Numerical Methods for Partial Differential Equations

CS555 / MATH552 / CSE510

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Spring 2022

Outline

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What's the point of this class?

PDEs describe lots of things in nature:

- Fluid flow (Navier-Stokes equations)
- Electromagnetism (Maxwell's equations)
- Waves (Elasticity, Acoustics)
- Plasmas (Magnetohydrodynamics)

Idea: Use them to

- Make predictions (and check them, to validate the model: science!)
- Use predictions (for design of cars, airplanes, reactors, . . .)

Survey

- Home dept
- Degree pursued
- Longest program ever written
  - in Python?
- Research area

Class web page

https://bit.ly/numpde-s22

- Book Draft
- Notes, Class Outline
- Assignments (submission and return)
- Piazza
- Grading Policies/Syllabus
- Video
- Scribbles
- Demos (binder)

Sources for these Notes

- Adler, James, Hans De Sterck, Scott MacLachlan, and Luke N. Olson. *Numerical Partial Differential Equations*, 2022. (draft)
- Strikwerda, John C. *Finite Difference Schemes and Partial Differential Equations*, Second Edition. Other Titles in Applied Mathematics. Society for Industrial and Applied Mathematics, 2004.
- LeVeque, Randall J. *Numerical Methods for Conservation Laws*. 2nd ed. Birkhäuser Basel, 1992.
- Braess, Dietrich. *Finite Elements: Theory, Fast Solvers, and Applications in Solid Mechanics*. Cambridge University Press, 2007.
- Shu, Chi-Wang. *Lecture Notes for AM257*, Brown University, Fall 2006.
- Heuveline, Vincent. *Lecture Notes for "Numerik für PDEs"*. Universität Karlsruhe, Summer 2005.
- Various prior bits of material by Luke Olson and Stephen Bond.

Open Source <3

These notes (and the accompanying demos) are open-source!

Bug reports and pull requests welcome:
https://github.com/inducer/numpde-notes

Outline

PDEs: Example I

What does this do? $\partial_t u = \partial_x u$

- Slope in x and t matches
- Single profile on an x/t diagonal
- Which one? (left-leaning)
- We'll deal with this a lot.
  - Advection equation, one-way wave equation
  - General solution: $u(x, t) = u_0(x + t)$

PDEs: Example II

What does this do? $\partial_x^2 u + \partial_y^2 u = 0$

- Second derivative measures "bendiness" of a function
- "Bendiness" in x and y need to add up to zero
- Can a function like this have a maximum?

Some good questions

- What is a time-like variable? (Variables labeled t?)

A variable across which information does not flow 'backward'.

- What if there are boundaries? (space/time)
- Existence and Uniqueness of Solutions?
  - Depends on where we look (the *function space*)
  - In the case of the two examples? (if there are no boundaries?)

Some general takeaways:

- Simple techniques can go a long way.
- Develop/make use of physical intuition.

PDEs: An Unhelpfully Broad Problem Statement

Looking for $u : \Omega \to R^n$ where $\Omega \subseteq \mathbb{R}^d$ so that $u \in V$ and

$$F(u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}, \dots, x, y, \dots) = 0$$

Notation

Used as convenient:

$$u_x = \partial_x u = \frac{\partial u}{\partial x}$$

Properties of PDEs

What is the order of the PDE?

> The highest (total, i.e. summing over axes) order of derivative occurring in F.

When is the PDE linear?

> If u and v are solutions, $\alpha u + \beta v$ are, too.

When is the PDE quasilinear?

> The dependency in F on the highest-order partial derivatives is linear in u.

When is the PDE semilinear?

Examples: Order, Linearity?

$$(xu^2)u_{xx} + (u_x + y)u_{yy} + u_x^3 + yu_y = f$$

Second-order quasilinear

$$(x + y + z)u_x + (z^2)u_y + (\sin x)u_z = f$$

First-order semilinear

Properties of Domains

- smooth
- with corners
- with *reentrant* corners
- with cusps

May influence existence/uniqueness of solutions!

Function Spaces: Examples

Name some function spaces with their norms.

$C(\Omega)$	f continuous, $\|f\|_\infty := \sup_{x\in\Omega} \lvert f(x)\rvert$
$C^k(\Omega)$	f k-times continuously differentiable
$C^{0,\alpha}(\Omega)$	$\|f\|_\alpha := \|f\|_\infty + \sup_{x\neq y} \frac{\lvert f(x)-f(y)\rvert}{\lvert x-y\rvert^\alpha}$ $(\alpha \in (0,1))$
$C_L(\Omega)$	$\lvert f(x) - (y)\rvert \le L \|x - y\|$
$L_p(\Omega)$	$\|f\|_{p,\Omega} := \sqrt[p]{\int_D \lvert f(x)\rvert^p dx} < \infty$
	Why do these only define equivalence classes?
	L_2 special because...?
$W_p^1(\Omega)$	$\|f\|_{W_1^p(\Omega)} := (\|f\|_{p,\Omega} + \|f'\|_{p,\Omega}) < \infty$
$H^1(\Omega)$	equivalent to $W_2^1(\Omega)$, also a Hilbert space

May *also* influence existence/uniqueness of solutions!

Solving PDEs

Closed-form solutions:

- If separation of variables applies to the domain: good luck with your ODE
- If not: Good luck! $\to$ Numerics

General Idea (that we will follow some of the time)

- Pick $V_h \subseteq V$ finite-dimensional
  - h is often a *mesh spacing*
- Approximate u through $u_h \in V_h$
- Show: $u_h \to u$ (in some sense) as $h \to 0$

Example

$u(x) = \sin x$ where V_h is piecewise constant functions with grid spacing h.

About grand big unifying theories

Is there a grand big unifying theory of PDEs?

No. Frustratingly, studying PDEs is a little bit like stamp collecting. For instance, there are broad classes of second-order PDEs that behave mostly alike.

Collect some stamps

$$a(x,y)u_{xx}+2b(x,y)u_{xy}+c(x,y)u_{yy}+d(x,y)u_x+e(x,y)u_y+f(x,y)u=g(x,y)$$

Discriminant value	Kind	Example
$b^2 - ac < 0$	Elliptic	Laplace $u_{xx} + u_{yy} = 0$
$b^2 - ac = 0$	Parabolic	Heat $u_t = u_{xx}$
$b^2 - ac > 0$	Hyperbolic	Wave $u_{tt} = u_{xx}$

Where do these names come from?

> Quadratic forms: $ax^2 + 2bxy + cy^2 +$ lower order terms
> Where does this come from? The search for *characteristic curves*.
> Will see these again later. See Hogg '17 for a good description.

PDE Classification in Other Cases

Scalar first order PDEs?

Classified as hyperbolic. (See later.)

First order systems of PDEs?

Can be classified into hyperbolic/elliptic/parabolic as well, using slightly more complicated method, depending on the direction of the characteristics. See Hogg '17 or Loret '08.

Classification in higher dimensions

$$Lu := \sum_{i=1}^{d} \sum_{j=1}^{d} a_{i,j}(x) \frac{\partial^2 u}{\partial x_i \partial x_j} + \text{lower order terms}$$

Consider the matrix $A(x) = (a_{ij}(x))_{i,j}$. May assume A symmetric. Why?

Schwarz's theorem. So: real-valued eigenvalues.

What cases can arise for the eigenvalues?

Case	Kind
$\lambda_j(x) = 0$ for some λ	parabolic
$\lambda_j(x)$ all have the same sign	elliptic
$\lambda_j(x)$ all but one have the same sign	hyperbolic
$\lambda_j(x) > 1$ eigenvalue per sign, nonsingular	ultra-hyperbolic

Elliptic PDE: Laplace/Poisson Equation

$$\triangle u = \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2} = \nabla \cdot \nabla u(x) \stackrel{\text{2D}}{=} u_{xx} + u_{yy} = f(x) \quad (x \in \Omega)$$

Called Laplace equation if $f = 0$. With Dirichlet boundary condition

$$u(x) = g(x) \qquad (x \in \partial\Omega).$$

Demo: Elliptic PDE Illustrating the Maximum Principle [cleared]

Elliptic PDEs: Singular Solution

Demo: Elliptic PDE Radially Symmetric Singular Solution [cleared]

Given $G(x) = C \log(|x|)$ as the free-space Green's function, can we construct the solution to the PDE with a more general f?

$$u(x) = (G * f)(x) = \int_{\mathbb{R}^d} G(x - y)f(y)dy$$

What can we learn from this?

Solutions to the Laplace equation are globally coupled. The value of f at any point influences the solution *everywhere* (if only a little)

Elliptic PDEs: Justifying the Singular Solution

$$u(x) = (G * f)(x) = \int_{\mathbb{R}^d} G(x-y)f(y)dy$$

Why?

$$\begin{aligned}\triangle u(x) = (\triangle G * f)(x) &= \int_{\mathbb{R}^d} (\triangle G(x-y))f(y)dy \\ &= \int_{\mathbb{R}^d} \delta(x-y)f(y)dy = f(x)\end{aligned}$$

Parabolic PDE: Heat Equation · Separation of Variables

$$u_t = u_{xx} \qquad ((x,t) \in [0,1] \times [0,T])$$
$$u(x,0) = g(x) \qquad (x \in [0,1])$$
$$u(0,t) = u(1,t) = 0 \qquad (t \in [0,T])$$

Looking for $u(x,t) = v(t) \cdot w(x)$.
Plug into PDE: $v'(t) \cdot w(x) = v(t) \cdot w''(x)$. Divide:

$$\frac{v'(t)}{v(t)} = C = \frac{w''(x)}{w(x)},$$

where C is constant since it is independent of x and t.

- $w'' = Cw$ with BCs yields $w(x) = \alpha \cdot \sin(m\pi x)$ and $C = -m^2\pi^2$ or any linear combination; Fourier to match g.
- Focus on specific value of m: $v' = Cv$ with ICs yields $v(t) = \exp(-m^2\pi^2 t)$.

Parabolic PDE: Solution Behavior

Demo: Parabolic PDE [cleared] What can we learn from analytic and numerical solution?

- Heat equation 'washes out' the solution
- Appears to obey a maximum principle
- Appears to smooth the data

Hyperbolic PDE: Wave Equation

$$
\begin{aligned}
u_{tt} &= c^2 u_{xx} \qquad ((x,t) \in \mathbb{R} \times [0, T]) \\
u(x,0) &= g(x) \qquad (x \in \mathbb{R})
\end{aligned}
$$

with $g(x) = \sin(\pi x)$.

Is this problem well-posed?

No, missing initial condition on u_t.

$$u_t(x,0) = 0 \qquad (x \in \mathbb{R})$$

Can be rewritten in conservation law form:

$$q_t(x) + \nabla \cdot F(q(x)) = s(x)$$

Hyperbolic Conservation Laws

$$\boldsymbol{q}_t(\boldsymbol{x}, t) + \nabla \cdot \boldsymbol{F}(\boldsymbol{q}(\boldsymbol{x}, t)) = \boldsymbol{s}(\boldsymbol{x})$$

Why is this called a (system of) conservation law(s)?

- Balance between a conserved quantity $\boldsymbol{q}$ and a flux $\boldsymbol{F}$.
  - Integrate, consider divergence theorem (for $n = 1$)
- Flux prescribes the 'flow direction'. When is flux divergence < 0?
- s is a source term.

$F :? \to ?$

- $\boldsymbol{q}(\boldsymbol{x}, t) \in \mathbb{R}^n$
- $\boldsymbol{F} : \mathbb{R}^n \to \mathbb{R}^n \times \mathbb{R}^d$

Wave Equation as a Conservation Law

Rewrite the wave equation in conservation law form:

Introduce a new variable v and let

$$
\begin{aligned}
u_t &= c v_x \\
v_t &= c u_x.
\end{aligned}
$$

Observe $u_{tt} = c v_{xt} = c^2 u_{xx}$. Define $\boldsymbol{q} := \begin{bmatrix} u & v \end{bmatrix}^T$.

Solving Conservation Laws

Solve

$$\begin{aligned} u_t &= c v_x \\ v_t &= c u_x. \end{aligned}$$

$$\boldsymbol{q}_t + \begin{bmatrix} 0 & -c \\ -c & 0 \end{bmatrix} \boldsymbol{q}_x = \boldsymbol{q}_t + A\boldsymbol{q}_x = 0$$

Diagonalize: Define $\tilde{\boldsymbol{q}} := V^{-1}\boldsymbol{q}$,

$$\tilde{\boldsymbol{q}}_t + V^{-1}AV\tilde{\boldsymbol{q}}_x = \tilde{\boldsymbol{q}}_t + \begin{bmatrix} c & 0 \\ 0 & -c \end{bmatrix} \tilde{\boldsymbol{q}}_x = 0$$

$\rightarrow$ two advection equations

Solution, for some ϕ_ℓ, ϕ_r: $u(t,x) = \phi_\ell(x+ct) + \phi_r(x-ct)$

Demo: Hyperbolic PDE [cleared]

Hyperbolic: Solution Properties

Properties of the solution for hyperbolic equations:

- Has *conserved quantities*
- q, “energy” ($\rightarrow$ HW1)
- Maintains smoothness of IC
- Typical trick: Project to one dimension, diagonalize, understand advection behavior.

Outline

Interpolation and Vandermonde Matrices

Limit the set of functions to a linear combination from an *interpolation basis* φ_i.

$$f(x) = \sum_{j=0}^{N_{\text{func}}} \alpha_j \varphi_j(x)$$

Interpolation becomes solving the linear system:

$$y_i = f(x_i) = \sum_{j=0}^{N_{\text{func}}} \alpha_j \underbrace{\varphi_j(x_i)}_{V_{ij}} \qquad \leftrightarrow \qquad V\boldsymbol{\alpha} = \boldsymbol{y}.$$

Want unique answer: Pick $N_{\text{func}} = N \to V$ square.
V is called the *(generalized) Vandermonde matrix*.

$$V\,(\text{coefficients}) = (\text{values at nodes})\,.$$

Numerical Differentiation: How?

How can we take derivatives numerically?

Let $\boldsymbol{x} = (x_i)_{i=1}^n$ be nodes and $(\varphi_i)_{i=1}^n$ an interpolation basis.
Find interpolation coefficients $\boldsymbol{\alpha} = (\alpha_i)_{i=1}^n = V^{-1}f(\boldsymbol{x})$. Then

$$f(\xi) \approx p_{n-1}(\xi) = \sum_{i=1}^n \alpha_i \varphi_i(\xi).$$

Then, simply take a derivative:

$$f'(\xi) \approx p'_{n-1}(\xi) = \sum_{i=1}^n \alpha_i \varphi'_i(\xi).$$

φ'_i are known because the interpolation basis φ_i is known!

Demo: Taking Derivatives with Vandermonde Matrices [cleared]

Finite Differences Numerically

Demo: Finite Differences [cleared]
Demo: Finite Differences vs Noise [cleared]
Demo: Floating point vs Finite Differences [cleared]

Taking Derivatives Numerically

Why *shouldn't* you take derivatives numerically?

- 'Unbounded'
  A function with small $\|f\|_\infty$ can have arbitrarily large $\|f'\|_\infty$
- Amplifies noise
  Imagine a smooth function perturbed by small, high-frequency wiggles
- Subject to cancellation error
- Inherently less accurate than integration
  - Interpolation: h^n
  - Quadrature: h^{n+1}
  - Differentiation: h^{n-1}

  (where n is the number of points)

Differencing Order of Accuracy Using Taylor

Find the order of accuracy of the finite difference formula $f'(x) \approx [f(x+h) - f(x-h)]/2h$.

$$
\begin{aligned}
& f'(x) - \frac{f(x+h) - f(x-h)}{2h} \\
=& f'(x) - \frac{1}{2h}\left[f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + O(h^4)\right] \\
& + \frac{1}{2h}\left[f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + O(h^4)\right] \\
=& \frac{1}{2h} \cdot \frac{h^3}{6}f'''(x) \quad \text{as } h \to 0.
\end{aligned}
$$

Outline

Truncation Error in Interpolation

If f is n times continuously differentiable on a closed interval I and $p_{n-1}(x)$ is a polynomial of degree at most n that interpolates f at n distinct points $\{x_i\}$ $(i = 1, ..., n)$ in that interval, then for each x in the interval there exists ξ in that interval such that

$$f(x) - p_{n-1}(x) = \frac{f^{(n)}(\xi)}{n!}(x - x_1)(x - x_2)\cdots(x - x_n).$$

Set the error term to be $R(x) := f(x) - p_{n-1}(x)$ and set up an auxiliary function:

$$Y_x(t) = R(t) - \frac{R(x)}{W(x)}W(t) \quad \text{where} \quad W(t) = \prod_{i=1}^{n}(t - x_i).$$

Note also the introduction of t as an additional variable, independent of the point x where we hope to prove the identity.

Truncation Error in Interpolation: cont'd.

$$Y_x(t) = R(t) - \frac{R(x)}{W(x)} W(t) \quad \text{where} \quad W(t) = \prod_{i=1}^{n} (t - x_i)$$

- Since x_i are roots of $R(t)$ and $W(t)$, we have $Y_x(x) = Y_x(x_i) = 0$, which means Y_x has at least $n+1$ roots.
- From Rolle's theorem, $Y_x'(t)$ has at least n roots, then $Y_x^{(n)}$ has at least one root ξ, where $\xi \in I$.
- Since $p_{n-1}(x)$ is a polynomial of degree at most $n-1$, $R^{(n)}(t) = f^{(n)}(t)$. Thus

$$Y_x^{(n)}(t) = f^{(n)}(t) - \frac{R(x)}{W(x)} n!.$$

- Plugging $Y_x^{(n)}(\xi) = 0$ into the above yields the result.

Error Result: Connection to Chebyshev

What is the connection between the error result and Chebyshev interpolation?

- The error bound suggests choosing the interpolation nodes such that the product $|\prod_{i=1}^{n}(x - x_i)|$ is as small as possible. The Chebyshev nodes achieve this.
- If nodes are edge-clustered, $\prod_{i=1}^{n}(x - x_i)$ clamps down the (otherwise quickly-growing) error there.
- Confusing: *Chebyshev approximating polynomial* (or "polynomial best-approximation"). Not the Chebyshev interpolant.
- Chebyshev nodes also do not minimize the Lebesgue constant.

Error Result: Simplified Form

Boil the error result down to a simpler form.

Assume $x_1 < \cdots < x_n$.

- $\left|f^{(n)}(x)\right| \leq M$ for $x \in [x_1, x_n]$,
- Set the interval length $h = x_n - x_1$.
  Then $|x - x_i| \leq h$.

Altogether–there is a constant C independent of h so that:

$$\max_x |f(x) - p_{n-1}(x)| \leq CMh^n.$$

For the grid spacing $h \to 0$, we have $E(h) = O(h^n)$. This is called *convergence of order n*.

- **Demo:** Interpolation Error [cleared]

Outline

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1D Advection Equation and Characteristics

$$u_t + au_x = 0, \quad u(0,x) = g(x) \qquad (x \in \mathbb{R})$$

Solution?

Generalize to 1D conservation law: $u_t + f(u)_x = 0$. Find solution.
Characteristic Curve: Define a function $x(t)$ so that $u(x(t),t) = u(x_0, 0)$. Suppose we consider x defined by the IVP

$$\begin{cases} \frac{\mathrm{d}x(t)}{\mathrm{d}t} = f'(u(x(t),t)), \\ x(0) = x_0. \end{cases}$$

Then

$$\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} = u_x x'(t) + u_t = u_x f'(u(x(t),t) + u_t = f(u)_x + u_t = 0.$$

So $u(x(t),t) = u(x(0),0) = g(x_0)$.

Solving Advection with Characteristics

$$u_t + a u_x = 0, \quad u(0, x) = g(x) \qquad (x \in \mathbb{R})$$

Find the characteristic curve for advection.

Here $x(t) = x_0 + at$.

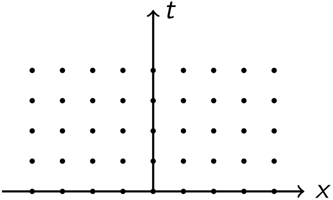
Generalize this to a solution formula.

General solution of advection: $u(t, x) = g(x - at)$. a: Advection speed.

Does the solution formula admit solutions that aren't obviously allowed by the PDE?

Solution formula allows nonsmooth profiles. Unclear: Those are not differentiable.

Finite Difference for Hyperbolic: Idea



$$\{(x_k, t_\ell) : x_k = kh_x, t_\ell = \ell h_t\}$$

If $u(x,t)$ is the exact solution, want

$$u_{k,\ell} \approx u(x_k, t_\ell).$$

Condition at each grid point?

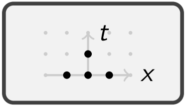
- Pick a derivative stencil for each derivative term in the PDE
- Get system of equations
- Solve

What are explicit/implicit schemes?

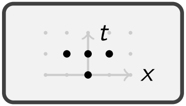
Implicit require solution of a system of equations

Designing Stencils

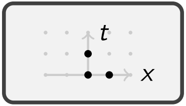
ETCS:



ITCS:



ETFS:



ETBS:

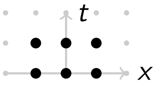
Terminology?

- E Explicit / I Implicit
- T Time / S Space
- F Forward: right
- B Backward: left
- Upwind: left if $a > 0$
- Downwind: right if $a > 0$

Write out ITCS:

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} + a\frac{u_{k+1,\ell+1} - u_{k-1,\ell+1}}{2h_x} = 0$$

Crank-Nicolson



Crank-Nicolson

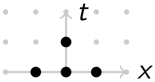
Write out Crank-Nicolson:

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} + \frac{a}{2}\left[\frac{u_{k+1,\ell+1} - u_{k-1,\ell+1}}{2h_x} + \frac{u_{k+1,\ell} - u_{k-1,\ell}}{2h_x}\right] = 0$$

Lax-Wendroff

What's the core idea behind Lax-Wendroff?

- Write out a Taylor expansion in time
- Use the PDE to replace time ∂ with space ∂
- Allows two-level schemes of any order of accuracy



Lax-Wendroff

Write out Lax-Wendroff.

$u_t = -au_x$ so also $u_{tt} = -a(u_x)_t = -a(u_t)_x = a^2 u_{xx}$.

$$
\begin{aligned}
u_{k,\ell+1} - u_{k,\ell} &\approx h_t u_t(x_k, t_\ell) + \frac{h_t^2}{2} u_{tt}(x_k, t_\ell) \\
&= -h_t a u_x(x_k, t_\ell) + \frac{h_t^2}{2} a^2 u_{xx}(x_k, t_\ell) \\
&\approx -h_t a \frac{u_{k+1,\ell} - u_{k-1,\ell}}{2h_x} + \frac{h_t^2 a^2}{2} \cdot \frac{u_{k+1,\ell} - 2u_{k,\ell} + u_{k-1,\ell}}{h_x^2}
\end{aligned}
$$

Exploring Advection Schemes

Demo: Methods for 1D Advection [cleared]

- Which of the schemes "work"?
- Any restrictions worth noting?

Outline

A Matrix View of Two-Level Stencil Schemes

Numerical solution vectors:

$$\boldsymbol{v}_\ell = \begin{bmatrix} u_{1,\ell} \\ \vdots \\ u_{N_x,\ell} \end{bmatrix}, \quad \boldsymbol{v} = \begin{bmatrix} \boldsymbol{v}_1 \\ \vdots \\ \boldsymbol{v}_{N_t} \end{bmatrix}.$$

True solution vectors:

$$\boldsymbol{u}_\ell = \begin{bmatrix} u(x_1, t_\ell) \\ \vdots \\ u(x_{N_x}, t_\ell) \end{bmatrix} \quad \boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_{N_t} \end{bmatrix}.$$

Definition (Two-Level Finite Difference Scheme)

A finite difference scheme that can be written as

$$\boxed{P_h \boldsymbol{v}_{\ell+1} = Q_h \boldsymbol{v}_\ell + h_t \boldsymbol{b}_\ell}$$

is called a two-level linear finite difference scheme.

- Mostly $\boldsymbol{b}_\ell = 0$, i.e. homogeneous schemes, no source terms.
- P_h and Q_h may depend on both h_x and h_t.
- P_h and Q_h and the spatial grid may also be infinite

Rewriting Schemes in Matrix Form (1/2)

$$P_h \boldsymbol{v}_{\ell+1} = Q_h \boldsymbol{v}_\ell + h_t \boldsymbol{b}_\ell$$

Find P_h and Q_h for ETCS:

ETCS:

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} + a\frac{u_{k+1,\ell} - u_{k-1,\ell}}{2h_x} = 0.$$

Equivalently:

$$u_{k,\ell+1} = u_{k,\ell} + \frac{ah_t}{2h_x}(-u_{k+1,\ell} + u_{k-1,\ell}).$$

So

$$P_h = I, \qquad Q_h = \operatorname{tridiag}\left(\frac{ah_t}{2h_x}, 1, -\frac{ah_t}{2h_x}\right).$$

Rewriting Schemes in Matrix Form (2/2)

Find P_h and Q_h for Crank-Nicolson:

$$P_h = \text{tridiag}\left(-\frac{ah_t}{4h_x}, 1, \frac{ah_t}{4h_x}\right),$$

and

$$Q_h = \text{tridiag}\left(\frac{ah_t}{4h_x}, 1, -\frac{ah_t}{4h_x}\right).$$

Truncation Error

Definition (Truncation Error)

The local truncation error $\tau_{k,\ell}$ is the error that remains when a finite difference method is applied to a smooth exact solution u at (x_k, t_ℓ).

Demo: Truncation Error Analysis via sympy [cleared]

Error and Error Propagation

Express definition of truncation error in our two-level framework:

$$P_h \boldsymbol{u}_{\ell+1} = Q_h \boldsymbol{u}_\ell + \underbrace{\boldsymbol{\tau}_\ell}_{\text{Trunc.Err.}} h_t.$$

Define $\boldsymbol{e}_\ell = \boldsymbol{u}_\ell - \boldsymbol{v}_\ell$. Understand the error as accumulation of truncation error:

Recall $P_h \boldsymbol{v}_{\ell+1} = Q_h \boldsymbol{v}_\ell$. Subtract from the truncation error definition to find:

$$\begin{aligned} \boldsymbol{e}_0 &= 0 \\ P_h \boldsymbol{e}_{\ell+1} &= Q_h \boldsymbol{e}_\ell + \boldsymbol{\tau}_\ell h_t \\ \boldsymbol{e}_{\ell+1} &= P_h^{-1} Q_h \boldsymbol{e}_l + P_h^{-1} \boldsymbol{\tau}_\ell h_t. \end{aligned}$$

Discrete and Continuous Norms

To measure properties of numerical solutions we need norms. Define a discrete L^∞ norm.

$$\|\boldsymbol{e}\|_\infty = \max_{k,\ell} |e_{k,\ell}|.$$

Define a discrete L^2 norm.

$$\|\boldsymbol{e}\|_2 = \sqrt{\sum_{k,\ell} e_{k,\ell}^2 h_x h_t}.$$

Unless otherwise given: $\|\cdot\| = \|\cdot\|_2$.

Important features:

- Value of discrete norm should not change wildly if h_x and h_t change (and, along with them, the number of nodes).

Consistency and Convergence

Assume $u, (\partial_x^{q_x})u, (\partial_t^{q_t})u \in L^2(\mathbb{R} \times [0, t^*])$.

Definition (Consistency)

A two-level scheme is consistent in the L^2-norm with order q_t in time and q_x in space if

$$\boxed{\max_{\ell, \ell h_t \leq t^*} \|\boldsymbol{\tau}_\ell\| = O(h_x^{q_x} + h_t^{q_t}) \qquad \text{as } (h_x, h_t) \to (0, 0).}$$

Definition (Convergence)

A two-level scheme is convergent in the L^2-norm with order q_t in time and q_x in space if

$$\boxed{\max_{\ell, \ell h_t \leq t^*} \|\boldsymbol{e}_\ell\| = O(h_x^{q_x} + h_t^{q_t}) \qquad \text{as } (h_x, h_t) \to (0, 0).}$$

Analyzing ETFS (1/2)

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} + a\frac{u_{k+1,\ell} - u_{k,\ell}}{h_x} = 0$$

Let's understand more precisely what happens for this scheme. Assume $a > 0$.

