Lecture Slides

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Math 228B Numerical Solutions of Differential Equations

Prerequisites

- MATLAB programming
  - Functions, loops, data structures, linear algebra, plotting
  - Possibly some knowledge of compiled languages (C or Fortran)
- Basic numerical analysis
  - Finite precision, root-finding, fixed point, Newton's method
  - Differentiation/integration, approximation/interpolation
  - Numerical linear algebra: Norms, linear systems
- Initial value problems (IVPs):
  - Explicit/implicit methods, Runge-Kutta/DIRK, Adams/BDF
  - Stability/convergence, absolute stability, stiff equations
  - Error estimation, stepsize control
  - Implementation, including Newton's method if nonlinear
- Boundary value problems (BVPs):
  - Finite difference approximations with arbitrary grid spacing
  - Global system of equations, with boundary conditions
- The finite difference method (FDM):
  - Elliptic equations: Formulation, analysis, implementaion
  - Some knowledge of schemes for parabolic/hyperbolic equations

Topics

- Finite difference methods for parabolic/hyperbolic equations (mostly review)
- Finite volume methods
- Finite element methods
- Discontinuous Galerkin methods
- Level set methods
- Unstructured grid generation
- Iterative methods for sparse equations, multigrid

Finite Difference Methods for Parabolic Problems

Parabolic equations

- Model problem: The *heat equation*:

$$\frac{\partial u}{\partial t} - \nabla \cdot (\kappa \nabla u) = f$$

  where
  - $u = u(\boldsymbol{x}, t)$ is the *temperature* at a given point and time
  - κ is the *heat capacity* (possibly $\boldsymbol{x}$- and t-dependent)
  - f is the *source term* (possibly $\boldsymbol{x}$- and t-dependent)
- Need *initial conditions* at some time t_0:

$$u(\boldsymbol{x}, t_0) = \eta(\boldsymbol{x})$$

- Need *boundary conditions* at domain boundary Γ:
  - *Dirichlet condition* (prescribed temperature): $u = u_D$
  - *Neumann condition* (prescribed heat flux): $\boldsymbol{n} \cdot (\kappa \nabla u) = g_N$

1D discretization

- Initial case: One space dimension, $\kappa = 1$, $f = 0$:

$$u_t = \kappa u_{xx}, \qquad 0 \le x \le 1$$

with boundary conditions $u(0,t) = g_0(t)$, $u(1,t) = g_1(t)$

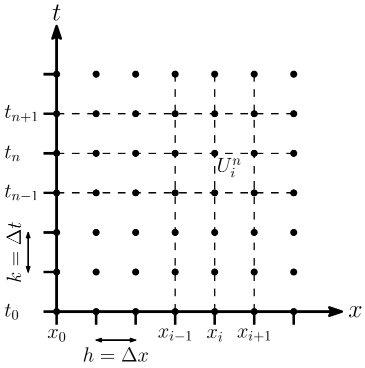
- Introduce finite difference grid:

$$x_i = ih, \quad t_n = nk$$

with *mesh spacing* $h = \Delta x$ and *time step* $k = \Delta t$.

- Approximate the solution u at grid point (x_i, t_n):

$$U_i^n \approx u(x_i, t_n)$$



Numerical schemes: FTCS

- FTCS (Forward in time, centered in space):

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{1}{h^2}\left(U_{i-1}^n - 2U_i^n + U_{i+1}^n\right)$$

or, as an explicit expression for U_i^{n+1},

$$U_i^{n+1} = U_i^n + \frac{k}{h^2}\left(U_{i-1}^n - 2U_i^n + U_{i+1}^n\right)$$

- Explicit one-step method in time
- Boundary conditions naturally implemented by setting

$$U_0^n = g_0(t_n), \qquad U_{m+1}^n = g_1(t_n)$$

FTCS, MATLAB implementation

ftcsdemo.m

```matlab
% 1D heat equation, FTCS scheme

% Discretization
m = 100;
h = 1 / (m+1);
x = h * (0:m)';
k = .5*h^2;
T = 0.2;

u = exp(-(x-0.25).^2 / .1^2) + 0.1*sin(10*2*pi*x); % Initial conditions
u([1,end]) = 0; % Dirichlet boundary conditions

for n=1:ceil(T/k)
    u(2:m) = u(2:m) + k/h^2 * (u(1:m-1) - 2*u(2:m) + u(3:m+1));
    plot(x,u), axis([0,1,-.1,1.1]), grid on, pause(0.05)
end
```

Numerical schemes: Crank-Nicolson

- Crank-Nicolson – like FTCS, but use average of space derivative at time steps n and $n+1$:

