

SAMMANFATTNING AV NUMDIFF (FMFF10)

Objectives

- Learn scientific computing
- Understand mathematics-numerics interaction
- Understand correspondence between math-physics
- Construct elementary MATLAB programs

Different equations

Initial value problems: $\frac{d}{dt}$ (IVP)

Boundary value problems: $\frac{d^2}{dx^2}, \frac{d}{dx}$ (BVP)

Partial differential equations: (PDE) ~~$\frac{\partial}{\partial t} \frac{\partial}{\partial x}$~~

- Parabolic: $\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}$



- Hyperbolic: $\frac{\partial}{\partial t} - \frac{\partial}{\partial x}$



Categories of mathematical problems:

	Algebra	Analysis
Linear	COMPUTABLE	NOT COMPUTABLE
nonlinear	NOT COMPUTABLE	NOT COMPUTABLE

Algebra: Only finite constructs

Analysis: Limits, derivates, integrals etc.

DEF: COMPUTABLE = Exact solution can be obtained with finite computations.

The four principles:

- Discretization : 
 - Linear algebra
 - Linearization
 - Iteration

Discretization (Yields computable problem)

Continuous function $f(x)$ is replaced by
the vector $F = \{f(x_k)\}_0^N$.

Taylor expansion

Approximate $f(x)$ with a polynomial

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \dots + \frac{f^{(n)}(a)}{n!}(x-a)^n + O(x^{n+1})$$

Derivate

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}, \text{ let } \Delta x = x_{k+1} - x_k$$

$$\Rightarrow f'(x_k) \approx \frac{f(x_k + x_{k+1} - x_k) - f(x_k)}{x_{k+1} - x_k} = \boxed{\frac{F_{k+1} - F_k}{x_{k+1} - x_k}} \boxed{f'(x_k)}$$

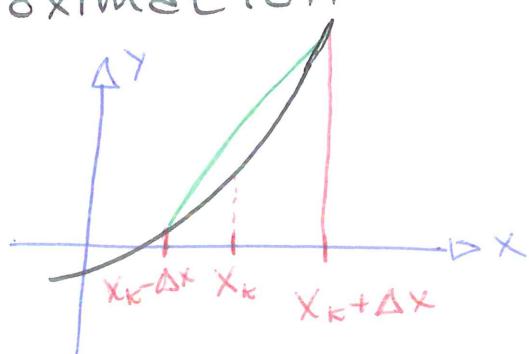
Testing the error: Plot error vs stepsize

in loglog and measure the slope.

$$\begin{aligned} r &= C \Delta x^p \\ \log(r) &= \log(C) + p \log(\Delta x) \end{aligned}$$

We can get faster convergence for $f'(x)$ if we use symmetric approximation

$$f'(x) = \boxed{\frac{F_{k+1} - F_{k-1}}{x_{k+1} - x_{k-1}}} + O(\Delta x^2).$$



Solving $\dot{Y} = q Y$

Analytical solution: $y(t) = y_0 e^{qt}$

Numerical approximation:

$$y_N = \left(1 + \frac{qT}{N}\right)^N y_0 \rightarrow e^{qT} \cdot y_0 \text{ when } N \rightarrow \infty$$

The numerical solution converges!

Summary of Chapter 1 slides - Numdiff

9/12-2015

Lipschitz condition

$$\|f(t, u) - f(t, v)\| \leq L[f] \cdot \|u - v\|$$

Δ — Lipschitz constant

If $L[f] < \infty$, then there exists a unique solution to the initial value problem on $[0, T]$ for every initial value $y(0) = y_0$.

The matrix norm $\|A\|$ is a Lipschitz constant for the equation $f(y) = Ay$

$$\text{Ex: } \dot{y} = Ay \Rightarrow L[f] = \max_{u \neq v} \frac{\|Au - Av\|}{\|u - v\|} = \left\| \begin{array}{l} y = u - v \\ y = Au - Av \end{array} \right\| = \max_{y \neq 0} \frac{\|Ay\|}{\|y\|} = \boxed{\|A\|}$$

Standard form

$$y'' = f, \quad y(0) = y_0, \quad y'(0) = y'_0$$

$$\text{Substitution: } \begin{cases} x_1' = x_2 \\ x_2' = f \end{cases}, \quad x_1(0) = y_0, \quad x_2(0) = y'_0$$

How should f be defined for this to work?

