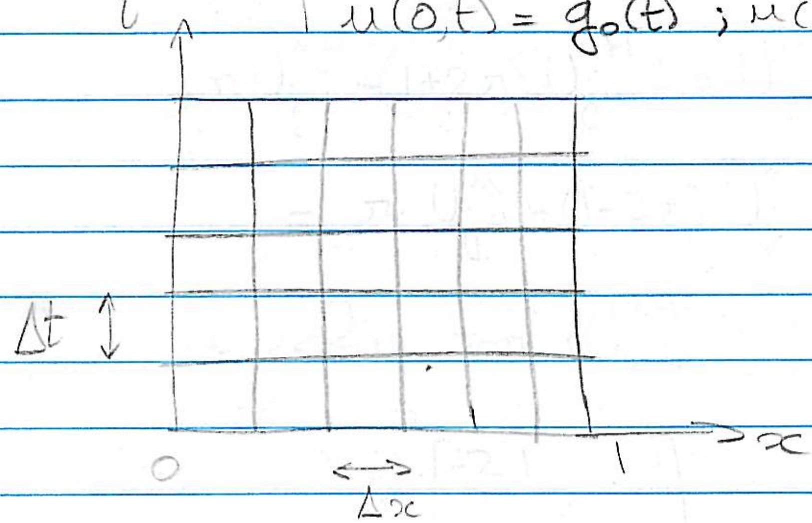
03/04 Initial-value problems (parabolic).

Heat/diffusion eqn: $u(x,t)$ s.t

$$\begin{cases} u_t = \alpha u_{xx} & x \in [0,1] \quad \alpha > 0. \\ u(x,0) = u_0(x) \\ u(0,t) = g_0(t) \ ; \ u(1,t) = g_1(t). \end{cases}$$



$x_j = j \Delta x$

$t_n = n \Delta t$

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

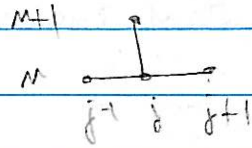
System of equations with a causal structure: once $U_j^0, U_j^1, \ldots, U_j^n$ are known, can get U_j^{n+1}.

→ solve by time marching

① Simplest/natural

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \underbrace{\frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{(\Delta x)^2}}_{D_{c,2} U_j^n}$$

Stencil:



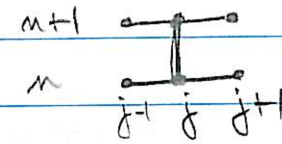
$$\rightarrow U_j^{n+1} = U_j^n + \boxed{\frac{\alpha \Delta t}{(\Delta x)^2}} \left(U_{j-1}^n - 2U_j^n + U_{j+1}^n \right)$$

→ explicit method.

2 Crank-Nicolson scheme

$$\frac{U_j^{n+1}-U_j^n}{\Delta t} = \alpha\left(\frac{D_{c,2}U_j^n + D_{c,2}U_j^{n+1}}{2}\right)$$

Implicit method



Call $r = \dfrac{\alpha \Delta t}{2(\Delta x)^2}$

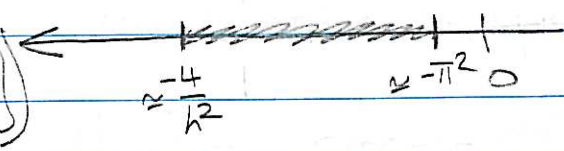
$$-rU_{j-1}^{n+1} + (1+2r)U_j^{n+1} - rU_{j+1}^{n+1}$$

$$= rU_{j-1}^{n} + (1-2r)U_j^{n} + rU_{j+1}^{n} \qquad + \text{B.C}$$

$\rightarrow$ solve for $\{U_j^{n+1} \; ; \; j = 1, \ldots, N\}$.

$$A = I - r\begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}$$

$\lambda\left(\begin{bmatrix} -2 & 1 & \\ 1 & \ddots & 1 \\ & 1 & -2 \end{bmatrix}\right)$



(neg. def.)

(pos. def.)

$\rightarrow$ invert with GE

Convergence: consistency and stability.

Local truncation error: insert solution into scheme and see by how much the discrete equation fails.

(1) $$\tau(x,t) = \frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} - \alpha\,\frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{(\Delta x)^2}$$

$$= \left(u_t + \frac{\Delta t}{2}u_{tt} + \cancel{\frac{(\Delta t)^2}{6}u_{ttt}} + \dots\right)$$

$$-\alpha\left(u_{xx} + \frac{(\Delta x)^2}{12}u_{xxxx} + \dots\right)$$

$$u_{tt} = \alpha u_{txx} = \alpha^2 u_{xxxx}$$

$$= \left[\frac{\alpha^2\Delta t}{2} - \frac{(\Delta x)^2}{12}\right]u_{xxxx} + O\left((\Delta t)^2 + (\Delta x)^4\right)$$
$$= O\left(\Delta t + (\Delta x)^2\right)$$

$\rightarrow$ first order in time, second order in space

(2) Crank-Nicolson: $\tau(x,t) = O\left((\Delta t)^2 + (\Delta x)^2\right)$
second order in space and time

Consistency: $\tau \rightarrow 0$ as $\Delta t, \Delta x \rightarrow 0$

Convergence: $U_j^n - u(x_j,t_n) \rightarrow 0$ as $\Delta t, \Delta x \rightarrow 0$
only happens when there is also stability

"Method of lines" — semidiscrete equations.

$$U_j'(t) = \frac{1}{(\Delta x)^2}\left(U^n_{j-1}(t) - 2U^n_j(t) + U^n_{j+1}(t)\right)$$

→ system of ODE

then discretize t using an ODE solver.

Say $y'(t) = f(y(t))$.

① Euler explicit: $\frac{y^{n+1}-y^n}{\Delta t} = f(y^n)$

→ simplest / natural

② Trapezoidal method: $\frac{y^{n+1}-y^n}{\Delta t} = \frac{f(y^{n+1})+f(y^n)}{2}$

→ Crank-Nicolson

③ Euler explicit: $\frac{y^{n+1}-y^n}{\Delta t} = f(y^{n+1})$

④ Midpoint method: $\frac{y^{n+1}-y^{n-1}}{2\Delta t} = f(y^n)$

→ Leap-frog method.

⑤ One-step Runge-Kutta.

⑥ Multistep

Heuristically, if $\frac{y^{n+1}-y^n}{\Delta t} = f(y^n) + O(\Delta t)$ → LTE

$\Rightarrow y^{n+1} = y^n + \Delta t\, f(y^n) + O((\Delta t)^2)$

→ one-step error on y^n

Global error: $O(\frac{1}{\Delta t})$ time steps

and assume one-step errors just add up without (too much) amplification
then global error $= O\left((\Delta t)^2 \times \frac{1}{\Delta t}\right) = O(\Delta t)$
like the LTE.

Make this more precise: non-blowup of the error owes to stability.

Def. A-stability / strong stability

⚠ Consider $y' = \lambda y$

⚠ Assume the num. method is linear and of the form

$$\underbrace{\frac{1}{\Delta t}\sum_{j=-r}^{1} \alpha_j y^{n+j}}_{\text{disc. of } y'} = \underbrace{\sum_{j=-r}^{1} \beta_j \lambda y^{n+j}}_{\text{evaluations of } \lambda y}$$

$$\Rightarrow \sum_{j=-1}^{r} (\alpha_j - \lambda \Delta t \beta_j) y^{n+j}$$

superscript

exponent

$$\Rightarrow y^{n} = \sum c_k \rho_k^{n} \quad \text{where } \rho$$

are the roots of

$$P(\rho) = \sum_{j=-r}^{1} (\alpha_j - \lambda \Delta t \beta_j) \rho^j$$

A-stability $=$ all $|\rho_k| \le 1$.

$\Rightarrow$ condition on $\lambda \Delta t$,

region of stability.