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{1}{2}\left(D^2 U_i^n + D^2 U_i^{n+1}\right)$$
$$= \frac{1}{2h^2}\left(U_{i-1}^n - 2U_i^n + U_{i+1}^n + U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}\right)$$

  or

$$-rU_{i-1}^{n+1} + (1+2r)U_i^{n+1} - rU_{i+1}^{n+1} = rU_{i-1}^n + (1-2r)U_i^n + rU_{i+1}^n$$

  where $r = k/2h^2$

- Implicit one-step method in time $\Longrightarrow$ need to solve tridiagonal system of equations

Crank-Nicolson, MATLAB implementation

cndemo.m

```
% 1D heat equation, Crank-Nicolson scheme

% Discretization
m = 99;
h = 1 / (m+1);
x = h * (0:m+1)';
k = .5*h^2;
T = 0.2;

u = exp(-(x-0.25).^2 / .1^2) + 0.1*sin(10*2*pi*x); % Initial conditions
u([1,end]) = 0; % Dirichlet boundary conditions

A = spdiags(ones(m,1) * [1,-2,1] / h^2, -1:1, m, m);
I = speye(m, m);

for n=1:ceil(T/k)
    u(2:m+1) = (I - k/2*A) \ ((I + k/2*A)*u(2:m+1)); % Zero-Dirichlet
    plot(x,u), axis([0,1,-.1,1.1]), grid on, pause(0.05)
end
```

Local truncation error

- LTE: Insert exact solution $u(x,t)$ into difference equations
- Ex: FTCS

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

Assume u smooth enough and expand in Taylor series:

$$\tau(x,t) = \left(u_t + \frac{1}{2}ku_{tt} + \frac{1}{6}k^2 u_{ttt} + \cdots\right) - \left(u_{xx} + \frac{1}{12}h^2 u_{xxxx} + \cdots\right)$$

Use the equation: $u_t = u_{xx}$, $u_{tt} = u_{txx} = u_{xxxx}$:

$$\tau(x,t) = \left(\frac{1}{2}k - \frac{1}{12}h^2\right) u_{xxxx} + O(k^2 + h^4) = O(k + h^2)$$

First order accurate in time, second order accurate in space

- Ex: For Crank-Nicolson, $\tau(x,t) = O(k^2 + h^2)$
- *Consistent* method if $\tau(x,t) \to 0$ as $k, h \to 0$

Method of Lines

- Discretize PDE in space, integrate resulting *semidiscrete* system of ODEs using standard schemes
- Ex: Centered in space

$$U_i'(t) = \frac{1}{h^2}(U_{i-1}(t) - 2U_i(t) + U_{i+1}(t)), \quad i = 1, \ldots, m$$

  or in matrix form: $U'(t) = AU(t) + g(t)$, where

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}, \quad g(t) = \frac{1}{h^2}\begin{bmatrix} g_0(t) \\ 0 \\ 0 \\ \vdots \\ 0 \\ g_1(t) \end{bmatrix}$$

- Solve the centered semidiscrete system using:
  - Forward Euler $U^{n+1} = U^n + kf(U^n)$
    $\Longrightarrow$ the FTCS method
  - Trapezoidal method $U^{n+1} = U^n + \frac{k}{2}(f(U^n) + f(U^{n+1}))$
    $\Longrightarrow$ the Crank-Nicolson method

Heat equation, method of lines with ode15s

heatdemo.m

```
% 1D heat equation, MATLAB ODE suite function ode15s
% With error and step size control

% Discretization
m = 99;
h = 1 / (m+1);
x = h * (0:m+1)';
T = 0.2;

u = exp(-(x-0.25).^2 / .1^2) + 0.1*sin(10*2*pi*x); % Initial conditions
u([1,end]) = 0; % Dirichlet boundary conditions

odeopts = odeset('reltol',1e-6, 'abstol', 1e-6);
fode = @(t,u) ([0;u(1:m-1)]-2*u+[u(2:m);0])/h^2; % Zero-Dirichlet
[ts,us] = ode15s(fode, [0,T], u(2:m+1), odeopts);

[tts,xxs]=meshgrid(ts,x(2:m+1));
surf(tts,xxs,us')
shading interp
camlight headlight
```

Method of Lines, Stability

- Stability requires $k\lambda$ to be inside the absolute stability region, for all eigenvalues λ of A
- For the centered differences, the eigenvalues are

$$\lambda_p = \frac{2}{h^2}(\cos(p\pi h) - 1), \quad p = 1, \ldots, m$$

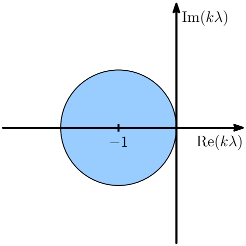
or, in particular, $\lambda_m \approx -4/h^2$