Rewrite as

$$u_{k,\ell+1} = u_{k,\ell} - \frac{ah_t}{h_x}(u_{k+1,\ell} - u_{k,\ell}) = (1+\lambda)u_{k,\ell} - \lambda u_{k+1,\ell}$$

for $\lambda = ah_t/h_x$.

Analyzing ETFS (2/2)

$$u_{k,\ell+1} = (1+\lambda)u_{k,\ell} - \lambda u_{k+1,\ell}$$

Consider $u(x,0) = 1_{[-1,0]}(x)$. Predict solution behavior.

$$\begin{aligned} u_{0,0} &= 1 & \qquad u_{1\ldots,0} &= 0 \\ u_{0,1} &= (1+\lambda) & \qquad u_{1\ldots,1} &= 0 \\ u_{0,2} &= (1+\lambda)^2 & \qquad u_{1\ldots,2} &= 0 \end{aligned}$$

So the right half never "sees" the traveling bump; this can't be convergent. Meanwhile,

$$u(0,t) \approx u_{0,t/h_t} = \left(1 + \frac{ah_t}{h_x}\right)^{t/h_t} = \left(1 + \frac{at/h_x}{t/h_t}\right)^{t/h_t} \overset{h_t \to 0}{\to} \exp\left(\frac{at}{h_x}\right)$$

Demo: Methods for 1D Advection [cleared] (Revisit ETFS)

Stability

$$P_h \boldsymbol{v}_{\ell+1} = Q_h \boldsymbol{v}_\ell$$

Write down a matrix product to bring $\boldsymbol{v}_0$ to $\boldsymbol{v}_\ell$:

$$\boldsymbol{v}_\ell = (P_h^{-1} Q_h)^\ell \boldsymbol{v}_0$$

Definition (Stability)

A two-level scheme is stable in the L^2-norm if there exists a constant $c > 0$ independent of h_t and h_x so that

$$\left\| (P_h^{-1} Q_h)^\ell P_h^{-1} \right\| \leq c$$

for all ℓ and h_t such that $\ell h_t \leq t^*$.

Lax Convergence Theorem

Theorem (Lax Convergence)

If a two-level FD scheme is

- *consistent in the L^2-norm with order q_t in time and q_x in space, and*
- *stable in the L^2-norm, then*

it is convergent in the L^2-norm with order q_t in time and q_x in space.

- A stronger result holds: The above is actually "if and only if". (called the Lax Equivalence Theorem or Lax-Richtmyer Theorem)
- Think of this as an important 'meta-theorem' of numerical analysis (or "fundamental theorem of NA"):

$$\text{Consistent} + \text{Stable} \Rightarrow \text{Convergent}$$

- A related result holds for ODEs, due to Dahlquist.

Lax Convergence: Proof (1/2)

Recall error propagation:

$$P_h \boldsymbol{e}_{\ell+1} = Q_h \boldsymbol{e}_\ell + \boldsymbol{\tau}_\ell h_t$$

So:

$$\boldsymbol{e}_{\ell+1} = P_h^{-1} Q_h \boldsymbol{e}_l + P_h^{-1} \boldsymbol{\tau}_\ell h_t.$$

Since $\boldsymbol{e}_0 = 0$,

$$\begin{aligned} \boldsymbol{e}_1 &= h_t P_h^{-1} \boldsymbol{\tau}_0, \\ \boldsymbol{e}_2 &= h_t (P_h^{-1} Q_h) P_h^{-1} \boldsymbol{\tau}_0 + h_t P_h^{-1} \boldsymbol{\tau}_1. \end{aligned}$$

By induction,

$$\boldsymbol{e}_\ell = h_t \sum_{m=1}^{\ell} (P_h^{-1} Q_h)^{\ell-m} P_h^{-1} \boldsymbol{\tau}_{m-1}.$$

Lax Convergence: Proof (2/2)

$$\boldsymbol{e}_\ell = h_t \sum_{m=1}^{\ell} (P_h^{-1} Q_h)^{\ell-m} P_h^{-1} \boldsymbol{\tau}_{m-1}.$$

Let $\ell h_t \leq t^*$. Taking the norm of both sides,

$$\begin{aligned}
\|\boldsymbol{e}_\ell\| &\leq h_t \sum_{m=1}^{\ell} \left\| (P_h^{-1} Q_h)^{\ell-m} P_h^{-1} \boldsymbol{\tau}_{m-1} \right\| \\
&\leq h_t \sum_{m=1}^{\ell} \underbrace{\left\| (P_h^{-1} Q_h)^{\ell-m} P_h^{-1} \right\|}_{\leq c \text{ (stab.)}} \|\boldsymbol{\tau}_{m-1}\| \\
&\leq h_t \ell c \cdot \max_{\ell : \ell h_t \leq t^*} \|\boldsymbol{\tau}_\ell\| \leq c t^* \max_{\ell : \ell h_t \leq t^*} \|\boldsymbol{\tau}_\ell\| \\
&\overset{\text{cons.}}{=} O(h_x^{q_x} + h_t^{q_t}).
\end{aligned}$$

Conditions for Stability

$$\left\|(P_h^{-1}Q_h)^\ell P_h^{-1}\right\| \leq c$$

Give a simpler, sufficient condition:

$$\left\|P_h^{-1}Q_h\right\| \leq 1, \qquad \left\|P_h^{-1}\right\| \leq c.$$

Also called Lax-Richtmyer stability.

How can we show bounds on these matrix norms?

- Observe: bounds have to hold for all h_t and h_x.
- Generally: cumbersome.
- Possibly easiest: approach via singular values.
- Bound singular values: For example using Gershgorin.

Stability of ETBS (1/3)

Theorem (Gershgorin)

For a matrix $A \in \mathbb{C}^{N\times N} = (a_{i,j})$,

$$\sigma(A) \subset \bigcup_{j=1}^{N} \bar{B}\left(a_{j,j}, \sum_{k\neq j} |a_{j,k}|\right).$$

ETBS:

$$\frac{u_{k,\ell+1} - u_{k,l}}{h_t} + a\frac{u_{k,\ell} - u_{k-1,\ell}}{h_x} = 0$$

Analyze stability of ETBS:

Let $\lambda = ah_t/h_x$. Then $u_{k,\ell+1} = \lambda u_{k-1,\ell} + (1-\lambda)u_{k,\ell}$.
So $P_h = I$ and $Q_h = \text{tridiag}(\lambda, 1-\lambda, 0)$. $\left\|P_h^{-1}\right\| \leq 1$ trivially.

Stability of ETBS (2/3)

$P_h = I$ and $Q_h = \text{tridiag}(\lambda, 1-\lambda, 0)$.

$$\|Q_h\| = \sqrt{\rho(Q_h^T Q_h)},$$

where $Q_h^T Q_h = \text{tridiag}(\lambda(1-\lambda), (1-\lambda)^2 + \lambda^2, \lambda(1-\lambda))$. Assume $0 \le \lambda \le 1$ for now, then $\lambda(1-\lambda) \ge 0$. Let $\Lambda \in \sigma(Q_h^T Q_h)$.

$$\begin{aligned} 2\lambda^2 - 2\lambda \le \quad & \Lambda - (1-\lambda)^2 - \lambda^2 & \le 2\lambda - 2\lambda^2, \\ 1 - 4\lambda + 4\lambda^2 \le \quad & \Lambda & \le 1, \\ 0 \le (1-2\lambda)^2 \le \quad & \Lambda & \le 1. \end{aligned}$$

So $|\Lambda| \le 1$, which implies $\left\|Q_h^T Q_h\right\| \le 1$, which means $\|Q_h\| \le 1$.
If $\lambda > 1$, analogously:
$|\Lambda| \ge 1$, which implies $\left\|Q_h^T Q_h\right\| \ge 1$, which means $\|Q_h\| \ge 1$.

Stability of ETBS (3/3)

Summarize ETBS stability:

We learn that ETBS is stable if $0 \leq \lambda \leq 1$. Rewriting, we obtain

$$\frac{ah_t}{h_x} < 1 \quad \Leftrightarrow \quad h_t \leq \frac{h_x}{a}.$$

This type of stability is called conditional stability, and the condition we found a Courant-Friedrichs-Lewy (CFL) condition.

Comments?

Way cumbersome to prove. Is there something easier that gives necessary/sufficient conditions?

Outline

Discrete (Space) Fourier Transform

Assume $\boldsymbol{x}$ infinitely long. Define:

$$\hat{\boldsymbol{x}}(\theta) = \sum_{k \in \mathbb{Z}} x_k e^{-i\theta k}$$

When is this well-defined?

$$|\hat{\boldsymbol{x}}(\theta)| = \left| \sum_k x_k e^{-i\theta k} \right| \leq \sum_k |x_k| ,$$

Well-defined if $\sum_k |x_k|$ is absolutely convergent. $(\sum_k = \sum_{k \in \mathbb{Z}})$

Inverting the Fourier Transform

To recover $\boldsymbol{x}$:

$$x_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\theta) e^{i\theta k} d\theta.$$

Proof?

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\sum_j x_j e^{-i\theta j} e^{i\theta k} d\theta = \frac{1}{2\pi}\sum_j x_j \int_{-\pi}^{\pi} e^{i\theta(k-j)} d\theta = \sum_j x_j \delta_{j,k} = x_k.$$

Getting to L^2

- Fourier Transform well defined for $\boldsymbol{x} \in \ell^1$.
- Problem: We care about L^2, not ℓ^1.

Theorem (Parseval)

If $\|\boldsymbol{x}\|_2 < \infty$, *then*

$$\|\boldsymbol{x}\|_2^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} |\hat{\boldsymbol{x}}(\theta)|^2 \, d\theta < \infty.$$

Impact?

Can extend definition of Fourier transform to L^2.

Toeplitz Operators

Definition (Toeplitz Operator)

An operator T is a Toeplitz operator if $(T\boldsymbol{x})_j = \sum_k x_k p_{j-k}$. In this case, $\boldsymbol{p}$ is called the Toeplitz vector.

Example: ETCS

Let $\lambda = ah_t/2h_x$. Then

$$u_{k,\ell+1} = \lambda u_{k-1,\ell} + u_{k,\ell} - \lambda u_{k+1,\ell}.$$

Is ETCS Toeplitz?

Is ETCS Toeplitz?

$$(P_h \boldsymbol{u}_{\ell+1})_j = u_{j,\ell+1} \stackrel{!}{=} \sum_k u_{k,\ell+1} p_{j-k}$$

$$p_{j-k} = \begin{cases} 1 & k = j, \\ 0 & \text{otherwise.} \end{cases} \qquad p_m = \delta_{0,m}.$$

$$(Q_h \boldsymbol{u}_\ell)_j = \lambda u_{j-1,\ell} + u_{j,\ell} - \lambda u_{j+1,\ell} \stackrel{!}{=} \sum_k u_{k,\ell} q_{j-k}$$

$$q_{j-k} = \begin{cases} \lambda & k = j-1, \\ 1 & k = j, \\ -\lambda & k = j+1, \\ 0 & \text{otherwise.} \end{cases} \qquad q_m = \begin{cases} \lambda & m = 1, \\ 1 & m = 0, \\ -\lambda & m = -1, \\ 0 & \text{otherwise.} \end{cases}$$

Both P_h and Q_h are Toeplitz.

Fourier Transforms of Toeplitz Operators (1/3)

$$y_j = \sum_k x_k p_{j-k}$$

$$\begin{aligned}
\hat{\boldsymbol{y}}(\theta) &= \sum_j \sum_k x_k p_{j-k} e^{-i\theta j} \\
&= \sum_j \sum_k \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi) e^{i\varphi k} d\varphi \right) p_{j-k} e^{-i\theta j} \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi) \sum_j \sum_k e^{i\varphi k} p_{j-k} e^{-i\theta j} d\varphi \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi) \sum_j \left(\sum_k e^{i\varphi(k-j)} p_{j-k} \right) e^{i(\varphi-\theta)j} d\varphi.
\end{aligned}$$

Fourier Transforms of Toeplitz Operators (2/3)

$$\hat{\boldsymbol{y}}(\theta) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi) \sum_j \left(\sum_k e^{i\varphi(k-j)} p_{j-k} \right) e^{i(\varphi-\theta)j} \, d\varphi.$$

Consider

$$\sum_k e^{i\varphi(k-j)} p_{j-k} = \sum_k e^{-i\varphi(j-k)} p_{j-k} \overset{\ell=j-k}{=} \hat{\boldsymbol{p}}(\varphi).$$

So

$$\hat{\boldsymbol{y}}(\theta) = \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi) \hat{\boldsymbol{p}}(\varphi) \frac{1}{2\pi} \sum_j e^{i(\varphi-\theta)j} \, d\varphi.$$

Fourier Transforms of Toeplitz Operators (3/3)

$$\hat{\boldsymbol{y}}(\theta) = \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi)\hat{\boldsymbol{p}}(\varphi)\frac{1}{2\pi}\sum_j e^{i(\varphi-\theta)j}\,d\varphi.$$

Define $w_j = (1/2\pi)e^{i\varphi j}$. Then $\hat{\boldsymbol{w}}(\theta) = \frac{1}{2\pi}\sum_k e^{i(\varphi-\theta)k}$. So

$$\hat{\boldsymbol{y}}(\theta) = \int_{-\pi}^{\pi} \hat{\boldsymbol{x}}(\varphi)\hat{\boldsymbol{p}}(\varphi)\hat{\boldsymbol{w}}(\theta)\,d\varphi.$$

To determine $\hat{\boldsymbol{w}}(\theta)$, consider

$$(1/2\pi)e^{i\varphi j} = w_j = \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{\boldsymbol{w}}(\theta)e^{i\theta j}\,d\theta.$$

Observe that (by uniqueness of the FT) $\hat{\boldsymbol{w}}(\theta) = \delta(\varphi-\theta)$ would do the trick. Therefore $\hat{\boldsymbol{y}}(\theta) = \hat{\boldsymbol{x}}(\theta)\hat{\boldsymbol{p}}(\theta)$.

Fourier Transforms of Inverse Toeplitz Operators

Recall $(P\boldsymbol{x})_j = \sum_k p_{j-k} x_k$.

What is the Fourier transform $\hat{\boldsymbol{z}}(\theta)$ of $P_h^{-1}\boldsymbol{x}$?

- Inverse is also Toeplitz (by linearity and translation invariance).
- Fourier transform of $P_h P_h^{-1}\boldsymbol{x}$ is $\hat{\boldsymbol{x}}$ for any $\boldsymbol{x}$.
- Therefore $\hat{\boldsymbol{p}}(\theta)\hat{\boldsymbol{z}}(\theta) = \hat{\boldsymbol{x}}(\theta)$.
- By uniqueness of Fourier t. (unproven): $\hat{\boldsymbol{z}}(\theta) = \frac{1}{\hat{\boldsymbol{p}}(\theta)}\hat{\boldsymbol{x}}(\theta)$.

Fourier transform $P_h^{-1}Q_h\boldsymbol{y}$?

$$\frac{\hat{\boldsymbol{q}}(\theta)}{\hat{\boldsymbol{p}}(\theta)}\hat{\boldsymbol{y}}(\theta).$$

Bounding the Operator Norm

Bound $\left\|P_h^{-1}Q_h\right\|_2^2$ using Fourier:

$$\left\|P_h^{-1}Q_h\right\|_2^2 = \sup_{\boldsymbol{x}\neq 0} \frac{\left\|P_h^{-1}Q_h\boldsymbol{x}\right\|_2^2}{\left\|\boldsymbol{x}\right\|_2^2} = \sup_{\boldsymbol{x}\neq 0} \frac{\frac{h_x}{2\pi}\int_{-\pi}^{\pi}\left|\frac{\hat{\boldsymbol{q}}(\theta)}{\hat{\boldsymbol{p}}(\theta)}\hat{\boldsymbol{x}}(\theta)\right|^2 d\theta}{\frac{h_x}{2\pi}\int_{-\pi}^{\pi}\left|\hat{\boldsymbol{x}}(\theta)\right|^2 d\theta}$$

$$\leq \sup_{\boldsymbol{x}\neq 0} \frac{\max_{\varphi\in[-\pi,\pi]}\left|\frac{\hat{\boldsymbol{q}}(\varphi)}{\hat{\boldsymbol{p}}(\varphi)}\right|^2 \int_{-\pi}^{\pi}\left|\hat{\boldsymbol{x}}(\theta)\right|^2 d\theta}{\int_{-\pi}^{\pi}\left|\hat{\boldsymbol{x}}(\theta)\right|^2 d\theta} = \max_{\varphi\in[-\pi,\pi]}\left|\frac{\hat{\boldsymbol{q}}(\varphi)}{\hat{\boldsymbol{p}}(\varphi)}\right|^2.$$

Similarly, $\quad \left\|P_h^{-1}\right\|_2^2 \leq \max_{\varphi\in[-\pi,\pi]} \left|1/\hat{\boldsymbol{p}}(\varphi)\right|^2.$

Is the upper bound attained?

If $\hat{\boldsymbol{x}}(\theta) = \delta(\theta-\varphi^*)$, where φ^* maximizes $|\hat{\boldsymbol{q}}(\theta)/\hat{\boldsymbol{p}}(\theta)|$, then yes. (So $x_k = (1/2\pi)e^{i\varphi^* k}$.)

von Neumann Stability

Two-level finite difference scheme

$$P_h \boldsymbol{v}_{\ell+1} = Q_h \boldsymbol{v}_\ell + h_t \boldsymbol{b}_\ell,$$

where P_h and Q_h are Toeplitz operators with vectors $\boldsymbol{p}$ and $\boldsymbol{q}$.

Definition (Symbol of a Two-Level Finite Difference Scheme)

Let

$$\hat{\boldsymbol{p}}(\theta) = \sum_k p_k e^{-i\varphi k}, \qquad \hat{\boldsymbol{q}}(\theta) = \sum_k q_k e^{-i\varphi k}.$$

Then the symbol of the two-level FD method is $s(\varphi) = \hat{\boldsymbol{q}}(\varphi)/\hat{\boldsymbol{p}}(\theta)$.

Definition (Von Neumann Stability)

If

$$\max_\varphi |s(\varphi)| \leq 1, \qquad \max_\varphi \left| \frac{1}{\hat{\boldsymbol{p}}(\varphi)} \right| \leq c$$

for some constant $c > 0$, we say the scheme is von Neumann stable.

Comparison with Lax-Richtmyer Stability

Need $\left\|(P_h^{-1}Q_h)^\ell P_h^{-1}\right\| \le c$.

Implied by von Neumann stability.

Why is bounding the symbol the most salient part?

If $\left\|P_h^{-1}Q_h\right\| \le 1$ encounters problems, there there often also doesn't exist a c so that $\left\|P_h^{-1}\right\| \le c$.

Main restriction of von Neumann stability?

- Only works on infinite/periodic grids.
- Have BCs? Analysis gets more difficult.

von Neumann Stability: ETBS (1/2)

ETBS: Let $\lambda = ah_t/h_x$. $u_{k,\ell+1} = \lambda u_{k-1,\ell} + (1-\lambda)u_{k,\ell}$.

$$P_h = I, \qquad Q_h = \text{tridiag}(\lambda, 1-\lambda, 0).$$

Auxiliary result: Fourier transform of $r_k = \delta_{k,j}$.

$$\hat{\boldsymbol{r}}(\varphi) = \sum_k r_k e^{-i\varphi k} = \sum_k \delta_{k,j} e^{-i\varphi k} = e^{-i\varphi j}.$$

$(Q_h\boldsymbol{x})_j = \sum_k q_{j-k}x_k$, so
$(Q_h\boldsymbol{x})_0 = q_0x_0 + x_{-1}q_1 + x_1q_{-1} + \cdots$, so
$\boldsymbol{q} = (\ldots, 0, 0, 1-\lambda, \lambda, 0, \ldots)$.

$$\hat{\boldsymbol{p}}(\varphi) = 1, \qquad \hat{\boldsymbol{q}}(\varphi) = \lambda e^{-i\varphi} + (1-\lambda) = 1 - \lambda(1 - e^{-i\varphi}).$$

$$\begin{aligned} |s(\varphi)|^2 &= \left|\frac{\hat{\boldsymbol{q}}(\varphi)}{\hat{\boldsymbol{p}}(\varphi)}\right|^2 = (1 - \lambda(1 - e^{-i\varphi}))(1 - \lambda(1 - e^{i\varphi})) \\ &= 1 + 2(\lambda - \lambda^2)(\cos\varphi - 1). \end{aligned}$$

von Neumann Stability: ETBS (2/2)

Found: $|s(\varphi)|^2 = 1 + 2(\lambda - \lambda^2)(\cos\varphi - 1)$.

Maximize: take derivative w.r.t. φ, set to 0:

$$\frac{d}{d\varphi}\left(1 + 2(\lambda - \lambda^2)(\cos\varphi - 1)\right) = -2(\lambda - \lambda^2)\sin\varphi = 0$$

if and only if $\varphi \in \mathbb{Z}\pi$.

For $m \in \mathbb{Z}$, $s(m\pi) = 1 + 2(\lambda - \lambda^2)((-1)^m - 1)$. For m even, $s(m\pi) = 1$.

For m odd, $s(m\pi) = 1 - 4(\lambda - \lambda^2) = (1 - 2\lambda)^2$.

Thus $|s(\varphi)|^2 \leq 1$ if and only if

$$|1 - 2\lambda| \leq 1 \quad \Leftrightarrow \quad 0 \leq \lambda \leq 1 \quad \Leftrightarrow \quad 0 \leq h_t \leq \frac{h_x}{a}.$$

Found: conditionally von Neumann stable with CFL as before.

von Neumann Stability: ETCS

Let $\lambda = ah_t/h_x$. Then

$$u_{k,\ell+1} = \frac{\lambda}{2} u_{k-1,\ell} + u_{k,\ell} - \frac{\lambda}{2} u_{k+1,\ell}.$$

$$P_h = I, \qquad Q_h = \operatorname{tridiag}(\lambda/2, 1, -\lambda/2).$$

So $\hat{\boldsymbol{p}}(\varphi) = 1$, and

$$\hat{\boldsymbol{q}}(\varphi) = \frac{\lambda}{2} e^{-i\varphi} + 1 - \frac{\lambda}{2} e^{-i\varphi(-1)} = 1 - \lambda \sin(\varphi) i.$$

So

$$\max_{\varphi} |s(\varphi)|^2 = \max_{\varphi} \left| \frac{\hat{\boldsymbol{q}}(\varphi)}{\hat{\boldsymbol{p}}(\varphi)} \right|^2 = 1 + \lambda^2 \sin^2(\varphi) \geq 1.$$

Not von Neumann stable $\Rightarrow$ not Lax-Richtmyer stable.

von Neumann Stability: Crank-Nicolson

Let $\lambda = ah_t/(4h_x)$

$$-\lambda u_{k-1,\ell+1} + u_{k,\ell+1} + \lambda u_{k+1,\ell+1} = \lambda u_{k-1,\ell} + u_{k,\ell} - \lambda u_{k+1,\ell}.$$

$$P_h = \text{tridiag}(-\lambda, 1, \lambda), \quad Q_h = \text{tridiag}(\lambda, 1, -\lambda).$$

$$\begin{aligned} \hat{\boldsymbol{p}}(\varphi) &= -\lambda e^{-i\varphi} + 1 + \lambda e^{i\varphi} = 1 + 2\lambda i \sin(\varphi), \\ \hat{\boldsymbol{q}}(\varphi) &= \lambda e^{-i\varphi} + 1 - \lambda e^{i\varphi} = 1 - 2\lambda i \sin(\varphi). \end{aligned}$$

$$|s(\varphi)|^2 = \frac{1 + 4\sin^2(\varphi)}{1 + 4\sin^2(\varphi)} = 1.$$

Crank-Nicolson is unconditionally von Neumann stable.

Outline

Studying Solutions of the PDE

Saw numerically: interesting dispersion/dissipation behavior.
Want: theoretical understanding.

Consider *linear*, *continuous* (not yet discrete) differential operators

$$
\begin{aligned}
L_1 u &= u_t + a u_x, \\
L_2 u &= u_t - D u_{xx} + a u_x \qquad (D > 0) \\
L_3 u &= u_t + a u_x - \mu u_{xxx}.
\end{aligned}
$$

What could we use as a prototype solution?

A Prototype Solution of the PDE

Observation: all these operators are diagonalized by complex exponentials. Come up with a 'prototype complex exponential solution'.

Let $z(x,t) = z_0 e^{i(kx-\omega t)}$.

What type of function is this?

- For k, ω real: traveling wave with speed $c = \omega/k$.
  $z(x-ct,0) = z_0 e^{i(k(x-ct))} = z(x,t)$.
- For k imaginary: an evanescent wave in x.
- For $\operatorname{Im}\omega < 0$: a wave decaying in time.

Wave-like Solutions of the PDE

$$z(x,t) = z_0 e^{i(kx-\omega t)}$$

$L_2 u = u_t - Du_{xx} + au_x$ $(D > 0)$. Plug in z.

$Lz = (-i\omega + iak + Dk^2)z.$

Observations in connection with L?

- $Lz = \lambda(\omega, k)z.$
- $z(x,t)$ is a solution iff $Lz = 0$ iff $\lambda(\omega, k) = 0.$

What is the dispersion relation?

The equation $\lambda(\omega, k) = 0$ is called the dispersion relation for the PDE L.

Picking Apart the Dispersion Relation

Consider $\omega(k) = \alpha(k) + i\beta(k)$. Rewrite the wave solution with this.

$$\begin{aligned} z(x,t) &= z_0 e^{i(kx-\omega(k)t)} \\ &= z_0 e^{i(kx-\alpha(k)t-i\beta(k)t)} \\ &= z_0 e^{\beta(k)t} e^{i(kx-\alpha(k)t)}. \end{aligned}$$

How can we recognize dissipation?

If $\beta(k) < 0$, we call the PDE dissipative.

What is the phase speed? How can we recognize dispersion?

- The phase speed of $z(x,t)$ is $v_{\text{ph}} = \alpha(k)/k$.
- If v_{ph} is a constant ($\Leftrightarrow \alpha(k)$ is linear in k), all waves move at the same speed.

Dispersion Relation: Examples

In each case, find the dispersion relation and identify properties.

$L_1 u = u_t + a u_x$

- $\lambda(\omega, k) = i(ak - \omega) = 0$, i.e. $\omega = ak$.
- Neither dissipative nor dispersive.

$L_2 u = u_t - D u_{xx} + a u_x$ $(D > 0)$

- $\lambda(\omega, k) = -i\omega + iak + Dk^2$, i.e. $\omega = ak - iDk^2$.
- Dissipative, but not dispersive.

$L_3 u = u_t + a u_x - \mu u_{xxx}$

- $\lambda(\omega, k) = -i\omega + iak + i\mu k^3$, i.e. $\omega = ak + \mu k^3$.
- Dispersive, but not dissipative.

Numerical Dissipation/Dispersion Analysis

Goal: Want discrete finite difference scheme to match dissipation/dispersion behavior of continuous PDE.

Define a discrete wave-like function:

$$z_{j,\ell} = z_0 e^{i(kjh_x - \omega \ell h_t)}$$

We want $\boldsymbol{z}$ to solve $P_h \boldsymbol{z}_{\ell+1} = Q_h \boldsymbol{z}_\ell$. How can we connect the operators to the wave solution?

P_h and Q_h consist of Toeplitz operators.