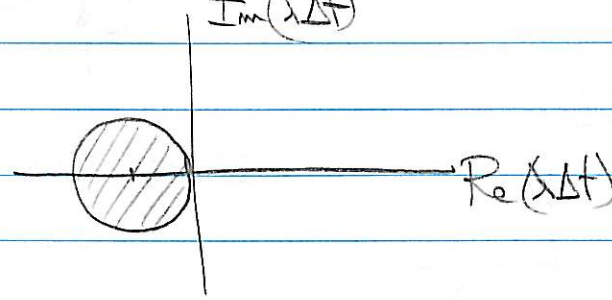
Ex. $y^{n+1} = y^n + \Delta t \lambda y^n$

$= (1 + \lambda \Delta t) y^n$

$y^{n+1} - (1+\lambda\Delta t)\, y^n = 0 \qquad y^n = \rho^n$

$\rho - (1+\lambda\Delta t) = 0, \qquad \rho = 1+\lambda\Delta t$

need $|\rho| \leq 1$:

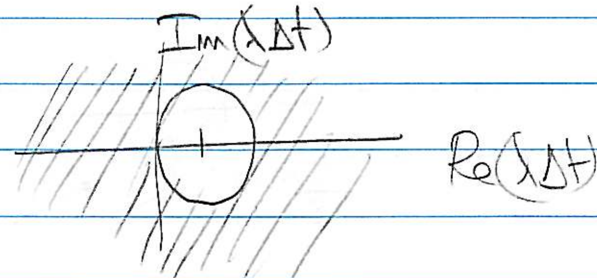


Ex. $y^{n+1} = y^n + \Delta t\, \lambda\, y^{n+1}$

$y^{n+1}(1-\Delta t\lambda) - y^n = 0 \qquad y^n = \rho^n$

$\rho(1-\Delta t\lambda) - 1 = 0$

$\rho = \dfrac{1}{1-\Delta t\lambda}, \qquad |\rho| \leq 1$:



Ex. $y^{n+1} = y^{n-1} + 2\Delta t\, \lambda y^n$ (midpoint)

$y^{n+1} - 2\lambda\Delta t\, y^n - y^{n-1} = 0 \qquad y^n = \rho^n$

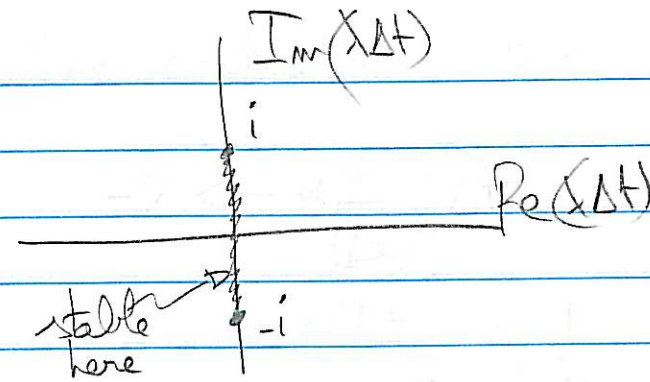
$\rho - 2\lambda\Delta t - \rho^{-1} = 0$

$\rho^2 - 2(\lambda\Delta t)\rho - 1 = 0$

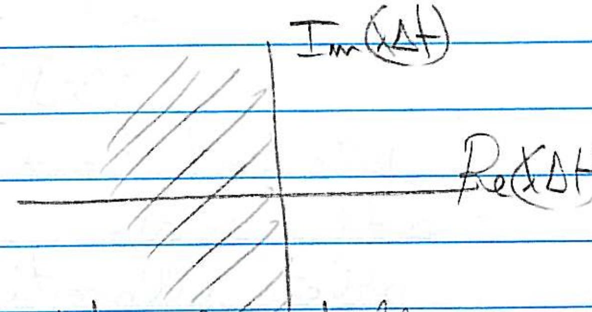
$\Rightarrow \rho = \lambda\Delta t \pm \sqrt{(\lambda\Delta t)^2 + 1}$

$|\rho| \geq 1$, $|\rho| = 1$ only if $\mathrm{Re}\,\lambda\Delta t = 0$

$-1 \leq \mathrm{Im}\,\lambda\Delta t \leq 1$

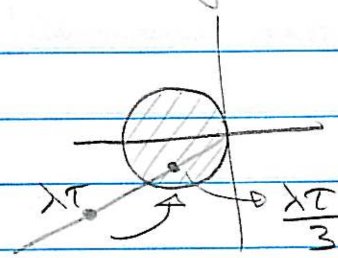


Ex. trapezoidal rule



unconditionally stable

Concl: ODE: choose Δt so small that λΔt is in the region of stability



Systems of ODE: same, but with $y' = Ay$ and let λ_j = eigenvalues of A

Then root condition should apply for all the λ_j

PDE: λ_j depend on Δx. !

$\lambda_j \Delta t$ obeys root condition

→ get relationship between Δt and Δx.

$u_t = \alpha u_{xx}$, $\lambda_N = -\alpha \cdot \frac{4}{(\Delta x)^2}$ such that $|\lambda_N|$ is max

Ex. Euler explicit: $-2 \leq \lambda_N \Delta t \leq 0$

$$-2 \leq -\alpha \frac{4}{(\Delta x)^2} \Delta t$$

$$\frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2}$$

$$\Rightarrow \Delta t = O((\Delta x)^2)$$

very small time step!

Ex. Trapezoidal rule: $-\infty < \lambda_N \Delta t \leq 0$

$\rightarrow$ unconditionally stable.

(only consistency matters)

Next: Lax equivalence theorem

Von Neumann analysis.

Stability / convergence for I.V.P. (Chap. 9) $\quad u_t = \mathcal{L}u$

Method of lines = discretization in space

$$U_j(t) \simeq u(x_j, t)$$

$$U_j'(t) = \sum_k A_{jk} U_k(t) + g_j(t)$$
$$\left(\Longleftrightarrow U'(t) = A\,U(t) + g(t) \right)$$

Use ODE solver with step Δt.

$$\Rightarrow U_j^{n+1} = \sum_k B(\Delta t)_{jk} U_k^n + b_j^n(\Delta t)$$
$$\left(\Longleftrightarrow U^{n+1} = B(\Delta t)\,U^n + b(\Delta t) \right)$$

Def. Stability (strong)

All $\lambda(B(\Delta t)) \le 1$ $\quad \Longleftrightarrow$

All $\lambda(A)\Delta t$ is in the region of stability of the ODE solver

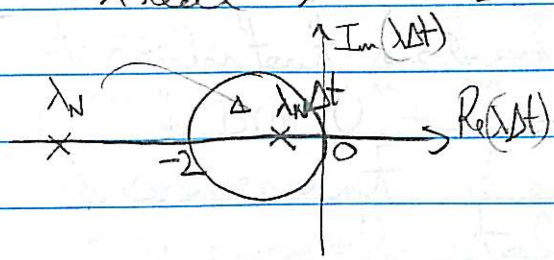
Rmk. A, $B(\Delta t)$ depend on Δx.

Ex. $u_t = u_{xx} \Rightarrow U'(t) = A\,U(t)$ $\quad A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}$

Euler explicit: $U^{n+1} = U^n + \Delta t\, A\, U^n$
$$= B(\Delta t)\,U^n \qquad B(\Delta t) = I + \Delta t A$$

$\Rightarrow$ need $|1 + \lambda \Delta t| \le 1$

λ real $\Rightarrow -2 \le \lambda \Delta t \le 0$ $\qquad \lambda_N \simeq \dfrac{-4}{(\Delta x)^2}$



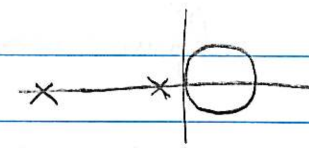
$$\Rightarrow \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2}$$

Ex. Same, Euler implicit

$$U^{n+1} = U^n + \Delta t\, A\, U^{n+1}$$

$$U^{n+1} = (I - \Delta t A)^{-1} U^n$$

$$\left|(1 - \lambda \Delta t)^{-1}\right| \leq 1$$



$\Rightarrow$ no restriction on Δt, Δx.

$\Rightarrow$ use implicit methods for parabolic problems.

Ex. (trapezoidal rule, Crank-Nicolson, same story)

Role of stability = key for convergence.

Def. Stability (weak, Lax-Richtmeyer)

$\forall T > 0 \;\; \exists C_T > 0$:

$$\|B(\Delta t)^n\|_2 \leq C_T$$

$\forall \Delta t > 0$, as long as $n \Delta t \leq T$

Ex. Could have $\|B(\Delta t)\|_2 \leq 1 + \alpha \cdot \Delta t$

$$\|B(\Delta t)^n\|_2 \leq \|B(\Delta t)\|_2^n \leq (1 + \alpha \Delta t)^n$$

$$\Delta t \leq \frac{T}{n}$$

$$\leq \left(1 + \alpha \frac{T}{n}\right)^n \leq \left(e^{\alpha T/n}\right)^n \leq e^{\alpha T} = C_T$$

Thm (Lax equivalence theorem)

A consistent method of the form

$$U^{n+1} = B(\Delta t) U^n + b^n(\Delta t)$$

is convergent if and only if it is weakly stable.

