\sqrt{N}\right)$$

In high-dimension (d) $1/\sqrt{N}$ is still powerful.

↘ # of points increase drastically!

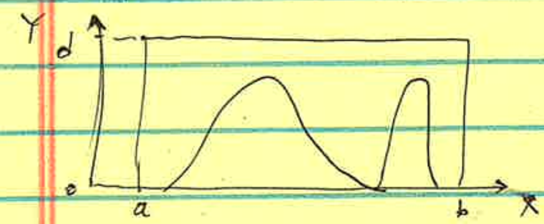
Standard integration (Riemann) $\sim \left(N^{-1/d}\right)^2 = N^{-2/d}$

Standard ~~Monte Carlo~~		Monte Carlo ~~Standard~~	
$1/N^{2/d}$	$\ngtr$	$1/N^{1/2}$	$(d \gg 1)$

- * String Methods for Diffusion Models.

• Acceptace / Rejection

$X \sim [a, b]$, $Y \sim [0, d]$



if X, Y above curve,

$Y > P(X) \rightarrow$ Reject

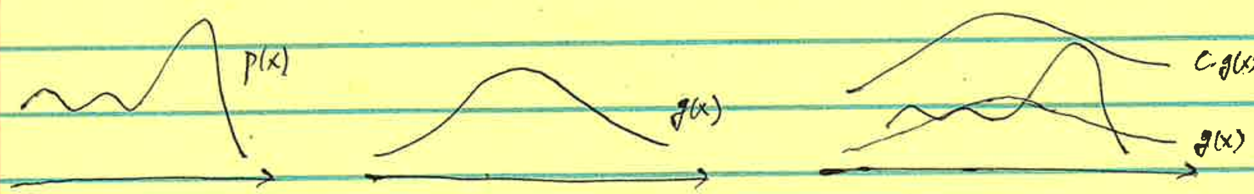
$Y < p(X) \rightarrow$ Accept

$\rightarrow$ Return X

problem 1) Infinite bound $p(X)$

problem 2) spike! in $p(X)$

Assume $g(x)$ ~~exists~~ (easy to sample, exists constant, $p(x) < C \cdot g(x)$)



1) $X \sim g(x)$

2) $Y \sim [0, C \cdot g(x)]$

3) If $Y \geq p(X)$, repeat

E.x)

$g(x) = k(x \rightarrow y)$

$p(x) = k(x \rightarrow y)\, I(y) / I(x)$

$p(x) < g(x) \cdot 1/I(x)$
$\quad\quad\quad\quad\quad\quad \parallel$
$\quad\quad\quad\quad\quad\quad C$

$Y \sim [0, k(x \rightarrow y) / I(x)]$

If $Y \geq$???

• Integration

$x \sim p \rightarrow E_{x \sim p} f(x)$

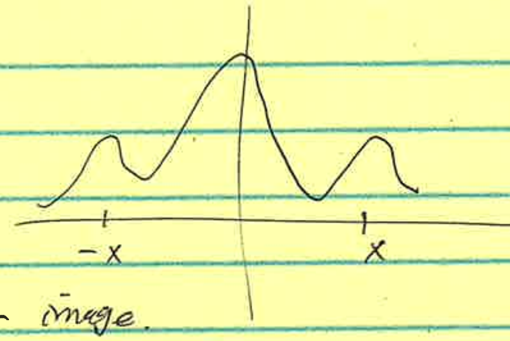
① Control variant

Suppose, $f(x) = h(x) + r(x) \Rightarrow E_{x \sim p} \{ h(x) + r(x) \}$ sometimes we know $E_{x \sim p} h(x) = A$

$= A + E_{x \sim p} \{ r(x) \}$

② Antithetic variables

$f(x)$ even $\rightarrow$ reduce variance
by choosing mirror image.