- Euler gives $-2 \leq -4k/h^2 \leq 0$, or

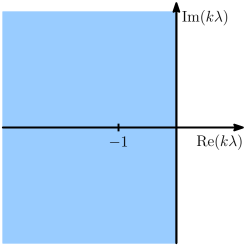
$$\frac{k}{h^2} \leq \frac{1}{2}$$

$\Longrightarrow$ time step restriction for FTCS

- Trapezoidal method A-stable $\Longrightarrow$ Crank-Nicolson is stable for any time step $k > 0$



Forward-Euler stability region



Trapezoidal method stability region

Convergence

- For convergence, k and h must in general approach zero at appropriate rates, for example $k \to 0$ and $k/h^2 \leq 1/2$
- Write the methods as

$$U^{n+1} = B(k)U^n + b^n(k) \qquad (*)$$

where, e.g., $B(k) = I + kA$ for forward Euler and $B(k) = \left(I - \frac{k}{2}A\right)^{-1}\left(I + \frac{k}{2}A\right)$ for Crank-Nicolson

Definition

A linear method of the form (*) is *Lax-Richtmyer stable* if, for each time T, these is a constant $C_T > 0$ such that

$$\|B(k)^n\| \leq C_T$$

for all $k > 0$ and integers n for which $kn \leq T$.

Theorem (Lax Equivalence Theorem)

A consistent linear method of the form (*) is convergent if and only if it is Lax-Richtmyer stable.

Lax Equivalence Theorem

Proof.

Consider the numerical scheme applied to the numerical solution U and the exact solution $u(x,t)$:

$$U^{n+1} = BU^n + b^n$$
$$u^{n+1} = Bu^n + b^n + k\tau^n$$

Subtract to get difference equation for the error $E^n = U^n - u^n$:

$$E^{n+1} = BE^n - k\tau^n, \quad \text{or} \quad E^N = B^N E^0 - k\sum_{n=1}^{N} B^{N-n}\tau^{n-1}$$

Bound the norm, use Lax-Richtmyer stability and $Nk \le T$:

$$\begin{aligned}\|E^N\| &\le \|B^N\|\|E^0\| + k\sum_{n=1}^{N}\|B^{N-n}\|\|\tau^{n-1}\| \\ &\le C_T\|E^0\| + TC_T \max_{1\le n\le N}\|\tau^{n-1}\| \to 0 \text{ as } k \to 0\end{aligned}$$

provided $\|\tau\| \to 0$ and that the initial data $\|E^0\| \to 0$. □

Convergence

Example

For the FTCS method, $B(k) = I + kA$ is symmetric, so $\|B(k)\|_2 = \rho(B) \leq 1$ if $k \leq h^2/2$. Therefore, it is Lax-Richtmyer stable and convergent, under this restriction.

Example

For the Crank-Nicolson method, $B(k) = \left(I - \frac{k}{2}A\right)^{-1}\left(I + \frac{k}{2}A\right)$ is symmetric with eigenvalues $(1 + k\lambda_p/2)/(1 - k\lambda_p/2)$. Therefore, $\|B(k)\|_2 = \rho(B) < 1$ for any $k > 0$ and the method is Lax-Richtmyer stable and convergent.

Example

$\|B(k)\| \leq 1$ is called *strong stability*, but Lax-Richtmyer stability is also obtained if $\|B(k)\| \leq 1 + \alpha k$ for some constant α, since then

$$\|B(k)^n\| \leq (1 + \alpha k)^n \leq e^{\alpha T}$$

Von Neumann Analysis

- Consider the *Cachy problem*, on all space and no boundaries ($-\infty < x < \infty$ in 1D)
- The grid function $W_j = e^{ijh\xi}$, constant ξ, is an eigenfunction of any translation-invariant finite difference operator
- Consider the centered difference $D_0 V_j = \frac{1}{2h}(V_{j+1} - V_{j-1})$:

$$D_0 W_j = \frac{1}{2h}\left(e^{i(j+1)h\xi} - e^{i(j-1)h\xi}\right) = \frac{1}{2h}\left(e^{ih\xi} - e^{-ih\xi}\right) e^{ijh\xi}$$
$$= \frac{i}{h}\sin(h\xi)e^{ijh\xi} = \frac{i}{h}\sin(h\xi)W_j,$$

  that is, W is an eigenfunction with eigenvalue $\frac{i}{h}\sin(h\xi)$
- Note that this agrees to first order with the eigenvalue $i\xi$ of the operator ∂_x