Outline of argument ($\Rightarrow$) functions of $\Delta t, \Delta x$.

$$LTE: \quad u^{n+1} = B\, u^n + b^n + \Delta t\, \tau^n$$

vector $u(x_j, t^n)$ of exact samples

$$E^n = U^n - u^n$$

$$\Rightarrow E^{n+1} = B E^n - \Delta t\, \tau^n \qquad n \geq 0$$

$$E^N = B^N E^0 - \Delta t \sum_{n=1}^{N} B^{N-n} \tau^{n-1}$$

power

superscript

$$\|E^N\| \leq \|B\|^N \|E^0\| + \Delta t \sum_{n=1}^{N} \|B\|^{N-n} \|\tau^{n-1}\|$$

weak stability $\Rightarrow$ $\leq C_T \|E^0\| + \Delta t N\, C_T \max_n \|\tau^{n-1}\|$

($N\Delta t \leq T$) $\leq C_T \|E^0\| + T C_T \max_n \|\tau^{n-1}\|$

$\to 0$ as $\Delta t \to 0$

when $\tau \to 0$ (consistency)

$E^0 \to 0$ (initial data properly discretized)

$\square$

Von Neumann analysis: - easier (no $\lambda(A)$)

- not as rigorous. (BC ignored)

Fourier analysis solves linear IVP

- with constant coefficients
- in periodic domains (or infinite domains)

both for the PDE and its numerical scheme.

Ex. $u_t = u_{xx}$ $\quad x \in [0, 2\pi]$, $\quad u(t=0) = u_0$

Fourier series:

$$u_0(x) = \sum_{k \in \mathbb{Z}} c_k e^{ikx}, \qquad c_k = \frac{1}{2\pi}\int_0^1 e^{-ikx} u_0(x)\,dx$$

$$u(x,t) = \sum_{k \in \mathbb{Z}} \hat{u}(k,t) e^{ikx}$$

$$u_t(x,t) = \sum_k \frac{\partial \hat{u}}{\partial t}(k,t) e^{ikx}$$

$$= u_{xx}(x,t) = \sum_k \hat{u}(k,t)\,(ik)^2 e^{ikx}$$

$$\Rightarrow \frac{\partial \hat{u}}{\partial t}(k,t) = -k^2 \hat{u}(k,t)$$

$$\Rightarrow \boxed{\hat{u}(k,t) = e^{-k^2 t} c_k}$$

one ODE for each k: the heat flow is diagonalized by the eigenfunctions e^{ikx} of d^2/dx^2

$$u(x,t) = \sum_k e^{-k^2 t} c_k e^{ikx}$$

Stability for the PDE: $\left| e^{-k^2 t} \right| \leq 1$

Ex. (vN analysis of Explicit Euler, heat equation)

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{(\Delta x)^2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right)$$

superscript

Anticipate a solution $U_j^n = \rho^n e^{ik(jh)}$ $\quad k \in \mathbb{Z}$, $h = \Delta x$

$$\rightarrow \rho^{n+1} = g(k)\,\rho^n$$

$g(k)$ → amplification factor of the k-th mode

put $\rho^n = 1$ without loss of generality

Require $|g(k)| \leq 1$ for all k.

$$U_j^{n+1} = U_j^n + \left(\frac{\Delta t}{h^2}\right)\left[U_{j-1}^n - 2U_j^n + U_{j+1}^n\right]$$

$$g(k)\,e^{ikjh} = e^{ikjh} + \frac{\Delta t}{h^2}\left[e^{ik(j-1)h} - 2e^{ikjh} + e^{ik(j+1)h}\right]$$

$$g(k) = 1 + \frac{\Delta t}{h^2}\Big[\underbrace{e^{-ikh} - 2 + e^{ikh}}_{2\cos kh - 2}\Big]$$

$$= 1 + 2\frac{\Delta t}{h^2}\left[\cos kh - 1\right]$$

$$= 1 - 4\frac{\Delta t}{h^2}\sin^2\left(\frac{kh}{2}\right) \qquad 0 \le \sin^2 \le 1 \ \text{(real)}$$

$$1 - 4\frac{\Delta t}{h^2} \le g(k) \le 1$$

Need $1 - 4\dfrac{\Delta t}{h^2} \ge -1$, $\quad \dfrac{\Delta t}{h^2} \le \dfrac{1}{2}$

(same result as previously)

von Neumann analysis:

* try $e^{ik(jh)}$ for the spatial part of the solution at t^n
* time t^{n+1} : amplification $g(k) \times e^{ikjh}$
* make sure $|g(k)| \le 1$

Stability in the l_2 sense: (because not every solution is a plane wave)

$$U_j^n = \sum_{k=-\pi N}^{\pi N} \hat{U}^n(k)\, e^{ikjh}$$

$$U_j^{n+1} = \sum_k g(k)\hat{U}^n(k)\, e^{ikjh}$$

Plancherel: $h\sum_{j=0}^{N-1} |U_j^n|^2 = \|U^n\|_2^2$

$$= \frac{1}{(2\pi)^2} \|\hat{U}^n\|_2^2$$

$$= \frac{1}{(2\pi)^2} \sum_{k=-\pi N}^{\pi N} |\hat{U}^n(k)|^2$$

Get $\|U^{n+1}\|_2$ as a function of $\|U^n\|_2$:

$$\|U^{n+1}\|_2^2 = \frac{1}{(2\pi)^2} \sum_k |g(k)|^2 |\hat{U}^n(k)|^2$$

$$\leq \max_k |g(k)|^2 \frac{1}{(2\pi)^2} \|\hat{U}^n\|_2^2$$

$$= \max_k |g(k)|^2 \|U^n\|_2^2$$

$\rightarrow$ stability when $|g(k)| \leq 1 \quad \forall k = -\pi N, \ldots, \pi N$

Ex. (Crank-Nicolson)

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{h^2}\left[\frac{1}{2} D_{c2} U_j^n + \frac{1}{2} D_{c2} U_j^{n+1}\right]$$

$$\Rightarrow g = 1 + \frac{\Delta t}{h^2}\left[e^{-ikh} - 2 + e^{ikh}\right]\left(\frac{1+g}{2}\right)$$

$$\Rightarrow g = \frac{1+\frac{1}{2}z}{1-\frac{1}{2}z} \quad \text{where } z = -4\frac{\Delta t}{h^2}\sin^2\left(\frac{kh}{2}\right)$$

$$\leq 0$$

$$\Rightarrow 1 + \frac{1}{2}z \leq 1 - \frac{1}{2}z$$

and $-1-\frac{1}{2}z \leq 1 - \frac{1}{2}z \quad \Rightarrow |1+\frac{1}{2}z| \leq |1-\frac{1}{2}z|$

$\Rightarrow |g| \leq 1$ always

$\Rightarrow$ unconditionally stable

03/11

Homework 1 q 2
Stability & Convergence of Jacobi.

- Stability: $AE = -\tau$, $E = -A^{-1}\tau$
  $\rightarrow$ control over A^{-1}
- Conv. Jacobi: $G = D^{-1}(D-A)$
  $e_k = G^k e_0$
  $\rightarrow$ control over G.

Ex. method A:
rule $u_0 - \frac{4}{3}u_1 + \frac{1}{3}u_2 = 0$
for Neumann

$$A = \frac{1}{h^2}\begin{bmatrix} T+\frac{4}{3}I & \frac{2}{3}I & & \\ I & T & I & \\ & I & \ddots & I \\ & & \frac{2}{3}I & T+\frac{4}{3}I \end{bmatrix}$$

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

each block: $N-1 \times N-1$
$N-1 \times N-1$ blocks

Ex. method B:

rule $u_{-1} - u_1 = 0$ for Neumann
+ equation $u_{-1} - 2u_0 + u_1 = 0$.

$$\begin{bmatrix} T & 2I & & & \\ I & T & I & & \\ & I & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & 2I & T \end{bmatrix}$$

each block. $N-1 \times N-1$
$N+1 \times N+1$ blocks

Method A:
$(N=32)$
(m script online)

$\rho(A^{-1}) = 0.1014$

$\|A^{-1}\|_2 = 0.1020$

$\rho(B^{-1}) = 0.1014$

$\|B^{-1}\|_2 = 0.1021$

$1/\pi^2 = 0.1013$

$\rho(G_A) = 0.9975$

$\|G_A\|_2 = 0.9975$

$\rho(G_B) = 0.9976$

$\|G_B\|_2 = 1.0056$

G_A is symmetric, the others (A, B, G_B) are not.