Toeplitz and Waves

$$z_{j,\ell} = z_0 e^{i(kjh_x - \omega \ell h_t)}.$$

Theorem (Waves Diagonalize Toeplitz Operators)

Let T be a Toeplitz operator. Then $T\boldsymbol{z}_\ell = \lambda(k)\boldsymbol{z}_\ell = \hat{\boldsymbol{t}}(kh_x)\boldsymbol{z}_\ell$.

$$\begin{aligned}
(T\boldsymbol{z}_\ell)_j &= \sum_m z_{m,\ell} t_{j-m} = \sum_m z_0 e^{i(kmh_x - \omega\ell h_t)} t_{j-m} \\
&= \sum_m z_0 e^{i(k(m-j)h_x)} e^{i(kjh_x - \omega\ell h_t)} t_{j-m} \\
&= \left(\sum_{m'} e^{-ikm'h_x} t_{m'} \right) z_0 e^{i(kjh_x - \omega\ell h_t)}.
\end{aligned}$$

$$\Rightarrow \lambda(k) = \sum_m e^{-ikmh_x} t_m = \hat{\boldsymbol{t}}(kh_x).$$

Waves and Two-Level Schemes

Since P_h and Q_h are Toeplitz, we must have

$$P_h \boldsymbol{z}_{\ell+1} = \lambda_P(k)\boldsymbol{z}_{\ell+1}, \qquad Q_h \boldsymbol{z}_\ell = \lambda_Q(k)\boldsymbol{z}_\ell.$$

What does that mean?

$$\begin{aligned}
\lambda_P(k)\boldsymbol{z}_{\ell+1} &= \lambda_Q(k)\boldsymbol{z}_\ell \\
\lambda_P(k) z_0 e^{i(kjh_x - \omega(\ell+1)h_t)} &= \lambda_Q(k) z_0 e^{i(kjh_x - \omega \ell h_t)} \\
e^{-i\omega h_t} &= \frac{\lambda_Q(k)}{\lambda_P(k)} = \frac{\hat{\boldsymbol{q}}(kh_x)}{\hat{\boldsymbol{p}}(kh_x)} = s(kh_x),
\end{aligned}$$

which is the symbol of of the finite difference method.

Seen before?

Used in von Neumann stability analysis.

Discrete Dispersion Relation (1/2)

So $\boldsymbol{z}_\ell$ is a solution of the finite difference scheme if $\omega = \omega(kh_x)$ satisfies

$$e^{-i\omega(\kappa)h_t} = s(\kappa),$$

where we let $\kappa = kh_x$. Interpret κ.

A number proportional to the number of wavelengths per point.

Let $s(\kappa) = |s(\kappa)|\, e^{i\varphi(\kappa)} = e^{\log|s(\kappa)|+i\varphi(\kappa)}$. $\omega(\kappa)$?

$$\omega(\kappa) = \frac{-\varphi(\kappa) + i\log|s(\kappa)|}{h_t}.$$

Discrete Dispersion Relation (2/2)

$$\omega(\kappa) = \frac{-\varphi(\kappa) + i \log|s(\kappa)|}{h_t}.$$

Plug that into the wave-like solution:

$$\begin{aligned} z_{j,\ell} &= z_0 e^{i(kjh_x - \omega \ell h_t)} \\ &= z_0 e^{i\left(kjh_x - \frac{-\varphi(\kappa)+i\log|s(\kappa)|}{h_t}\ell h_t\right)} \\ &= z_0 e^{\log|s(\kappa)|\ell} e^{ik\left(jh_x - \frac{-\varphi(\kappa)}{kh_t}\ell h_t\right)} \end{aligned}$$

Criterion for stability?

$|s(\kappa)| \leq 1$ (as before)

Numerical Dispersion/Dissipation

Finite difference scheme $P_h \boldsymbol{u}_{\ell+1} = Q_h \boldsymbol{u}_\ell$ with symbol $s(k)$.

$$z_{j,\ell} = z_0 e^{\log|s(\kappa)|\ell} e^{ik\left(jh_x - \frac{-\varphi(\kappa)}{kh_t}\ell h_t\right)}$$

When is the scheme dissipative?

> If $|s(kh_x)| < 1$, the scheme is called dissipative. Dissipation occurs exponentially in time, with factor $s(kh_x)$.

What is the phase speed?

> The scheme has phase speed $v_{\text{ph}} = \frac{-\varphi(kh_x)}{kh_t}$.

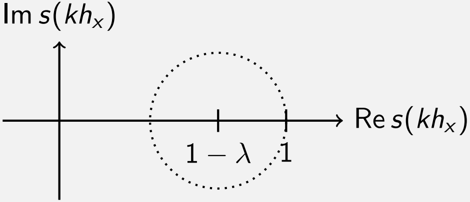
Dispersion?

> If v_{ph} is independent of k, all waves move with the same speed. If not, the scheme is called dispersive.

Dispersion/Dissipation Analysis of ETBS

Let $\lambda = ah_t/h_x$. Shown earlier: $s(kh_x) = 1 - \lambda(1 - e^{-ikh_x})$.

$s(\kappa) = (1-\lambda) + \lambda e^{-i\kappa}$. If we sweep κ, $s(\kappa)$ traces a circle:



For small λ, the circle moves towards $s(kh_x) = 1$, implying lower dissipation per step.

Overall, we obtain

$$e^{-i\omega(\kappa)h_t} = 1 - \lambda(1 - e^{-ikh_x}).$$

Dispersion/Dissipation Analysis of ETBS: Fine Grid

$$e^{-i\omega(\kappa)h_t} = 1 - \lambda(1 - e^{-ikh_x})$$

If kh_x is small, $e^{-ikh_x} \approx 1 - ikh$, so that

$$s(kh_x) \approx (1-\lambda) + \lambda(1 - ikh_x) = 1 - i\lambda kh_x.$$

For small $\omega(kh_x)$, approximate $e^{-i\omega(kh_x)h_t} = 1 - i\omega(kh_x)h_t$.
Setting the two (approximately) equal yields

$$1 - i\omega(kh_x)h_t \approx 1 - i\lambda kh_x \qquad \Rightarrow \qquad \omega(kh_x)h_t \approx \lambda kh_x = \frac{ah_t}{h_x}kh_x,$$

i.e. $\omega(kh_x) \approx ak$, or $v_{\text{ph}} \approx (-ak)/(kh_t) = -a/h_t$, which is independent of k. Thus we expect little dispersion for waves with low number of wavelengths per point.

Dispersion/Dissipation: Demo

- **Demo:** Experimenting with Dispersion and Dissipation [cleared]
- **Demo:** Dispersion and Dissipation [cleared]

Outline

Heat Equation

Heat equation $(D > 0)$:

$$\begin{aligned} u_t &= Du_{xx}, \qquad (x,t) \in \mathbb{R} \times (0,\infty), \\ u(x,0) &= g(x) \qquad x \in \mathbb{R}. \end{aligned}$$

Fundamental solution $(g(x) = \delta(x))$:

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t}.$$

Why is this a weird model?

Infinite speed of propagation of information

Schemes for the Heat Equation

Cook up some schemes for the heat equation.

Explicit Euler:

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} - D\frac{u_{k+1,\ell} - 2u_{k,\ell} + u_{k-1,\ell}}{h_x^2} = 0$$

Implicit Euler:

$$\frac{u_{k,\ell+1} - u_{k,\ell}}{h_t} - D\frac{u_{k+1,\ell+1} - 2u_{k,\ell+1} + u_{k-1,\ell+1}}{h_x^2} = 0$$

Von Neumann Analysis of Explicit Euler for Heat (1/2)

Let $\lambda = Dh_t/h_x^2$.

$$u_{k,\ell+1} = u_{k,\ell} + \lambda(u_{k+1,\ell} - 2u_{k,\ell} + u_{k-1,\ell}).$$

$$P_h = I, \qquad Q_h = \operatorname{tridiag}(\lambda, 1-2\lambda, \lambda).$$

Thus

$$\begin{aligned} \hat{\boldsymbol{p}}(\varphi) &= 1, \\ \hat{\boldsymbol{q}}(\varphi) &= \lambda e^{-i\varphi} + (1-2\lambda) + \lambda e^{i\varphi} = 1 - 2\lambda + 2\lambda\cos(\varphi). \end{aligned}$$

We want $|s(\varphi)| \leq 1$, thus we need

$$\begin{aligned} -1 \leq & \quad 1 + 2\lambda(\cos(\varphi) - 1) & \leq 1 \\ \Leftrightarrow \quad -2 \leq & \quad 2\lambda(\cos(\varphi) - 1) & \leq 0. \end{aligned}$$

Von Neumann Analysis of Explicit Euler for Heat (2/2)

$$-2 \leq 2\lambda(\cos(\varphi) - 1) \leq 0.$$

Since $|\cos(\varphi)| \leq 1$, also $-2 \leq \cos(\varphi) - 1 \leq 0$. For the lower bound,

$$-2 \leq -4\lambda \quad \Leftrightarrow \quad \frac{1}{2} \geq \frac{D h_t}{h_x^2} \quad \Leftrightarrow \quad h_t \leq \frac{h_x^2}{2D}.$$

Observe $h_t = O(h_x^2)$, which is often prohibitively small.

Comment on the stability region found regarding speeds of propagation.

- Saw: heat equation has infinite speed of information propagation
- Explicit Euler has finite speed of information propagation (how fast?)

Von Neumann Analysis of Implicit Euler for Heat

Let $\lambda = Dh_t/h_x^2$.

$$u_{k,\ell+1} - \lambda(u_{k+1,\ell+1} - 2u_{k,\ell+1} + u_{k-1,\ell+1}) = u_{k,\ell}$$

$$P_h = \operatorname{tridiag}(-\lambda, 1+2\lambda, -\lambda), \qquad Q_h = I.$$

$$\hat{\boldsymbol{p}}(\varphi) = 1 + 2\lambda(1-\cos(\varphi)), \quad \hat{\boldsymbol{q}}(\varphi) = 1.$$

To obtain $|s(\varphi)| \leq 1$, consider $1 \leq |1 + 2\lambda(1-\cos(\varphi))|$, which is always true.

Does the type of system we need to solve for implicit+parabolic correspond to another PDE?

- Yes, elliptic.
- Focus on solving those later.

Outline

Outline

Conservation Laws: Recap

$$u_t + f(u)_x = 0,$$

where u is a function of x and $t \in \mathbb{R}_0^+$.

Rewrite in integral form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b u(x,t)\mathrm{d}x + f(u(b,t)) - f(u(a,t)) = 0 \qquad \text{for any } a,\ b.$$

Recall: Characteristic Curve: a function $x(t)$ so that $u(x(t),t) = u(x_0, 0)$.

$$\begin{cases} \frac{\mathrm{d}x(t)}{\mathrm{d}t} = f'(u(x(t),t)), \\ x(0) = x_0. \end{cases}$$

What assumption underlies all this?

Smooth Solution.

Going Nonlinear: Burgers' Equation

Make a simple modification to advection $u_t + au_x = 0$ to make it nonlinear.

$$u_t + uu_x = 0$$

Is that a sensible modification?

Yes: it is the core part of the momentum equation in Euler's equations of gas dynamics in 1D.

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \frac{\nabla p}{\rho} = \boldsymbol{g}$$

Is that still a conservation law?

Yes: $u_t + (u^2/2)_x = 0$. Called Burgers' Equation.

Burgers' Equation: Try FD Numerics

Demo: ETBS for Volume Burgers [cleared]

What do you think of these results?

No good, very bad. Conservation of $\int u$ should hold at least to the order of accuracy of the scheme!

We clearly need to rethink our plan here. We will begin by learning about the theory of conservation laws.

Burgers' Equation

$$\begin{cases} u_t + \left(\frac{u^2}{2}\right)_x = 0, \\ u(x,0) = g(x) = \sin(x). \end{cases}$$

Interpret Burgers' equation.

> $f(u) = u^2/2$. So $f'(u) = u$.
> Characteristic speed is given by 'how much stuff there is'/'the density'

Consider the characteristics at $\pi/2$ and $3\pi/2$.

> $f(u) = u^2/2$. So $f'(u) = u$.
> - $x = \pi/2$: $f'(\sin x) = 1$.
> - $x = 3\pi/2$: $f'(\sin x) = -1$.
>
> They intersect!

Weak Solutions

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b u(x,t)\mathrm{d}x = f(u(a,t)) - f(u(b,t))$$

Define a weak solution:

- If u satisfies the integral form for almost all (a,b) then u is called a weak solution. (physically meaningful)
- If for any $\varphi \in C_0^1(\mathbb{R}\times[0,\infty))$ (compact support),

  $$-\int_0^\infty \int_{-\infty}^\infty (u\varphi_t + f(u)\varphi_x)\mathrm{d}x\mathrm{d}t - \int_{-\infty}^\infty u^0(x)\varphi(x,0)\mathrm{d}x = 0,$$

  then in u is called a weak solution. (more meaningful mathematically)

Turns out: equivalent. (not shown)

Rankine-Hugoniot Condition (1/2)

Consider: Two C^1 segments separated by a curve $x(t)$ with no regularity.

$$(d/dt)\Bigg(\underbrace{\int_a^{x(t)} u(x,t)dx}_{G_a(x(t),t):=} + \underbrace{\int_{x(t)}^{b} u(x,t)dx}_{G_b(x(t),t):=}\Bigg) + f(u(b,t)) - f(u(a,t)) = 0.$$

$$\begin{aligned}\frac{d}{dt}G_a(x(t),t) &= \frac{\partial G_a(x(t),t)}{\partial x}\cdot\frac{dx(t)}{dt} + \frac{\partial G_a}{\partial t}\\ &= u(x(t),t)x'(t) + \int_a^{x(t)} u_t(x,t)dx\\ &= u(x(t),t)x'(t) - \int_a^{x(t)} f(u)_x(x,t)dx\\ &= u(x(t),t)x'(t) - (f(u(x(t),t)) - f(u(a,t))),\end{aligned}$$

and $dG_b(x(t),t)/dt$ analogously.

Rankine-Hugoniot Condition (2/2)

$$(d/dt)G_a(x(t),t) = u(x(t),t)x'(t) - (f(u(x(t),t)) - f(u(a,t))).$$

Discontinuity at $u(x(t),t)$: $(d/dt)G_a$ doesn't exist. One-sided limits:

$$\begin{aligned}
\left[\frac{dG_a(x(t),t)}{t}\right]^- &= u^- x'(t) - (f(u^-) - f(u(a,t))), \\
\left[\frac{dG_b(x(t),t)}{t}\right]^+ &= -u^+ x'(t) - (f(u(b,t)) - f(u^+)).
\end{aligned}$$

Adopted shorthand: $u^- := u(x(t)^-, t)$, $\qquad u^+ := u(x(t)^+, t)$.
Plug into integral form: $u^- x'(t) - f(u^-) - u^+ x'(t) + f(u^+) = 0$.

$$x'(t) = \frac{f(u^+) - f(u^-)}{u^+ - u^-}.$$

This is the called the Rankine-Hugoniot Condition.

Rankine-Hugoniot and Weak Solutions

Theorem (Rankine-Hugoniot and Weak Solutions)

If u is piecewise C^1 and is discontinuous only along isoated curves, and if u satisfies the PDE when it is C^1, and the Rankine-Hugoniot condition holds along all discontinuous curves, then u is a weak solution of the conservation law.

Riemann Problems: Example 1

Consider the following Riemann problem:

$$u_t + \left(\frac{u^2}{2}\right)_x = 0,$$

$$u(x,0) = \begin{cases} 1 & x < 0, \\ -1 & x \geq 0. \end{cases}$$

The IC is just propagated in time (at "speed 0") to form a weak solution (a shock).

Riemann Problems: Example 2

$$u_t + \left(\frac{u^2}{2}\right)_x = 0,$$
$$u(x,0) = \begin{cases} -1 & x < 0, \\ 1 & x \geq 0. \end{cases}$$

(IC sign flip compared to previous slide)

The propagated ICs also form a weak solution. But consider

$$u(x,t) = \begin{cases} -1 & x \leq -t, \\ x/t & -t < x < t, \\ 1 & x > t. \end{cases}$$

This is also a weak solution (a rarefaction wave).
Conclusion: Our current notion of weak solution is *too* weak.

Bad Shocks and Good Shocks

In the shock version of the ‘ambiguous’ Riemann problem, where do the characteristics go?

- Out of the shock.
- In the first example, the shock is self-steepening.
- In the second example, it is not.

Comment on the stability of that situation.

Smearing out the initial profile or adding viscosity would wash out the solution into a rarefaction fan.

Ad-Hoc Idea: Ban Bad Shocks

Recall: what is $f'(u)$?

> Characteristic speed.

Devise a way to ban unstable shocks.

> A discontinuity propagating with speed s (cf. Rankine-Hugoniot) satsifes the entropy condition if
>
> $$f'(u^-) > s > f'(u^+).$$
>
> If f is convex, f' is monotonically non-decreasing, and the Rankine-Hugoniot speed automatically falls between $f'(u^-)$ and $f'(u^+)$. So for convex f, $f'(u^-) > f'(u^+)$ is sufficient (and implies $u^- > u^+$ by convexity).

Vanishing Viscosity Solutions

Goal: neither uniqueness nor existence poses a problem.

How?

Consider adding an artificial viscosity:

$$u_t^\varepsilon + f(u^\varepsilon)_x = \varepsilon u_{x,x}^\varepsilon \qquad \text{with small } \varepsilon > 0.$$

By ‘washing out’ the solution, the viscous term increases smoothness, and, we hope, restores uniqueness.

Then we would wish to define an vanishing viscosity weak solution as

$$\lim_{\varepsilon \to 0} u^\varepsilon(x,t) = u(x,t)$$

in some norm.

Entropy-Flux Pairs

What are features of (physical) entropy?

- Constant along particle paths in smooth flow
- Jumps to higher values across a shock

Definition (Entropy/Entropy Flux)

An entropy $\eta(u)$ and an entropy flux $\psi(u)$ are functions so that η is convex and

$$\eta(u)_t + \psi(u)_x = 0$$

for smooth solutions of the conservation law.

Finding Entropy-Flux Pairs

$\eta(u)_t + \psi(u)_x = 0$. Find conditions on η and ψ.

For smooth u, the chain rule gives $\eta'(u)u_t + \psi'(u)u_x = 0$. Similarly, we can rewrite the conservation law:

$$\begin{aligned} u_t + f'(u)u_x &= 0 \\ \Leftrightarrow \quad \eta'(u)u_t + \eta'(u)f'(u)u_x &= 0. \end{aligned}$$

This gives us $\psi'(u) = -\eta'(u)(u_t/u_x) = \eta'(u)f'(u)$.
Lots of solutions for scalar conservation laws. For systems and in multiple dimensions: may have no solutions.

Come up with an entropy-flux pair for Burgers.

$f(u) = u^2/2$. If we take $\eta(u) = u^2$, then $\psi'(u) = 2u \cdot u$, i.e. $\psi(u) = 2u^3/3$.

Back to Vanishing Viscosity (1/2)

$$u_t + f(u)_x = \varepsilon u_{xx}$$

What's the evolution equation for the entropy?

Note: Viscosity solutions are always smooth. Allowed to do derivative gymnastics. Multiply by $\eta'(u)$:

$$\begin{aligned} \eta'(u)u_t + \eta'(u)f'(u)u_x &= \varepsilon\eta'(u)u_{xx} \\ \Leftrightarrow \quad \eta(u)_t + \psi(u)_x &= \varepsilon(\eta'(u)u_x)_x - \varepsilon\eta''(u)u_x^2. \end{aligned}$$

Back to Vanishing Viscosity (2/2)

$$\eta(u)_t + \psi(u)_x = \varepsilon(\eta'(u)u_x)_x - \varepsilon\eta''(u)u_x^2.$$

Integrate this over $[x_1, x_2] \times [t_1, t_2]$, with x_1, x_2 on either side of jump.

$$\begin{aligned} & \int_{t_1}^{t_2} \int_{x_1}^{x_2} \eta(u)_t + \psi(u)_x dxdt \\ = \quad & \varepsilon \int_{t_1}^{t_2} [\eta'(u(x_2,t))u_x(x_2,t) - \eta'(u(x_1,t))u_x(x_1,t)]dt \\ & -\varepsilon \int_{t_1}^{t_2} \int_{x_1}^{x_2} \underbrace{\eta''(u)u_x^2}_{\geq 0} dxdt. \end{aligned}$$

As $\varepsilon \to 0$, the first term goes to zero. The second term involves an integral over the square of the derivative of a steepening u (as $\varepsilon \to 0$), and so will not vanish. Accordingly, $\eta(u)_t + \psi(u)_x \leq 0$ weakly.

Entropy Solution

Definition (Entropy solution)

The function $u(x, t)$ is the entropy solution of the conservation law if for all convex entropy functions and corresponding entropy fluxes, the inequality

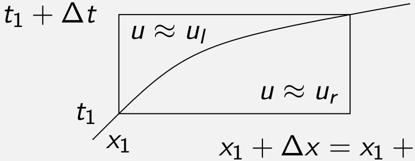
$$\eta(u)_t + \psi(u)_x \leq 0$$

is satisfied in the weak sense.

Entropy Solution vs Entropy Condition

Relate entropy solutions $\eta(u)_t + \psi(u)_x \le 0$ back to the entropy condition.

Consider Burgers, integrate the entropy ineq. over a small box:



$$x_1 + \Delta x = x_1 + s_1 \Delta t$$

$$\begin{aligned}
0 &\ge \left[\int_{x_1}^{x_1+\Delta x} u^2\right]_{t_1}^{t_1+\Delta t} + \left[\int_{t_1}^{t_1+\Delta t} 2u^3/3\right]_{x_1}^{x_1+\Delta x} \\
&= s_1 \Delta t(u_l^2 - u_r^2) + 2/3 \Delta t(u_r^3 - u_l^3) + O(\Delta t^2) \\
&= \Delta t(u_l^2 - u_r^2)(s_1 - s_2) + O(\Delta t^2) \\
&= -1/6(u_l - u_r)^3 \Delta t + O(\Delta t^2) \quad \rightarrow \quad u_l > u_r,
\end{aligned}$$

with $s_1 = [u^2/2]/[u]$, $s_2 = [2u^3/3]/[u^2]$, $s_2 - s_1 = [u]^2/(6(u_l + u_r))$.

Conservation of Entropy?

What can you say about conservation of entropy in time?

$$
\begin{aligned}
0 &\geq \int_{t_1}^{t_2}\int_{x_1}^{x_2} \eta(u)_t + \psi(u)_x \, dxdt \\
&= \left[\int_{x_1}^{x_2} \eta(u(x,t))dx\right]_{t_1}^{t_2} + \left[\int_{t_1}^{t_2} \psi(u(x,t))dt\right]_{x_1}^{x_2},
\end{aligned}
$$

so that

$$
\int_{x_1}^{x_2} \eta(u(x,t_2))dx \leq \int_{x_1}^{x_2} \eta(u(x,t_1))dx - \underbrace{\left[\int_{t_1}^{t_2} \psi(u(x,t))dt\right]_{x_1}^{x_2}}_{\text{Outflow/Inflow}}
$$

If u is compactly supported, then we can choose x_1 and x_2 so that $\psi(u(x_1,t)) \equiv \text{const}(t) \equiv \psi(u(x_2,t))$ and entropy can only decrease. (fluid flow: math. entropy $= -\rho \cdot$ phys. entropy)

Total Variation

$$\mathrm{TV}(u) = \limsup_{\varepsilon \to 0} \frac{1}{\varepsilon} \int |u(x+\varepsilon) - u(x)| \, dx.$$

Simpler form if u is differentiable?

$$\mathrm{TV}(u) = \int \left| u'(x) \right| \, dx$$

Hiking analog?

Elevation change

Total Variation and Conservation Laws

Theorem (Total Variation is Bounded [Dafermos 2016, Thm. 6.2.6])

Let u be a solution to a conservation law with $f''(u) \geq 0$. Then:

$$\mathrm{TV}(u(t+\Delta t, \cdot)) \leq \mathrm{TV}(u(t, \cdot)) \quad \textit{for } \Delta t \geq 0.$$

- For smooth solutions (and non-crossing characteristics), all function values live $\Rightarrow$ TV stays unchanged.
- For solutions with shocks, local minima and maxima may disappear into the shock $\Rightarrow$ TV decreases.

Theorem (L^1 contraction [Dafermos 2016, Thm. 6.3.2])

Let u, v be viscosity solutions of the conservation law. Then

$$\|u(t+\Delta, \cdot) - v(t+\Delta t, \cdot)\|_{L^1(\mathbb{R})} \leq \|u(t, \cdot) - v(t, \cdot)\|_{L^1(\mathbb{R})} \quad \textit{for } \Delta t \geq 0$$

Outline

Finite Difference for Conservation Laws? (1/2)

$$\begin{cases} u_t + \left(\frac{u}{2}\right)^2_x = 0 \\ u(x,0) = \begin{cases} 1 & x < 0, \\ 0 & x \geq 0. \end{cases} \end{cases}$$

Entropy Solution?

$$u(x,t) = \begin{cases} 1 & x \leq \frac{1}{2}t, \\ 0 & x > \frac{1}{2}t. \end{cases}$$

Rewrite the PDE to 'match' the form of advection $u_t + au_x = 0$:

$$u_t + uu_x = 0.$$

Equivalent?

Finite Difference for Conservation Laws? (2/2)

Recall the *upwind scheme* for $u_t + au_x = 0$:

$$u_{j,\ell+1} = u_{j,\ell} - a \cdot \frac{\Delta t}{\Delta x}(u_{j,\ell} - u_{j-1,\ell}).$$

Write the upwind FD scheme for $u_t + uu_x = 0$:

$$u_{j,\ell+1} = u_{j,\ell} - \frac{\Delta t}{\Delta x} u_{j,\ell}(u_{j,\ell} - u_{j-1,\ell}).$$

- For $j \neq 0$, $u_{j,0} - u_{j-1,0} = 0$
- For $j = 0$, $u_{j,0} = 0$.

Altogether,

$$u_{j,\ell+1} = u_{j,\ell}.$$

Bad.

Schemes in Conservation Form

Definition (Conservative Scheme)

A conservation law scheme is called conservative iff it can be written as

$$u_{j,\ell+1} = u_{j,\ell} - \frac{\Delta t}{\Delta x}[f^*_{j+1/2}(\boldsymbol{u}_\ell) - f^*_{j-1/2}(\boldsymbol{u}_\ell)],$$

where $f^*\dots$

- is Lipschitz continuous,
- satisfies $f^*(u, \cdots, u) = f(u)$ (consistency).

Theorem (Lax-Wendroff)

If the solution $\{u_{j,\ell}\}$ to a conservative scheme converges (as $\Delta t, \Delta x \to 0$) boundedly almost everywhere to a function $u(x,t)$, then u is a weak

Lax-Wendroff Theorem: Proof

Summation by parts: With $\Delta^+ a_k = a_{k+1} - a_k$ and $\Delta^- a_k = a_k - a_{k-1}$:

$$\sum_{k=1}^{N} a_k(\Delta^- \varphi_k) + \sum_{k=1}^{N} \varphi_k(\Delta^+ a_k) = -a_1\varphi_0 + \varphi_N a_{N+1}.$$

Let $\varphi_{j,\ell} = \varphi(x_j, t_\ell)$ for $\varphi \in C_0^1$ (compact support). Then, by conservativity,

$$0 = \sum_{\ell=1}^{\infty} \sum_{j} \left(\frac{\Delta_2^+ u_{j,\ell}}{h_t} + \frac{\Delta^+ f^*_{j-1/2}}{h_x} \right) \varphi_{j,\ell} h_x h_t$$

$$= \quad -\sum_{\ell=1}^{\infty} \sum_{j} \left(\frac{\Delta_2^- \varphi_{j,\ell}}{h_t} u_{j,\ell} + \frac{\Delta_1^- \varphi_{j,\ell}}{h_x} f^*_{j-1/2} \right) h_x h_t - \sum_{j} u_{j,1}\phi_{j,0} h_x$$

$$\underset{f^*(u,u)=u}{\overset{\text{DCT}}{\longrightarrow}} \quad -\int_0^\infty \int_{-\infty}^\infty (\varphi_t u + \varphi_x f(u)) \mathrm{d}x\mathrm{d}t - \int_{-\infty}^\infty u(x,0)\phi(x,0)\mathrm{d}x = 0.$$

Finite Volume Schemes

Finite volume: Idea?

- Consider the solution constant in each cell: $\bar{u}_j$
- $\bar{u}_j$ is the cell average of cell I_j:

$$\bar{u}_j = (1/h_x) \int_{x_{j-1/2}}^{x_{j+1/2}} u(x)dx$$

- Choose h_x, h_t so that $\max|f'(u)|h_t < h_x$.

Idea: Solve Riemann problem at each cell interface.