Von Neumann Analysis

- Consider a function V_j on the grid $x_j = jh$, with finite 2-norm

$$\|V\|_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{1/2}$$

- Express V_j as linear combination of $e^{ijh\xi}$ for $|\xi| \le \pi/h$:

$$V_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{V}(\xi) e^{ijh\xi}\, d\xi, \quad \text{where } \hat{V}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} V_j e^{-ijh\xi}$$

- *Parseval's relation*: $\|\hat{V}\|_2 = \|V\|_2$ in the norms

$$\|V\|_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{1/2}, \quad \|\hat{V}\|_2 = \left(\int_{-\pi/h}^{\pi/h} |\hat{V}(\xi)|^2 d\xi \right)^{1/2}$$

Von Neumann Analysis

- Using Parseval's relation, we can show Lax-Richtmyer stability

$$\|U^{n+1}\|_2 \leq (1+\alpha k)\|U^n\|_2$$

in the Fourier transform of U^n:

$$\|\hat{U}^{n+1}\|_2 \leq (1+\alpha k)\|\hat{U}^n\|_2$$

- This decouples each $\hat{U}^n(\xi)$ from all other wave numbers:

$$\hat{U}^{n+1}(\xi) = g(\xi)\hat{U}^n(\xi)$$

with *amplification factor* $g(\xi)$.

- If $|g(\xi)| \leq 1+\alpha k$, then

$$|\hat{U}^{n+1}(\xi)| \leq (1+\alpha k)|\hat{U}^n(\xi)| \quad \text{and} \quad \|\hat{U}^{n+1}\|_2 \leq (1+\alpha k)\|\hat{U}^n\|_2$$

Von Neumann Analysis

Example (FTCS)

For the FTCS method,

$$U_i^{n+1} = U_i^n + \frac{k}{h^2}\left(U_{i-1}^n - 2U_i^n + U_{i+1}^n\right)$$

we get the amplification factor

$$g(\xi) = 1 + 2\frac{k}{h^2}(\cos(\xi h) - 1)$$

and $|g(\xi)| \leq 1$ if $k \leq h^2/2$

Example (Crank-Nicolson)

For the Crank Nicolson method,

$$-rU_{i-1}^{n+1} + (1+2r)U_i^{n+1} - rU_{i+1}^{n+1} = rU_{i-1}^n + (1-2r)U_i^n + rU_{i+1}^n$$

we get the amplification factor

$$g(\xi) = \frac{1+\frac{1}{2}z}{1-\frac{1}{2}z} \quad \text{where} \quad z = \frac{2k}{h^2}(\cos(\xi h) - 1)$$

and $|g(\xi)| \leq 1$ for any k, h

Multidimensional Problems

- Consider the heat equation in two space dimensions:

$$u_t = u_{xx} + u_{yy}$$

with initial conditions $u(x,y,0) = \eta(x,y)$ and boundary conditions on the boundary of the domain Ω.

- Use e.g. the 5-point discrete Laplacian:

$$\nabla_h^2 U_{ij} = \frac{1}{h^2}(U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{ij})$$

- Use e.g. the trapezoidal method in time:

$$U_{ij}^{n+1} = U_{ij}^n + \frac{k}{2}\left[\nabla_h^2 U_{ij}^n + \nabla_h^2 U_{ij}^{n+1}\right]$$

or

$$\left(I - \frac{k}{2}\nabla_h^2\right) U_{ij}^{n+1} = \left(I + \frac{k}{2}\nabla_h^2\right) U_{ij}^n$$

- Linear system involving $A = I - k\nabla_h^2/2$, not tridiagonal
- But condition number $= O(k/h^2)$, $\Longrightarrow$ fast iterative solvers

Locally One-Dimensional and Alternating Directions

- Split timestep and decouple u_{xx} and u_{yy}:

$$U_{ij}^* = U_{ij}^n + \frac{k}{2}(D_x^2 U_{ij}^n + D_x^2 U_{ij}^*)$$
$$U_{ij}^{n+1} = U_{ij}^* + \frac{k}{2}(D_y^2 U_{ij}^* + D_x^2 U_{ij}^{n+1})$$

or, as in the *alternating direction implicit* (ADI) method,

$$U_{ij}^* = U_{ij}^n + \frac{k}{2}(D_y^2 U_{ij}^n + D_x^2 U_{ij}^*)$$
$$U_{ij}^{n+1} = U_{ij}^* + \frac{k}{2}(D_x^2 U_{ij}^* + D_y^2 U_{ij}^{n+1})$$