$f(t, y, y')$ \Rightarrow GREAT

$f(t, y)$ \Rightarrow PROBLEMATIC

The explicit Euler method,

$$\left\{ \begin{array}{l} Y_{n+1} = Y_n + h \cdot f(t_n, Y_n) \\ t_{n+1} = t_n + h \end{array} \right.$$

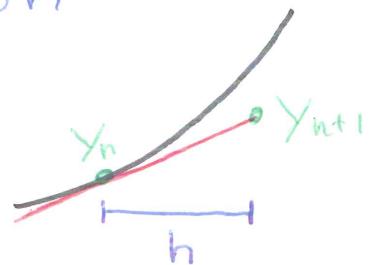
Solution

$$y' = f(t, y)$$

Equation

Taylor: $y(t+h) = y(t) + hy'(t) + O(h^2)$

$f(t, y)$



Local error

Error caused by one step.

Global error

Total error caused by multiple steps.

Convergent: $\lim_{N \rightarrow \infty} \|Y_{N,h} - y(T)\| = 0$ for every $T = N \cdot h$.

Is explicit Euler convergent?

Lemma: assume $a_{n+1} \leq (1+h\mu) a_n + ch^2$
 then $a_n \leq \frac{ch}{\mu} ((1+h\mu)^n - 1)$

Apply the lemma to global error recursion, to get:

$$\|\text{error}_{n,h}\| \leq \frac{C}{L[f]} \cdot h \left[(1 + hL[f])^n - 1 \right] = C(T) \cdot h \xrightarrow{h \rightarrow 0} 0, \quad h \rightarrow 0$$

THE ERROR GOES TO ZERO ~~as~~

WHEN THE STEPSIZE GOES TO ZERO!

Theoretical error bound:

Eq: $y' = -100y$, $y(0) = 1$

$$L[f] \geq \frac{\| -100u - (-100v) \|}{\| u - v \|} = \frac{\| -100y \|}{\| y \|} = 100 L[f]$$

exact solution: $y(t) = e^{-100t}$ exact sol.

$$\begin{aligned} \| \text{error} \| &\leq \frac{c}{L[f]} \cdot h \left((1 + hL[f])^n - 1 \right) = \\ &= \frac{100^2/2}{100} \cdot h \left(e^{100T} - 1 \right) \stackrel{T=1}{\leq} 5e^{100} \cdot h \approx 1.4 \cdot 10^{45} h \end{aligned}$$

A LOT

Actual error: $y_n = (1 - 100h)^n$, $T = 1$, $h \leq 1/50$

$$\Rightarrow \| \text{actual error} \| = \left\| \left(1 - \frac{100}{N} \right)^N - e^{-100} \right\| \leq 3.7 \cdot 10^{-44}$$

THE ERROR IS OVERESTIMATED BY
AT LEAST 89 ORDERS OF MAGNITUDE.

~~This is why "real" math sucks. // Numdiffers~~

~~order of consistency~~

~~The OOC (order of consistency) p is given in~~

The order of Consistency is P if

$$Y(t_{n+1}) - \Phi_h(f, h, Y(t_n), Y(t_{n+1}), \dots) = O(h^{P+1})$$

Just insert monomes to test this.

The linear test equation

$$\text{Eq: } y' = \lambda y, y(0) = 1, t \geq 0, \lambda \in \mathbb{C}$$

Bounded sols if $\boxed{\operatorname{Re}(\lambda) \leq 0}$

DOES NOT IMPLY NUMERICAL STABILITY!

$$\text{DEF: } |y_n| \leq \tilde{K}, \text{ ex: } y_{n+1} = (1+h\lambda)y_n \Rightarrow |1+h\lambda| \leq 1$$

small $h \Rightarrow$ stability

Numerical instability increases exponentially and have oscillatory behaviour!

DEF: A-stability

Stiff equations

"If explicit solvers need very small stepsize to solve the eq., then the eq is stiff."

Homogenius sols are very damped.

Implicit methods with unbounded stability regions put no stability restrictions on h.