Developing Finite Volume

$$\int_{t_\ell}^{t^{\ell+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} (u_t + f(u)_x)\mathrm{d}x\mathrm{d}t = 0$$

$$\begin{aligned}
\frac{1}{h_x}\int_{x_{j-1/2}}^{x_{j+1/2}} u^{\ell+1}\mathrm{d}x - \frac{1}{h_x}\int_{x_{j-1/2}}^{x_{j+1/2}} u^{\ell}\mathrm{d}x & & \\
+\frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j+1/2})\mathrm{d}t - \frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j-1/2})\mathrm{d}t &=& 0 \\
\Leftrightarrow \quad \bar{u}_{j,\ell+1} - \bar{u}_{j,\ell} & & \\
+\frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j+1/2})\mathrm{d}t - \frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j-1/2})\mathrm{d}t &=& 0.
\end{aligned}$$

Flux Integrals?

$$\frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j+1/2})\mathrm{d}t?$$

The substitution

$$\bar{x} = ax, \qquad \bar{t} = at.$$

leaves the conservation law and the Riemann ICs invariant.
$\Rightarrow$ The Riemann solution must be self-similar under scaling.

Thus: the Riemann solution $u(x,t)$ can be viewed as function of only one variable $\xi = x/t$.

Thus u is constant along $x = x_{j\pm1/2}$, so that

$$\frac{1}{h_x}\int_{t_\ell}^{t_{\ell+1}} f(u_{j+1/2})\mathrm{d}t = \frac{h_t}{h_x} f(u_{j+1/2}).$$

The Godunov Scheme

Altogether:

$$\bar{u}_{j,\ell+1} = \bar{u}_{j,\ell} - \frac{h_t}{h_x}(f(u_{j+1/2,\ell}) - f(u_{j-1/2,\ell})).$$

Overall algorithm?

- Reconstruct $u^-_{j\pm 1/2,\ell}$ and $u^+_{j\pm 1/2,\ell}$
- Evolve the Riemann problem at $x_{j\pm 1/2}$:
- Average the Riemann solutions to obtain $\bar{u}_{j,\ell+1}$

$\to$ Numerical flux / Riemann solver: $f^*(u^-_{j\pm 1/2,\ell}, u^+_{j\pm 1/2,\ell})$

Heuristic time step restriction?

Will run into problems if wave from one cell interface interacts with other interface: $h_t \le h_x / \max_j |f'(u_j)|$

Riemann Problem

$$\begin{cases} u_t + f(u)_x = 0, \\ u(x,0) = \begin{cases} u_l & x < 0, \\ u_r & x \geq 0 \end{cases} \end{cases}$$

Exact solution in the Burgers case?

$$u(x,t) = \begin{cases} \begin{cases} u_l & x < st, \\ u_r & x \geq st, \end{cases} & u_l \geq u_r, \\ \begin{cases} u_l & x < u_l t, \\ x/t & u_l t \leq x < u_r t, \\ u_r & x \geq u_r t, \end{cases} & u_l < u_r, \end{cases}$$

$$s = \frac{f(u_r) - f(u_l)}{u_r - u_l} = \frac{\frac{1}{2}[u_r^2 - u_l^2]}{u_r - u_l} = \frac{1}{2}(u_l + u_r).$$

Why is the rarefaction part independent of u_l and u_r?

Riemann Solver for a General Conservation Law

To complete the scheme: Need $f^*(u^-, u^+)$. For Burgers: already known. For a general convex ($f''(u) > 0$) conservation law?

Let u_s such that $f'(u_s) = 0$ (called the stagnation state: why?)

$$f(u(0,t)) = f^*(u^-, u^+) = \begin{cases} f(u^-) & \text{if shock with } s > 0, \\ f(u^+) & \text{if shock with } s \le 0, \\ f(u^-) & \text{if raref. with } f'(u^-) \ge 0, \\ f(u^+) & \text{if raref. with } f'(u^+) \le 0, \\ f(u_s) & \text{if raref. with } f'(u^-) \le 0 \le f'(u^+). \end{cases}$$

Equivalent to

$$f^*(u^-, u^+) = \begin{cases} \max_{u^+ \le u \le u^-} f(u) & \text{if } u^- > u^+, \\ \min_{u^- \le u \le u^+} f(u) & \text{if } u^- \le u^+. \end{cases}$$

More Riemann Solvers

Downside of Godunov Riemann solver?

> Not easy/efficient to implement in general. Want simpler Riemann solvers.

Back to Advection

Consider only $f(u) = au$ for now. Riemann solver inspiration from FD?

For $a \geq 0$, want ETBS:

$$\begin{aligned} 0 &= \frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + a\frac{u_{j,\ell} - u_{j-1,\ell}}{h_x} \\ &= \frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + \frac{f(u_{j,\ell}) - f(u_{j-1,\ell})}{h_x} \\ &= \frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + \frac{f^*(u_{j,\ell}, u_{j+1,\ell}) - f^*(u_{j-1,\ell}, u_{j,\ell})}{h_x}. \end{aligned}$$

Clearly equivalent to a finite volume scheme! Upwind numerical flux?

$$f^*(u^-, u^+) = \begin{cases} au^- & a \geq 0 \\ au^+ & a < 0 \end{cases} = \frac{au^- + au^+}{2} - \frac{|a|}{2}(u^+ - u^-).$$

Side Note: First Order Upwind, Rewritten

$$\frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + \frac{f^*(u_{j,\ell}, u_{j+1,\ell}) - f^*(u_{j-1,\ell}, u_{j,\ell})}{h_x}$$

with

$$f^*(u^-, u^+) = \frac{au^- + au^+}{2} - \frac{|a|}{2}(u^+ - u^-).$$

$$\frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + a\frac{u_{j+1,\ell} - u_{j-1,\ell}}{2h_x} = \frac{|a|\, h_x}{2} \cdot \frac{u_{j+1,\ell} - 2u_{j,\ell} + u_{j-1,\ell}}{h_x^2},$$

i.e. it is equivalent to ETCS (unstable!) with a second-order discretization of ∂_x^2, i.e. a dissipation, with a coefficient that vanishes as $h_x \to 0$.

Lax-Friedrichs

Generalize linear upwind flux for a nonlinear conservation law:

$$f^*(u^-, u^+) = \frac{au^- + au^+}{2} - \frac{|a|}{2}(u^+ - u^-).$$

$$f^*(u^-, u^+) = \frac{f(u^-) + f(u^+)}{2} - \frac{\alpha}{2}(u^+ - u^-).$$

Choice of α (consistent with linear)? Idea: $\alpha = |f'((u^- + u^+)/2)|$
Unfortunately: may converge to a weak solution that violates the entropy condition (not shown). Better:

$$\alpha = \max\left(\left|f'(u^-)\right|, \left|f'(u^+)\right|\right).$$

Called local Lax-Friedrichs. Global variant (with global max) also OK.

Demo: Finite Volume Burgers [cleared] (Part I)

Outline

Improving Accuracy

Consider our existing discrete FV formulation:

$$\bar{u}_{j,\ell+1} = \bar{u}_{j,\ell} - \frac{h_t}{h_x}(f(u_{j+1/2,\ell}) - f(u_{j-1/2,\ell})).$$

What obstacles exist to increasing the order of accuracy?

- Temporal Accuracy
- Spatial Accuracy
- Nonsmoothness (in both space and time)

What order of accuracy can we expect?

- Near shocks: no convergence in L^∞, first-order in L^2.
- Elsewhere: hopefully, as high as we would like

Improving the Order of Accuracy

Improve temporal accuracy.

Rewrite FV using the method of lines:

$$\frac{d\bar{u}_j(t)}{dt} + \frac{f^*(u^-_{j+1/2}(t), u^+_{j+1/2}(t)) - f^*(u^-_{j-1/2}(t), u^+_{j-1/2}(t))}{h_x} = 0.$$

What's the obstacle to higher spatial accuracy?

Letting $u^-_{j+1/2} = \bar{u}_j = u^+_{j-1/2}$.

How can we improve the accuracy of that approximation?

Include more cells in the reconstruction of the state $u^\pm_{j+1/2}$.

Increasing Spatial Accuracy

Temporary Assumptions:

- $f'(u) \geq 0$
- $f^*_{j+1/2}(u^-, u^+) = f(u^-)$ (e.g. Godunov in this situation)

Reconstruct $u_{j+1/2}$ using $\{\bar{u}_{j-1}, \bar{u}_j, \bar{u}_{j+1}\}$. Accuracy? Names?

$$\begin{aligned} u^{-,(1)}_{j+1/2} &= \frac{1}{2}(\bar{u}_j + \bar{u}_{j+1}), && \text{(2nd order central)} \\ u^{-,(2)}_{j+1/2} &= \frac{3}{2}\bar{u}_j - \frac{1}{2}\bar{u}_{j-1}, && \text{(2nd order upwind)} \end{aligned}$$

Compute fluxes, use increments over cell average:

$$f^{*,(1)}_{j+1/2} = f\Big(\bar{u}_j + \underbrace{\frac{1}{2}(\bar{u}_{j+1} - \bar{u}_j)}_{\tilde{u}^{(1)}_j}\Big), \qquad f^{*,(2)}_{j+1/2} = f\Big(\bar{u}_j + \underbrace{\frac{1}{2}(\bar{u}_j - \bar{u}_{j-1})}_{\tilde{u}^{(2)}_j}\Big).$$

Demos: Spatial Accuracy

- **Demo:** Higher-Order Reconstruction [cleared]
- **Demo:** Finite Volume Burgers [cleared] (Part II)

Lax-Wendroff

Another scheme for high-order. For $u_t + au_x$, from finite difference:

$$f^*(u^-, u^+) = \frac{au^- + au^+}{2} - \frac{a^2}{2} \cdot \frac{\Delta t}{\Delta x}(u^+ - u^-).$$

Taylor in time: $u_{\ell+1} = u_\ell + \partial_t u_\ell \cdot h_t + \partial_t^2 u_\ell \cdot h_t^2/2 + O(h_t^3)$.

$$\begin{aligned} u_t &= -f(u)_x, \\ u_{tt} &= -f(u)_{xt} = -(f(u)_t)_x = -(f'(u)u_t)_x = (f'(u)f(u)_x)_x. \end{aligned}$$

Then use central differences to discretize derivatives:

$$\frac{u_{j,\ell+1} - u_{j,\ell}}{h_t} + \frac{f(u_{j+1,\ell}) - f(u_{j-1,\ell})}{2h_x}$$

$$= \frac{h_t}{2h_x}\left[f'(u_{j+1/2,\ell})\frac{f(u_{j+1,\ell}) - f(u_{j,\ell})}{h_x} - f'(u_{j-1/2,\ell})\frac{f(u_{j,\ell}) - f(u_{j-1,\ell})}{h_x}\right]$$

As Riemann solver: $f^*(u^-, u^+) = \dfrac{f(u^-) + f(u^+)}{2} - \dfrac{h_t}{h_x}[f'(u^\circ)(f(u^+) - f(u^-))]$.

Monotone Schemes

Definition (Monotone Scheme)

A scheme

$$\begin{aligned} u_{j,\ell+1} &= u_{j,\ell} - \lambda(f^*(u_{j-p},\ldots,u_{j+q}) - f^*(u_{j-p-1},\ldots,u_{j+q-1})) \\ &=: G(u_{j-p-1},\ldots,u_{j+q}) \end{aligned}$$

is called a montone scheme if G is a monotonically nondecreasing function $G(\uparrow,\uparrow,\ldots,\uparrow)$ of each argument.

Monotonicity for Three-Point Schemes

Three-Point Scheme:

$$G(u_{j-1}, u_j, u_{j+1}) = u_j - \lambda[f^*(u_j, u_{j+1}) - f^*(u_{j-1}, u_j)].$$

When is this monotone?

If $f^*(\uparrow, \downarrow)$, then $G(\uparrow, ?, \uparrow)$. To clean up the second argument, consider

$$\frac{\partial G}{\partial u_j} = 1 - \lambda[\underbrace{f_1^* - f_2^*}_{\geq 0}] \geq 0.$$

(The subscripts indicate partial derivatives with respect to the first and second argument.)

If $\lambda(f_1^* - f_2^*) \leq 1$, then $G(\uparrow, \uparrow, \uparrow)$.

Note: Also obtain a time-step restriction.

Lax-Friedrichs is Monotone

$$f^*(u^-, u^+) = \frac{f(u^-) + f(u^+)}{2} - \frac{\alpha}{2}(u^+ - u^-).$$

Show: This is monotone.

Let $\alpha = \max_u |f'(u)|$.

$$\begin{aligned} f_1^* &= \frac{1}{2}[f'(u^-) + \alpha] \geq 0, \\ f_2^* &= \frac{1}{2}[f'(u^+) - \alpha] \leq 0. \end{aligned}$$

So $f^*(\uparrow, \downarrow)$. Assume h_t is chosen small enough so that $\lambda(f_1^* - f_2^*) \leq 1$ is satisfied.

Monotone Schemes: Properties

Theorem (Good properties of monotone schemes)

- *Local maximum principle*:

$$\min_{i \in \text{stencil around } j} u_i \leq G(u)_j \leq \max_{i \in \text{stencil around } j} u_i.$$

- *L^1-contraction:*

$$\|G(u) - G(v)\|_{L^1} \leq \|u - v\|_{L^1}.$$

- *TVD:*

$$TV(G(u)) \leq TV(u).$$

- *Solutions to monotone schemes satisfy all entropy conditions.*

Godunov's Theorem

Theorem (Godunov, see also Harten/Hyman/Lax/Keyfitz '76)

Monotone schemes are at most first-order accurate.

What now?

Maybe relax this condition? Maybe only ask for TVD?

Linear Schemes

Definition (Linear Schemes)

A scheme is called a linear scheme if it is linear when applied to a linear PDE:

$$u_t + au_x = 0,$$

where a is a constant.

Write the general case of a linear scheme for $u_t + u_x = 0$:

$$u_{j,\ell+1} = \sum_{k=-K}^{K} c_k(\lambda) u_{j-k,\ell},$$

where $c_k(\lambda)$ are constants which may depend on $\lambda = h_t/h_x$. Such a linear scheme is monotone iff $c_k(\lambda) \geq 0$ for all k.

Also called positive schemes.

Linear + TVD = ?

Theorem (TVD for linear Schemes)

For linear schemes, TVD $\Rightarrow$ monotone.

What does that mean?

Linear TVD schemes are at most first order accurate.

Now what?

Not all bad: Implies that *nonlinear* TVD schemes at least stand a chance.

Harten's Lemma

Theorem (Harten's Lemma)

If a scheme can be written as

$$\bar{u}_{j,\ell+1} = \bar{u}_{j,\ell} + \lambda(C_{j+1/2}\Delta_+\bar{u}_j - D_{j-1/2}\Delta_-\bar{u}_j)$$

with $C_{j+1/2} \geq 0$, $D_{j+1/2} \geq 0$, $1 - \lambda(C_{j+1/2} + D_{j+1/2}) \geq 0$ *and* $\lambda = h_t/h_x$, *then it is TVD.*

As a matter of notation, we have

$$\begin{aligned}\Delta_+ u_j &= u_{j+1} - u_j,\\ \Delta_- u_j &= u_j - u_{j-1}.\end{aligned}$$

We have omitted the time subscript for the time level ℓ.

Harten's Lemma: Proof

$$
\begin{aligned}
\Delta_+\bar{u}_{j,\ell+1} &= \Delta_+\bar{u}_{j,\ell} + \lambda\Delta_+\big(C_{j+1/2}\Delta_+\bar{u}_j - D_{j-1/2}\Delta_-\bar{u}_j\big)\\
&= \Delta_+\bar{u}_{j,\ell} + \lambda\big(C_{j+3/2}\Delta_+\bar{u}_{j+1} - D_{j+1/2}\underbrace{\Delta_+\bar{u}_j}_{=\Delta_-\bar{u}_{j+1}}\\
&\quad -C_{j+1/2}\Delta_+\bar{u}_j + D_{j-1/2}\Delta_-\bar{u}_j\big)\\
&= [1-\lambda(C_{j+1/2}+D_{j+1/2})]\Delta_+\bar{u}_j\\
&\quad +\lambda C_{j+3/2}\Delta_+\bar{u}_{j+1} + \lambda D_{j-1/2}\Delta_-\bar{u}_j.\\
|\Delta_+\bar{u}_{j,\ell+1}| &\overset{C,D,\cdots\geq 0}{\leq} [1-\lambda(C_{j+1/2}+D_{j+1/2})]|\Delta_+\bar{u}_j|\\
&\quad +\lambda\underbrace{C_{j+3/2}|\Delta+\bar{u}_{j+1}|}_{C_{j'+1/2}|\Delta_+\bar{u}_{j'}|}+\lambda\underbrace{D_{j-1/2}|\Delta_-\bar{u}_j|}_{D_{j''+1/2}|\Delta_+\bar{u}_{j''}|}.\\
\mathrm{TV}(\bar{u}_{\ell+1}) &= \sum_j|\Delta_+\bar{u}_{j,\ell+1}| \leq \sum_j\Big[1-\lambda(C_{j+1/2}+D_{j+1/2})\\
&\quad +\lambda C_{j+1/2}+\lambda D_{j+1/2}\Big]|\Delta_+\bar{u}_j| \leq \mathrm{TV}(u_\ell).
\end{aligned}
$$

Minmod Scheme

Still assume $f'(u) \geq 0$.

$$f^{*,(1)}_{j+1/2} = f\Big(\bar{u}_j + \underbrace{\frac{1}{2}(\bar{u}_{j+1} - \bar{u}_j)}_{\tilde{u}_j^{(1)}}\Big), \qquad f^{*,(2)}_{j+1/2} = f\Big(\bar{u}_j + \underbrace{\frac{1}{2}(\bar{u}_j - \bar{u}_{j-1})}_{\tilde{u}_j^{(2)}}\Big).$$

Design a 'safe' thing to use for $\tilde{u}$:

$$\operatorname{minmod}(a,b) := \begin{cases} a & |a| < |b|, ab > 0, \\ b & |b| < |a|, ab > 0, \\ 0 & ab \leq 0, \end{cases} \qquad \tilde{u}_j := \operatorname{minmod}(\tilde{u}_j^{(1)}, \tilde{u}_j^{(2)}).$$

Intuition: TV growth driven by local extrema
$\rightarrow$ if slopes have different signs, revert to first order.

Then consider $f^{*,(3)}_{j+1/2} = f(\bar{u}_j + \tilde{u}_j)$. Called a slope limiter.

Minmod is TVD

Show that Minmod is TVD:

Rewrite

$$\bar{u}_{j,\ell+1} = \bar{u}_j - \lambda[f(\bar{u}_j + \tilde{u}_j) - f(\bar{u}_{j-1} + \tilde{u}_{j-1})] = \bar{u}_j - \lambda[-D_{j-1/2}\Delta_-\bar{u}_j],$$

with

$$\begin{aligned} D_{j-1/2} &= \frac{f(\bar{u}_j + \tilde{u}_j) - f(\bar{u}_{j-1} + \tilde{u}_{j-1})}{\bar{u}_j - \bar{u}_{j-1}} = f'(\xi)\frac{\bar{u}_j - \bar{u}_{j-1} + \tilde{u}_j - \tilde{u}_{j-1}}{\bar{u}_j - \bar{u}_{j-1}} \\ &= \underbrace{f'(\xi)}_{\geq 0 (\text{by ass.})} \left[1 + \underbrace{\frac{\tilde{u}_j}{\bar{u}_j - \bar{u}_{j-1}}}_{0 \leq \cdot \leq \frac{1}{2}} - \underbrace{\frac{\tilde{u}_{j-1}}{\bar{u}_j - \bar{u}_{j-1}}}_{0 \leq \cdot \leq \frac{1}{2}} \right] \geq 0. \end{aligned}$$

Minmod: CFL restriction?

Derive a time step restriction for Minmod.

$$D_{j-1/2} \leq 3/2 f'(\xi) \leq \frac{3}{2} \max_u |f'(u)|.$$

Plugging this into the Harten CFL bound gives:

$$1 - \lambda D_{j-1/2} \geq 1 - \frac{3}{2} \lambda \max_u |f'(u)| \geq 0 \Leftarrow \boxed{\lambda \max_u |f'(u)| \leq \tfrac{2}{3}.}$$

What about Time Integration?

$$u^{(1)} = u_\ell + h_t L(u_\ell), \qquad u_{\ell+1} = \frac{u_\ell}{2} + \frac{1}{2}(u^{(1)} + h_t L(u^{(1)})).$$

Above: A version of RK2 with L the ODE RHS. Will this cause wrinkles?

- $\mathrm{TV}(\boldsymbol{u} + h_t L(\boldsymbol{u})) \le \mathrm{TV}(\boldsymbol{u})$ (via Harten's L.)
- TV convex. $TV(\alpha \boldsymbol{u} + (1-\alpha)\boldsymbol{v}) \le \alpha TV(\boldsymbol{u}) + (1-\alpha) TV(\boldsymbol{v})$

$$\begin{aligned}
\mathrm{TV}(u_{\ell+1}) &= \mathrm{TV}\left(\frac{u_\ell}{2} + \frac{1}{2}(u^{(1)} + h_t L(u^{(1)}))\right) \\
&\le \frac{1}{2}\mathrm{TV}(u_\ell) + \frac{1}{2}\mathrm{TV}(u^{(1)} + h_t L(u^{(1)})) \\
&\overset{\mathrm{TVD}}{\le} \frac{1}{2}\mathrm{TV}(u_\ell) + \frac{1}{2}\mathrm{TV}(u^{(1)}) \overset{\mathrm{TVD}}{\le} \frac{1}{2}\mathrm{TV}(u_\ell) + \frac{1}{2}\mathrm{TV}(u_\ell) = \mathrm{TV}(u_\ell).
\end{aligned}$$

General idea: time steppers out of convex comb. of Fw Euler.
(SSP / Strong-Stability Preserving Schemes) Above: SSPRK(2,2)

Total Variation is Convex

Show: $\mathrm{TV}(\cdot)$ is a convex functional.

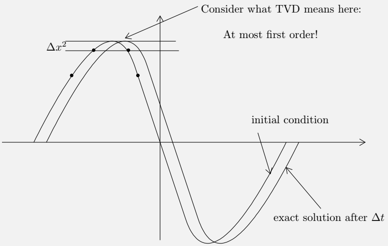
With $0 \le \alpha \le 1$:

$$
\begin{aligned}
& \mathrm{TV}(\alpha u + (1-\alpha) v) \\
\le\ & \sum_j |\alpha(u_j - u_{j-1}) + (1-\alpha)(v_j - v_{j-1})| \\
\le\ & \sum_j \alpha\,|u_j - u_{j-1}| + (1-\alpha)\,|v_j - v_{j-1}| \\
=\ & \alpha\,\mathrm{TV}(u) + (1-\alpha)\,\mathrm{TV}(v).
\end{aligned}
$$

TVD and High Order

Can TVD schemes be high order everywhere? (aside from near shocks)

Consider $u_t + u_x = 0$.



Clearly $f'(u) \neq 0$ near local max. (otherwise assume) Everything smooth: use derivatives. According to picture, $u_h - u = O(h^2)$. Plausibly, then $f(u_h)_x - f(u)_x = f'(u)(u - u_h)_x = O(h)$, yielding first-order accuracy. See also [Osher/Chakravarthy '84, Lemma 2.3].

High Order at Smooth Extrema

- TVB Schemes [Shu '87]
- ENO [Harten/Engquist/Osher/Chakravarthy '87]
  - Define $W_j = w(x_{j+1/2}) = \int_{x_{1/2}}^{x_{j+1/2}} u(\xi, t) d\xi = h_x \sum_{i=1}^{j} \bar{u}_i$
    - Observe $u_{j+1/2} = w'(x_{j+1/2})$.
    - Approximate by interpolation/numerical differentiation.
  - Start with the linear function $p^{(1)}$ through W_{j-1} and W_j
  - Compute divided differences on (W_{j-2}, W_{j-1}, W_j)
  - Compute divided differences on (W_{j-1}, W_j, W_{j+1})
  - Use the one with the smaller magnitude (of the divided differences) to extend $p^{(1)}$ to quadratic
  - (and so on, adding points on the side with the lowest magnitude of the divided differences)
- WENO [Liu/Osher/Chan '94]

Outline

Systems of Conservation Laws

Linear system of hyperbolic conservation laws, $A \in \mathbb{R}^{m \times m}$:

$$\begin{aligned} \boldsymbol{u}_t + A\boldsymbol{u}_x &= 0, \\ \boldsymbol{u}(x,0) &= \boldsymbol{u}_0(x). \end{aligned}$$

Assumptions on A?

System is hyperbolic [cf. Hogg '17] if A is diagonalizable with real eigenvalues.

Let $A\boldsymbol{r}_p = \lambda_p \boldsymbol{r}_p$ $(p = 1, \ldots, m)$. Called strictly hyperbolic if the eigenvalues are distinct. $AR = R\Lambda$.

Substitution $\boldsymbol{v} = R^{-1}\boldsymbol{u}$ attains $\boldsymbol{v}_t + \Lambda \boldsymbol{v}_x = 0$, called characteristic variables.

Recall: Rewrote wave equation in this form early on.

Linear System Solution

$$\boldsymbol{v} = R^{-1}\boldsymbol{u}, \qquad \boldsymbol{v}_t + \Lambda \boldsymbol{v}_x = 0.$$

Write down the solution.

$$u(x,t) = \sum_p \boldsymbol{r}_p v_p(x - \lambda_p t, 0),$$

where

$$\boldsymbol{v}(x,0) = R^{-1}\boldsymbol{u}(x,0).$$

What is the impact on boundary conditions? E.g. $(\lambda_p) = (-c, 0, c)$ for a BC at $x = 0$ for $[0,1]$?

Can only impose BCs on incoming waves! E.g. only one BC (on v_3) at $x = 0$.

Characteristics for Systems (1/2)

Consider system $\boldsymbol{u}_t + \boldsymbol{f}(\boldsymbol{u})_x = 0$. Write in quasilinear form:

$$\boldsymbol{u}_t + A(\boldsymbol{u})\boldsymbol{u}_x = 0 \qquad \text{with} \quad A(\boldsymbol{u}) = J_{\boldsymbol{f}}(\boldsymbol{u}).$$

When hyperbolic?

A diagonalizable w/real eigenvalues. "Strictly" hyperbolic for distinct eigenvalues. Both now local properties.

Characteristics for Systems (2/2)

What about characteristics/shock speeds?

- By considering eigenstates: can still define characteristics.
  m characteristics through each point.
- Characteristic locations no longer obey an ODE.

Are values of $\boldsymbol{u}$ still constant along characteristics?

No, only the coefficients of the eigenstates are constant along characteristics, and only locally.

Shocks and Riemann Problems for Systems

$$
\begin{aligned}
\boldsymbol{u}_t + A\boldsymbol{u}_x &= 0, \\
\boldsymbol{u}(x,0) &= \begin{cases} \boldsymbol{u}_l & x < 0, \\ \boldsymbol{u}_r & x > 0. \end{cases}
\end{aligned}
$$

Solution? (Assume strict hyperbolicity with $\lambda_1 < \lambda_2 < \cdots < \lambda_m$.)

$$
\boldsymbol{u}_l = \sum_{p=1}^{m} \alpha_p \boldsymbol{r}_p, \quad \boldsymbol{u}_r = \sum_{p=1}^{m} \beta_p \boldsymbol{r}_p. \qquad \text{Then} \quad v_p(x,0) = \begin{cases} \alpha_p & x < 0, \\ \beta_p & x > 0. \end{cases}
$$

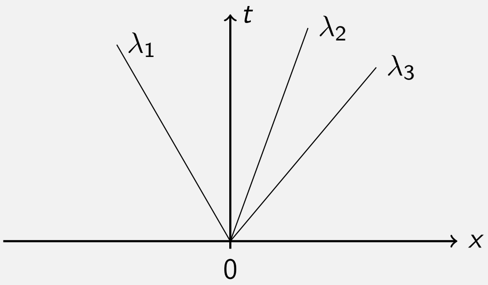
Let $P(x,t)$ be the maximum value of p for which $x - \lambda_p t > 0$, then

$$
\boldsymbol{u}(x,t) = \sum_{p=1}^{P(x,t)} \beta_p \boldsymbol{r}_p + \sum_{p=P(x,t)+1}^{m} \alpha_p \boldsymbol{r}_p.
$$

Shock Fans (1/2)

What does the solution look like?