SDEs 03/10/2025

- $dx = v(x)\, dt$
  $df(x) = f'(x)\, v(x)\, dx$ } ODE (Newton Calculus)

- $dx = v(x)\,dt + dW$
  $df(x) = f'(x)\,dx + 1/2\, f''(x)\,(dx)^2$ } SDE

$$= f'(x)\{v(x)dt + dW\} + 1/2\, f''(x)\{v(x)dt + dW\}\{v(x)dt + dW\}$$

$$= \quad " \quad + \quad " \quad \{\cancel{v^2 dt^2} + \cancel{2v\, dt\, dW} + (dW)^2\}$$

Keep first order (Riemann sum)

$$= \{f'(x)\, v(x) + \tfrac{1}{2} f''(x)\} dt + f'(x)\, dW \quad \text{(Ito's formula)}$$

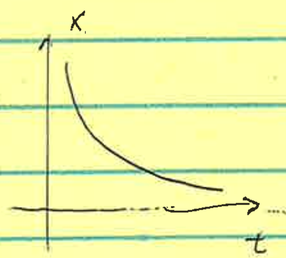
(Ito Calculus)

- Examples

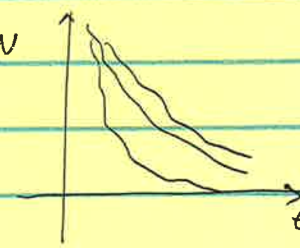
$dx = -x\,dt$

$x(0) = 1$

$x(t) = e^{-t}$



$dx = -x\,dt + dW$



How to solve? (Integrating factor)

$e^t dx + e^t x\,dt = 0$

$\Rightarrow d(e^t x) = 0$

$\Rightarrow x = e^{-t}$

$e^t dx + x e^t dt = dW e^t$

$\Rightarrow \int_0^T d(e^t x) = \int_0^T dW\, e^t$ (correct because no higher order in Ito)

$\Rightarrow e^T x(T) - x(0) = \int_0^T e^t\, dW$

$\Rightarrow x(T) = e^{-T} x(0) + e^{-T} \int_0^T e^t\, dW$

• Example (Geometric Brownian Motion) $\qquad df(x) = 1/x \, dx$

check,

$$\frac{dX}{X} = + dt + dW$$

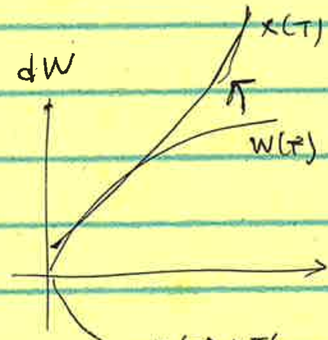
$$df(x) = \frac{1}{x} dx + 1/2\left(-1/x^2\right)(dx)^2$$

$$= 1/x \, dx - 1/2\left(\frac{dx}{x}\right)^2$$

$$= 1/x \, dx - 1/2 \, dt$$

Guess

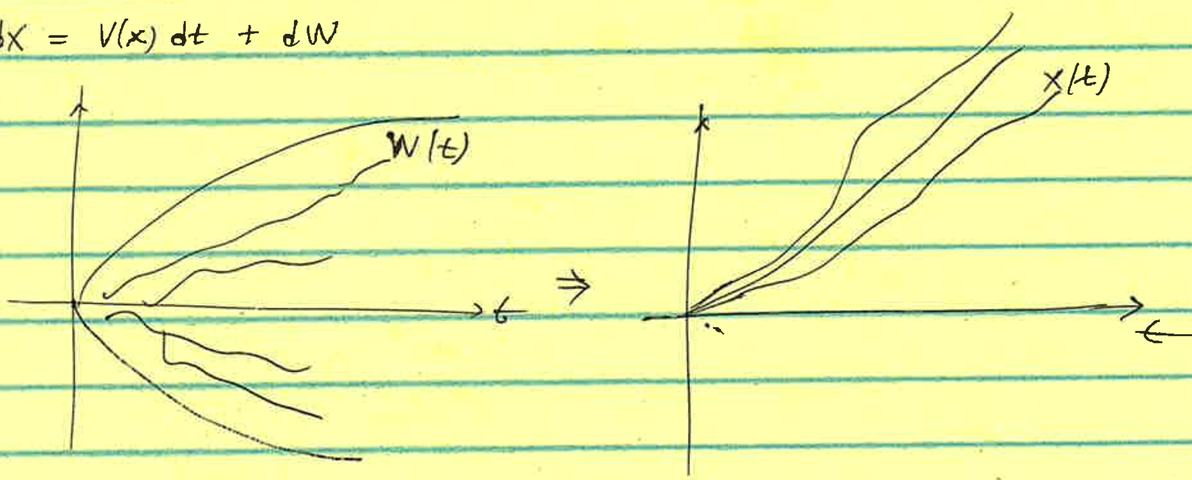
$d(f(x))$



$$X(T) = X(0) \cdot e^{W(T) + T/2}$$

• Numerical methods (SDE)

$$dX = V(x)\, dt + dW$$



"Find Transformation"