If $\rho(M) \neq \|M\|_2$ or $M^*M \neq MM^*$, then no relabeling / reordering of the unknowns would make M symmetric. (does not change orthog. of eigenvectors)

<u>Stability</u>, A symmetric:

$$\|E\|_2 \leq \|A^{-1}\|_2 \, \|\tau\|_2 = \frac{1}{\min|\lambda_j(A)|} \|\tau\|_2$$

$\rightarrow$ need $\min|\lambda_j(A)| \geq c > 0$
with c independent of h.

<u>Stability</u>, A not symmetric:

$$\|E\|_2 \leq \|A^{-1}\|_2 \, \|\tau\|_2$$

Either

(i) $A = P\Lambda P^{-1}$ $\qquad A^{-1} = P\Lambda^{-1}P^{-1}$

$$\|E\|_2 \leq \|P\Lambda^{-1}P^{-1}\|_2 \, \|\tau\|_2$$
$$\leq \underbrace{\|P\|_2 \|P^{-1}\|_2}_{\kappa(P)} \, \underbrace{\|\Lambda^{-1}\|_2}_{=\max|\lambda_j(A)|^{-1} = 1/\min|\lambda_j(A)|} \|\tau\|_2$$

Or

(ii) $\|A^{-1}\|_2 = 1/\sigma_{min}(A) = 1/\sqrt{\lambda_{min}(A^TA)}$

Get $\lambda_j(A^TA)$ numerically using the shifted power method $\rightarrow$ no need for computing A^{-1} explicitly

Convergence of Jacobi, $G = G^*$

$$\|e_k\|_2 \le \|G\|_2^k \|e_0\|_2$$
$$\le \max |\lambda_j(G)|^k \|e_0\|_2$$
$$\Rightarrow \text{need } \max |\lambda_j(G)| < 1.$$

Convergence of Jacobi, $G \neq G^*$.

$$e_k = G^k e_0$$

$\|G\|_2$ could be > 1 yet Jacobi converges

$$G = Q \Lambda Q^{-1}$$
$$G^k = Q \Lambda^k Q^{-1}$$
$$\|G^k\|_2 \le \kappa(Q) \max |\lambda_j(G)|^k$$
$$\to 0 \text{ if } \max |\lambda_j(G)| < 1$$

Answering a homework question

- be candid: say if you can't solve.
- be critical of your results:
  - nonrigorous but true? 99/100
  - nonrigorous and false
    → make another claim.
  - nonrigorous and unclear whether true or false
    → figure out true vs. false before trying to be rigorous.
- assume the TA does not need to be educated.
- nothing should get in the way of asking the right questions.

J. Tukey, 1962
"Far better an approx. answer to the right question than the exact answer to the wrong question"

von Neumann analysis

| $x_j = jh$, $j \in \mathbb{Z}$ $h = 1/N = \Delta x$
| Linear PDE with uniform coeff.
| Disregard B.C.

superscript

$\Rightarrow$ Let $U_j^n = \rho^n e^{ik(jh)}$ $k \in \mathbb{Z}$: called <u>wave number</u>

Get $\rho^{n+1} = g(k)\,\rho^n$
$\hookrightarrow$ amplification factor of the k-th mode.

(Put $\rho^n = 1$ wlog.)
Require $|g(k)| \le 1$ for all $k \in \mathbb{Z}$

Ex. $U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta x^2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right)$

Continue on p. 5 of previous lecture.
& do p. 6

Multi-D problems (2D)

LOD : $U_{ij}^{*} = U_{ij}^{n} + \frac{\Delta t}{2}\left(D_{c,2,x} U_{ij}^{n} + D_{c,2,x} U_{ij}^{*}\right)$
(locally 1D) $U_{ij}^{n+1} = U_{ij}^{*} + \frac{\Delta t}{2}\left(D_{c,2,y} U_{ij}^{*} + D_{c,2,y} U_{ij}^{n+1}\right)$

ADi : $U_{ij}^{*} = U_{ij}^{n} + \frac{\Delta t}{2}\left(D_{c,2,y} U_{ij}^{n} + D_{c,2,x} U_{ij}^{*}\right)$
(alt. dir. implicit) $U_{ij}^{n+1} = U_{ij}^{*} + \frac{\Delta t}{2}\left(D_{c,2,x} U_{ij}^{*} + D_{c,2,y} U_{ij}^{n+1}\right)$

$\rightarrow$ tridiagonal systems only! (ADi better for B.C.)

03/16 Advection equations / von Neumann.

Num XP: heat_CN(1) 1e-2
heat_CN_conv.
heat_EE(0.5). 0.51

adv_LF(1), 1.01
adv_LF_conv
adv_EE(0.5) → unstable
adv_LaxF(1)

$u_t = u_{xx}$	$u_t + u_x = 0$
$a = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$	$a = \frac{\Delta t}{\Delta x} \leq 1$ (CFL)
Stiff, need implicit	Explicit OK. Stability: leap-frog, etc.

Advection eqn / hyperbolic eqns.

$u_t + a u_x = 0$, $x \in [0,1]$
$u(x,0) = u_0(x)$
$\Rightarrow u(x,t) = u_0(x - at)$
Left B.C. $u(0,t) = u_0(-at)$ (inflow)
$u(1,t) = u_0(1-at)$ (outflow)

1) Simplest (forward in time, centered in space)

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = (-a)\,\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$\Rightarrow \quad U_j^{n+1} = U_j^n - a\frac{\Delta t}{2\Delta x}\left(U_{j+1}^n - U_{j-1}^n\right)$$

von Neumann: $U_j^n = e^{ik(jh)}$

$$U_j^{n+1} = g(k)\, e^{ik(jh)}$$

$$\Rightarrow \quad g(k) = 1 - \frac{a\Delta t}{2\Delta x}\left(e^{ikh} - e^{-ikh}\right)$$

$$= \underbrace{1}_{\mathrm{Re}\, g} \underbrace{-ia\frac{\Delta t}{\Delta x}\sin kh}_{\mathrm{Im}\, g}$$

$|g(k)| \geq 1$, unstable

2) Method of lines, centered in space
Assume periodic B.C.

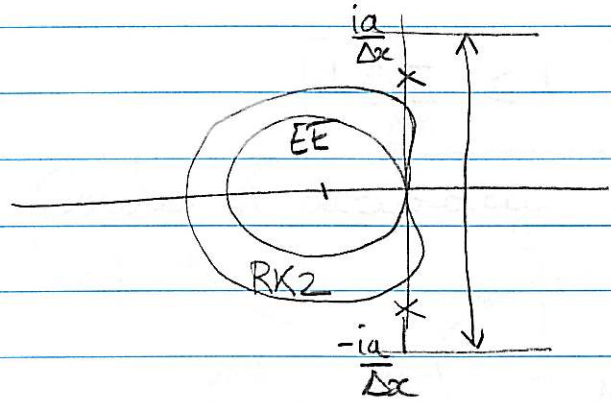
$$U_j'(t) = \frac{-a}{2\Delta x}\left(U_{j+1} - U_{j-1}\right)$$

$$= -\frac{a}{2\Delta x}\underbrace{\begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{bmatrix}}_{A}\begin{bmatrix} U_1 \\ \vdots \\ U_{N-1} \end{bmatrix}$$

$A^T = -A \Rightarrow \lambda(A)$ are purely imaginary
(skew symmetric)

In fact, $u_j^p = e^{2\pi i p (jh)}$ $\quad (k = 2\pi p)$

$\lambda_p = -\frac{ia}{\Delta x} \sin(2\pi p h)$



Need $\lambda_p \Delta t \in$ Region of stab. $\forall p$.