Fan of values constant between each characteristic.



Jump across the characteristic associated with λ_p?

$$[\boldsymbol{u}] = (\beta_p - \alpha_p)\boldsymbol{r}_p.$$

Shock Fans (2/2)

Do those jumps satisfy Rankine-Hugoniot?

$$[\boldsymbol{f}] = A[\boldsymbol{u}] = (\beta_p - \alpha_p)A\boldsymbol{r}_p = \lambda_p[\boldsymbol{u}],$$

where λ_p is the propagation speed of the jump.

How can we find intermediate values of $\boldsymbol{u}$?

"Split up" the jump into a sum of jumps:

$$\boldsymbol{u}_r - \boldsymbol{u}_l = (\beta_1 - \alpha_1)\boldsymbol{r}_1 + \cdots + (\beta_m - \alpha_m)\boldsymbol{r}_m.$$

Use Rankine-Hugoniot as a constraint.
This works much the same way in the nonlinear case.

Two Dimensions

$u_t + f(u)_x + g(u)_y = 0$. Finite volume methods generalize in principle:

$$\frac{d\bar{u}_{ij}(t)}{\mathrm{dt}} + \frac{1}{h^2}\int_{y_{j-1/2}}^{y_{j+1/2}} f(u(x_{i+1/2}, y, t)) - f(u(x_{i-1/2}, y, t))dy$$
$$+ \frac{1}{h^2}\int_{x_{i-1/2}}^{x_{i+1/2}} g(u(x, y_{j+1/2}, t)) - g(u(x, y_{j-1/2}, t))dx$$

Downside: Stencil full ($n \times n$), not star-shaped (cf. FD)

However:

- If a method is TVD in two dimensions, it is at most first order accurate except in trivial cases. [Goodman/Leveque '85].
- The 'reconstruction' idea in complex geometry can become computationally expensive at high order.

Later: discontinuous Galerkin (DG) for high order with c. laws

Outline

Outline

Function Spaces

Consider

$$f_n(x) = \begin{cases} -1 & x \leq -\frac{1}{n}, \\ \frac{3n}{2}x - \frac{n^3}{2}x^3 & -\frac{1}{n} < x < \frac{1}{n}, \\ 1 & x \geq 1/n. \end{cases}$$

Converges to the step function. Problem?

f_n continuous, step function not. Want: limits that preserve smoothness properties. Limits defined by norms.

Norms

Definition (Norm)

A norm $\|\cdot\|$ maps an element of a *vector space* into $[0, \infty)$. It satisfies:

- $\|x\| = 0 \Leftrightarrow x = 0$
- $\|\lambda x\| = |\lambda| \|x\|$
- $\|x + y\| \leq \|x\| + \|y\|$ (triangle inequality)

Convergence

Definition (Convergent Sequence)

$x_n \to x :\Leftrightarrow \|x_n - x\| \to 0$ (convergence in norm)

Definition (Cauchy Sequence)

For all $\epsilon > 0$ there exists an n for which $\|x_\nu - x_\mu\| \leq \epsilon$ for $\mu, \nu \geq n$.

Banach Spaces

Definition (Complete/"Banach" space)

Cauchy $\Rightarrow$ Convergent

What's special about Cauchy sequences?

Limits appear out of thin air. Can be used to construct things.

Counterexamples?

- $\mathbb{Q}$ with absolute value
- C^0 with L^2 norm

More on C^0

Let $\Omega \subseteq \mathbb{R}^n$ be open. Is $C^0(\Omega)$ with $\|f\|_\infty := \sup_{x\in\Omega} |f(x)|$ Banach?

$f(x) = 1/x$ clearly satisfies $f \in C^0(\Omega)$, but its norm is unbounded, so $\|\cdot\|_\infty$ is not a norm on this space.

Is $C^0(\bar{\Omega})$ with $\|f\|_\infty := \sup_{x\in\Omega} |f(x)|$ Banach?

Assume $(f_i)_i$ is Cauchy.

- For each x, $(f_i(x))_i$ is Cauchy, so a pointwise limit exists. Call that f.
- Let $\varepsilon > 0$. There exists N so that $|f_n(x) - f_m(x)| < \varepsilon$ for all $n, m \geq N$ and $x \in \bar{\Omega}$. Taking the limit $m \to \infty$ yields $|f_n(x) - f(x)| < \varepsilon$, i.e. uniform convergence, forcing f to be continuous.

C^m Spaces

Let $\Omega \subseteq \mathbb{R}^n$.

Consider a multi-index $\boldsymbol{k} = (k_1, \ldots, k_n) \in \mathbb{N}_0^n$ and define the symbols

$$D^{\boldsymbol{k}} f = \frac{\partial^{|\boldsymbol{k}|}}{\partial x_1^{k_1} \cdots \partial x_n^{k_n}}, \qquad |\boldsymbol{k}| = k_1 + \cdots + k_n.$$

Definition (C^m Spaces)

$$C^m(\Omega) = \left\{ f \in C^0(\Omega) : D^{\boldsymbol{k}} f \in C^0 \text{ for all } \boldsymbol{k} \text{ with } |\boldsymbol{k}| \leq m \right\},$$

$$C^\infty(\Omega) = \left\{ f \in C^0(\Omega) : D^{\boldsymbol{k}} f \in C^0(\Omega) \text{ for all } \boldsymbol{k} \right\},$$

$$C_0^m(\Omega) = \{ f \in C^m(\Omega) : f \text{ has compact support} \},$$

where compact support means that there is a compact (closed and bounded) set $S \subset \Omega$ for which $f(x) = 0$ if $x \notin S$.

L^p Spaces

Let $1 \leq p < \infty$.

Definition (L^p Spaces)

$$L^p(\Omega) := \left\{ u : (u : \mathbb{R} \to \mathbb{R}) \text{ measurable}, \int_\Omega |u|^p \, dx < \infty \right\},$$

$$\|u\|_p := \left(\int_\Omega |u|^p \, dx \right)^{1/p}.$$

Definition (L^∞ Space)

$$L^\infty(\Omega) := \left\{ u : (u : \mathbb{R} \to \mathbb{R}), |u(x)| < \infty \text{ almost everywhere} \right\},$$

$$\|u\|_\infty = \inf \left\{ C : |u(x)| \leq C \text{ almost everywhere} \right\}.$$

L^p Spaces: Properties

Theorem (Hölder's Inequality)

For $1 \leq p, q \leq \infty$ *with* $1/p + 1/q = 1$ *and measurable* u *and* v,

$$\|uv\|_1 \leq \|u\|_p \|v\|_q .$$

Theorem (Minkowski's Inequality (Triangle inequality in L^p))

For $1 \leq p \leq \infty$ *and* $u, v \in L^p(\Omega)$,

$$\|u + v\|_p \leq \|u\|_p + \|v\|_p .$$

Inner Product Spaces

Let V be a vector space.

Definition (Inner Product)

An inner product is a function $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ such that for any $f, g, h \in V$ and $\alpha \in \mathbb{R}$

$$\begin{aligned} \langle f, f \rangle &\geq 0, \\ \langle f, f \rangle &= 0 \Leftrightarrow f = 0, \\ \langle f, g \rangle &= \langle f, g \rangle, \\ \langle \alpha f + g, h \rangle &= \alpha \langle f, h \rangle + \langle g, h \rangle. \end{aligned}$$

Definition (Induced Norm)

$$\|f\| = \sqrt{\langle f, f \rangle}.$$

Hilbert Spaces

Definition (Hilbert Space)

An inner product space that is complete under the induced norm.

Let Ω be open.

Theorem (L^2)

$L^2(\Omega)$ equals the closure of (set of all limits of Cauchy sequences in) $C_0^\infty(\Omega)$ under the induced norm $\|\cdot\|_2$.

Theorem (Hilbert Projection (e.g. Yosida '95, Thm. III.1))

Let $M \subseteq V$ be a closed subspace of a Hilbert space V. For any $u \in V$ there exists a unique $v \in M$ such that $u = v + w$ with $w \in M^\perp$.

Weak Derivatives

Define the space L^1_{loc} of locally integrable functions.

$$L^1_{\text{loc}}(\Omega) = \Big\{ u : (u : \mathbb{R} \to \mathbb{R}) \text{ measurable}, \\ \int_\Omega |u(x)\varphi(x)|\, dx < \infty \text{ for every } \varphi \in C_0^\infty(\Omega) \Big\}$$

Definition (Weak Derivative)

$v \in L^1_{\text{loc}}(\Omega)$ is the weak partial derivative of $u \in L^1_{\text{loc}}(\Omega)$ of multi-index order $\boldsymbol{k}$ if

$$\int_\Omega v\varphi dx = (-1)^{|\boldsymbol{k}|} \int_\Omega u D^{\boldsymbol{k}} \varphi dx \qquad \text{for all } \varphi \in C_0^\infty(\Omega).$$

In this case, $D^{\boldsymbol{k}}_w u := v$.

Weak Derivatives: Examples (1/2)

Consider all these on the interval $[-1, 1]$.

$$f_1(x) = 4(1 - x)x$$

$D_w f_1(x) = 4 - 8x$. For ("strongly") differentiable functions, weak and strong derivatives coincide.

$$f_2(x) = \begin{cases} 2x & x \leq 1/2, \\ 2 - 2x & x > 1/2. \end{cases}$$

"Kinks" in the function are allowed (but jumps are not):

$$D_w f_2(x) = \begin{cases} 2 & x \leq 1/2, \\ -2 & x > 1/2. \end{cases}$$

Weak Derivatives: Examples (2/2)

$$f_3(x) = \sqrt{\frac{1}{2}} - \sqrt{|x - 1/2|}$$

Even cusps are allowed:

$$D_w f_3(x) = \begin{cases} \frac{1}{2\sqrt{1/2 - x}} & x < 1/2, \\ -\frac{1}{2\sqrt{x - 1/2}} & x > 1/2. \end{cases}$$

Sobolev Spaces

Let $\Omega \subset \mathbb{R}^n$, $k \in \mathbb{N}_0$ and $1 \leq p < \infty$.

Definition ((k, p)-Sobolev Norm/Space)

$$\|u\|_{k,p} := \sqrt[p]{\sum_{|\boldsymbol{\alpha}| \leq k} \|D_w^{\boldsymbol{\alpha}} u\|_p^p},$$

$$|u|_{k,p} := \sqrt[p]{\sum_{|\boldsymbol{\alpha}| = k} \|D_w^{\boldsymbol{\alpha}} u\|_p^p}.$$

$$W^{k,p}(\Omega) := \left\{ u : (u : \Omega \to \mathbb{R}), \|u\|_{k,p} < \infty \right\}.$$

More Sobolev Spaces

$W^{0,2}$?

Equal to L^2.

$W^{s,2}$?

Also called H^s, a Hilbert space, with an induced norm. From what scalar product?

$H_0^1(\Omega)$?

Closure of the space $C_0^\infty(\Omega)$ under $\|u\|_{k,p}$.
The Sobolev way of saying zero on the boundary.

Outline

An Elliptic Model Problem

Let $\Omega \subset \mathbb{R}^n$ open, bounded, $f \in H^1(\Omega)$.

$$\begin{aligned} -\nabla \cdot \nabla u + u &= f(x) \quad (x \in \Omega), \\ u(x) &= 0 \qquad (x \in \partial\Omega). \end{aligned}$$

Let $V := H_0^1(\Omega)$. Integration by parts? (Gauss's theorem applied to $a\boldsymbol{b}$):

$$\int_\Omega \nabla a \cdot \boldsymbol{b} + \int_\Omega a \nabla \cdot \boldsymbol{b} = \int_\Omega \nabla \cdot (a\boldsymbol{b}) = \int_{\partial\Omega} \hat{\boldsymbol{n}} \cdot (a\boldsymbol{b}).$$

Weak form?

Multiply by test function $v \in V$, integrate by parts:

$$\int_\Omega \nabla u \cdot \nabla v - \underbrace{\int_{\partial\Omega} \hat{n} \cdot (v \nabla u)}_{=0\ (v \in H_0^1)} + \int_\Omega uv = \int_\Omega fv.$$

Motivation: Bilinear Forms and Functionals

$$\int_\Omega \nabla u \cdot \nabla v + \int_\Omega uv = \int fv.$$

This is the weak form of the strong-form problem. The task is to find a $u \in V$ that satisfies this for all test functions $v \in V$.

Recast this in terms of bilinear forms and functionals:

$$\begin{aligned} a(u, v) &= \langle \nabla u, \nabla v \rangle + \langle u, v \rangle, \\ g(v) &= \langle f, v \rangle, \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the L^2 inner product. Then the weak form is equivalent to

$$a(u, v) = f(v) \qquad \text{for all } v \in V.$$

This motivates further study of Hilbert spaces and objects in them.

Dual Spaces and Functionals

Bounded Linear Functional

Let $(V, \|\cdot\|)$ be a Banach space. A linear functional is a linear function $g : V \to \mathbb{R}$. It is bounded ($\Leftrightarrow$ continuous) if there exists a constant C so that $|g(v)| \leq C \|v\|$ for all $v \in V$.

Dual Space

Let $(V, \|\cdot\|)$ be a Banach space. Then the dual space V' is the space of bounded linear functionals on V.

Dual Space is Banach (cf. e.g. Yosida '95 Thm. IV.7.1)

V' is a Banach space with the dual norm

$$\|g\|_{V'} = \sup_{v \in V \setminus \{0\}} \frac{|g(v)|}{\|v\|_V}.$$

Functionals in the Model Problem

Is g from the model problem a bounded functional? (In what space?)

Must use same space as rest of problem: $H^1(\Omega)$.

$$\|g\|_{V'} = \sup_{v \in H^1 \setminus \{0\}} \frac{|\langle f, v\rangle_{L^2}|}{\|v\|_{H^1}} \le \frac{\|f\|_{L^2}\|v\|_{L^2}}{\|v\|_{L^2} + \|D_w v\|_{L^2}} \le \frac{\|f\|_{L^2}\|v\|_{L^2}}{\|v\|_{L^2}} = \|f\|_{L^2}$$

using Cauchy-Schwarz. Find: $f \in L^2$ leads to bounded g in H^1.

That bound felt loose and wasteful. Can we do better?

Define negative-index Sobolev norms:

$$\|f\|_{H^{-1}} = \sup_{v \in H^1(\Omega) \setminus \{0\}} \frac{|\langle f, v\rangle_{L^2}|}{\|v\|_{H^1}}.$$

Bound (by definition) $|g(v)| \le \|f\|_{H^{-1}}\|v\|_{H^1}$. Allows $f \in H^{-1}$.

Riesz Representation Theorem (1/3)

Let V be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$.

Theorem (Riesz)

Let g be a bounded linear functional on V, i.e. $g \in V'$. Then there exists a unique $u \in V$ so that $g(v) = \langle u, v \rangle$ for all $v \in V$.

Let $g \in V'$. $N(\cdot)$ below represents the nullspace.
Case 1. $N(g) = V$. $u = 0$ works, unique by scalar product axioms.
Case 2. $N(g) \neq V$. Let $w \in N(g)^\perp \setminus \{0\}$. Let $\alpha = g(w) \neq 0$.

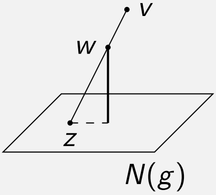
$$g\left(\frac{g(v)}{\alpha} w\right) = \frac{g(v)}{\alpha} g(w) = g(v) \qquad \text{for all } v \in V.$$

Let $v \in V$ be arbitrary, and let $z := v - (g(v)/\alpha)w$. (Feel reminded of Gram-Schmidt?) Then $g(z) = g(v) - g(v) = 0$, i.e. $z \in N(g)$, i.e. $\langle z, w \rangle_V = 0$ since $w \in N(g)^\perp$.

Riesz Representation Theorem: Proof (2/3)

Have $w \in N(g)^\perp \setminus \{0\}$, $\alpha = g(w) \neq 0$, and $z := v - (g(v)/\alpha)w \perp w$.

$$0 = \left\langle v - \frac{g(v)}{\alpha} w, w \right\rangle \quad \Leftrightarrow \quad \left\langle \frac{g(v)}{\alpha} w, w \right\rangle = \langle v, w \rangle \qquad \text{for all } v \in V.$$



Multiplying by $\alpha / \langle w, w \rangle$ yields

$$g(v) = \left\langle v, \underbrace{\frac{\overbrace{g(w)}^{=\alpha}}{\langle w, w \rangle_V} w}_{u:=} \right\rangle .$$

Riesz Representation Theorem: Proof (3/3)

Uniqueness of u?

Suppose we have two: u and $\hat{u}$ so that

$$g(v) = \langle u, v \rangle = \langle \hat{u}, v \rangle \quad \Rightarrow \quad \langle u - \hat{u}, v \rangle = 0 \quad \text{for all } v \in V,$$

Plugging in $v = u - \hat{u}$ yields $u - \hat{u} = 0$ by the properties of the inner product.

Back to the Model Problem

$$\begin{aligned} a(u,v) &= \langle \nabla u, \nabla v \rangle_{L^2} + \langle u, v \rangle_{L^2} \\ g(v) &= \langle f, v \rangle_{L^2} \\ a(u,v) &= g(v) \end{aligned}$$

Have we learned anything about the solvability of this problem?

In this particular case, observe that $a(u,v) = \langle u, v \rangle_{H^1}$. By the Riesz Representation theorem and knowing that g is a bounded linear functional in H^1, we know that there exists a unique u so that

$$a(u,v) = \langle u, v \rangle_{H^1} = g(v).$$

Poisson

Let $\Omega \subset \mathbb{R}^n$ open, bounded, $f \in H^{-1}(\Omega)$.

$$\begin{aligned} -\nabla \cdot \nabla u &= f(x) \quad (x \in \Omega), \\ u(x) &= 0 \qquad (x \in \partial\Omega). \end{aligned}$$

This is called the Poisson problem (with Dirichlet BCs).

Weak form?

$$\underbrace{\int_\Omega \nabla u \cdot \nabla v dx}_{a(u,v)} = \underbrace{\int_\Omega f(x) v(x) dx}_{g(v)} \quad \text{for all } v \in V.$$

We know that g is a bounded linear functional in H_0^1, but $a(u, v)$ is no longer identical to our inner product. Maybe we can come up with some conditions that make a 'sufficiently similar' to an inner product?

Ellipticity

Let V be Hilbert space.

V-Ellipticity

A bilinear form $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ is called coercive if there exists a constant $c_0 > 0$ so that

$$\boxed{c_0 \left\| u \right\|_V^2 \leq a(u,u) \quad \text{for all } u \in V,}$$

and a is called continuous if there exists a constant $c_1 > 0$ so that

$$\boxed{|a(u,v)| \leq c_1 \left\| u \right\|_V \left\| v \right\|_V \quad \text{for all } u, v \in V.}$$

If a is both coercive and continuous on V, then a is said to be V-elliptic.

Lax-Milgram Theorem

Let V be Hilbert space with inner product $\langle \cdot, \cdot \rangle$.

Lax-Milgram, Symmetric Case

Let a be a V-elliptic bilinear form that is also symmetric, and let g be a bounded linear functional on V.
Then there exists a unique $u \in V$ so that $a(u, v) = g(v)$ for all $v \in V$.

a defines an inner product $\langle u, v \rangle_a = a(u, v)$ on V, with linearity and symmetry trivial, and:

- Show $a(u, u) \geq 0$.
  $a(u, u) \geq c_0 \|u\|_V^2 \geq 0$ by coercivity,
- Show $a(u, u) = 0 \Rightarrow u = 0$.
  $0 = a(u, u) \geq c_0 \|u\|_V^2 \geq 0$, i.e. $\|u\|_V = 0$, i.e. $u = 0$.

From the Riesz representation theorem, there exists a unique $u \in V$ so that $a(u, v) = \langle u, v \rangle_a = g(v)$.

Back to Poisson

Can we declare victory for Poisson?

Continuity of a holds:

$$\left|\int_\Omega \nabla u \cdot \nabla v dx\right| = |\langle \nabla u, \nabla v\rangle_{L^2}| \leq \|\nabla u\|_{L^2} \|\nabla v\|_{L^2} \leq \|u\|_{H^1} \|v\|_{H^1} .$$

However coercivity is less clear:

$$\int_\Omega \nabla u \cdot \nabla u dx \overset{?}{\geq} c_1 \left(\int_\Omega \nabla u \cdot \nabla u dx + \int_\Omega u^2 dx\right) .$$

Can this inequality hold in general, without further assumptions?

No: a constant would violate it.

Poincaré-Friedrichs Inequality (1/3)

Theorem (Poincaré-Friedrichs Inequality)

Suppose $\Omega \subset \mathbb{R}^n$ is bounded and $u \in H_0^1(\Omega)$. Then there exists a constant $C > 0$ such that

$$\|u\|_{L^2} \leq C \|\nabla u\|_{L^2} .$$

Outline: Helpful identity, result in $C_0^\infty(\Omega)$, result in $H_0^1(\Omega)$.

A helpful identity. For $u \in C_0^\infty(\Omega)$,

$$\begin{aligned} \nabla \cdot (u^2 \boldsymbol{x}) &= \partial_{x_1}(u^2 x_1) + \cdots + \partial_{x_n}(u^2 x_n) \\ &= u^2 + 2(u\partial_{x_1} u)x_1 + \cdots + u^2 + 2(u\partial_{x_n} u)x_n \\ &= nu^2 + 2u(\nabla u \cdot \boldsymbol{x}). \\ \Rightarrow \quad u^2 &= \frac{1}{n}\nabla \cdot (u^2 \boldsymbol{x}) - \frac{2}{n} u(\nabla u \cdot \boldsymbol{x}). \end{aligned}$$

Poincaré-Friedrichs Inequality (2/3)

Prove the result in $C_0^\infty(\Omega)$.

$$
\begin{aligned}
\|u\|_{L^2}^2 &= \int_\Omega u^2 d\boldsymbol{x} = \int_\Omega \frac{1}{n}\nabla\cdot(u^2\boldsymbol{x}) - \frac{2}{n}u(\nabla u\cdot\boldsymbol{x})d\boldsymbol{x} \\
&= \frac{1}{n}\int_{\partial\Omega} \underbrace{\hat{\boldsymbol{n}}\cdot(u^2\boldsymbol{x})}_{0} ds_{\boldsymbol{x}} - \frac{2}{n}\int_\Omega u(\nabla u\cdot\boldsymbol{x})d\boldsymbol{x} \\
&\leq \frac{2}{n}\max_{\boldsymbol{x}\in\Omega}|\boldsymbol{x}|\int_\Omega |u\nabla u|\, d\boldsymbol{x} \leq \frac{2}{n}\max_{\boldsymbol{x}\in\Omega}|\boldsymbol{x}|\,\|u\|_{L^2}\,\|\nabla u\|_{L^2} \\
\Rightarrow \|u\|_{L^2} &\leq \underbrace{\frac{2}{n}\max_{\boldsymbol{x}\in\Omega}|\boldsymbol{x}|}_{C}\,\|\nabla u\|_{L^2}\,.
\end{aligned}
$$

Poincaré-Friedrichs Inequality (3/3)

Prove the result in $H_0^1(\Omega)$.

Let $u \in H_0^1(\Omega)$. Since $C_0^\infty(\Omega)$ is dense in $H_0^1(\Omega)$, let $(u_k) \subset C_0^\infty$. Then the inequality holds for each u_k, and $\|u_k\|_{L^2} \to \|u\|_{L^2}$ and $\|\nabla u_k\|_{L^2} \to \|\nabla u\|_{L^2}$.

Back to Poisson, Again

Show that the Poisson bilinear form is coercive.

$$\frac{1}{C^2+1}\|u\|_{H^1(\Omega)}^2 = \frac{1}{C^2+1}\left(\|u\|_{L^2(\Omega)}^2 + \|\nabla u\|_{L^2}^2\right) \le \|\nabla u\|_{L^2}^2 = a(u,u).$$

Draw a conclusion on Poisson:

Because of coercivity and continuity of a, the Poisson weak form admits a unique solution in $H_0^1(\Omega)$.

Outline

Ritz-Galerkin

Some key goals for this section:

- How do we use the weak form to compute an approximate solution?
- What can we know about the accuracy of the approximate solution?

Can we pick one underlying principle for the construction of the approximation?

Considered: Weak form $a(u, v) = g(v)$ for all $v \in V \subseteq H$, where H is a Hilbert space. (Think of V as H_0^1 for example.)
Idea: Choose a finite-dimensional subspace $V_h \subset V$, find a solution $u_h \in V_h$ to the weak-form problem

$$a(u_h, v_h) = g(v_h) \qquad \text{for all } v_h \in V_h.$$

This is called Ritz-Galerkin approximation.

Galerkin Orthogonality

$$a(u,v) = g(v) \qquad \text{for all } v \in V, a(u_h, v_h) \quad = g(v_h) \qquad \text{for all } v_h \in V_h.$$

Observations?

Observe that the 'continuous' weak form also allows v_h to be plugged in:

$$a(u, v_h) = g(v_h) \qquad \text{for all } v_h \in V_h.$$

Subtracting the two leads to Galerkin Orthgonality:

$$a(u_h - u, v_h) = 0 \qquad \text{for all } v_h \in V_h,$$

i.e. using $a(\cdot,\cdot)$ as a (sort of) inner product, the error $u - u_h$ is orthogonal to the space of test functions.

Céa's Lemma

Let $V \subset H$ be a closed subspace of a Hilbert space H.

Céa's Lemma

Let $a(\cdot, \cdot)$ be a coercive and continuous bilinear form on V. In addition, for a bounded linear functional g on V, let $u \in V$ satisfy

$$a(u, v) = g(v) \qquad \text{for all } v \in V.$$

Consider the finite-dimensional subspace $V_h \subset V$ and $u_h \in V_h$ that satisfies

$$a(u_h, v_h) = g(v_h) \qquad \text{for all } v_h \in V_h.$$

Then

$$\boxed{\|u - u_h\|_V \leq \frac{c_1}{c_0} \inf_{v_h \in V_h} \|u - v_h\|_V .}$$

Céa's Lemma: Proof

Recall Galerkin orthgonality: $a(u_h - u, v_h) = 0$ for all $v_h \in V_h$. Show the result.

For any $v_h \in V_h$,

$$
\begin{aligned}
c_0 \|u - u_h\|_V^2 &\le a(u - u_h, u - u_h) \qquad \text{(coercivity)} \\
&= a(u - u_h, u - v_h) + a(u - u_h, v_h - u_h) \\
&= a(u - u_h, u - v_h) \qquad \text{(Galerkin orth.)} \\
&\le c_1 \|u - u_h\|_V \|u - v_h\|_V .
\end{aligned}
$$

Dividing by $\|u - u_h\|_V$ completes the proof.

Elliptic Regularity

Definition (H^s Regularity)

Let $m \geq 1$, $H_0^m(\Omega) \subseteq V \subseteq H^m(\Omega)$ and $a(\cdot,\cdot)$ a V-elliptic bilinear form. The bilinear form $a(u,v) = \langle f, v \rangle$ for all $v \in V$ is called H^s regular, if for every $f \in H^{s-2m}$ there exists a solution $u \in H^s(\Omega)$ and we have with a constant $C(\Omega, a, s)$,

$$\|u\|_{H^s} \leq C(\Omega, a, s) \, \|f\|_{H^{s-2m}} .$$

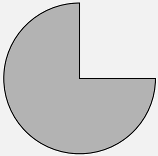
Theorem (Elliptic Regularity (cf. Braess Thm. 7.2))

Let a be a H_0^1-elliptic bilinear form with sufficiently smooth coefficient functions.

- *If Ω is convex, then then Dirichlet problem is H^2 regular.*
- *Let $s \geq 2$. If $\partial\Omega$ is C^s, the Dirichlet problem is H^s regular.*

Elliptic Regularity: Counterexamples

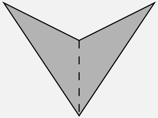
Are the conditions on the boundary essential for elliptic regularity?