SUMMARY OF CHAPTER 3 SLIDES - NUMDIFF

10/12-2015

First order approximations:

- Forward difference: $y'(x) = \frac{y(x+\Delta x) - y(x)}{\Delta x} + O(\Delta x)$

- Backward difference: $y'(x) = \frac{y(x) - y(x-\Delta x)}{\Delta x} + O(\Delta x)$

Second order approximations:

- $y'(x) = \frac{y(x+\Delta x) - y(x-\Delta x)}{2\Delta x} + O(\Delta x^2)$

$$- y''(x) = \frac{\frac{y_{n+1} - y_n}{\Delta x} - \frac{y_n - y_{n-1}}{\Delta x}}{\Delta x} = \frac{y(x+\Delta x) - 2y(x) + y(x-\Delta x)}{\Delta x^2} + O(\Delta x^3)$$

From derivate to matrices

All operators can be represented by a matrix.

Example: forward difference: $\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_N \end{bmatrix} \approx \frac{1}{\Delta x} \begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix} \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_N \end{bmatrix}$

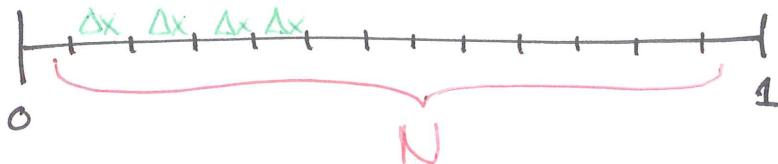
Nullspace: $y = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$

DEFINITION

Nullspace: For which x is $Ax = 0$?

Finite difference methods for 2 p-BVP.

Grid with stepsize $\Delta x = \frac{1}{N+1}$



To discretize, always write the following:

- $y'' = f(x, y) , y(0) = \alpha , y(1) = \beta$

ALWAYS

$$\left\{ \begin{array}{l} \bullet F_1(y) = \frac{\alpha - 2y_1 + y_2}{\Delta x^2} - f(x_1, y_1) \\ \bullet F_i(y) = \frac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} - f(x_i, y_i) \\ \bullet F_N(y) = \frac{y_{N-1} - 2y_N + \beta}{\Delta x^2} - f(x_N, y_N) \end{array} \right.$$

Boundary conditions

Dirchlet: $y(0) = \alpha , y(1) = \beta$

Neumann: $y'(0) = \gamma , y'(1) = \beta$

Robin: $y(0) + c y'(0) = \gamma , y(1) = \beta$

Remember: $\Delta x = \frac{L}{N+0,5}$ for Neumann problems!

Sturm-Liouville eigenvalue problem

DEF: $\frac{d}{dx} \left(p(x) \frac{d}{dx} y(x) \right) = \lambda y$

Example: $y'' = \lambda y \Rightarrow y = A \sin(\sqrt{\lambda}x) + B \cos(\sqrt{\lambda}x)$

$$y(0) = 0 \Rightarrow B = 0$$

$$y(1) = 0 \Rightarrow A \sin(\sqrt{\lambda}) = 0 \Rightarrow \lambda_k = -(k\pi)^2, k=1,2,\dots$$

$$\Rightarrow Y_k(x) = A \sin(k\pi x)$$

Discretization of $y'' = \lambda y$ with BCs

$$\frac{Y_{i-1} - 2Y_i + Y_{i+1}}{\Delta x^2} = \lambda \Delta x Y_i$$

Dirichlet!

$$Y_0 = Y_{N+1} = 0, \Delta x = \frac{1}{N+1}$$

Toeplitz matrix

$$T_{\Delta x} = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & & \ddots & \\ & & & 1 & -2 \end{bmatrix} = \text{tridiag}(1, -2, 1)$$

$$\Rightarrow T_{\Delta x} y = \lambda_{\Delta x} y \quad \text{MATLAB: } \lambda_{\Delta x} = \text{eig}(T_{\Delta x})$$

Note: { Lowest λ more accurate
Good approximation for \sqrt{N} eigenvalues.

DEF: Toeplitz matrix is constant along its diagonals.