→ Euler-Maruyama method (discrete time)

$$\Rightarrow \Delta X = V(x)\, \Delta t + \sqrt{\Delta t}\, \xi, \quad \xi \sim N(0,1)$$

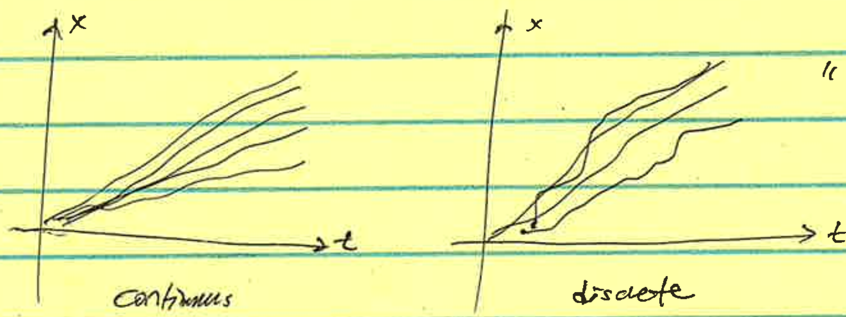
- $dx = b(x)\,dt + \sigma(x)\,dW$, how to numerically ?

$$\Delta X = b(x)\Delta t + \sigma(x)\cdot\sqrt{\Delta t}\,\xi \quad , \quad \xi \sim N(0,1)$$

- Accuracy ? (weak & strong) purposes : ① Get correct trajectory
② Get distribution at time t

1) Strong error ✓ 2) Weak error ✓

For purpose ②



" If each trajectory match, the distribution will match. Reverse does not hold! "

Match distribution = sampling

The scheme of X_n has strong error order α if,

$$\mathbb{E}\,|X_n - X(n\Delta t)| \leq \Delta t^{\alpha}$$

or,

$$\mathbb{E}\{|X_n - X(n\Delta t)|^2\} = O(\Delta t^{2\alpha})$$

Weak error order β if,

$\cancel{\text{dist}\left(\rho_{X(T)}, \rho_{X_N}\right) \sim \Delta t^{\beta}}$ (we don't use this!)

For any smooth function F

$$\left|\mathbb{E}\{F(X_N) - F(X_T)\}\right| \leq C_F\,\Delta t^{\beta}$$

· Conclusion on E.M.

$$\begin{cases} \text{Strong error} : \alpha = 1/2 & \begin{cases} \text{Special} \cdot \sigma(x) = \text{constant}. \\ \text{then, } \alpha = 1 \end{cases} \\ \text{Weak error} : \beta = 1 \end{cases}$$

Can we improve E.M ? $\rightarrow$ Milstein method

$$X_{n+1} = X_n + b(X_n)\Delta t + \sigma(X_n)\Delta W_n + \tfrac{1}{2}\sigma(X_n)\sigma'(X_n)\left((\Delta W_n)^2 - \Delta t\right)$$

$\searrow$ $\alpha = 1$

See in Milstein $\sigma = \text{const}$, $\sigma' = 0 \Rightarrow$ Milstein = E.M.

#

$$\begin{cases} \text{SDE} : X(t_{n+1}) = X(t_n) + \int_{t_n}^{t_{n+1}} b(X(t))dt + \Delta W_n \\ \text{EM} : \bar{X}_{n+1} = \bar{X}_n + \int_{t_n}^{t_{n+1}} b(\bar{X}_n)\,dt + \Delta W_n \end{cases}$$

03/12/2026

- $X_{n+1} = X_n + \Delta t\, b(X_n) + \Delta W_n$ Euler – Maruyama (EM)