Consider $\triangle u = 0$, $u(e^{i\phi}) = \sin(2/3\phi)$, $u = 0$ elsewhere.

- $u(z) = \mathrm{Im}(z^{2/3})$ with $z = x + iy \in \mathbb{C}$.
- Derivative: $(2/3)z^{-1/3}$: unbounded $\Rightarrow$ $u \notin H^2$!

Are there any particular concerns for mixed boundary conditions?



Homogeneous Neumann on dashed line with (e.g.) left half, Dirichlet elsewhere.

- Solution could be found by solving on whole domain using reflected Dirichlet BCs.
- Reentrant corner $\Rightarrow$ $u \notin H^2$ (in gen.)

Estimating the Error in the Energy Norm

Come up with an idea of a bound on $\|u - u_h\|_{H^1}$.

$$\|u - u_h\|_{H^1} \underset{\text{Céa}}{\leq} C \inf_{v_h \in V_h} \|u - v_h\|_{H^1} \leq C \|u - I_h u\|_{H^1}$$
$$\underset{\text{TBD}}{\leq} C_1 h \|u\|_{H^2} \underset{H^2 \text{ reg.}}{\leq} c_2 h \|f\|_{L^2}.$$

What's still to do?

- we still need to figure out what V_h will be,
- I_h is some interpolation operator that we will define more precisely later, and
- we need to worry about the interpolation error bound ("TBD")
- Finally, H^1 is kind of a weird norm. Can we get an error estimate in L^2?

L^2 Estimates

Let H be a Hilbert space with the norm $\|\cdot\|_H$ and the inner product $\langle \cdot, \cdot \rangle$.
(Think: $H = L^2$, $V = H^1$.)

Theorem (Aubin-Nitsche)

Let $V \subseteq H$ be a subspace that becomes a Hilbert space under the norm $\|\cdot\|_V$. Let the embedding $V \to H$ be continuous. Then we have for the finite element solution $u \in V_h \subset V$:

$$\|u - u_h\|_H \leq c_1 \|u - u_h\|_V \sup_{g \in H} \left[\frac{1}{\|g\|_H} \inf_{v_h \in V_h} \|\varphi_g - v_h\|_V \right],$$

if with every $g \in H$ we associate the unique (weak) solution φ_g of the equation (also called the dual problem)

$$a(w, \varphi_g) = \langle g, w \rangle \quad \text{for all } w \in V,$$

Aubin-Nitsche: Proof

The norm of an element in a Hilbert space can be determined via the scalar product: $\|w\|_H = \sup_{g \in H} \langle g, w \rangle \, / \, \|g\|_H$.

$$
\begin{aligned}
\langle g, u - u_h \rangle \quad & \underset{\text{Def. } \varphi_g}{=} \quad a(u - u_h, \varphi_g) \underset{\text{Galerkin orth.}}{=} a(u - u_h, \varphi_g - v_h) \\
& \underset{\text{cont. } a}{\leq} \quad c_1 \|u - u_h\|_V \, \|\varphi_g - v_h\|_V \, .
\end{aligned}
$$

Since this argument is valid for any $v_h \in V_h$, we obtain

$$
\langle g, u - u_h \rangle \leq c_1 \|u - u_h\|_V \inf_{v_h \in V_h} \|\varphi_g - v_h\|_V \, .
$$

Plugging into the norm relationship yields

$$
\|u - u_h\|_H = \sup_{g \in H} \frac{\langle g, w \rangle}{\|g\|_H} \leq c_1 \|u - u_h\|_V \sup_{g \in H} \left[\frac{1}{\|g\|_H} \inf_{v_h \in V_h} \|\varphi_g - v_h\|_V \right] .
$$

L^2 Estimates using Aubin-Nitsche

$$\|u - u_h\|_H \leq c_1 \|u - u_h\|_V \sup_{g \in H} \left[\frac{1}{\|g\|_H} \inf_{v_h \in V_h} \|\varphi_g - v_h\|_V \right],$$

If $u \in H_0^1(\Omega)$, what do we get from Aubin-Nitsche?

E.g. Poisson+$u \in H_0^1$: symmetry of a: primal prob. = dual prob.:

$$\inf_{v_h \in V_h} \|\varphi_g - v_h\|_{H^1} \leq C \|\varphi_g - I_h \varphi_g\|_{H^1} \leq C_1 h \|\varphi_g\|_{H^2} \leq c_2 h \|g\|_{L^2},$$

i.e. same bounds as before. So $\|u - u_h\|_{L^2} \leq Ch \|u - u_h\|_{H^1}$.

So does Aubin-Nitsche give us an L^2 estimate?

Had (aside from missing pieces): $\|u - u_h\|_{H^1} \leq c_2 h \|f\|_{L^2}$.
If we have $f \in L^2(\Omega)$ and hence $u \in H^2(\Omega)$ (H^2 regularity), then

$$\|u - u_h\| \leq C h^2 \|f\|$$

Outline

Finite Elements in 1D: Discrete Form

$\Omega := [\alpha, \beta]$. Look for $u \in H_0^1(\Omega)$, so that $a(u, \varphi) = \langle f, \varphi \rangle$ for all $\varphi \in H_0^1(\Omega)$. Choose $V_h = \operatorname{span}\{\varphi_1, \ldots, \varphi_n\}$ and expand $u_h = \sum_{i=1}^n u_h^i \varphi_i \in V_h$. Find the discrete system.

$$a\left(\sum_{i=1}^{n} u_h^i \varphi_i, \varphi\right) = \langle f, \varphi \rangle \quad \text{for all } \varphi \in V_h,$$

We may as well choose the basis (φ_i) to represent $\varphi \in V_h$:

$$a\left(\sum_{i=1}^{n} u_h^i \varphi_i, \varphi_j\right) = \langle f, \varphi_j \rangle \quad \text{for all } j \in \{1, \ldots, n\}.$$

This *could* lead to a linear system $A\boldsymbol{u} = \boldsymbol{b}$, where $A = \{a_{i,j}\} \in \mathbb{R}^{n \times n}$ with $a_{i,j} = a(\varphi_i, \varphi_j)$, $u = \{u_h^i\}$, $b_j = \langle f, \varphi_j \rangle$, but we choose not to go this route.

Grids and Hats

Let $I_i := [\alpha_i, \beta_i]$, so that $\bar{\Omega} = \bigcup_{i=0}^N I_i$ and $I_i^\circ \cap I_j = \emptyset$ for $i \neq j$. Consider a grid

$$\alpha = x_0 < \cdots < x_N < x_{N+1} = \beta,$$

i.e. $\alpha_i = x_i$, $\beta_i = x_{i+1}$ for $i \in \{0, \ldots, N\}$. The $\{x_i\}$ are called nodes of the grid. $h_i := x_{i+1} - x_i$ for $i \in \{0, \ldots, N\}$ and $h := \max_i h_i$. V_h? Basis?

$$P_h^1 := \{v_h \in C^0(\bar{\Omega}) : \text{for all } i \in \{0, \ldots, N\}, v_h|_{I_i} \in \mathbb{P}_1\}.$$

For $i \in \{0, \ldots, N+1\}$, let

$$\varphi_i(x) := \begin{cases} \frac{1}{h_{i-1}}(x - x_{i-1}) & x \in I_{i-1}, \\ \frac{1}{h_i}(x_{i+1} - x) & x \in I_i, \\ 0 & \text{otherwise} \end{cases} \quad \in P_h^1.$$

Observe: The set $\{\varphi_i\}_i$ forms a basis of P_h^1.

Degrees of Freedom and Matrices

Define something more general than basis coefficients to solve for.

- For $i \in \{0, \ldots, N+1\}$, let $\gamma_i : C(\bar{\Omega}) \to \mathbb{R}$.
  Here: $v \mapsto \gamma_i(v) := v(x_i) \in \mathbb{R}$.
  Generally: could be derivatives etc. (cf. splines).
- $\{\gamma_i\}_{i=0}^{N+1}$ are global degrees of freedom in P_h^1.
- $\{\gamma_i\}_{i=0}^{N+1}$ forms a basis of the dual space $(P_h^1)'$.
  (i.e. uniquely determine $\varphi \in V_h$, global unisolvence)

Define shape functions and assemble the stiffness matrix:

Shape functions $\hat{\varphi} \in V_h$ satisfy $\gamma_j(\hat{\varphi}_i) = \delta_{i,j}$ for $i, j \in \{0, \ldots, N+1\}$.

$$a(u_h, \hat{\varphi}_i) = \langle f, \varphi_i \rangle \Leftrightarrow \sum_{j=1}^{N} \underbrace{\gamma_j(u_h)}_{=u_h^i} \underbrace{a(\hat{\varphi}_j, \hat{\varphi}_i)}_{(A_h)_{i,j}} = \underbrace{\langle f, \varphi_i \rangle}_{(\boldsymbol{b}_h)_i} (j = 1, \ldots, N)$$

A Matrix Property for Efficiency

$$(A_h)_{i,j} = a(\hat{\varphi}_j, \hat{\varphi}_i).$$

Anything special about the matrix?

Only $a_{i,i}, a_{i,i+1}, a_{i,i-1} \neq 0$ in the ith row of A is nonzero. Sparse.

Error Estimation

According to Céa, what's our main missing piece in error estimation now?

An interpolation operator

$$\begin{aligned} I_h^1 : C^0(\bar{\Omega}) &\to P_h^1, \\ v &\mapsto \sum_{i=0}^{N+1} \gamma_i(v)\hat{\varphi}_i \in P_h^1. \end{aligned}$$

Next: need to estimate its accuracy.

Interpolation Error (1D-only)

For $v \in H^2(\Omega)$,

$$\begin{aligned} \left\| v - I_h^1 v \right\|_{L^2} &\leq h^2 \left| v \right|_{H^2} \quad \text{for all } h > 0, \\ \left| (v - I_h^1 v) \right|_{H^1} &\leq h \left| v \right|_{H^2} \quad \text{for all } h > 0. \end{aligned}$$

If $v \in H^1(\Omega) \setminus H^2(\Omega)$,

$$\begin{aligned} \left\| v - I_h^1 v \right\|_{L^2} &\leq h \left| v \right|_{H^1} \quad \text{for all } h > 0, \\ \lim_{h \to 0} \left| (v - I_h^1 v) \right|_{H^1} &= 0. \end{aligned}$$

In general (not just 1D), is I_h^1 defined for $v \in H^2$? for $v \in H^1 \setminus H^2$?

Depends on the dimension n and the domain Ω. Need to consider the Sobolev Embedding Theorem.

Interpolation Error: Towards an Estimate

Provide an a-priori estimate.

$$\left\| u - u_h \right\|_{H^1} \le \frac{c_1}{c_0} \inf_{v_h \in P_h^1} \left\| u - v_h \right\|_{H^1} \le \frac{c_1}{c_0} \left\| u - I_h^1 u \right\|_{H^1} \le \frac{c_1}{c_0} h \left| u \right|_{H^2} .$$

What's the relationship between $I_h^1 u$ and u_h?

None!

Local-to-Global

Is there a simple way of constructing the polynomial basis?

The basis functions $\{\varphi_i\}_{i=1}^N$ can be viewed as a composition of

- grid-independent reference basis functions on a reference element, and
- geometric transformations from the reference element to the grid.

Local-to-Global: Math

Construct a polynomial basis using this approach.

Let $\hat{\kappa} = [0,1]$ be the reference interval and consider the affine transformations $T_I : \hat{x} \in \hat{\kappa} \mapsto x = x_i + \hat{x} h_i$ for $i \in \{0, \dots, N\}$. Define the shape functions

$$\begin{aligned} \hat{\varphi}_0(\hat{x}) &:= 1 - \hat{x} \quad \text{for all } \hat{x} \in \hat{\kappa}, \\ \hat{\varphi}_1(\hat{x}) &:= \hat{x} \quad \text{for all } \hat{x} \in \kappa. \end{aligned}$$

These functions form a basis of $P_1(\hat{\kappa})$. Then

$$\varphi_i(x) = \begin{cases} (\hat{\varphi}_1 \circ T_{i-1}^{-1})(x) & x \in [x_{i-1}, x_i], \\ (\hat{\varphi}_0 \circ T_i^{-1})(x) & x \in [x_i, x_{i+1}]. \end{cases}$$

Demo

Demo: Developing FEM in 1D [cleared]

Going Higher Order

$\Omega \subset \mathbb{R}$ with a grid as above.

Possible extension:

$$P_h^k := \{v_h \in C^0(\bar{\Omega}) : \text{for all } i \in \{1, \ldots, N\}, v_h|_{I_i} \in \mathbb{P}_k\}.$$

Higher Order Approximation

Let $0 \le \ell \le k$. Then for $v \in H^{\ell+1}(\Omega)$,

$$\left\| v - I_h^k v \right\|_{L^2} + h \left| (v - I_h^k v) \right|_{H^1} \le C h^{\ell+1} \left| v \right|_{H^{\ell+1}}.$$

High-Order: Degrees of Freedom

Define some degrees of freedom (or DoFs) for high-order 1D FEM.

Let $\{\gamma_j\}_{j=0}^{N+1} \in (V_h^1)'$ be the linear functionals so that

$$\gamma_j(v_h) = v_h(x_j) \quad \text{for all } v_h \in V_h^1.$$

Using terminology from classical mechanics, these functions are called (global) degrees of freedom. The functions $\{\varphi_i\}_{i=0}^{N+1}$ that are defined so that

$$\gamma_j(\varphi_i) = \delta_{i,j} \quad (i, j \in \{0, \ldots, N+1\}, \varphi_i \in V_h^1)$$

holds are called (global) shape functions. One can also define local shape functions on the reference element.

High-Order: Local Basis

Define local form functions for high-order 1D FEM.

The local form functions are typically chosen to be Lagrange polynomials:

$$\hat{\varphi}_i^k(\hat{x}) = \frac{\prod_{j=0,j\neq i}^{k}(\hat{x}-\hat{x}_j)}{\prod_{j=0,j\neq i}^{k}(\hat{x}_i-\hat{x}_j)},$$

where $\hat{x}_j = j/k$ for $i = 0, \ldots, k$.
$x_{i,j} := x_i + (j/k)h_i$ for $i = 0, \ldots, N$ and $j = 0, \ldots, k-1$, further $x_{N+1,0} = 0$. Then

$$\dim(V_h^k) = k(N+1) + 1.$$

High-Order: Global Basis

Obtain the global shape functions for high-order 1D FEM.

Define

$$\varphi_{i,0}(x) := \begin{cases} \hat{\varphi}_k^k \circ T_{i-1}^{-1}(x) & x \in [x_{i-1}, x_i], \\ \hat{\varphi}_0^k \circ T_i^{-1}(x) & x \in [x_i, x_{i+1}], \\ 0 & \text{otherwise}, \end{cases}$$

and

$$\varphi_{i,j}(x) := \begin{cases} \hat{\varphi}_j^k \circ T_i^{-1}(x) & x \in [x_i, x_{i+1}], \\ 0 & \text{otherwise}. \end{cases}$$

for $j = 0, \ldots, k-1$ und $i = 0, \ldots, N$.

Outline

A Boundary Value Problem

Consider the following elliptic PDE

$$-\nabla \cdot (\kappa(\boldsymbol{x}) \nabla u) = f(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^2,$$
$$u(\boldsymbol{x}) = 0 \quad \text{when} \quad \boldsymbol{x} \in \partial\Omega.$$

Weak form?

Multiply by a test function $v \in H_0^1(\Omega)$ and integrate by parts:

$$\int_\Omega [-\nabla \cdot (\kappa(\boldsymbol{x}) \nabla u) - f(\boldsymbol{x})] \, v \, \mathrm{d}\boldsymbol{x} = 0$$

$$\Leftrightarrow -\int_{\partial\Omega} v \, [\kappa \widehat{\boldsymbol{n}} \cdot \nabla u] \, \mathrm{d}\Gamma + \int_\Omega [\kappa(\boldsymbol{x}) \nabla u \cdot \nabla v - f(\boldsymbol{x}) \, v] \, \mathrm{d}\boldsymbol{x} = 0.$$

The boundary integral vanishes since $v \in H_0^1$ and we find

$$\int_\Omega \kappa(\boldsymbol{x}) \nabla u \cdot \nabla v \, \mathrm{d}\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) \, v \, \mathrm{d}\boldsymbol{x}.$$

Weak Form: Bilinear Form and RHS Functional

Hence the problem is to find $u \in V$, such that

$$a(u, v) = g(v), \quad \text{for all } v \in V = H_0^1(\Omega)$$

where...

$$a(u, v) := \int_\Omega \kappa(\boldsymbol{x}) \nabla u \cdot \nabla v \, \mathrm{d}\boldsymbol{x},$$

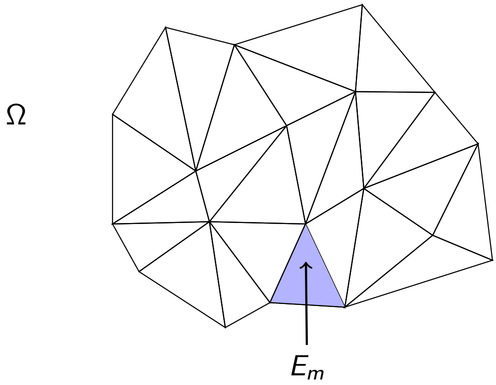
$$g(v) := \int_\Omega f(\boldsymbol{x}) v \, \mathrm{d}\boldsymbol{x},$$

Is this symmetric, coercive, and continuous?

- Symmetric: yes.
- Coercive: When there exists c so that $0 < c \leq \kappa(\boldsymbol{x})$ for all $\boldsymbol{x}$.
- Continuous: When there exists C so that $\kappa(\boldsymbol{x}) \leq C < \infty$ for all $\boldsymbol{x}$.

Triangulation: 2D

Suppose the domain is a union of triangles E_m, with vertices x_i.



$$\bar{\Omega} = \bigcup_{i=1}^{M} E_m.$$

Elements and the Bilinear Form

If the domain, Ω, can be written as a disjoint union of elements, E_k,

$$\Omega = \cup_{m=1}^{M} E_m \quad \text{with} \quad E_i^\circ \cap E_j^\circ = \emptyset \text{ for } i \neq j,$$

what happens to a and g?

$$a(u, v) = \sum_{m=1}^{M} \int_{E_m} \kappa(\boldsymbol{x}) \nabla u \cdot \nabla v \, \mathrm{d}\boldsymbol{x},$$

$$g(v) = \sum_{m=1}^{M} \int_{E_m} q(\boldsymbol{x}) \, v \, \mathrm{d}\boldsymbol{x}.$$

Basis Functions

Expand

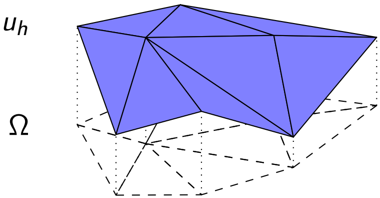
$$u_N(\boldsymbol{x}) = \sum_{i=1}^{N_p} u_i \varphi_i,$$

and plug into the weak form.

$$\sum_{j=1}^{N_p} u_j a(\varphi_j, \varphi_i) = g(\varphi_i), \quad \text{for } i = 1 \dots N_p.$$

Global Lagrange Basis

Approximate solution u_h: Piecewise linear on Ω



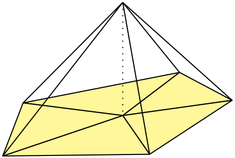
The Lagrange basis for V_h consists of piecewise linear φ_i, with...

$$\varphi_i(\boldsymbol{x}_i) = 1 \quad \text{and} \quad \varphi_i(\boldsymbol{x}_j) = 0, \quad \text{for} \quad i \neq j.$$

Basis Functions Features

Features of the basis?

- For the piecewise linear Lagrange basis, each φ_i is continuous on Ω.
- Restricted to E_m, each φ_i is linear.



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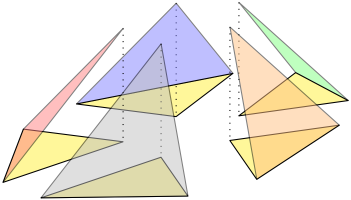
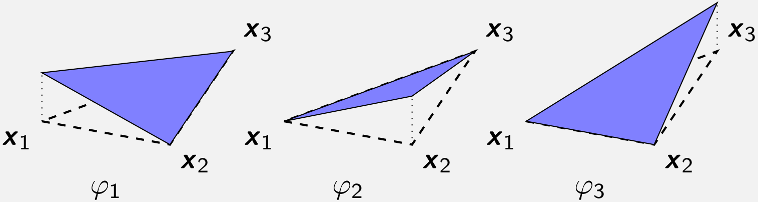


Local Basis

What basis functions exist on each triangle?

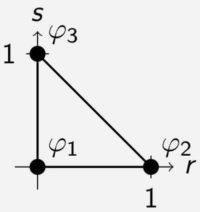
On each triangle, E_m, we have three non-zero basis functions, one for each vertex of the triangle:



In the Figure, $\varphi_1(\boldsymbol{x}_1) = 1$, $\varphi_1(\boldsymbol{x}_2) = 0$, and $\varphi_1(\boldsymbol{x}_3) = 0$.

Local Basis Expressions

Write expressions for the nodal linear basis in 2D.



- $\varphi_1(r, s) = 1 - r - s$
- $\varphi_2(r, s) = r$
- $\varphi_3(r, s) = s$

Higher-Order, Higher-Dimensional Simplex Bases

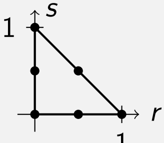
What's an n-simplex?

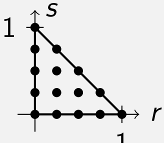
$r_i \geq 0$, $\sum r_i \leq 1$. ($\rightarrow$ barycentric) Interval, $\triangle$, tetrahedron, ...

Give a higher-order polynomial space on the n-simplex:

$$P^N := \operatorname{span}\left\{\prod_{i=1}^{d} x_i^{n_i} : \sum n_i \leq N\right\}$$

Give nodal sets (on the $\triangle$) for P^N and $\dim P^N$ in general.





$$\dim P^N = N_p = \frac{(N+1)(N+2)}{2}$$

Avoiding Runge: e.g. Warburton '06

Finding a Nodal/Lagrange Basis in General

Given a nodal set $(\xi_i)_{i=1}^{N_p} \subset \hat{E}$ (where $\hat{E}$ is the reference element) and a basis $(\varphi_j)_{j=1}^{N_p} : \hat{E} \to \mathbb{R}$, find a Lagrange basis.

Set up a Vandermonde matrix:

$$V := \begin{bmatrix} \varphi_1(\xi_1) & \cdots & \varphi_{N_p}(\xi_1) \\ \vdots & \ddots & \vdots \\ \varphi_1(\xi_{N_p}) & \cdots & \varphi_{N_p}(\xi_{N_p}) \end{bmatrix}.$$

Then $\ell_i := \sum_{j=1}^{N^p} (V^{-T})_{i,j} \varphi_j$ is a Lagrange basis.

Higher-Order, Higher-Dimensional Tensor Product Bases

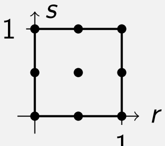
What's a tensor product element?

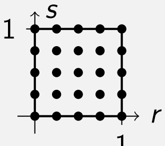
$[0,1]^n \subset \mathbb{R}^n$. Interval, quad, hexahedron.

Give a higher-order polynomial space on the n-simplex:

$$Q^N := \operatorname{span}\left\{\prod_{i=1}^{d} x_i^{n_i} : \max n_i \leq N\right\}$$

Give the nodal sets (on the quad) for Q^N.



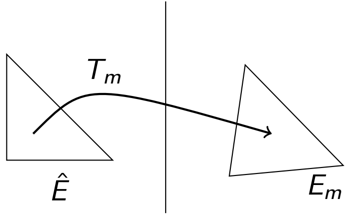


Tensor Product Elements: Lagrange Basis

Lagrange Basis for Tensor Product Elements?

> Can use tensor product of one-dimensional basis $\Rightarrow$ Lower complexity for this and many other operations.

Element Mappings



Construct a mapping $T_m : \hat{E} \to E_m$. Reference element $\hat{E}$, global $\triangle$ E_m.

$$T_m(r, s) = (\boldsymbol{x}_2 - \boldsymbol{x}_1)r + (\boldsymbol{x}_3 - \boldsymbol{x}_1)s + \boldsymbol{x}_1.$$

What is the Jacobian of T_m?

$$J_T = \begin{bmatrix} \partial x/\partial r & \partial x/\partial s \\ \partial y/\partial r & \partial y/\partial s \end{bmatrix} = \begin{bmatrix} \dfrac{\partial T}{\partial r} & \dfrac{\partial T}{\partial s} \end{bmatrix}$$
$$= \begin{bmatrix} (\boldsymbol{x}_2 - \boldsymbol{x}_1) & (\boldsymbol{x}_3 - \boldsymbol{x}_1) \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

More on Mappings

Is an affine mapping sufficient for a tensor product element?

No, because affine mappings preserve parallel lines: Global elements could only be parallelograms.
Idea: Consider a mapping $T_m \in (Q^1)^n$.

How might we accomplish curvilinear elements using the same idea?

- Use isoparametric mappings $T_m \in (P^N)^n$ (if FEM basis is P^N)
- Use subparametric mappings $T_m \in (P^M)^n$
  ($M < N$ if FEM basis is P^N)
- Use superparametric mappings $T_m \in (P^M)^n$
  ($M > N$ if FEM basis is P^N)

Constructing the Global Basis

Construct a basis on the element E_m from the reference basis $(\hat{\varphi}_j)_j : \hat{E} \to \mathbb{R}$.

$$\varphi_j(\boldsymbol{x}) = \hat{\varphi}_j(T_m^{-1}(\boldsymbol{x})).$$

What's the gradient of this basis?

$$\begin{aligned}
\nabla_{\boldsymbol{x}} \varphi_j(T^{-1}(\boldsymbol{x})) &= \left[\frac{d}{d\boldsymbol{x}} \varphi_j(T^{-1}(\boldsymbol{x}))\right]^T \\
&= \left[\left(\frac{d\varphi_j}{d\boldsymbol{r}}\right)_{T^{-1}(\boldsymbol{x})} J_T^{-1}(\boldsymbol{x})\right]^T \\
&= J_T^{-T}(\boldsymbol{x}) \nabla_{\boldsymbol{r}} \varphi_j(T^{-1}(\boldsymbol{x})).
\end{aligned}$$

Assembling a Linear System

Express the matrix and vector elements in

$$\sum_{j=1}^{N_p} u_j a(\varphi_j, \varphi_i) = g(\varphi_i) \quad \text{for } i = 1, \dots, N_p.$$

$$a(\varphi_i, \varphi_j) = \sum_{m=1}^{M} \int_{E_m} \kappa(\boldsymbol{x}) \nabla\varphi_i \cdot \nabla\varphi_j \, \mathrm{d}\boldsymbol{x},$$

$$g(\varphi_i) = \sum_{m=1}^{M} \int_{E_m} f(\boldsymbol{x}) \varphi_i \, \mathrm{d}\boldsymbol{x}.$$

Integrals on the Reference Element

Evaluate

$$\int_E \kappa(\boldsymbol{x})\nabla_{\boldsymbol{x}}\varphi_i(\boldsymbol{x})^T\nabla_{\boldsymbol{x}}\varphi_j(\boldsymbol{x})d\boldsymbol{x}.$$

$$\begin{aligned}
&\int_E \kappa(\boldsymbol{x})\nabla_{\boldsymbol{x}}\varphi_i(\boldsymbol{x})^T\nabla_{\boldsymbol{x}}\varphi_j(\boldsymbol{x})d\boldsymbol{x} \\
&= \int_E \kappa(\boldsymbol{x})(J_T^{-T}\nabla_{\boldsymbol{r}}\varphi_i)^T(J_T^{-T}\nabla_{\boldsymbol{r}}\varphi_j)d\boldsymbol{x} \\
&\overset{P^1}{=}(J_T^{-T}\nabla_{\boldsymbol{r}}\varphi_i)^T(J_T^{-T}\nabla_{\boldsymbol{r}}\varphi_j)|J_T|\int_{\hat{E}} \kappa(T(\boldsymbol{r}))d\boldsymbol{r}
\end{aligned}$$

And now the RHS functional.

$$\int_E f(\boldsymbol{x})\varphi_i(\boldsymbol{x})d\boldsymbol{x} = |J_T|\int_{\hat{E}} f(T(\boldsymbol{r}))\varphi_i(\boldsymbol{r})d\boldsymbol{r}.$$

Inhomogeneous Dirichlet BCs

Handle an inhomogeneous boundary condition $u(\boldsymbol{x}) = \eta(\boldsymbol{x})$ on $\partial\Omega$.