Eigenvalues to Toeplitz matrices

$$p(\lambda) = \det(T - \lambda I), \text{ assume } T = S - 2I$$

$$\Rightarrow \det(T - \lambda I) = \det(S - 2I - \lambda I) = \det(S - (\lambda + 2)I)$$

$$\text{Note } \lambda[T] = -2 + \lambda[S] \quad \text{Important}$$

$$\text{Now, find eigenvalues to } S = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & 0 \end{bmatrix}$$

$$\text{Solve } Sy = \lambda y \Leftrightarrow y_{n+1} + y_{n-1} = \lambda y_n$$

Remember function: This is a linear diff. eq.

$$\text{Char eq: } z^2 - \underline{\lambda} z + \underline{1} = 0$$

$$\text{Compare with: } (z-\alpha)(z-\beta) = z^2 - (\underline{\alpha+\beta})z + \underline{\alpha\beta}$$

$$\Rightarrow \begin{cases} \alpha\beta = 1 \\ \alpha + \beta = \lambda \end{cases}, \lambda \text{ is } \cancel{\text{imaginary}} \Rightarrow \text{Roots: } \begin{cases} z \\ 1/z \end{cases}$$

$$y_n = Az^n + Bz^{-n}$$

$$y_0 = 0 \Rightarrow y_n = A(z^n - z^{-n})$$

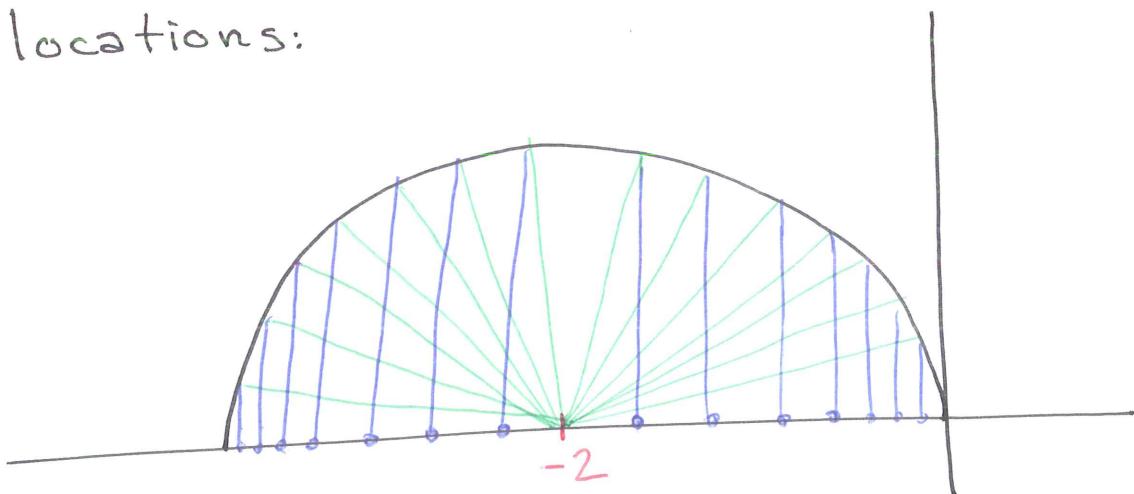
$$y_{N+1} = 0 = A(z^{N+1} - z^{-N-1})$$

$$\Rightarrow z^{(N+1)} = 1 \Rightarrow z_k = e^{\frac{k\pi i}{N+1}}, k=1, \dots, N$$

$$\Rightarrow \lambda_k[s] = z_k + \frac{1}{z_k} = 2 \cos\left(\frac{k\pi i}{N+1}\right)$$

$$\Rightarrow \boxed{\lambda_k[T] = -4 \sin^2\left(\frac{k\pi i}{2(N+1)}\right)} \quad \boxed{\text{eig}(T)}$$

locations:



Norms

$$A \text{ symmetric} \Rightarrow \|A\|_2 = \max_k |\lambda_k|$$

$$A \text{ symmetric} \Rightarrow \mu_2[A] = \max_k \lambda_k$$

Logarithmic norm.

DEF: $\mu_2[A] = \max_{x^T x \neq 0} \left(\frac{x^T A x}{x^T x} \right)$

Th: $\|T_{\Delta x}\|_2 = \frac{4}{\Delta x^2}, \mu_2[T_{\Delta x}] = -5t^2$

Root mean square norm (RMS):

$$\|u\|_{\Delta x}^2 = \sum_{i=1}^N u(x_i)^2 \Delta x = \frac{1}{N+1} \sum_{i=1}^N u(x_i)^2 = \frac{1}{N+1} \|u\|_2^2$$