→ Euler explicit KO

→ RK2 OK.

$$\boxed{\Delta t \frac{a}{\Delta x}} \leq C.$$

CFL number,

Courant-Friedrichs-Levy

3) Lax-Friedrichs

$$U_j^{n+1} = \frac{U_{j-1}^n + U_{j+1}^n}{2} - a\Delta t \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$U_j^n = e^{ik(jh)} \quad ; \quad U_j^{n+1} = g(k)\, e^{ikjh}$$

$$g(k) = \frac{e^{ikh} + e^{-ikh}}{2} - \frac{a\Delta t}{\Delta x}\left(\frac{e^{ikh} - e^{-ikh}}{2}\right)$$

$$= \cos kh - i\frac{a\Delta t}{\Delta x} \sin kh$$

$$|g(k)|^2 = \cos^2 kh + (CFL)^2 \sin^2 kh$$

$\Rightarrow$ need CFL ≤ 1 for $|g(k)| \leq 1$.

$$\boxed{\frac{a\Delta t}{\Delta x} \leq 1} \qquad a = \text{wave speed}$$

Order of accuracy $O(\Delta t + (\Delta x)^2)$

4) Leap-frog

previous time step

$$U_j^{n+1} = U_j^{n-1} - 2a\Delta t \, \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$U_j^{n-1} = e^{ikjh}$$

$$U_j^n = g(k)\, e^{ikjh}$$

$$U_j^{n+1} = g^2(k)\, e^{ikjh}$$

$$g^2(k) = 1 - g(k)\left[\frac{a\Delta t}{\Delta x}\right]\underbrace{\left(e^{ikh} - e^{-ikh}\right)}_{2i\sin kh}$$

$$g^2(k) + 2i\overbrace{\left[\frac{a\Delta t}{\Delta x}\right]}^{C}\sin kh \; g(k) - 1 = 0$$

$$g(k) = \frac{-2iC\sin kh \pm \sqrt{-4C^2\sin^2 kh + 4}}{2}$$

$$= -iC\sin kh \pm \sqrt{1 - C^2\sin^2 kh}$$

- If $C \leq 1$, $1 - C^2\sin^2 kh \geq 0$,

$$|g(k)|^2 = C^2\sin^2 kh + 1 - C^2\sin^2 kh$$

$$= 1$$ (marginally stable)

(watch out if variable coeff. or nonlinearities)

- If $C>1$ and $1-C^2\sin^2 kh<0$ for some k,

$$g(k) = -iC\sin kh \pm i\sqrt{C^2\sin^2 kh-1}$$

$$|g(k)|^2 = \left(C\sin kh \pm \sqrt{C^2\sin^2 kh-1}\right)^2$$

↳ choose same sign as $\sin kh$ (worst case)

$$= C^2\sin^2 kh + 2C\sin kh\sqrt{C^2\sin^2 kh-1} + (C^2\sin^2 kh - 1)$$

$$> 1 + 0 + 0$$

→ unstable.

Order of accuracy: $O((\Delta t)^2 + (\Delta x)^2)$

5) Lax-Wendroff:

2nd order, but no need for 3 levels.

$$u_t + a u_x = 0$$

Taylor series: $u(t+\Delta t) = u(t) + \Delta t\, u'(t) + \frac{(\Delta t)^2}{2}u''(t) + O(\Delta t^3)$

$$u(t+\Delta t) = u(t) - a\Delta t\, u_x(t) + \frac{(\Delta t)^2}{2}a^2 u_{xx}(t) + O((\Delta t)^3)$$

because $u_{tt} = -a u_{xt} = a^2 u_{xx}$

→ use
$$U_j^{n+1} = U_j^n - \frac{a\Delta t}{2\Delta x}\left(U_{j+1}^n - U_{j-1}^n\right) + \frac{a^2(\Delta t)^2}{2(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

Accuracy: $O((\Delta t)^2 + \Delta x^2)$ (LTE)

Stability: $C = a\frac{\Delta t}{\Delta x}$

$$g(k) = 1 - C\left(\frac{e^{ikh} - e^{-ikh}}{2}\right) + C^2\left(\frac{e^{ikh} - 2 + e^{-ikh}}{2}\right)$$

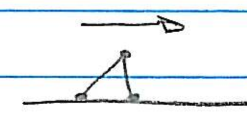
$$= 1 - iC\sin kh + C^2(\cos kh - 1)$$

$$= 1 - iC\left[2\sin\frac{kh}{2}\cos\frac{kh}{2}\right] + C^2\left[2\sin^2\frac{kh}{2}\right]$$

$$|g(k)|^2 = \dots = 1 - 4\underbrace{C^2(1-C^2)}_{\substack{\le \frac{1}{4} \\ \text{when} \\ 0 \le C \le 1}}\underbrace{\sin^4\frac{kh}{2}}_{\le 1}$$

$\Rightarrow$ stable when $C \le 1$.

6) Upwind method:



$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = -a\frac{U_j^n - U_{j-1}^n}{\Delta x}$$

accuracy: $O(\Delta t + \Delta x)$

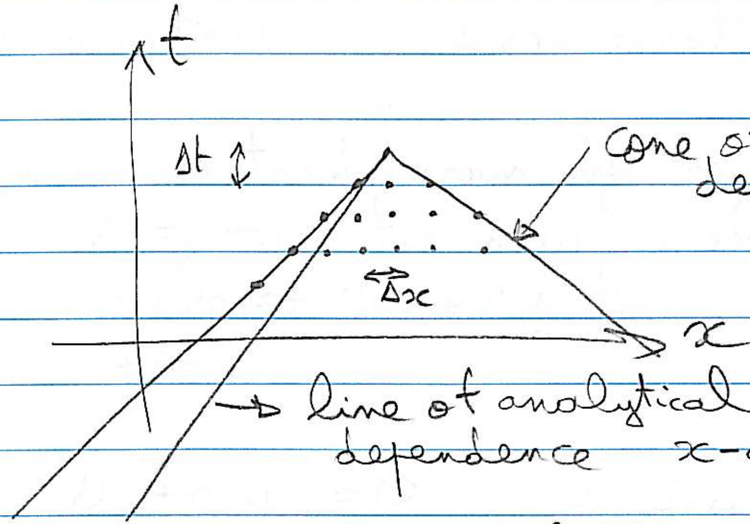
stability: $0 \le a\frac{\Delta t}{\Delta x} \le 1$

$\Rightarrow$ good only for $a \ge 0$

Also called upstream differencing.

(This idea comes back for nonlinear conservation laws)

About the CFL condition:



$a\frac{\Delta t}{\Delta x} = C \leq 1$

$\Rightarrow \Delta x - a\Delta t \geq 0.$

$x - at = \text{const}.$

Need line $\subset$ cone.

$\rightarrow$ need $CFL = a\frac{\Delta t}{\Delta x} \leq 1.$

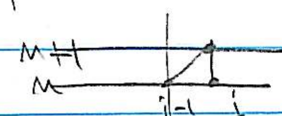
Next: modified equations.

03/18

Modified equations, dispersion relations

Idea: understand error by formulating PDE that the numerical solution is closer to obey than the original PDE.

Ex. $u_t + a u_x = 0$, Upwind method
$(a>0)$



$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = -a \frac{U_j^n - U_{j-1}^n}{\Delta x}$$

$\Rightarrow$ find $u(x,t)$ such that

$$\frac{u(x+\Delta t) - u(x,t)}{\Delta t} = -a \frac{u(x,t) - u(x-\Delta x, t)}{\Delta x}$$

at (x,t), $u_t + \frac{\Delta t}{2} u_{tt} + O((\Delta t)^2)$

$$= -a\left[u_x - \frac{\Delta x}{2} u_{xx} + O((\Delta x)^2)\right]$$

$$u(x-\Delta x) = u(x) - \Delta x\, u_x(x) + \frac{(\Delta x)^2}{2} u_{xx}(x)$$

$$\Rightarrow u(x) - u(x-\Delta x) = \Delta x\, u_x - \frac{(\Delta x)^2}{2} u_{xx} + \frac{(\Delta x)^3}{6} u_{xxx}$$

$$u(x+\Delta x) = u(x) + \Delta x\, u_x(x) + \frac{(\Delta x)^2}{2} u_{xx} + \frac{(\Delta x)^3}{6} u_{xxx}$$

$$u(x+\Delta x) - u(x-\Delta x) = 2\Delta x\, u_x + \frac{(\Delta x)^3}{3} u_{xxx}$$

$$\Rightarrow u_t + a u_x = \frac{1}{2}\left(-\Delta t\, u_{tt} + a \Delta x\, u_{xx}\right) + \text{h.o.t}$$

now $u_{tt} \simeq -a u_{xt} \simeq a^2 u_{xx}$ (up to $O(\Delta t)$)

modified eq.:

$$\Rightarrow u_t + a u_x = \frac{1}{2} a \Delta x \Big(1 - \underbrace{a\frac{\Delta t}{\Delta x}}_{\nu,\ \text{CFL number}}\Big) u_{xx}$$

$$= \varepsilon u_{xx} \qquad \varepsilon > 0$$

numerical dissipation/diffusion

Ex. $u_t + a u_x = 0$, Simplest $\quad \nu = \frac{a\Delta t}{\Delta x}$

$$\frac{u(x+\Delta t) - u(x)}{\Delta t} = -a \frac{u(x+\Delta x, t) - u(x-\Delta x, t)}{2\Delta x}$$

$$u_t + \frac{\Delta t}{2} u_{tt} + \frac{(\Delta t)^2}{6} u_{ttt} + \ldots$$

$$= -a\left[u_x + \frac{(\Delta x)^2}{6} u_{xxx} + \ldots \right]$$

and $\left\{ \begin{array}{l} u_{tt} = a^2 u_{xx} + h.o.t. \\ u_{ttt} = -a^3 u_{xxx} \end{array} \right.$

mod-eq:

$$u_t + a u_x = \boxed{-\frac{a^2}{2}(\Delta t) u_{xx}}$$

$$- \frac{1}{6} a (\Delta x)^2 \left(1 - \nu^2\right) u_{xxx} + h.o.t.$$

$\Rightarrow$ anti-diffusion (instability)

Ex. Lax-Wendroff.

$$\frac{u(x+\Delta t) - u(x)}{\Delta t} = -a \frac{u(x+\Delta x, t) - u(x-\Delta x, t)}{2\Delta x}$$

$$+ \frac{a^2}{2} \Delta t \frac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{(\Delta x)^2}.$$

modified eqn:

$$u_t + a u_x = -\frac{1}{6} a (\Delta x)^2 \left(1 - \nu^2\right) u_{xxx} + h.o.t.$$

$- \varepsilon u_{xxxx}$, $\varepsilon > 0$ and $O((\Delta t)^3 + (\Delta x)^3)$

$\Rightarrow$ dispersion / phase errors

Dispersive waves.

$$\begin{cases} u_t = u_{xxx} & x \in \mathbb{R}. \\ u(x,0) = u_0(x) \end{cases}$$

Fourier transform in space: $x \to \xi \in \mathbb{R}$.

$$\hat{u}(\xi,t) = \int_{-\infty}^{\infty} e^{-i\xi x} u(x,t)\,dx$$

$$\Rightarrow \hat{u}_t(\xi,t) = (i\xi)^3 \hat{u}(\xi,t) = -i\xi^3 \hat{u}(\xi,t)$$

$$\hat{u}(\xi,t) = e^{-i\xi^3 t} \hat{u}_0(\xi). \qquad \text{(dispersion)}$$

note $|\hat{u}(\xi,t)| = |\hat{u}_0(\xi)|$

[Compare with: - advection $e^{\pm i\xi t}$ (translation)
- diffusion $e^{-\xi^2 t}$
(damping of high frequency modes)]

$$u(x,t) = \frac{1}{2\pi}\int e^{i\xi x} e^{-i\xi^3 t} \hat{u}_0(\xi)\,d\xi.$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi(x-\xi^2 t)} \hat{u}_0(\xi)\,d\xi.$$

$\to$ like $x - ct$ with $c = \xi^2$

mode $e^{i\xi x}$ travels with speed ξ^2.

other ex. $u_t + a u_x + b u_{xxx} = 0$

leads to $u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi(x-(a-b\xi^2)t)} \hat{u}_0(\xi)d\xi$

$\rightarrow e^{i\xi x}$ propagates with speed $a - b\xi^2$.

Advection / hyperbolic eq. / wave eq.:
- all components travel at the same speed.
- singularities propagate (along characteristics)

Dispersive wave eq. (incl. Schrödinger / water waves / etc.)
- speed depends on wave number / freq.
- singularities break down

ex. Schrödinger $iu_t = -u_{xx}$

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi(x-\xi t)} \hat{u}_0(\xi)d\xi$$

$\rightarrow e^{i\xi x}$ propagates w/ speed ξ.
(momentum).

More generally, $u_t + a_1 u_x + a_2 u_{xx} + a_3 u_{xxx} + \dots = 0$

$$\omega(\xi) = a_1\xi + i a_2 \xi^2 - a_3\xi^3 - i a_4 \xi^4 + \dots$$

$$u(x,t) = \frac{1}{2\pi}\int e^{i(\xi x - \omega(\xi)t)} \hat{u}_0(\xi)d\xi.$$

$$= \frac{1}{2\pi}\int e^{i\xi(x - \frac{\omega(\xi)}{\xi}t)} \hat{u}_0(\xi)d\xi.$$

ξ is the wave number of the wave $e^{i\xi x}$

ω real: $\omega(\xi)$ is the frequency of the wave $e^{i\xi x}$
(called dispersion relation)

Def. $c_p = \frac{\omega(\xi)}{\xi}$ is the phase velocity of the wave. $e^{i\xi x}$
($\omega = ck$)

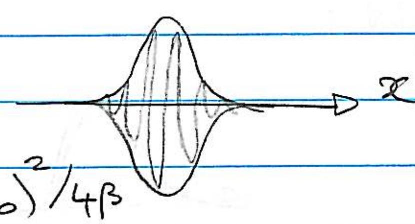
(ω complex · real part gives freq. / phase velocity
· imag. part gives damping / growth.)

Def. $c_g = \frac{d\omega(\xi)}{d\xi}$ is the group velocity of the wave

→ velocity at which energy travels

e.g. $c_p = a - b\xi^2$, $\omega(\xi) = a\xi - b\xi^3$
$c_g = a - 3b\xi^2 \neq c_p$.

Ex. $u_0(x) = e^{i\xi_0 x} e^{-\beta x^2}$ (wave packet)



$$\hat{u}_0(\xi) = \sqrt{\frac{\pi}{\beta}}\, e^{-(\xi-\xi_0)^2/4\beta}$$

$$u(x,t) = c \int e^{i(\xi x - \omega(\xi)t)}\, e^{-(\xi-\xi_0)^2/4\beta}\, d\xi$$

oscillations cancel out at most points, except those where the phase is stationary:

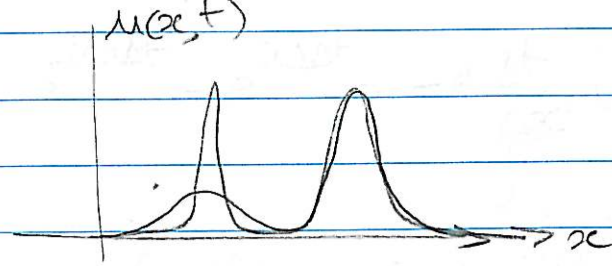
$$\frac{d}{d\xi}\left(\xi x - \omega(\xi)t\right) \Rightarrow x = \frac{d\omega}{d\xi}t.$$

and $\xi \simeq \xi_0 \Rightarrow x = \frac{d\omega}{d\xi}(\xi_0)\, t$

is the point around which the Gaussian is centered.

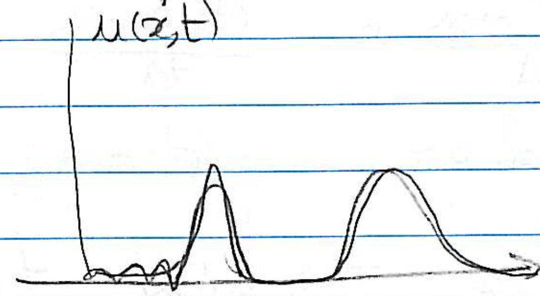
$\rightarrow c_g = \frac{d\omega}{d\xi}$ is the wave packet speed.

Numerical dissipation:



(high freq. are damped out)

Numerical dispersion:



(high freq. are trailing)

Upwind (num. dissipation) may be preferable to Lax-Wendroff or Leap Frog (num. dispersion)

Dispersion relation (curve): $\omega(\xi)$ for a PDE
or $\omega(k)$ for a numerical scheme.