- Find a function $u^0 \in H^1(\Omega)$ with boundary values $u^0(\boldsymbol{x}) = \eta(\boldsymbol{x})$ on $\partial\Omega$. ("lifted" from boundary to volume)
- Define $\hat{u} := u - u^0 \in H_0^1(\Omega)$.
- Insert $u = \hat{u} + u^0$ into the weak form:

$$\begin{aligned} a(\hat{u} + u^0, v) = a(\hat{u}, v) + a(u^0, v) &= g(v), \\ a(\hat{u}, v) &= \underbrace{g(v) - a(u^0, v)}_{\hat{g}(v):=}, \end{aligned}$$

  where still $\hat{u} \in H_0^1$.

Altogether:

- Inhomogeneous BC just leads to extra term on RHS.
- No change in function spaces.

Demo

- **Demo:** Meshing and Connectivity for FEM in 2D [cleared]
- **Demo:** Developing FEM in 2D [cleared]
- **Demo:** 2D FEM Using Firedrake [cleared]
- **Demo:** Rates of Convergence [cleared]

Outline

Conditions on the Mesh

Let Ω be a polygonal domain.

Admissibility (Braess, Def. II.5.1)

A partition (mesh) $\mathcal{T} = \{E_1, \ldots, E_M\}$ of Ω into triangular or quadrilateral elements is called admissible if

- $\bar{\Omega} = \bigcup_{i=1}^{M} E_i$.
- If $E_i \cap E_j$ consists of exactly one point, then it is a common vertex of E_i and E_j.
- If $E_i \cap E_j$ consists of more than one point for $i \neq j$, then $E_i \cap E_j$ is a common edge of E_i and E_j.

Give an example of a non-admissible partition.

One with a hanging node.

Mesh Resolution, Shape Regularity

Definition (Diameter)

A bounded set Ω has diameter $d(\Omega) = \sup\{|x - y| : x, y \in \Omega\}$.

Mesh Resolution

When every element of a partition has diameter at most $2h$, we write $\mathcal{T}_h$ instead of $\mathcal{T}$.

Definition (Shape Regularity (Braess, Def. II.5.1))

A family of partitions $\{\mathcal{T}_h\}$ is called shape regular if

there exists a number $\kappa > 0$ so that every $E \in \mathcal{T}_h$ contains a circle

Cone Conditions

Definition (Lipschitz Domain)

A bounded domain $\Omega \subset \mathbb{R}^n$ is called a Lipschitz domain provided that...

> for every $x \in \partial\Omega$ there exists a neighborhood of x within which $\partial\Omega$ can be represented as the graph of a Lipschitz function.

Lipschitz domains satisfy a cone condition:

> The interior angles at vertices are positive, so that a cone can be placed in Ω with its tip at the vertex.

Theorem (Rellich Selection Theorem (Braess, Thm. II.1.9))

Let $m \geq 0$, let Ω be Lipschitz. Then the imbedding $H^{m+1}(\Omega) \to H^m(\Omega)$ is compact, i.e. any bounded sequence in the range of the imbedding has a

The Interpolation Operator

Theorem (Interpolation Operator (Braess, Lemma II.6.2))

Let $\Omega \subset \mathbb{R}^2$ be Lipschitz. Let $t \geq 2$, and $z_1, z_2, \ldots, z_s$ are $s := t(t+1)/2$ prescribed points in $\bar{\Omega}$ such that the interpolation operator $I : H^t \to \mathbb{P}^{t-1}$ is well-defined. Then there exists a constant c so that for $u \in H^t(\Omega)$

$$\|u - Iu\|_{H^t} \leq c(\Omega, (z_i)) \, |u|_{H^t} \, .$$

Theorem (Approx. for Congruent △ (Braess, Remark II.6.5))

Let $E_h := h\hat{E}$, i.e. a scaled version of a reference triangle, with $h \leq 1$. Then, for $0 \leq m \leq t$, there exists a C so that

$$\|u - Iu\|_{H^m(E_h)} \leq C h^{t-m} \, |u|_{H^t(E_h)} \, .$$

Approximation for Congruent Triangles: Proof (1/2)

Set up a function on E_h and $\hat{E}$. Work out the scaling for the derivative.

Let $u \in H^t(E_h)$. Define $v \in H^t(\hat{E})$ by $v(y) := u(hy)$.
Then $D_w^\alpha v = h^{|\alpha|} D_w^\alpha u$ for $|\alpha| \le t$.

Work out the scaling for the Sobolev seminorm.

$$|v|^2_{H^\ell(\hat{E})} = \sum_{|\alpha|=\ell} \int_{\hat{E}} (D_w^\alpha v)^2 = \sum_{|\alpha|=\ell} \int_{E_h} h^{2\ell} (D_w^\alpha u)^2 h^{-2} = h^{2\ell-2} |u|^2_{H^\ell(E_h)}.$$

Work out the scaling for the Sobolev norm. Recall $h \le 1$.

$$\|u\|^2_{H^m(E_h)} = \sum_{\ell \le m} |u|^2_{H^\ell(E_h)} = \sum_{\ell \le m} h^{-2\ell+2} |v|^2_{H^\ell(E_h)} \le C' h^{-2m+2} \|v\|^2_{H^m(\hat{E})}.$$

Approximation for Congruent Triangles: Proof (1/2)

$$\|u - Iu\|_{H^m(E_h)} \leq Ch^{t-m} |u|_{H^t(E_h)} \quad (0 \leq m \leq t)$$

- $|v|^2_{H^\ell(\hat{E})} = |u|^2_{H^\ell(E_h)}$
- $\|u\|^2_{H^m(E_h)} \leq C' h^{-2m+2} \|v\|^2_{H^m(\hat{E})}$

Prove the estimate.

Inserting $u - Iu$ into this estimate in place of u:

$$\begin{aligned} \|u - Iu\|_{H^m(E_h)} &\leq C' h^{-m+1} \|v - Iv\|_{H^m(\hat{E})} \leq C' h^{-m+1} \|v - Iv\|_{H^t(\hat{E})} \\ &\leq C' c h^{-m+1} |v|_{H^t(\hat{E})} \leq C' c h^{t-m} |u|_{H^t(E_h)} . \end{aligned}$$

H^m Polynomial Approximation on Meshes

Definition (Broken Norm)

Given a partition $\mathcal{T}_h = \{E_i\}_{i=1}^M$ and a function u such that $u \in H^m(E_i)$,

$$\boxed{\|u\|_{H^m,h} := \sqrt{\sum_{i=1}^{M} \|u\|^2_{H^m(E_i)}}.}$$

Approximation Theorem (Braess, Theorem II.6.4)

Let $t \geq 2$, suppose $\mathcal{T}_h$ is a shape-regular triangulation of Ω. Then there exists a constant c such that, for $0 \leq m \leq t$ and $u \in H^t(\Omega)$,

$$\boxed{\|u - I_h u\|_{H^m,h} \leq c(\Omega, \kappa, t) h^{t-m} |u|_{H^t(\Omega)},}$$

Outline

Weak Forms as Minimization Problems

Let V be a linear space, and $a : V \times V \to \mathbb{R}$ a bilinear form, and $g \in V'$.

Theorem (Solutions of Weak Forms are Quadratic Form Minimizers)

If a is SPD, then

$$J(v) := \tfrac{1}{2} a(v,v) - g(v)$$

attains its minimum over V at u iff $a(u,v) = g(v)$ for all $v \in V$.

$$\begin{aligned} J(u+tv) &= \frac{1}{2} a(u+tv, u+tv) - g(u+tv) \\ &= J(u) + t[a(u,v) - g(v)] + \frac{t^2}{2} a(v,v). \end{aligned}$$

for $u, v \in V$ and $t \in \mathbb{R}$.
If u satisfies $a(u,v) = g(v)$, $J(u+v) > J(u)$.
If J has a min at u, derivative of $t \mapsto J(u+tv)$ must vanish at $t = 0$

Example: Lagrange Multipliers in $\mathbb{R}^2$

$$\begin{aligned} f(x,y) = x^2 + y^2 &\quad \rightarrow \quad \text{min!} \\ g(x,y) = x + y &\quad = \quad 2 \end{aligned}$$

Write down the Lagrangian.

$$\mathcal{L}(x,y,\lambda) = f(x,y) + \lambda g(x,y) = x^2 + y^2 + \lambda(x + y - 2).$$

Write down a necessary condition for a constrained minimum.

$$0 = \nabla \mathcal{L} = \begin{bmatrix} \nabla f + \lambda \nabla g \\ g \end{bmatrix}.$$

Saddle Point Problems

X, M Hilbert spaces. $a : X \times X \to \mathbb{R}$ and $b : X \times M \to \mathbb{R}$ continuous bilinear forms, $f \in X'$, $g \in M'$. Minimize

$$J(u) = \frac{1}{2}a(u,u) - \langle f, u\rangle \qquad \text{subject to} \qquad b(u,\mu) = \langle g, \mu\rangle \quad (\mu \in M).$$

Apply the method of the Lagrange multipliers.

$$\mathcal{L}(u,\lambda) = J(u) + [b(u,\lambda) - \langle g, \lambda\rangle] \quad (\lambda \in M).$$

- J and $\mathcal{L}(\cdot,\lambda)$ agree when constraint is satisfied.
- Idea: Select $\lambda \in M$ to 'tweak' $\mathcal{L}$ so that minimizer of $\mathcal{L}(\cdot,\lambda)$ satsifies the constraints. (Finite-dim: $-\nabla f = J_g^T \boldsymbol{\lambda}$)

Yields saddle point problem: find $(u,\lambda) \in X \times M$ so that

$$\begin{aligned} a(u,v) + b(v,\lambda) &= \langle f, v\rangle \quad (v \in X),\\ b(u,\mu) &= \langle g, \mu\rangle \quad (\mu \in M). \end{aligned}$$

Example: Saddle Point Problem in $\mathbb{R}^2$

$$\begin{aligned} f(x,y) = x^2 + y^2 &\quad\rightarrow\quad \text{min!} \\ g(x,y) = x + y &\quad=\quad 2 \end{aligned}$$

Lagrangian: $\mathcal{L}(x,y,\lambda) = f(x,y) + \lambda g(x,y) = x^2 + y^2 + \lambda(x+y-2)$.

Show that $x = y = 1$, $\lambda = -2$ is a saddle point.

The Hessian has the form

$$\mathcal{H}_{\mathcal{L}} = \begin{bmatrix} H_f & \nabla g \\ \nabla g^T & 0 \end{bmatrix}.$$

$$\mathcal{H}_{\mathcal{L}} = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} = M \begin{bmatrix} A & \\ & -BA^{-1}B^T \end{bmatrix} M^T,$$

demonstrating indefiniteness using Sylvester's Law of Inertia.
(cf. Benzi et al. '05, Section 3.4)

Stokes Equation

$$
\begin{aligned}
\Delta \boldsymbol{u} + \nabla p &= -\boldsymbol{f} \quad (x \in \Omega), \\
\nabla \cdot \boldsymbol{u} &= 0 \quad (x \in \Omega), \\
\boldsymbol{u} &= \boldsymbol{u}_0 \quad (x \in \partial\Omega).
\end{aligned}
$$

What are the pieces?

- $\boldsymbol{u}$ is the velocity field,
- p is the pressure,
- $\boldsymbol{f}$ is an externally applied force field,
- Pressure gradient gives rise to an additional force that prevents a density change.
- $\nabla \cdot \boldsymbol{u} = 0$ is the incompressibility constraint:
  Pressure falls/rises where a source/sink would be created.

Stokes: Properties

$$\begin{aligned} \Delta \boldsymbol{u} + \nabla p &= -\boldsymbol{f} \quad (x \in \Omega), \\ \nabla \cdot \boldsymbol{u} &= 0 \quad (x \in \Omega), \\ \boldsymbol{u} &= \boldsymbol{u}_0 \quad (x \in \partial\Omega). \end{aligned}$$

Can we choose any $\boldsymbol{u}_0$?

$$\int_{\partial\Omega} \boldsymbol{u}_0 \cdot \hat{\boldsymbol{n}} dS_{\boldsymbol{x}} = \int_{\partial\Omega} \boldsymbol{u} \cdot \hat{\boldsymbol{n}} dS_{\boldsymbol{x}} = \int_{\Omega} \nabla \cdot \boldsymbol{u} d\boldsymbol{x} = 0$$

is a compatibility condition. Satisfied e.g. for $\boldsymbol{u}_0 \equiv 0$.

Does Stokes fully determine the pressure?

Only up to an additive constant. Additionally demand $\int_\Omega p dx = 0$.

Stokes: Variational Formulation

$$\Delta \boldsymbol{u} + \nabla p = -\boldsymbol{f}, \qquad \nabla \cdot \boldsymbol{u} = 0 \quad (x \in \partial\Omega).$$

Choose some function spaces (for homogeneous $\boldsymbol{u}_0 = 0$).

$$X = H_0^1(\Omega)^n, \qquad M = L_0^2(\Omega) := \left\{ q \in L^2(\Omega) : \int_\Omega q dx = 0 \right\}$$

Derive a weak form.

$$a(\boldsymbol{u}, \boldsymbol{v}) = \int_\Omega J_{\boldsymbol{u}} : J_{\boldsymbol{v}}, \qquad b(\boldsymbol{v}, q) = \int_\Omega \nabla \cdot \boldsymbol{v} q,$$

$A : B = \mathrm{tr}(AB^T) = \sum_{i,j} A_{i,j} B_{i,j}$. Find $(\boldsymbol{u}, p) \in X \times M$ so that

$$\begin{aligned} a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) &= \langle \boldsymbol{f}, \boldsymbol{v} \rangle_{L^2} \quad (\boldsymbol{v} \in X), \\ b(\boldsymbol{u}, q) &= 0 \quad (q \in M), \end{aligned}$$

where in reusing b, we used that $(-\operatorname{div})^* = \operatorname{grad}$ are adjoint.

Solvability of Saddle Point Problems

The Stokes weak form is clearly in saddle-point form.
Do all saddle point problems have unique solutions?

$$\begin{aligned} f(x,y) = x^2 + y^2 &\to \text{min!}, \\ x + y &= 2, \\ 3x + 3y &= 6. \end{aligned}$$

$\mathcal{L}(x,y,\lambda) = x^2 + y^2 + \lambda(x + y - 2) + \mu(3x + 3y - 6)$. (λ, μ) no longer uniquely determined.

$\to$ Need a criterion.

The inf-sup Condition

$$\begin{aligned} a(u,v) + b(v,\lambda) &= \langle f, v\rangle \quad (v \in X), \\ b(u,\mu) &= \langle g, \mu\rangle \quad (\mu \in M). \end{aligned}$$

Theorem (Brezzi's splitting theorem (Braess, III.4.3))

The saddle point problem has a unique solution if and only if

- *The bilinear form $a(\cdot,\cdot)$ is V-elliptic, where* $V = \{u : b(u,\mu) = 0 \text{for all } \mu \in M\}$, *i.e. there exists $c_0 > 0$ so that*

$$\boxed{a(v,v) \geq c_0 \|v\|_X^2 \qquad (v \in V).}$$

- *There exists a constant $c_2 > 0$ so that (inf-sup or LBB condition):*

$$\boxed{\inf_{\mu \in M} \sup_{v \in X} \frac{b(v,\mu)}{\|v\|_X \|\mu\|_M} \geq c_2.}$$

Interpreting the inf-sup Condition

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} = M \begin{bmatrix} A & \\ & -BA^{-1}B^T \end{bmatrix} M^T$$

$$a(v,v) \ge c_0 \|v\|_X^2, \qquad \inf_{\mu\in M} \sup_{v\in X} \frac{b(v,\mu)}{\|v\|_X \|\mu\|_M} \ge c_2.$$

For any given v, can we expect $b(v,\mu)$ to be nonzero for all μ?

> No! E.g. for Stokes, the B block is short-and-fat $\Rightarrow \exists$ nullspace.

What is the inf-sup condition saying?

> "b has no μ-nullspace."

Why does it suffice for a to be V-elliptic?

> True in the linear algebra, too! (Think Schur complements.) (Benzi et al. '05, Thm. 3.2)

inf-sup and Stokes

$$
\begin{aligned}
a(\boldsymbol{u}, \boldsymbol{v}) &= \int_\Omega J_{\boldsymbol{u}} : J_{\boldsymbol{v}}, \qquad \text{where } A : B = \operatorname{tr}(AB^T),\\
b(\boldsymbol{v}, q) &= \int_\Omega \nabla \cdot \boldsymbol{v} q.
\end{aligned}
$$

Find $(\boldsymbol{u}, p) \in X \times M$ so that

$$
\begin{aligned}
a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) &= \langle \boldsymbol{f}, \boldsymbol{v} \rangle_{L^2} \quad (\boldsymbol{v} \in X),\\
b(\boldsymbol{u}, q) &= 0 \quad (q \in M).
\end{aligned}
$$

Theorem (Existence and Uniqueness for Stokes (Braess, III.6.5))

There exists a unique solution of this system when $\boldsymbol{f} \in H^{-1}(\Omega)^n$.

(based on results due to Ladyšenskaya, Nečas)

Discretizations for Stokes

Demo: 2D Stokes Using Firedrake [cleared] (P^1-P^1)

Give a heuristic reason why P^1-P^1 might not be great.

> The differential operators being applied to $\boldsymbol{u}$ and p in the Stokes system are of different order.

Demo: Bad Discretizations for 2D Stokes [cleared]

Establishing a Discrete inf-sup Condition

Suppose $b : X \times M \to \mathbb{R}$ satisfies inf-sup. Subspaces $X_h \subseteq X$, $M_h \subseteq M$.

Fortin's Criterion ([Fortin 1977])

Suppose there exists a bounded projector $\Pi_h : X \to X_h$ so that

$$b(v - \Pi_h v, \mu_h) = 0 \quad (\mu_h \in M_h).$$

If $\|\Pi_h\| \leq c$ for some constant c independent of h, then b satisfies the inf-sup-condition on $X_h \times M_h$.

Let $\mu_h \in M_h$. By assumption, $b(v, \mu_h) = b(\Pi_h v, \mu_h)$ for $v \in X$.

$$\sup_{v_h \in X_h} \frac{b(v_h, \mu_h)}{\|v_h\|} \geq \sup_{v_h \in \Pi_h X} \frac{b(v_h, \mu_h)}{\|v_h\|} = \sup_{v \in X} \frac{b(\Pi_h v, \mu_h)}{\|\Pi_h v\|}$$
$$\geq \frac{1}{c} \sup_{v \in X} \frac{b(v, \mu_h)}{\|v\|} \geq c_2 \|\mu_h\|.$$

H^1-Boundedness of the L^2-Projector

Assume H^2-regularity and a uniform triangulations $\mathcal{T}_h$. (Not in general!)

H^1-Boundedness of the L^2-Projector (Braess Corollary II.7.8)

Let π_h^0 be the L_2-projector onto a finite element space $V_h \subset H^1(\Omega)$. Then, for an h-independent constant c,

$$\left\|\pi_h^0 v\right\|_{H^1} \leq c \left\|v\right\|_{H^1} .$$

Ingredients?

- Regularity
- Aubin-Nitsche
- Inverse estimates (For affine, pw. polynomial family V_h: $\left\|v_h\right\|_{H^t,h} \leq Ch^{m-t} \left\|v_h\right\|_{H^m,h}$ with $0 \leq m \leq t$, e.g. $\left\|v_h\right\|_{H^1,h} \leq Ch^{-1} \left\|v_h\right\|_{L^2,h}$)

H^1-Boundedness of the L^2-Projector

Does H^1 boundedness of the H^1 projector hold?

Yes, any Hilbert space projection is bounded. (Pythagoras)

How would this break down without the uniformity assumption?

On a graded mesh, where L^2 projection introduces $O(1/h)$ growth in the H^1 seminorm (which measures oscillation, in a way).

Bubbles and the MINI Element

What is a bubble function?

$\varphi_b(r,s) = rs(1-r-s)$. (see figure on next slide)

Let B^3 be the span of the bubble function and $\mathcal{T}_h$ the triangulation.

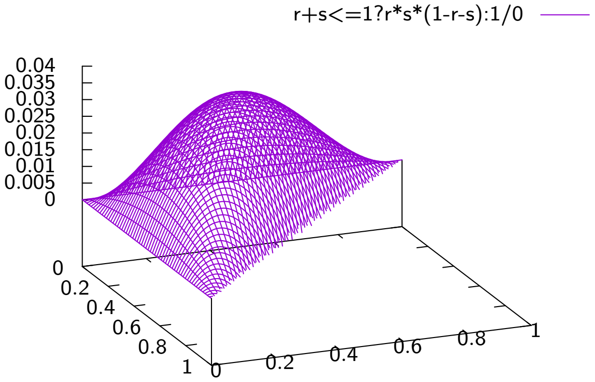
Define the MINI variational space $X_h \times M_h$.

$$
\begin{aligned}
X_h &:= \left\{ v_h \in C(\bar{\Omega})^2 \cap H_0^1(\Omega)^2 : v_h|_E \in (P^1 \oplus B^3)^2 \text{ for } E \in \mathcal{T}_h \right\} \\
M_h &:= \left\{ q_h \in C(\bar{\Omega}) \cap L_0^2(\Omega) : v_h|_E \in P^1 \text{ for } E \in \mathcal{T}_h \right\}
\end{aligned}
$$

Computational impact of the bubble DOF?

Not coupled to DOFs outside the element; can use static condensation to eliminate.

The Bubble in Pictures



MINI Satisifies an inf-sup Condition (1/4)

MINI satisifes inf-sup (Braess Theorem III.7.2)

Assume Ω is convex or has a smooth boundary. Then the MINI variational space satisfies an inf-sup condition for every variational form that itself satisfies one.

Assume uniform meshes (can generalize). Let

$$\mathcal{M}_h := \left\{ v_h \in C(\bar{\Omega}) \cap H_0^1(\Omega) : v_h|_E \in P^1 \text{ for } E \in \mathcal{T}_h \right\}.$$

Let $\pi_h^0 : H_0^1 \to \mathcal{M}_h$ be the L^2 projector.
Then $\left\| \pi_h^0 v \right\|_{H^1} \leq c_1 \left\| v \right\|_{H^1}$ from its H^1-boundedness and, from the interpolation estimate,

$$\begin{aligned}\left\| v - \pi_h^0 v \right\|_{L^2} &\leq \left\| v - \mathcal{I} v \right\|_{L^2} + \left\| \mathcal{I} v - \pi_h^0 v \right\|_{L^2} \\ &= \left\| v - \mathcal{I} v \right\|_{L^2} + \left\| \pi_h^0 (\mathcal{I} v - v) \right\|_{L^2} \leq c_2 h \left| v \right|_{H^1}.\end{aligned}$$

MINI Satisifies an inf-sup Condition (2/4)

Create a projector onto the bubble space B^3.

Let $\pi_h^1 : L^2 \to B^3$ be linear so that

$$\int_E (\pi_h^1 v - v) dx = 0 \quad \text{for } E \in \mathcal{T}_h.$$

What does this bubble projector do?

- Project onto piecewise constant functions.
- Replace the constant by a bubble with the same integral.

Do we have an estimate for the bubble projector?

$$\left\| \pi_h^1 v \right\|_{L^2} \leq c_3 \left\| v \right\|_{L^2}.$$

MINI Satisifies an inf-sup Condition (3/4)

Make an overall projector Π_h onto X_h.

Define $\Pi_h v := \pi_h^0 v + \pi_h^1(v - \pi_h^0 v)$. By construction, Π_h preserves the constant mode, i.e. $\int(\Pi_h v - v)dx = 0$.

Show Fortin's criterion for Π_h.

Extend Π_h to vector-valued component-by-component.
$q_h \in M_h$ is continuous, so we may apply Gauss's theorem.

$$
\begin{aligned}
& b(\boldsymbol{v} - \Pi_h \boldsymbol{v}, q_h) \\
= & \int \nabla \cdot (\boldsymbol{v} - \Pi_h \boldsymbol{v}) q_h dx \\
= & \int_{\partial\Omega} (\boldsymbol{v} - \Pi_h \boldsymbol{v}) \cdot \hat{\boldsymbol{n}} \underbrace{q_h}_{0} dS_x - \int_\Omega (v - \Pi_h v) \cdot \underbrace{\nabla q_h}_{\text{const}} dx = 0.
\end{aligned}
$$

MINI Satisifies an inf-sup Condition (4/4)

- $\left\|\pi_h^0 v\right\|_{H^1} \leq c_1 \|v\|_{H^1}$ for L^2 projector $\pi_h^0 : H_0^1 \to \mathcal{M}_h$.
- $\left\|v - \pi_h^0 v\right\|_{L^2} \leq c_2 h |v|_{H^1}$.
- $\left\|\pi_h^1 v\right\|_{L^2} \leq c_3 \|v\|_{L^2}$.

Show H^1-boundedness of Π_h.

$$
\begin{aligned}
\|\Pi_h v\|_{H^1} &\leq \left\|\pi_h^0 v\right\|_{H^1} + \left\|\pi_h^1(v - \pi_h^0 v)\right\|_{H^1} \\
&\underset{\text{inv.est.}}{\leq} c_1 \|v\|_{H^1} + c_4 h^{-1} \left\|\pi_h^1(v - \pi_h^0 v)\right\|_{L^2} \\
&\leq c_1 \|v\|_{H^1} + c_4 h^{-1} c_3 \left\|v - \pi_h^0 v\right\|_{L^2} \\
&\leq c_1 \|v\|_{H^1} + c_4 c_3 c_2 \|v\|_{H^1} .
\end{aligned}
$$

Demo

Demo: 2D Stokes Using Firedrake [cleared] (MINI and Taylor-Hood)

Outline

Lax-Milgram, General Case

Let V be Hilbert space with inner product $\langle \cdot, \cdot \rangle$.

Theorem (Lax-Milgram, General Case)

Let a be a V-elliptic bilinear form, and let g be a bounded linear functional on V.
Then there exists a unique $u \in V$ so that $a(u, v) = g(v)$ for all $v \in V$.

Let $u \in V$ and observe $a_u(v) := a(u, v)$ is a bounded linear functional (due to continuity of a). Let $t_u \in V$ be the Riesz representer of a_u with $a_u(v) = \langle v, t_u \rangle$ for all $v \in V$. Consider the mapping defined by that:

$$T : V \to V, \qquad u \mapsto Tu := t_u.$$

We show that T is linear, bounded, has closed range, and is onto V.

Lax-Milgram Proof (2/5)

$a(u, v) = \langle v, Tu \rangle$. Show linearity of T.

For $u, v, w \in V$ and $\alpha \in \mathbb{R}$:

$$\langle v, T(\alpha u + w) \rangle = a(\alpha u + w, v) = \alpha \langle v, Tu \rangle + \langle v, Tw \rangle .$$

Show boundedness $\Leftrightarrow$ continuity of T.

$$\| Tu \|^2 = \langle Tu, Tu \rangle = a_u(Tu) = a(u, Tu) \leq c_1 \| Tu \| \, \| u \| \quad \text{(continuity)}.$$

Lax-Milgram Proof (3/5)

$a(u, v) = \langle v, Tu \rangle$. Show that T has closed range. (Needed for Hilbert projection, which is needed for onto.)