RMS: $\|u\|_{\Delta x} = \sqrt{\frac{1}{N+1} \sum_{i=1}^N u(x_i)^2}$

square
Root Mean

The Lax principle

Fundamental theorem of numerical analysis

Consistency + Stability \Rightarrow Convergence

Local error $\rightarrow 0$

Bounded second derivative
 $(\|T_{\Delta x}\|_2 \leq C)$

Global error $\rightarrow 0$

SUMMARY OF CHAPTER 4 SLIDES - NUMDIFF

10/12-2015

FROM FINITE DIFFERENCES TO FINITE ELEMENTS

Inner product: $\langle u, v \rangle = \int_0^1 u \cdot v \, dx \Rightarrow \|u\|_2^2 = \langle u, u \rangle$

Can we find a constant such that:

$$\langle u, u'' \rangle \leq M_2 \left[\frac{d^2}{dx^2} \right] \cdot \|u\|_2^2$$

YES, $M_2 \left[\frac{d^2}{dx^2} \right] = -\pi^2$

Awesome formula

$$\langle u, v' \rangle = -\langle u', v \rangle$$

Because $u(0) = u(1)$

$$\langle u, v' \rangle = \int_0^1 uv' \, dx = [uv]_0^1 - \int_0^1 u'v \, dx = -\langle u', v \rangle$$

Sobolov's lemma

For all functions u with $u(0) = u(1) = 0$ it holds that

$$\|u'\|_2 \geq \pi \|u\|_2$$

Proof with Parseval's theorem:

$$u = \sqrt{2} \sum_{k=1}^{\infty} c_k \sin k\pi x \Rightarrow u' = \sqrt{2} \sum_{k=1}^{\infty} k\pi c_k \cos(k\pi x) \quad \square$$

Equality for $u(x) = \sin(\pi x)$.

$$Th: M_2 \left[\frac{d^2}{dx^2} \right] = -\pi^2$$

DEF: if $\langle v, Au \rangle = \langle A^*v, u \rangle$, then A^* is the adjoint operator.

DEF: self-adjoint $\Rightarrow A = A^*$.

All self-adjoint operators have real eigenvalues!

Anti self-adjoint op. ($A^* = -A$) have imaginary λ .

$\frac{d^2}{dx^2}$ - Self-adjoint , $\frac{d}{dx}$ - Anti self-adjoint

This means that diffusion problems have real λ and wave problems have imaginary λ .

Orthogonal eigenvectors: Let $Au = \lambda u$ & $Av = \mu v$

$$\Rightarrow \lambda \langle v, u \rangle = \langle v, Au \rangle = \langle A^*v, u \rangle = \langle Av, u \rangle = \mu \langle v, u \rangle$$

$$\lambda \neq \mu \Rightarrow \langle v, u \rangle = 0. \quad \square$$

Elliptic operators

expectation value of A is the same as λ . $\Rightarrow \lambda_k > 0$

DEF: $\langle u, Au \rangle > 0$, ex: $-\Delta$ is elliptic

DEF: An operator is positive definite if it is self-adjoint and elliptic

Finite difference method

- Replace u and f by vectors
- Replace A by a matrix
- Obtain linear system of equations

Weak formulation

$$\langle v', u' \rangle = \langle v, f \rangle \quad \forall v \quad (\text{several } f \text{ may satisfy this})$$

Energy norm

DEF: $a(v, u) = \langle v', u' \rangle$

The weak formulation can be written: $a(v, u) = \langle v, f \rangle$.

Finite element method

Choose ~~*~~ piecewise linear basis polynomials.

$$v(x) = \sum_{j=1}^n c_j \ell_j(x), \text{ Note: } v(x_i) = c_i \approx u(x_i)$$

Galerkin continuous G(1) method

Best approx: $a(v, u) = \langle v, f \rangle$ with $u, v \in V$

$$\Rightarrow a(u_i, \sum_{j=1}^n c_j \ell_j) = \langle \ell_i, f \rangle$$

which is equivalent to $Kc = b$.