Assume a solution $U_j^n = e^{i(kx_j - \omega t_n)}$

(so $g(k) \to e^{-i\omega\Delta t}$ where $\omega(k)$)

eg Leap-frog for $u_t + a u_x = 0$

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = -a \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$\Rightarrow e^{-i\omega\Delta t} - e^{i\omega\Delta t} = -\underbrace{a\frac{\Delta t}{\Delta x}}_{=\nu}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right),$$

$h = \Delta x$

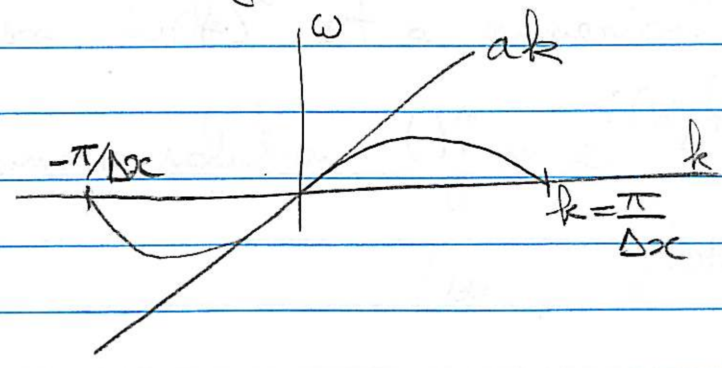
$$\boxed{\sin(\omega\Delta t) = \nu \sin(k\Delta x)} \qquad \nu = a\frac{\Delta t}{\Delta x}$$

or $\dfrac{\sin(\omega\Delta t)}{\Delta t} = a\dfrac{\sin(k\Delta x)}{\Delta x} \Rightarrow \omega(k)$ nonlinear

(ODE (exact): $\omega = ak$)

Note that $|k\Delta x| \le \pi$ for the well-resolved wave numbers.

Δt very small $\Rightarrow \omega \simeq a \dfrac{\sin k\Delta x}{\Delta x}$



$$\frac{d\omega}{dk} = \pm \frac{a\cos kh}{\sqrt{1 - \nu\sin^2 kh}}$$

can become negative, unlike a.

03/30 | Dispersion curves
Spectral methods.

Recall
$$\begin{cases} u_t + a u_x + b u_{xxx} = 0 & x \in \mathbb{R} \\ u(x,0) = u_0(x) \end{cases}$$

where $b u_{xxx}$ could be numerical dispersion in a modified equation

$$\Rightarrow u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(x\xi - \omega(\xi)t)}\, \hat{u}_0(\xi)\, d\xi$$

with the dispersion relation

$$\omega(\xi) = a\xi - b\xi^3$$

$$\Rightarrow x\xi - \omega(\xi)t = \xi\left(x - \frac{\omega(\xi)}{\xi}t\right)$$

(i.e. $e^{i(x\xi - \omega t)}$ is a solution only for some ω)

$$C_p = \frac{\omega(\xi)}{\xi} = a - b\xi^2 \qquad \text{phase velocity}$$

$$C_g = \frac{d\omega}{d\xi} = a - 3b\xi^2 \qquad \text{group velocity}$$

Dispersion: | different $e^{ix\xi}$ travel at different speeds C_p.

Can also directly consider the dispersion relation $\omega(k)$ of a numerical scheme

$\rightarrow$ assume a solution $U_j^n = e^{i(x_j k - \omega t_n)}$ $\qquad x_j = j\Delta x$, $t_n = n\Delta t$

$$\left(\text{so } \rho_n = e^{-i\omega t_n}, \quad g(k) = e^{-i\omega \Delta t}\right)$$

→ Determine $\omega(k)$ from the scheme

eg leap-frog for $u_t + a u_x = 0$ $(a>0)$

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = -a \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$e^{-i\omega\Delta t} - e^{i\omega\Delta t} = -a\frac{\Delta t}{\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)$$

$$\sin(\omega\Delta t) = \nu \sin(k\Delta x) \qquad \nu = a\frac{\Delta t}{\Delta x}$$

or $$\frac{\sin(\omega\Delta t)}{\Delta t} = a\frac{\sin(k\Delta x)}{\Delta x} \rightarrow \omega(k)$$

Contrast with dispersion relation for the ODE:

$$\omega = ak.$$

Cutoff on wave vectors: $|k\Delta x| \leq \pi$,

such that if $k = \pi/\Delta x$,

$$e^{ikj\Delta x} = e^{i\pi j} = (-1)^j \rightarrow U_j = [1,-1,1,-1,\ldots]$$

(flip-flop)

Modes such that $|k| \leq \pi/\Delta x$

are resolved / properly sampled

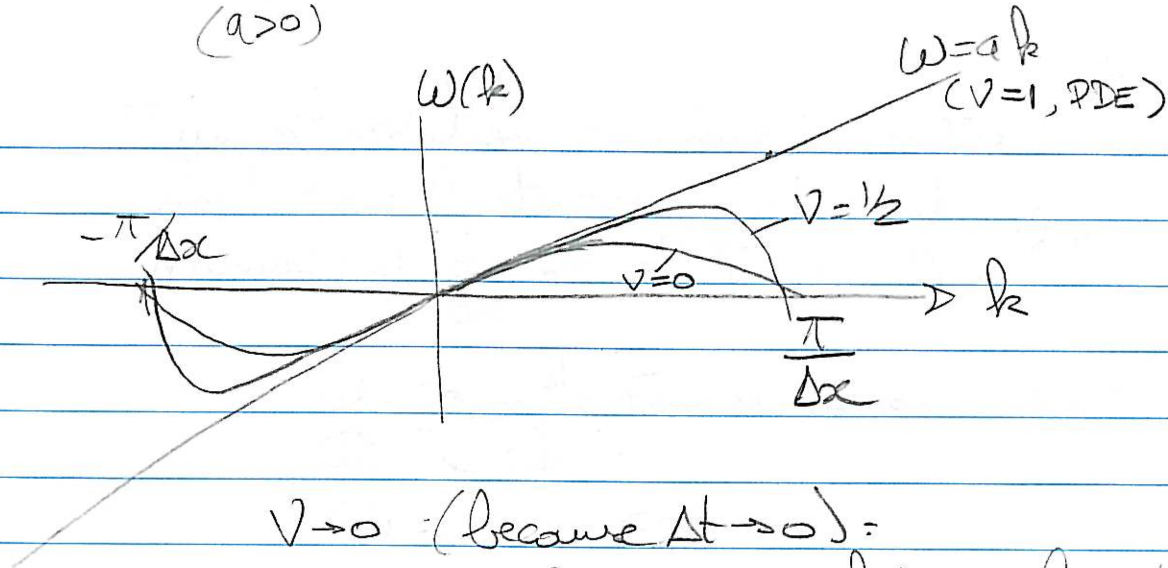
Modes such that $|k| > \pi/\Delta x$ are aliases:

eg. $k = \frac{2\pi}{\Delta x}$: $e^{i(2\pi/\Delta x)j\Delta x} = e^{2\pi i j} = 1^j = 1$

equivalent to $k=0$

$k = \frac{3}{2}\frac{\pi}{\Delta x}$ equivalent to $k = -\frac{\pi}{2\Delta x}$

→ periodicity in k, with period $\frac{2\pi}{\Delta x}$.



$V \to 0$ (because $\Delta t \to 0$):

$$\omega(k) \to a \frac{\sin k\Delta x}{\Delta x}$$ = big dispersion errors.

$V=1$: $\omega(k) = ak$ (coincidence, almost)

$V>1$: unstable

In general, $\frac{d\omega}{dk} = a\frac{\cos k\Delta x}{\cos \omega\Delta t} = a\frac{\cos k\Delta x}{\sqrt{1-V^2\sin^2 k\Delta x}}$

can become negative! (a>0)

→ high frequency numerical pollution can travel left

(e.g. $|k| \geq \frac{1}{2}\frac{\pi}{\Delta x}$ when V very small)

Concl. FD methods for hyperbolic/advection eq. in general incur significant dispersion-based errors.

Remedy: Higher-order methods
Spectral methods

→ enlarge the bandwidth (range in k) for which $\omega(k)$ is close to that of the PDE.