- Implicit scheme with only tridiagonal systems
- Remains second order accurate

Finite Difference Methods for Hyperbolic Problems

Advection

- The *scalar advection equation*, with constant velocity a:

$$u_t + au_x = 0$$

- Cauchy problem needs initial data $u(x,0) = \eta(x)$, and the exact solution is

$$u(x,t) = \eta(x - at)$$

- FTCS scheme:

$$\frac{U_j^{n+1} - U_j^n}{k} = -\frac{a}{2h}\left(U_{j+1}^n - U_{j-1}^n\right)$$

or

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

- Stability problems – more later

The Lax-Friedrichs Method

- Replace U_j^n in FTCS by the average of its neighbors:

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

- Lax-Richtmyer stable if

$$\left|\frac{ak}{h}\right| \leq 1,$$

or $k = \mathcal{O}(h)$ – *not stiff*

Method of Lines

- With bounded domain, e.g. $0 \leq x \leq 1$, if $a > 0$ we need an *inflow* boundary condition at $x = 0$:

$$u(0,t) = g_0(t)$$

  and $x = 1$ is an *outflow* boundary
- Opposite if $a < 0$
- Need one-sided differences – more later

Periodic Boundary Conditions

- For analysis, impose the *periodic boundary conditions*

$$u(0,t) = u(1,t), \qquad \text{for } t \geq 0$$

- Equivalent to Cauchy problem with periodic initial data
- Introduce one boundary value as an unknown, e.g. $U_{m+1}(t)$:

$$U(t) = (U_1(t), U_2(t), \dots, U_{m+1}(t))^T$$

- Use periodicity for first and last equations:

$$U_1'(t) = -\frac{a}{2h}(U_2(t) - U_{m+1}(t))$$
$$U_{m+1}'(t) = -\frac{a}{2h}(U_1(t) - U_m(t))$$

Periodic Boundary Conditions

- Leads to Method of Lines formulation $U'(t) = AU(t)$, where

$$A = -\frac{a}{2h}\begin{bmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{bmatrix}$$

- *Skew-symmetric* matrix ($A^T = -A$) $\Longrightarrow$ purely imaginary eigenvalues:

$$\lambda_p = -\frac{ia}{h}\sin(2\pi p h), \qquad p = 1, 2, \ldots, m+1$$

with eigenvectors

$$u_j^p = e^{2\pi i p j h}, \qquad p, j = 1, 2, \ldots, m+1$$

Forward Euler

- Use Forward Euler in time $\Longrightarrow$ FTCS scheme:

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

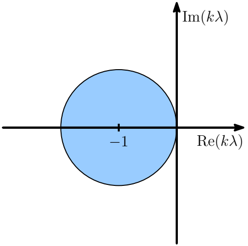
- Stability region $\mathcal{S}$: $|1 + k\lambda| \leq 1 \Longrightarrow$ imaginary $k\lambda_p$ will always be outside $\mathcal{S} \Longrightarrow$ unstable for fixed k/h
- However, if e.g. $k = h^2$, we have

$$\begin{aligned} |1 + k\lambda_p|^2 &\leq 1 + \left(\frac{ka}{h}\right)^2 \\ &= 1 + a^2h^2 = 1 + a^2k \end{aligned}$$

  which gives Lax-Richtmyer stability

$$\|(I + kA)^n\|_2 \leq (1 + a^2k)^{n/2} \leq e^{a^2T/2}$$

- Not used in practice – too strong restriction on timestep k



Forward-Euler stability region

Leapfrog

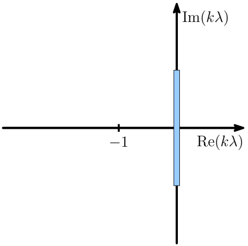
- Consider using the midpoint method in time:

$$U^{n+1} = U^{n-1} + 2kAU^n$$

- For the centered differences in space, this gives the *leapfrog method*:

$$U_j^{n+1} = U_j^{n-1} - \frac{ak}{h}\left(U_{j+1}^n - U_{j-1}^n\right)$$

- Stability region $\mathcal{S}$: $i\alpha$ for $-1 < \alpha < 1$ $\implies$ stable if $|ak/h| < 1$
- Only marginally stable $\implies$ *nondissipative*



Midpoint method stability region

Lax-Friedrichs

- Rewrite the average as:

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

to obtain

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

or

$$\frac{U_j^{n+1} - U_j^n}{k} + a\left(\frac{U_{j+1}^n - U_{j-1}^n}{2h}\right) = \frac{h^2}{2k}\left(\frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2}\right)$$

- Like a discretization of the *advection-diffusion* equation

$$u_t + au_x = \epsilon u_{xx}$$

where $\epsilon = h^2/(2k)$.