~~Reaktionen~~

Stiffness matrix: $K_{\Delta x} = \frac{1}{\Delta x} \text{tridiag}(-1, 2, -1)$

Mass matrix: $B_{\Delta x} = \frac{\Delta x}{6} \text{tridiag}(1, 4, 1)$

SUMMARY OF CHAPTER 5 SLIDES - NUMDIFF

Elliptic and Parabolic PDEs

10/12-2015

CLASSIFICATION

Poisson eq: $-\Delta u = f + BC$ ELLIPTIC

Diffusion eq: $u_t = \Delta u + BC \& IV$ PARABOLIC

Wave eq: $u_{tt} = \Delta u + BC \& IV$ HYPERBOLIC

Advection eq: $u_t + a(u) \cdot \nabla u = 0 + BC \& IV$ HYPERBOLIC

Classical approach

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + L(u_x, u_y, u, x, y) = 0$$

DEF: $\Delta = \det \begin{pmatrix} A & B \\ B & C \end{pmatrix} = AC - B^2$

$\Delta > 0 \Rightarrow$ Elliptic

$\Delta = 0 \Rightarrow$ Parabolic

$\Delta < 0 \Rightarrow$ Hyperbolic

How can we try this out?

EXAMPLE:

Hyperbolic if $p+q$ is even.
Parabolic if $p+q$ is odd.

Highest real order terms!

$$\frac{\partial^p u}{\partial t^p} = \frac{\partial^q u}{\partial x^q}$$

$$u_t = u_x$$

Hyperbolic

$$u_t = u_{xx}$$

Parabolic

$$u_t = u_{xx}$$

Hyperbolic

↑ not real!

$$u_t = u_{xxx}$$

Hyperbolic

$$u_t = -u_{xxxx}$$

Parabolic

$$u_{tt} = u_{xx}$$

Hyperbolic

$$u_{tt} = -u_{xxxx}$$

Hyperbolic

Strong form: $-\Delta u = f$; $u=0$ on $\partial\Omega$

Irreversability: $u_t = -\Delta u$ is not well posed
 \Rightarrow We cannot run diffusion problems in backward time.

Method of lines (MOL)

In $u_t = u_{xx}$, discretize $\frac{\partial^2}{\partial x^2}$ by:

$$u_{xx} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}$$

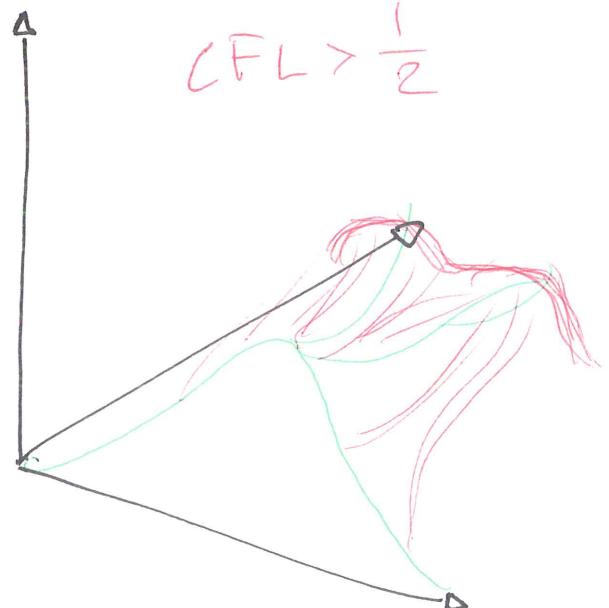
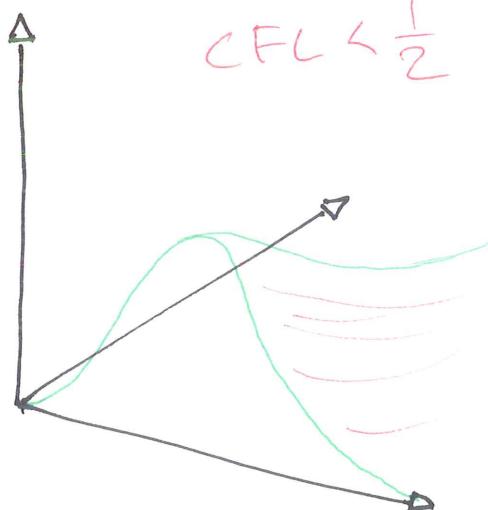
Note: $u_i(t) \approx u(t, x_i)$ along the line $x=x_i$ in (t, x) plane.

Courant number: $\mu = \frac{\Delta t}{\Delta x^2}$

CFL-condition:

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

Important!



Ellen

Crank-Nicolson method (solves $U_t = \alpha U_{xx}$)

Same as the trapezoidal rule for PDEs.