Type of solution considered in the next few lectures: such that numerical $\frac{d}{dx}$ of e^{ikx_j} is ike^{ikx_j}

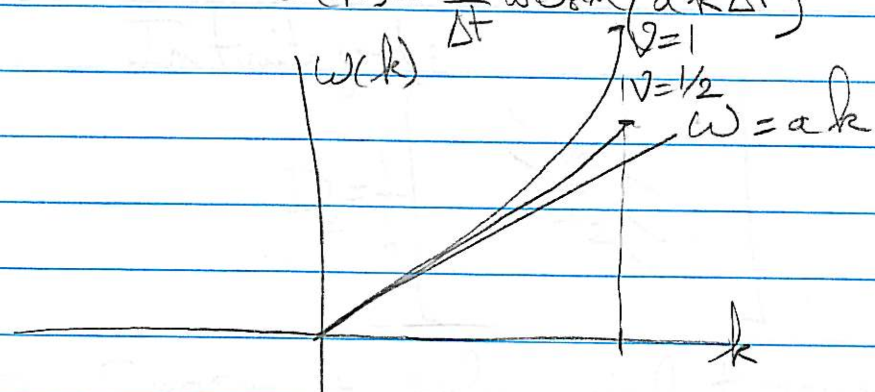
1. go in the Fourier domain (FT)
2. $\times\, ik$
3. inverse FT

Then, if $U_j^n = e^{i(kx_j - \omega t_n)}$,

$$\frac{U_j^{n+1} - U_j^{n-1}}{2\Delta t} = -a(ik)\,U_j^n$$

$$\Rightarrow \frac{\sin(\omega\Delta t)}{\Delta t} = ak$$

$$\omega(k) = \frac{1}{\Delta t}\arcsin(ak\Delta t)$$



Correct behavior (limit) as $\nu \to 0$

Better: use higher order in t.

Questions:
- how: range of discrete k
- how accurate: relation btw k and ξ
  - Taylor $\to$ Fourier series
- boundary conditions: beyond periodic

Part III (Trefethen)

Differentiation - spectral accuracy. (Chap. 1)
Derivative from interpolant (local)

$$\{x_j, u(x_j)\} \longrightarrow u'(x_j) \qquad\qquad x_j = jh$$

ex: For each j, pass a parabola through

$$\left\{\begin{array}{l} x_{j-1}, u(x_{j-1}) \\ x_j, u(x_j) \\ x_{j+1}, u(x_{j+1}) \end{array}\right. \longrightarrow p(x)$$

Differentiate at x_j:

$$u'(x_j) \simeq p'(x_j)$$
$$= \frac{u(x_{j+1}) - u(x_{j-1})}{2h} \quad \to \text{order } 2$$

Infinite grid:

$$D_2 = \frac{1}{h}\begin{bmatrix} \ddots & & \\ \ddots & 1/2 & \\ \ddots & 0 & \ddots \\ & -1/2 & \ddots \\ & & \ddots \end{bmatrix} \qquad \text{(circulant matrix)}$$

ex. Degree 4 polynomial through

$$\left\{\begin{array}{l} x_{j\pm 2}, u(x_{j\pm 2}) \\ x_{j\pm 1}, u(x_{j\pm 1}) \\ x_j, u(x_j) \end{array}\right.$$

Diff. at x_j $\quad u'(x_j) \simeq p'(x_j)$

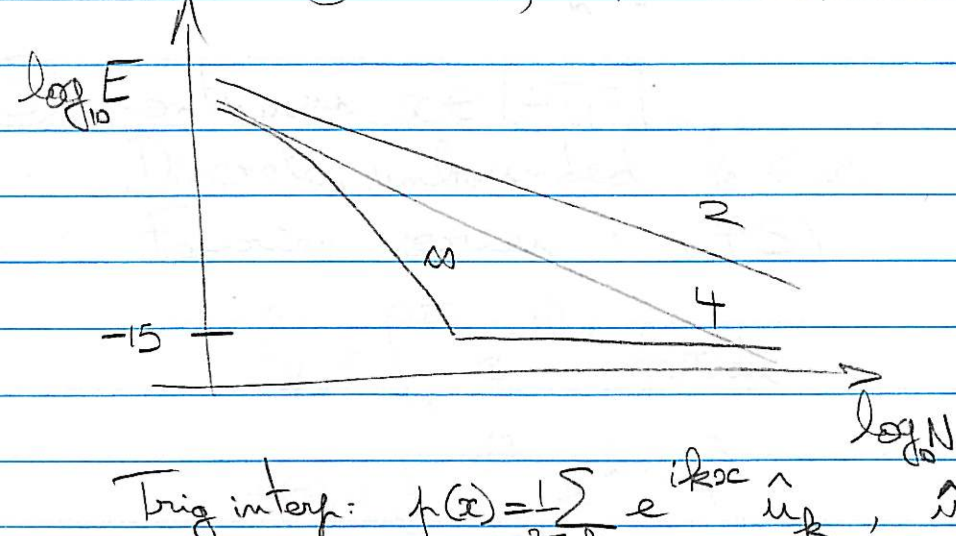
Now $D_4 = \frac{1}{h}\begin{bmatrix} & \ddots & \\ & -1/12 & \\ & 2/3 & \\ & 0 & \\ & -2/3 & \\ & 1/12 & \\ & \ddots & \end{bmatrix}$ → order 4.

ex. take the limit deg (polynomial) → ∞.

$$D_N \to \frac{1}{h}\begin{bmatrix} & \vdots & \\ & 1/3 & \\ \ddots & -1/2 & \\ & 1 & \\ & 0 & \\ & -1 & \\ & 1/2 & \ddots \\ & -1/3 & \\ & \vdots & \end{bmatrix} = D_\infty$$

D_∞ is also the result of differentiating the trigonometric interpolant of $\{x_j, u(x_j)\}$. (on an infinite grid).

Spectral accuracy: error decays like $O(C^N)$, $C<1$, instead of the usual $O(N^{-m})$, $m = 2$ or 4.



Trig interp: $p(x) = \frac{1}{2\pi}\sum_k e^{ikx}\,\hat{u}_k$, $\hat{u}_k = \sum_j e^{-ikx_j} u(x_j)$

→ periodic grid.

Different kinds of Fourier transforms:

① Continuous $x \in \mathbb{R}$
Continuous $\xi \in \mathbb{R}$, Fourier transform: (FT)

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} f(x)\,dx$$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi x} \hat{f}(\xi)\,d\xi$$

ξ = wave number
$= 2\pi/\lambda$,
λ = wavelength

② Discrete, unbounded $x_j = jh$, $f_j = f(x_j)$, $j \in \mathbb{Z}$
Continuous $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$ (fundamental cell)
"Semidiscrete" Fourier transform (SFT)

$$\hat{f}(\xi) = h \sum_{j=-\infty}^{\infty} e^{-i\xi x_j} f_j$$

$$f_j = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} e^{i\xi x_j} \hat{f}(\xi)\,d\xi.$$

Rmk: $\hat{f}\left(\xi + \frac{2\pi m}{h}\right) = \hat{f}(\xi)$ when $m \in \mathbb{Z}$.

③ Continuous $x \in [-\pi, \pi]$
Discrete, unbounded $k \in \mathbb{Z}$
Fourier series: (FS)

$$\hat{f}_k = \int_{-\pi}^{\pi} e^{-ikx} f(x)\,dx$$

$$f(x) = \frac{1}{2\pi}\sum_{k=-\infty}^{\infty} e^{ikx} \hat{f}_k$$

Rmk: $f(x+2\pi m) = f(x)$

Justification: $\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} \right\}$ are orthonormal on $[-\pi,\pi]$

+ completeness.

(4) Discrete, bounded $x_j = jh$, $j = 1, \dots, N$.

with $x_0 = 0$ and $x_N = 2\pi$, identified by periodicity ($j=0$ not part of the grid)

$\Rightarrow$ $Nh = 2\pi$

$$\boxed{h = \frac{2\pi}{N}} \quad \left(\text{instead of } \frac{1}{N}\right)$$

Discrete, bounded $k = -\frac{N}{2}, -\frac{N}{2}+1, \dots, 0, \dots, \frac{N}{2}-1$.

(assume N even)

with $k = -\frac{N}{2}$ and $\frac{N}{2}$ identified by periodicity.

(could also write $k = 1, \dots, N$).

Discrete Fourier transform (DFT):

$$\hat{f}_k = h \sum_{j=1}^{N} e^{-ikx_j} f_j$$

$$f_j = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2-1} e^{ikx_j} \hat{f}_k$$

Concl: Discretize in x $\Longleftrightarrow$ Bound, periodize in ξ, k

ξ, k $\qquad\qquad$ x

Trig. interpolant: morally, $u(x_j) \xrightarrow{SFT} \hat{u}(\xi) \xrightarrow{IFT} p(x)$

or $u(x_j) \xrightarrow{DFT} \hat{u}_k \xrightarrow{IFS} p(x)$