Lax-Friedrichs

- The Lax-Friedrichs method can then be written as $U'(t) = A_\epsilon U(t)$ with

$$A_\epsilon = -\frac{a}{2h}\begin{bmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{bmatrix} + \frac{\epsilon}{h^2}\begin{bmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ 1 & & & & 1 & -2 \end{bmatrix}$$

where $\epsilon = h^2/(2k)$

Lax-Friedrichs

- The eigenvalues of A_ϵ are shifted from the imaginary axis into the left half-plane:

$$\mu_p = -\frac{ia}{h}\sin(2\pi p h) - \frac{2\epsilon}{h^2}(1-\cos(2\pi p h))$$

- Ellipse centered at $-2ka/h^2$, semi-axes $2k\epsilon/h^2$, ak/h
- For Lax-Friedrichs, $\epsilon = h^2/(2k)$ and $-2k\epsilon/h^2 = -1 \Longrightarrow$ stable if $|ak/h| \leq 1$

The Lax-Wendroff Method

- Use Taylor series method for higher order accuracy in time
- For $U'(t) = AU(t)$, we have $U'' = AU' = A^2U$ and the second-order Taylor method

$$U^{n+1} = U^n + kAU^n + \frac{1}{2}k^2A^2U^n$$

- Note that

$$(A^2U)_j = \frac{a^2}{4h^2}\left(U_{j-2} - 2U_j + U_{j+2}\right)$$

so the method can be written

$$U_j^{n+1} = U_j^n - \frac{ak}{2h}\left(U_{j+1}^n - U_{j-1}^n\right) + \frac{a^2k^2}{8h^2}\left(U_{j-2}^n - 2U_j^n + U_{j+2}^n\right)$$

- Replace last term by 3-point discretization of $a^2k^2u_{xx}/2 \Longrightarrow$ the *Lax-Wendroff method*:

$$U_j^{n+1} = U_j^n - \frac{ak}{2h}\left(U_{j+1}^n - U_{j-1}^n\right) + \frac{a^2k^2}{2h^2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right)$$

Stability analysis

- The Lax-Wendroff method is Euler's method applied to $U'(t) = A_\epsilon U(t)$, with $\epsilon = a^2k/2 \implies$ eigenvalues

$$k\mu_p = -i\left(\frac{ak}{h}\right)\sin(p\pi h) + \left(\frac{ak}{h}\right)^2(\cos(p\pi h) - 1)$$

- On ellipse centered at $-(ak/h)^2$ with semi-axes $(ak/h)^2$, $|ak/h|$
- Stable if $|ak/h| \leq 1$

- Consider *one-sided approximations* for u_x, e.g. for $a > 0$:

$$U_j^{n+1} = U_j^n - \frac{ak}{h}(U_j^n - U_{j-1}^n), \text{ stable if } 0 \leq \frac{ak}{h} \leq 1$$

or, if $a < 0$:

$$U_j^{n+1} = U_j^n - \frac{ak}{h}(U_{j+1}^n - U_j^n), \text{ stable if } -1 \leq \frac{ak}{h} \leq 0$$

- Natural with asymmetry for the advection equation, since the solution is translating at speed a

Stability analysis

- The upwind method for $a > 0$ can be written

$$U_j^{n+1} = U_j^n - \frac{ak}{2h}(U_{j+1}^n - U_{j-1}^n) + \frac{ak}{2h}(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$$

- Again like a discretization of advection-diffusion $u_t + au_x = \epsilon u_{xx}$, with $\epsilon = ah/2 \implies$ stable if

$$-2 < -2\epsilon k/h^2 < 0, \quad \text{or} \quad 0 \leq \frac{ak}{h} \leq 1$$

- The three methods, Lax-Wendroff, upwind, Lax-Friedrichs, can all be written as advection-diffusion with

$$\epsilon_{LW} = \frac{a^2k}{2} = \frac{ah\nu}{2}, \quad \epsilon_{up} = \frac{ah}{2}, \quad \epsilon_{LF} = \frac{h^2}{2k} = \frac{ah}{2\nu}$$

where $\nu = ak/h$. Stable if $0 < \nu < 1$.