Let $\rho(n\Delta t, x)$ be dist. of $X(n\Delta t)$

" $\rho_n(x)$ " $\bar{X}_n$

$e_n = x(t_n) - \bar{X}_n$ (error)

$$e_{n+1} = e_n + \int_{t_n}^{t_{n+1}} \left[b(X(t)) - b(\bar{X}_n) \right] dt$$

$$\parallel$$

$$\begin{bmatrix} b(X(t)) - b(X(t_n)) \\ + b(X(t_n)) - b(\bar{X}_n) \end{bmatrix}$$

$$\mathbb{E}[e_{n+1}] = \mathbb{E}[e_n] + \int_{t_n}^{t_{n+1}} \mathbb{E}[b(X(t)) - b(X(t_n))]\, dt$$

$$+ \int_{t_n}^{t_{n+1}} \mathbb{E}[b(X(t_n)) - b(\bar{X}_n)]\,dt$$

By Lipschitz,

$$= \mathbb{E}[e_n] + L\,\mathbb{E}\left[\int_{t_n}^{t_{n+1}} |X(t) - X(t_n)|\,dt\right] + L\,\mathbb{E}\left[\int_{t_n}^{t_{n+1}} \underbrace{|X(t_n) - \bar{X}_n|}_{\text{error}}\,dt\right]$$

Recall,

$$\mathbb{E}\,|X(t) - X(t_n)| = \mathbb{E}\left|\int_{t_n}^{t} b(X_s)\,ds\right| + \mathbb{E}\left|W(t) - W(t_n)\right|$$

$\to \sim N(0, t-t_n)$

$$\le c \cdot \Delta t + \sqrt{\Delta t}$$

S.D. $\sigma \sim \sqrt{\Delta t}$

after taking expectation.

$$\therefore\ E\{e_{n+1}\} \le (1 + L\Delta t)\, E\{e_n\} + L\cdot\Delta t^{1/2}\,\Delta t$$

$$\Rightarrow E\{e_{n+1}\} \le (1+L\Delta t)\, E\{e_n\} + L\Delta t^{1.5} + \Delta t^{0.5}$$

$$+ \Delta t^{0.5}$$

$$\Rightarrow \text{Recursive!} \rightarrow \left(E\{e_{n+1}\} + \sqrt{\Delta t}\right) \le (1+L\Delta t)^{T/\Delta t\ (n)} \left(\underbrace{E\{e_0\}}_{=\text{const}=0} + \sqrt{\Delta t}\right) \quad (0+\sqrt{\Delta t})$$

$$\approx e^{LT}\sqrt{\Delta t} \qquad \boxed{(\alpha = 1/2)}$$

- What if, $\sigma \ne$ constant? $\qquad E\{\bar{X}_n - x(n\Delta t)\} \le |\Delta t|^{\alpha}$

$$dx = b(x)\,dt + \sigma(x)\,dW$$

$$\bar{X}_{n+1} = \bar{X}_n + b(\bar{X}_n)\Delta t + \sigma(\bar{X}_n)\Delta W_n \qquad \text{(EM)}$$

$$= \bar{X}_n + b(\bar{X}_n)\Delta t + \sigma(\bar{X}_n)\Delta W_n \qquad \text{(Milstein)}$$

$$+ \frac{1}{2}\sigma(x_n)\cdot\sigma'(x_n)\left(\Delta W_n^2 - \Delta t\right)$$

↳ This has $(\alpha = 1)$

- Weak convergence of EM

Idea: Given $F(x)$, study

$$E\left\{F(\bar{X}_n) - F(X(n\Delta t))\right\} \le |\Delta t|^{\alpha}$$

By Ito, $dX = b(x)\,dt + dW$

$$d(F(X)) = F'(x)\,b(x)\,dt + F'(x)\,dW + \frac{1}{2}F''(x)\,dt$$

Take expectation to Ito,

$$d\,\mathbb{E}\{F(x)\} = \{F'(x)\,b(x) + 1/2\,F''(x)\}\,dt + \mathbb{E}\{F'(x)\}\,dW$$

independent.

$\parallel$

0

$$= \underbrace{\{E(F(x))'\,b(x) + 1/2\,E(F(x))''\}}\,dt$$

operator $\mathcal{L}[f] = bf' + \frac{1}{2}f''$

$$\Rightarrow \boxed{\frac{\partial}{\partial t}\mathbb{E}\{F(x)\} = \mathcal{L}[\mathbb{E}\{F(x)\}]}$$ PDE for $\mathbb{E}\{F(x)\}$

Kolmogorov Equation.