There is no CFL condition on the time-step Δt which is why the Crank-Nicolson method is preferable.

$$\text{Th: } 2[A_\mu] = \frac{1 + \frac{\mu}{2} \lambda[T]}{1 - \frac{\mu}{2} \lambda[T]}$$

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

For every explicit method, there is a CFL-condition.

The convection-diffusion equation

$$U_t = U_{xx} + \alpha U_x - f$$

convection = transport.

Diffusion = concentration loss.

Well-posedness

Suppose $u(x,t) = \mathcal{E}(t) \cdot g(x)$

DEF: The eq. is well-posed for every $t^* > 0$ if there is a constant $0 < C(t^*) < \infty$ such that $\|\mathcal{E}(t)\| \leq C(t^*)$ for all $0 \leq t \leq t^*$.

A well posed eq. has a solution that:

- Depends continuously on the initial value.
- Is uniformly bounded in any compact interval.

Do this:

* Prove that $U_t = U_{xx}$ is well posed!

SUMMARY OF CHAPTER 6 SLIDES - NUMOIFF

11/12-2015

Waves and hyperbolics

Wave equation: $u_{tt} = c^2 u_{xx}$ or $u_t + cu_x = 0$

Conservation law: $u_t + (f(u))_x = 0$ (inviscid flow)

This equation is solved by d'Alembert:

$$u(x,t) = g(x-ct)$$

d'Alembert solution

The solution is constant on the characteristics:

$$x - ct = \text{constant}$$

The advection equation

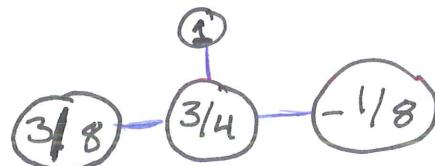
$$u_t + vu_x = 0$$

This can be solved by upwind, downwind and symmetric schemes.

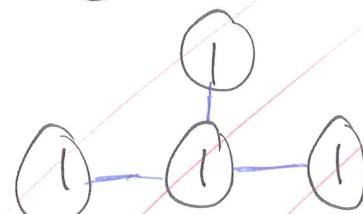
Lax-Wendroff scheme solves this,

$$u_x^{n+1} = \frac{\alpha\mu}{2} (1+\alpha\mu) u_{x-1}^n + (-\alpha^2\mu^2) u_x^n - \frac{\alpha\mu}{2} (1-\alpha\mu) u_{x+1}^n$$

$$\alpha\mu = 1/2 \Rightarrow$$



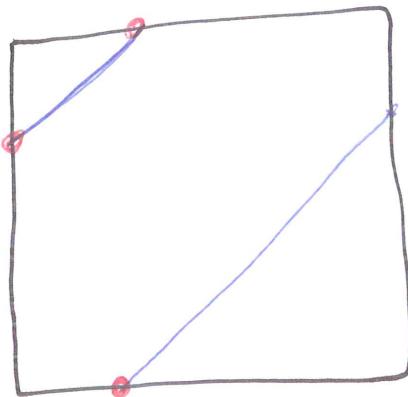
$$\alpha\mu = 1 \Rightarrow$$



Characteristic!

Periodic BV conditions

$$u(t,0) = u(t,1) \quad \text{for all } t \geq 0.$$



$u^{n+1} = A(\alpha\mu)u^n$, where
 $A(\alpha\mu)$ is a circulant
matrix given by the
corner expressions.

$$A(\alpha\mu) = \begin{pmatrix} 1 - \alpha^2\mu^2 & \frac{\alpha\mu}{2}(\alpha\mu - 1) & & \\ \frac{\alpha\mu}{2}(\alpha\mu + 1) & \ddots & & \\ & \ddots & \ddots & \\ & & \frac{\alpha\mu}{2}(\alpha\mu + 1) & 1 - \alpha^2\mu^2 \end{pmatrix}$$

$$A(1) = \begin{pmatrix} 0 & 0 & \dots & 1 \\ 1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & \vdots & \vdots & 0 \end{pmatrix} \Rightarrow u_2^{n+1} = u_{\ell-1}^n$$

Th: Let c be a circular $N \times N$ -matrix,

$$\text{then } \lambda_k[c] = \sum_{j=0}^{N-1} x_j e^{\frac{2kj\pi i}{N}}$$

A finite difference scheme with periodic BCs is stable iff $|\lambda_k[A(\alpha\mu)]| \leq 1$

If characteristics collide, we get a discontinuity. • ~~(shock)~~

shock!