The Beam-Warming method

- Like upwind, but use second-order one-sided approximations:

$$
\begin{aligned}
U_j^{n+1} = & U_j^n - \frac{ak}{2h}(3U_j^n - 4U_{j-1}^n + U_{j-2}^n) \\
& + \frac{a^2k^2}{2h^2}(U_j^n - 2U_{j-1}^n + U_{j-2}^n) \quad \text{for } a > 0
\end{aligned}
$$

and

$$
\begin{aligned}
U_j^{n+1} = & U_j^n - \frac{ak}{2h}(-3U_j^n + 4U_{j+1}^n - U_{j+2}^n) \\
& + \frac{a^2k^2}{2h^2}(U_j^n - 2U_{j+1}^n + U_{j+2}^n) \quad \text{for } a < 0
\end{aligned}
$$

- Stable if $0 \le \nu \le 2$ and $-2 \le \nu \le 0$, respectively

Von Neumann analysis

Example (The upwind method)

$$g(\xi) = (1 - \nu) + \nu e^{-i\xi h}$$

where $\nu = ak/h$, stable if $0 \leq \nu \leq 1$

Example (Lax-Friedrichs)

$$g(\xi) = \cos(\xi h) - \nu i \sin(\xi h) \Longrightarrow |g(\xi)|^2 = \cos^2(\xi h) + \nu^2 \sin^2(\xi h),$$

stable if $|\nu| \leq 1$

Von Neumann analysis

Example (Lax-Wendroff)

$$g(\xi) = 1 - i\nu[2\sin(\xi h/2)\cos(\xi h/2)] - \nu^2[2\sin^2(\xi h/2)]$$
$$\implies |g(\xi)|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4(\xi h/2)$$

stable if $|\nu| \leq 1$

Example (Leapfrog)

$$g(\xi)^2 = 1 - 2\nu i \sin(\xi h) g(\xi),$$

stable if $|\nu| < 1$ (like the midpoint method)

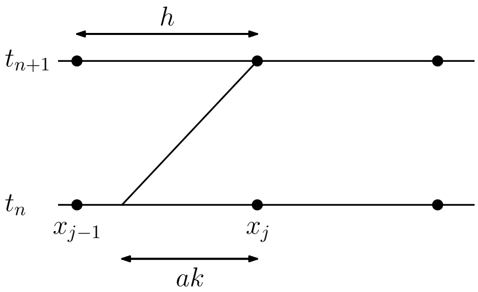
Characteristic tracing and interpolation

- Consider the case $a > 0$ and $ak/h < 1$
- Trace characteristic through x_j, t_{n+1} to time t_n
- Find U_j^{n+1} by linear interpolation between U_{j-1}^n and U_j^n:

$$U_j^{n+1} = U_j^n - \frac{ak}{h}(U_j^n - U_{j-1}^n)$$

$\Longrightarrow$ first order upwind method

- Quadratic interpolating U_{j-1}^n, U_j^n, U_{j+1}^n $\Longrightarrow$ Lax-Wendroff
- Quadratic interpolating U_{j-2}^n, U_{j-1}^n, U_j^n $\Longrightarrow$ Beam-Warming



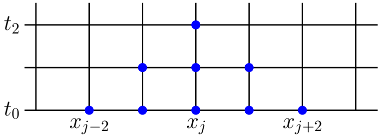
The CFL condition

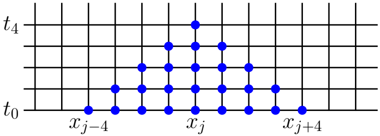
- For the advection equation, $u(X,T)$ depends only on the initial data $\eta(X-aT)$
- The *domain of dependence* is $\mathcal{D}(X,T) = \{X-aT\}$
- Heat equation $u_t = u_{xx}$, $\mathcal{D}(X,T) = (-\infty,\infty)$
- Domain of dependence for 3-point explicit FD method: Each value depends on neighbors at previous timestep
- Refining the grid with fixed $k/h \equiv r$ gives same interval
- This region must contain the true $\mathcal{D}$ for the PDE:

$$X - T/r \le X - aT \le X + T/r$$

$\implies |a| \le 1/r$ or $|ak/h| \le 1$

- The *Courant-Friedrichs-Lewy* (CFL) condition: Numerical domain of dependence must contain the true $\mathcal{D}$ as $k,h \to 0$





The CFL condition

Example (FTCS)

The centered-difference scheme for the advection equation is unstable for fixed k/h even if $|ak/h| \leq 1$

Example (Beam-Warming)

3-point one-sided stencil, CFL condition gives $0 \leq ak/h \leq 2$ (for left-sided, used when $a > 0$)

Example (Heat equation)

- $\mathcal{D}(X, T) = (-\infty, \infty) \implies$ any 3-point explicit method violates CFL condition for fixed k/h
- However, with $k/h^2 \leq 1/2$, all of $\mathbb{R}$ is covered as $k \to 0$

Example (Crank-Nicolson)

Any implicit scheme satisfies the CFL condition, since the tridiagonal linear system couples all points.