$\mathcal{I}$ of E.M. is frozen version.

$$\bar{A}f(x) = b(\bar{X}_n)\,f'(x) + 1/2\,f''(x)$$

$$\left.\begin{aligned} d/dt\ F &= AF \\ d/dt\ F_{EM} &= \mathcal{I}F_{EM} \end{aligned}\right) \to \text{Do something} \ldots$$

$$F(\Delta t) \doteq F(0) + A(F(0))\Delta t + 1/2\,AA(F))\Delta t^2$$

$$F_{EM}(\Delta t) = F_{EM}(0) + \bar{A}F_{EM}\Delta t + 1/2\,\bar{A}\bar{A}(F_{EM})\Delta t^2$$

$$\mathcal{L}\mathcal{L}F = b(bf' + 1/2 f'')' + 1/2(bf' + 1/2 f'')''$$

$$|F(\Delta t) - F_{EM}(\Delta t)| \leq \Delta t \cdot \Delta t$$

Multistep, $\Delta t^2\ T/\Delta t \doteq T(\Delta t)$ $\quad \alpha = 1$

* Final

1. Hamiltonian systems — prove symplectic
   — equations.

2. Elliptic equations.
   - Finite difference
   - Finite element — write formulation
     - bounded, coersive
     - $AU = F$

3. Parabolic equations.
   - $u_t = u_{xx}$
   - finite difference
   - Fourier methods — stability $h/s << 1$?

4. Wave equations.
   - finite difference

~~(4) Conservation laws~~

5. Conservation laws
   - convex, concave, burgers
   - weak formulation — finite volume
     - → Godonov
     - → L-F
     - → L-L-F
   - → Monotonic, $U_n = G(U_{n-1}, U_n, U_{n+1})$
     - → for G, L-F, L-L-F

6. Monte Carlo — detailed balance

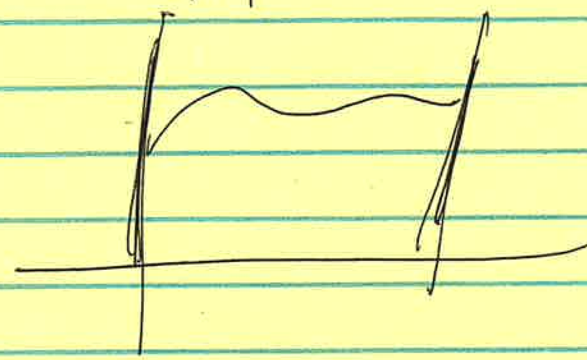
7. SPE — not on final

Office Hour — prof. Ying

- $dx = \underbrace{-\nabla U(x)\,dt}_{①} + \underbrace{\sqrt{2\beta^{-1}}\,dW_t}_{②}$

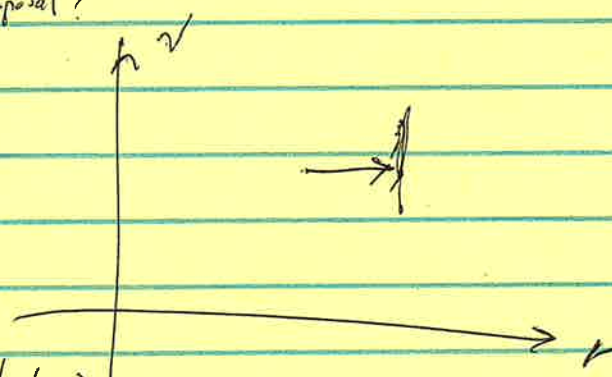
1) Error from both ① and ② ?

$\tau \wedge T$



2) How to reject (MALA)?

$\alpha = \min\left[1, \frac{q\,\pi}{q\,\pi}\right]$ Gaussian proposal ?



3) Markovian ? → True. (phys)

$$\begin{cases} \dot r = v \\ \dot v = -\nabla U(r) - \gamma \dot r + \sqrt{2\beta^{-1}}\,dW_t \end{cases}$$

$$\begin{pmatrix} \dot r \\ \dot v \end{pmatrix} = \begin{bmatrix} 0 & 1 \\ -\nabla U + \gamma & 0 \end{bmatrix} \begin{pmatrix} r \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ \sqrt{2\beta^{-1}} \end{pmatrix} dW_t$$

long lag time, τ — T

Markovian in R

4) kernel representation

$K_{\Delta t}(y|x)$ $\quad y = x - \nabla U(x)\Delta t + \sqrt{2\beta^{-1}\Delta t}\,\xi$

$K_\tau(y|x)$?