Modified equations

- Find a PDE $v_t = \cdots$ that the numerical approximation U_j^n satisfies *exactly*, or at least better than the original PDE

Example (Upwind method)

To second order accuracy, the numerical solution satisfies

$$v_t + av_x = \frac{1}{2}ah\left(1 - \frac{ak}{h}\right)v_{xx}$$

Advection-diffusion equation

Example (Lax-Wendroff)

To third order accuracy,

$$v_t + av_x + \frac{1}{6}ah^2\left(1 - \left(\frac{ak}{h}\right)^2\right)v_{xxx} = 0$$

Dispersive behavior, leading to a *phase error*. To fourth order,

$$v_t + av_x + \frac{1}{6}ah^2\left(1 - \left(\frac{ak}{h}\right)^2\right)v_{xxx} = -\epsilon v_{xxxx}$$

where $\epsilon = O(k^3 + h^3) \implies$ highest modes damped

Modified equations

Example (Beam-Warming)

To third order,

$$v_t + av_x = \frac{1}{6}ah^2\left(2 - \frac{3ak}{h} + \left(\frac{ak}{h}\right)^2\right)v_{xxx}$$

Dispersive, similar to Lax-Wendroff

Example (Leapfrog)

Modified equation

$$v_t + av_x + \frac{1}{6}ah^2\left(1 - \left(\frac{ak}{h}\right)^2\right)v_{xxx} = \epsilon v_{xxxxx} + \cdots$$

where $\epsilon = O(h^4 + k^4) \implies$ only odd-order derivatives, *nondissipative* method

Hyperbolic systems

- The methods generalize to first order linear systems of equations of the form
$$u_t + Au_x = 0,$$
$$u(x,0) = \eta(x),$$
where $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}^s$ and a constant matrix $A \in \mathbb{R}^{s\times s}$
- *Hyperbolic* system of conservation laws, with *flux function* $f(u) = Au$, if A diagonalizable with real eigenvalues:
$$A = R\Lambda R^{-1} \quad \text{or} \quad Ar_p = \lambda_p r_p \text{ for } p = 1, 2, \ldots, s$$
- Change variables to eigenvectors, $w = R^{-1}u$, to decouple system into s independent scalar equations
$$(w_p)_t + \lambda_p (w_p)_x = 0, \quad p = 1, 2, \ldots, s$$
with solution $w_p(x,t) = w_p(x - \lambda_p t, 0)$ and initial condition the pth component of $w(x,0) = R^{-1}\eta(x)$.
- Solution recovered by $u(x,t) = Rw(x,t)$, or
$$u(x,t) = \sum_{p=1}^{s} w_p(x - \lambda_p t, 0) r_p$$

Numerical methods for hyperbolic systems

- Most methods generalize to systems by replacing a with A

Example (Lax-Wendroff)

$$U_j^{n+1} = U_j^n - \frac{k}{2h}A(U_{j+1}^n - U_{j-1}^n) + \frac{k^2}{2h^2}A^2(U_{j-1}^n - 2U_j^n + U_{j+1}^n)$$

Second-order accurate, stable if $\nu = \max_{1 \leq p \leq s} |\lambda_p k/h| \leq 1$

Example (Upwind methods)

$$U_j^{n+1} = U_j^n - \frac{k}{h}A(U_j^n - U_{j-1}^n)$$
$$U_j^{n+1} = U_j^n - \frac{k}{h}A(U_{j+1}^n - U_j^n)$$

Only useful if all eigenvalues of A have same sign. Instead, decompose into scalar equations and upwind each one separately $\Longrightarrow$ *Godunov's method*

Initial boundary value problems

- For a bounded domain, e.g. $0 \leq x \leq 1$, the advection equation requires an *inflow* condition $x(0,t) = g_0(t)$ if $a > 0$
- This gives the solution

$$u(x,t) = \begin{cases} \eta(x - at) & \text{if } 0 \leq x - at \leq 1, \\ g_0(t - x/a) & \text{otherwise.} \end{cases}$$

- First-order upwind works well, but other stencils need special cases at inflow boundary and/or outflow boundary
- von Neumann analysis not applicable, but generally gives necessary conditions for convergence
- Method of Lines applicable if eigenvalues of discretization matrix are known