Let $z_n = Tu_n$ be a sequence in range(T). By definition, $a(u_n, v) = \langle v, Tu_n \rangle = \langle v, z_n \rangle$ for all $v \in V$, so that

$$
\begin{aligned}
a(u_n - u_m, v) &= \langle v, z_n - z_m \rangle \\
\Rightarrow \quad a(u_n - u_m, u_n - u_m) &= \langle u_n - u_m, z_n - z_m \rangle \\
\Rightarrow \quad c_0 \|u_n - u_m\|^2 &\le \|u_n - u_m\| \, \|z_n - z_m\| \quad \text{(coercivity)} \\
\Rightarrow \quad c_0 \|u_n - u_m\| &\le \|z_n - z_m\| .
\end{aligned}
$$

If $z_n \to z$, (u_n) must be Cauchy, so has a limit (because V is Hilbert). Let u be the limit. Next: Show $z = Tu$.
Let $v \in V$ be arbitrary. $a(u_n, v) \to a(u, v)$ by continuity. Also: $|\langle Tu_n - z, v \rangle| \to 0$, so that $\langle v, Tu_n \rangle \to \langle v, z \rangle$, so $a(u, v) = \langle v, z \rangle$, and by definition of T, $z = Tu$.

Lax-Milgram Proof (4/5)

$a(u, v) = \langle v, Tu \rangle$. Show that T is onto V.

Suppose not. By the Hilbert projection theorem, there exists $w \in \operatorname{range}(T)^{\perp} \setminus \{0\}$. Therefore $\langle w, Tu \rangle = 0$ for all $u \in V$. Choosing $u = w$ gives $0 = \langle w, Tw \rangle = a(w, w)$, a contradiction.

Lax-Milgram Proof (5/5)

Show existence of the solution u.

Let z be the Riesz representer of g: $g(v) = \langle v, z \rangle$ for all $v \in V$. Since $T : V \to V$ is onto, there exists a $u \in V$ so that $z = Tu$, i.e. $g(v) = \langle v, Tu \rangle = a(u, v)$ for all $v \in V$.

Show uniqueness of the solution u.

Suppose we have a second $\hat{u}$ with $z = T\hat{u}$. Then $a(u - \hat{u}, v) = 0$ for all $v \in V$, particularly $a(u - \hat{u}, u - \hat{u}) = 0$, i.e. $u = \hat{u}$.

Outline

Outline

Conservation laws

Goal: Solve *conservation laws* on bounded domain $\Omega \subset \mathbb{R}^n$:

$$\boldsymbol{q}_t + \nabla \cdot \boldsymbol{F}(\boldsymbol{q}) = 0$$

Example: Maxwell's Equations

$$\begin{aligned} \partial_t \boldsymbol{D} - \nabla \times \boldsymbol{H} &= -\boldsymbol{j}, & \partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} &= 0, \\ \nabla \cdot \boldsymbol{D} &= \rho, & \nabla \cdot \boldsymbol{B} &= 0. \end{aligned}$$

What do we do with the divergence constraints?

Ignore them. If satisfied at initial condition, they continue to be satisfied.

Rewriting Maxwell's

Let $\boldsymbol{q} = (D_x, D_y, D_z, B_x, B_y, B_z)^T$. Consider $\boldsymbol{D} = \epsilon \boldsymbol{E}$ and $\boldsymbol{B} = \mu \boldsymbol{H}$.

$$\partial_t \boldsymbol{D} - \nabla \times \boldsymbol{H} = -0, \qquad \partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0.$$

Assume ϵ, μ constant. Rewrite in conservation law form: $\boldsymbol{q}_t + \nabla \cdot F(\boldsymbol{q}) = 0$

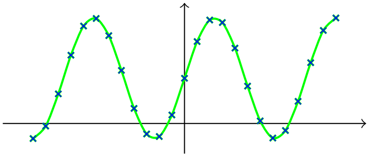
$$\boldsymbol{q}_t + \nabla \cdot \begin{pmatrix} 0 & -\frac{B_z}{\varepsilon} & \frac{B_y}{\varepsilon} \\ \frac{B_z}{\varepsilon} & 0 & -\frac{B_x}{\varepsilon} \\ -\frac{B_y}{\varepsilon} & \frac{B_x}{\varepsilon} & 0 \\ 0 & \frac{D_z}{\mu} & -\frac{D_y}{\mu} \\ -\frac{D_z}{\mu} & 0 & \frac{D_x}{\mu} \\ \frac{D_y}{\mu} & -\frac{D_x}{\mu} & 0 \end{pmatrix} = 0$$

Could we also define $\boldsymbol{q} = (E_x, E_y, E_z, H_x, H_y, H_z)^T$?

No: coeff. on the wrong side of the $\nabla \cdot$. Only OK for constant-coeff.

Outline

Solving $q_t + aq_x = 0$: Finite Differences

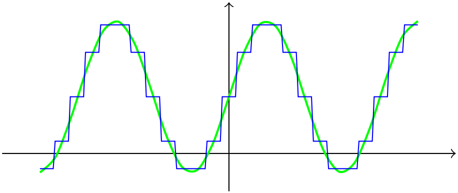


- Simple to implement
- High-order
- Local and explicit in time
- Theory available
- High-order/geometry: pick one.
  - Upwind/downwind differencing?
    - How about in a system?
  - Boundaries?
  - Discontinuities?

$$D_t^- + aD_x^- = 0$$

$$D_t^+ f := \frac{f(t + \Delta t) - f(t)}{\Delta t}$$

Solving $q_t + aq_x = 0$: Finite Volume



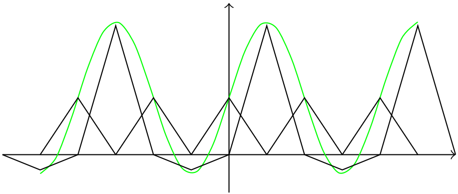
- Robust, fast, good for c.laws
- Local and explicit in time
- Solid theory
- High-order/geometry: pick one.

$$\bar{q}_k := \int_{(k-1/2)\Delta x}^{(k+1/2)\Delta x} q(x)dx$$

$$\Delta x \partial_t \bar{q}_k + f^{k+1/2} - f^{k-1/2} = 0$$

$f^{k\pm1/2}$: flux "reconstructions"

Solving $q_t + aq_x = 0$: Finite Elements

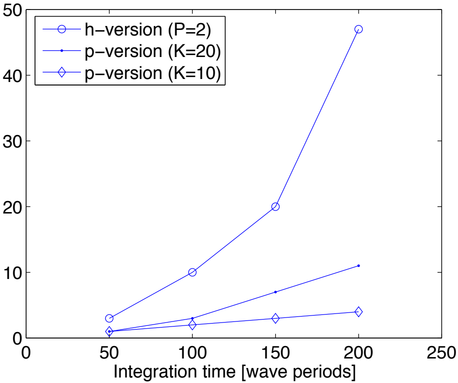


- ⊕ High-order
- ⊕ geom. flexible
- ⊕ Non-local and implicit in time
- ⊕ Solid theory
- ⊖ Not nonlinearly robust
- ⊖ Not fast: Mass matrix solve

$$\int_\Omega q_t^N \phi + a q_x^N \phi dx = 0$$

for ϕ in a test space.

Do we really want high order?



Time to compute solution at 5% error

Big assumption?

Spectral expansion of solution decays quickly
(i.e. solution smooth)

Figure from talk by Jan Hesthaven

Summarizing

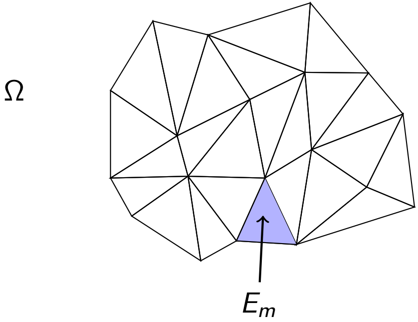
Want flexibility of finite elements *without* the drawbacks.

Let's redevelop finite elements, with a bit more care.
Strategy:

- Use n-dimensional POV for a while to expose geometric issues more clearly.
- Reduce to 1D when necessary.
- Mop up remaining issues later.

Outline

Developing the Scheme



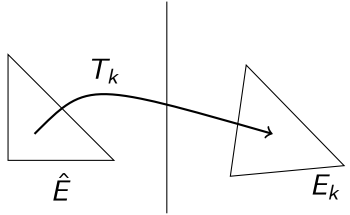
What do do about unbounded domains?

Need to truncate domain, e.g.:

- Special boundary conditions (e.g. Engquist/Majda '77, Hagstrom/Warburton '04)
- Perfectly Matched Layers (PMLs, Berenger '94)

Dealing with the Mesh, Part I

For each cell E_k, find a ref-to-global map T_k:



$$T_k : \hat{E} \to E_k$$
$$\boldsymbol{x} = (x, y, z) = T_k(r, s, t) = T_k(\boldsymbol{r})$$

- T_k affine for straight-sided simplices: $T_k(\boldsymbol{r}) = A\boldsymbol{r} + \boldsymbol{b}$
- Curved elements also possible: iso/sub/super-parametric

Dealing with the Mesh, Part II

Based on knowledge of how to do this on $\hat{E}$:

Can now *integrate* on Ω:

$$\int_\Omega f dx = \sum_{E_k} \int_{E_k} f dx = \sum_{E_k} \int_{\hat{E}} f \left| \frac{d\boldsymbol{x}}{d\boldsymbol{r}} \right| dr$$

and *differentiate* on Ω:

$$\frac{\partial f}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{x}} \frac{\partial f}{\partial \boldsymbol{r}}$$

Jacobian of T_k^{-1}?

$$\frac{d\boldsymbol{x}}{d\boldsymbol{r}} \frac{d\boldsymbol{r}}{d\boldsymbol{x}} = \mathrm{Id} \quad \Leftrightarrow \quad \left(\frac{d\boldsymbol{x}}{d\boldsymbol{r}} \right)^{-1} = \frac{d\boldsymbol{r}}{d\boldsymbol{x}}$$

Dealing with the Mesh, Part III

Approximation basis set on E_k?

Use the one we have on $\hat{E}$:

$$\phi_i^k(x) := \phi_i(T_k^{-1}(x))$$

What function space do we get if T_k is non-affine?

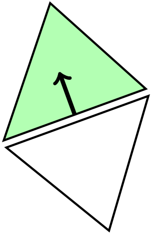
- Complicated. Often: A basis of rational functions.
- Approximation results nontrivial.

Going Galerkin

$$\int_{E_k} q_t^k \phi + (\nabla \cdot F^k)\phi dx = 0$$

Integrate by parts:

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k \cdot \nabla \phi dx + \int_{\partial E_k} (F^k \cdot \hat{\boldsymbol{n}}) \phi dx$$



Problem?

- Problem: Two values to choose from on boundary.
- Don't choose (for now).
- Call chosen answer numerical flux $(F^k \cdot n)^*$
- Feel vaguely reminded of finite volume

Strong-Form DG

Weak form:

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k \cdot \nabla \phi dx + \int_{\partial E_k} (F^k \cdot \hat{\boldsymbol{n}})^* \phi dx$$

Integrate by parts *again*:

$$0 = \int_{E_k} q_t^k \phi + (\nabla \cdot F^k) \phi dx + \int_{\partial E_k} (F^k \cdot \hat{\boldsymbol{n}})^* - (F^k \cdot \hat{\boldsymbol{n}})^- \phi dx$$

- Strong-form DG
- Same solution as weak for linear, constant-coefficient problems.

Outline

Accuracy and Stabillity

In DG: what provides accuracy? what provides stability?

- Local approximation space provides *accuracy*
- Fluxes provide *stability*

Lax equivalence: Accuracy + Stability = Convergence

$\rightarrow$ Let flux choice be guided by stability.

Following slides based on material by Tim Warburton

Stability: Basic Setup (1/2)

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k \cdot \nabla \phi dx + \int_{\partial E_k} (F^k \cdot \hat{\boldsymbol{n}}) \phi dS_x$$

Trick: Set $\phi = q$. Specialize $F(u) := (au, 0, 0)^T = a\boldsymbol{e}_x u$.

$$\begin{aligned}
0 &= \int_{E_k} q_t^k q_k dx - \int_{E_k} a q_k \boldsymbol{e}_x \cdot \nabla q_k dx + \int_{\partial E_k} (a q_k \boldsymbol{e}_x \cdot \hat{\boldsymbol{n}})^* q_k dS_x \\
&= \int_{E_k} q_t^k q_k dx - \int_{E_k} a q_k \partial_x q_k dx + \int_{\partial E_k} (a q_k n_x)^* q_k dS_x \\
&= \frac{\partial_t}{2} \int_{E_k} q_k q_k dx - \int_{E_k} a q_k \partial_x q_k dx + \int_{\partial E_k} (a q_k n_x)^* q_k dS_x
\end{aligned}$$

$$\Rightarrow \frac{\partial_t \|q_k\|_{2,E_k}^2}{2} = \int_{E_k} a q_k \partial_x q_k dx - \int_{\partial E_k} (a q_k n_x)^* q_k dS_x \overset{!}{\leq} 0$$

Stability: Basic Setup (2/2)

$$\frac{\partial_t \|q_k\|_{2,E_k}^2}{2} = \int_{E_k} a q_k \partial_x q_k dx - \int_{\partial E_k} (a q_k n_x)^* q_k dS_x$$

Integrate by parts:

$$\int f \partial_x f = -\int f \partial_x f + \int_\partial f^2 n_x$$

to see:

$$\frac{\partial_t \|q_k\|_{2,E_k}^2}{2} = \int_{\partial E_k} \frac{a(q_k)^2 n_x}{2} - (a q_k n_x)^* q_k dS_x$$

This depends on neighbors–end of element-local analysis!

Stability: Going Global

$$\frac{\partial_t \|q_k\|^2_{2,E_k}}{2} = \int_{\partial E_k} \frac{a(q_k)^2 n_x}{2} - (aq_k n_x)^* q_k dS_x$$

$$\frac{\partial_t \|q_k\|^2_{2,\Omega}}{2} = \sum_k \int_{\partial E_k} \frac{a(q_k)^2 n_x}{2} - (aq_k n_x)^* q_k dS_x$$

$$= \sum_{f \in \text{faces}} \left(\int_f \frac{a(q_k^+)^2 n_x^+}{2} - (aq_k n_x)^*_+ q_k^+ dS_x \right.$$

$$\left. + \int_f \frac{a(q_k^-)^2 n_x^-}{2} - (aq_k n_x)^*_- q_k^- dS_x \right)$$

- Assumption: $(aq_k n_x)^*_+ + (aq_k n_x)^*_- = 0$ ("no accumulation on interface")
- a is constant
- Neglect domain boundaries

Gather up

$$\frac{\partial_t \|q_k\|_{2,\Omega}^2}{2} = \sum_{f \in \text{faces}} \left(\int_f \frac{a(q_k^+)^2 n_x^+}{2} - (a q_k n_x)_+^* q_k^+ dS_x \right.$$
$$\left. + \int_f \frac{a(q_k^-)^2 n_x^-}{2} - (a q_k n_x)_-^* q_k^- dS_x \right)$$

$$\frac{\partial_t \|q_k\|_{2,\Omega}^2}{2} = \sum_{f \in \text{faces}} \int_f a n_x^- \frac{(q_k^-)^2 - (q_k^+)^2}{2} - (a q_k n_x)_-^* (q_k^- - q_k^+) dS_x$$
$$= \sum_{f \in \text{faces}} \int_f \left(a n_x^- \frac{q_k^- + q_k^+}{2} - (a q_k n_x)_-^* \right) (q_k^- - q_k^+) dS_x$$

Want all that non-positive. So demand:

$$\left(a n_x^- \frac{q_k^- + q_k^+}{2} - (a q_k n_x)_-^* \right) (q_k^- - q_k^+) \overset{!}{\leq} 0$$

Picking a Flux

Want:

$$(*) = \left(a n_x^- \frac{q_k^- + q_k^+}{2} - (a q_k n_x)^*_- \right) (q_k^- - q_k^+) \overset{!}{\leq} 0$$

Ideas?

One possible choice:

$$(a q_k n_x)^*_- := a n_x^- \frac{q_k^- + q_k^+}{2}$$

- Called the *central flux*.
- Observe: $(*) = 0 \Rightarrow L^2$-norm exactly conserved!
- The lazy man's flux.
- Works.
- Problematic! Why?

Picking a flux, attempt two

Want:

$$(*) = \left(a n_x^- \frac{q_k^- + q_k^+}{2} - (a q_k n_x)^*_- \right) (q_k^- - q_k^+) \overset{!}{\leq} 0$$

More ideas?

$$(a q_k n_x)^*_- := a n_x^- \frac{q_k^- + q_k^+}{2} + \alpha \frac{q_k^- - q_k^+}{2}$$

(with $\alpha \geq 0$)

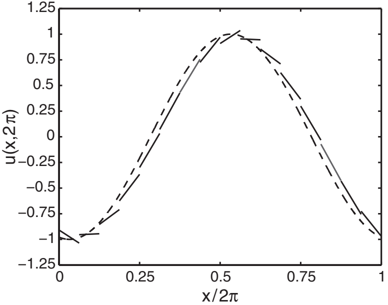
Unit considerations suggest: $\alpha = \pm a n_x^- \overset{!}{\geq} 0$.

Familiar as Rusanov or Local Lax-Friedrichs. In this simple case: also the upwind flux.

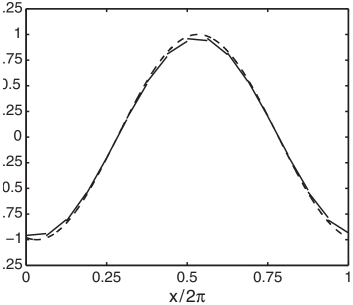
- Observe: $(*) < 0 \Rightarrow$ dissipative!
- Quite good in practice.

Comparing Fluxes (1/3)

Central



Upwind



Upwind penalizes jumps!

Figure from talk by Jan Hesthaven

Comparing Fluxes (2/3)

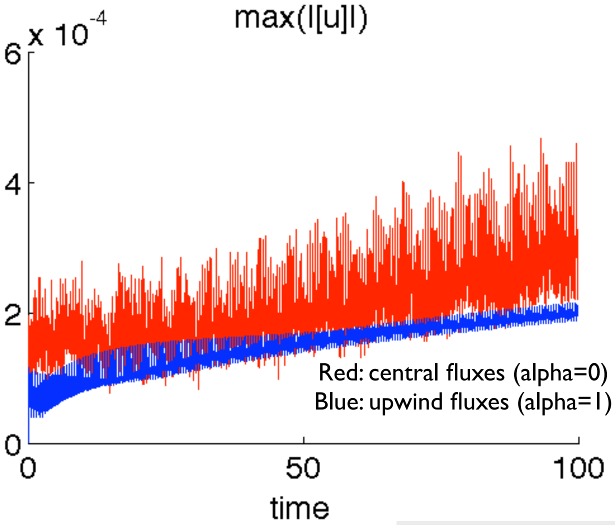


Figure from lecture by Tim Warburton

Comparing Fluxes (3/3)

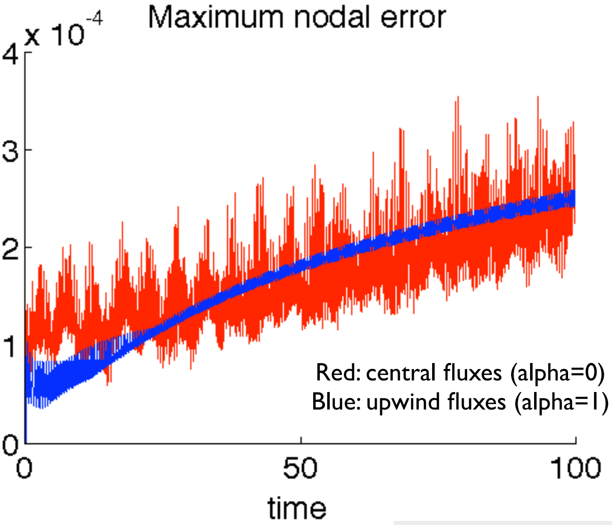


Figure from lecture by Tim Warburton

Stability Analysis

Clif notes on flux choice?

> 'Pick the average' or 'pick the upwind value'

Swept under the rug: Boundary conditions

> Also important for stability!

Element coupling (and BCs) done *weakly*

> - Numerical solution really is discontinuous
> - Hence "discontinuous Galerkin"

Accuracy

Stability: (preliminary version) done!
Accuracy: Depends on approximation properties!

Need approximation space: polynomials of (total) degree at most N on the reference element.

So, expect h^{N+1} residual.

Practically often true. Theoretically:

- Lesaint, Raviart '74:
  - h^N in the general case
  - h^{N+1} for special grids
- Johnson '86: $h^{N+1/2}$

Systems of Conservation Laws

What to do about systems?

- Consider Riemann (jump) problem
  - Obtain 'fan' of different wave speeds
- *Rankine-Hugoniot condition*:

$$[\![F(q)]\!] = (\text{wave speed})\,[\![q]\!]$$

- Number states across fan $q_0, q_{-1}, q_1, \ldots$
- Set up Rankine-Hugoniot at each state boundary
- Solve for rest-state flux $F(q_0)$
- Just like Finite Volume

What about multiple dimensions?

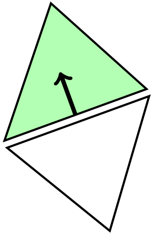
We've dealt with 1D systems.

How about the move to multiple dimensions?

In principle there is (almost) nothing to see.

Recipe:

- Reduce nD c.law to 1D c.law across boundary
- Diagonalize
- Play Rankine-Hugoniot game as before
- Transform back



Simultaneous Diagonalization

2D second-order wave equation across a boundary with normal n:

$$q_t + \begin{pmatrix} 0 & -c\,n_x & -c\,n_y \\ -c\,n_x & 0 & 0 \\ -c\,n_y & 0 & 0 \end{pmatrix} \partial_n q = 0$$

Must simultaneously diagonalize for all $(n_x, n_y)^T$ to obtain generic expression!

More symbolically:

$$q_t + (An_x)\partial_x q + (Bn_y)\partial_y q$$

Need to find matrix S that simultaneously diagonalizes An_x and Bn_y!

Demo: Finding Numerical Fluxes for DG [cleared] (Part 1)

Jumps and Averages

Jump and average of a scalar quantity:

$$\{q\} := \frac{q^- + q^+}{2}$$
$$[\![q]\!] := q^+ \boldsymbol{n}^+ + q^- \boldsymbol{n}^-$$

Jump and average of a vector quantity:

$$\{\boldsymbol{q}\} := \frac{\boldsymbol{q}^- + \boldsymbol{q}^+}{2}$$
$$[\![\boldsymbol{q}]\!] := \boldsymbol{q}^+ \cdot \boldsymbol{n}^+ + \boldsymbol{q}^- \cdot \boldsymbol{n}^-$$

A Flux for Maxwell's

Wanted to solve Maxwell's equation in the time domain. Numerical flux?

Either look in the literature:

$$\hat{\boldsymbol{n}} \cdot (\boldsymbol{F}_N - \boldsymbol{F}_N^*) := \frac{1}{2} \begin{pmatrix} \{Z\}^{-1} \hat{\boldsymbol{n}} \times (Z^+ [\![\boldsymbol{H}]\!] - \alpha \hat{\boldsymbol{n}} \times [\![\boldsymbol{E}]\!]) \\ \{Y\}^{-1} \hat{\boldsymbol{n}} \times (-Y^+ [\![\boldsymbol{E}]\!] - \alpha \hat{\boldsymbol{n}} \times [\![\boldsymbol{H}]\!]) \end{pmatrix}.$$

or derive yourself: **Demo: Finding Numerical Fluxes for DG** [cleared] (Part 2)

Good news: Scheme mathematically complete.

Outline

Implementing DG

Weak form:

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k \cdot \nabla \phi dx + \int_{\partial E_k} (F^k \cdot n)^* \phi dx$$

What do the DoFs mean?

Two main choices:

- *Modal* DG (expansion coefficients)
- *Nodal* DG (point values at nodal locations)

We choose to use nodal DG here.

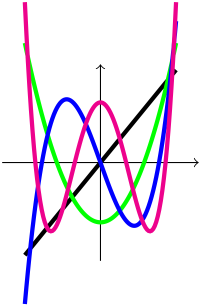
Need: set of basis functions, set of nodes

Modes

Function spaces same as for FEM: P^N, Q^N.

Numerically: better to use orthogonal polynomials with

$$\int_{\hat{E}} \phi_i \phi_j = \delta_{i,j}$$



- 1D: Legendre polys
- nD: Proriol '57/Koornwinder '75/Dubiner '93

Notation: $(\phi_i)_{i=1}^{N_p}$.

Nodes

Define set of interpolation nodes $(\xi_i)_{i=1}^{N_p}$ and ℓ_i their Lagrange basis.

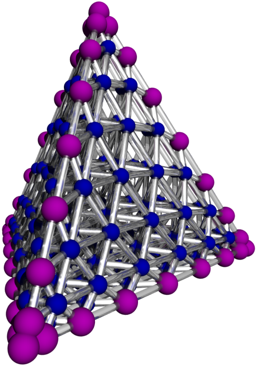
Define *generalized Vandermonde matrix*

$$V_{ij} := \phi_j(\xi_i)$$

$$V(\text{modal coeff.}) = (\text{nodal coeff.})$$

ξ_i determine cond(V)!

- Equispaced nodes: cond. exponential in N
- 1D: Gauß-Lobatto or Chebyshev
- nD: cottage industry (e.g. [Warburton '06])



In Matrix Form

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k \cdot \nabla \phi dx + \int_{\partial E_k} (F^k \cdot n)^* \phi dx$$

Write in matrix form:

$$\mathcal{M}_{ij}^k := \int_{E_k} \ell_i \ell_j dx = |A_k| \mathcal{M} := |A_k| \int_{\hat{E}} \ell_i \ell_j dx = |A_k| V^{-T} V^{-1}$$

$$\mathcal{S}_{ij}^{k,\partial\nu} := \int_{E_k} \ell_i \partial_{x_\nu} \ell_j \mathrm{d}x,$$

$$\mathcal{M}_{ij}^{k,A} := \int_{A \subset \partial E_k} \ell_i \ell_j \mathrm{d}S_x.$$

$$0 = \mathcal{M}^k \partial_t u^k - \sum_{\nu} \mathcal{S}^{k,\partial_\nu} [F(u^k)] + \sum_{A \subset \partial E_k} \mathcal{M}^{k,A} (\hat{n} \cdot F)^*$$

Explicit Time Integration

$$0 = \mathcal{M}^k \partial_t u^k - \sum_{\nu} \mathcal{S}^{k,\partial_\nu}[F(u^k)] + \sum_{A \subset \partial E_k} \mathcal{M}^{k,A} (\hat{n} \cdot F)^*$$

How can we do time integration on this weak form?

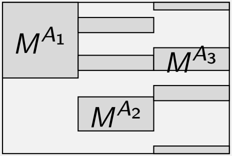
Goal: Dig out $\partial_t u$! Must invert $\mathcal{M}$.

- In 'normal' finite elements: large, unstructured, sparse matrix
- In DG: Block-diagonal
- In simplicial DG: Templated block-diagonal
- In curvilinear DG: *Still* templated block-diagonal
  e.g.: [Warburton '08], [Chan, Hewett, Warburton '17]

Trick: Multiple face mass matrices

Applying multiple face mass matrices at once:

$$\int_{\partial E_k} \hat{n} \cdot (F^*) \phi \mathrm{d}S =$$



$$\left(J_1 \hat{n} \cdot (F^*)|_{A_1} \middle| \cdots \middle| J_3 \hat{n} \cdot (F^*)|_{A_3} \right).$$

Dealing with Nonlinearity

$$0 = \int_{E_k} q_t^k \phi dx - \int_{E_k} F^k(q_k) \cdot \nabla \phi dx + \int_{\partial E_k} (F^k(q_k) \cdot n)^* \phi dx$$

What happens if F is nonlinear (in volume/surface)?

- Good news: Stability proof stays largely intact
  - But: requires that integrals are evaluated exactly. A tall order.
- Inexact quadrature (a variational crime) drives aliasing instabilities
  - Overintegration: Use higher-order quadrature. (But what about terms like $q^{1.4}$?)
  - Filtering: Damp out the highest polynomial modes
  - Make the scheme discretely stable $\rightarrow$ Entropy-stable DG
- Shocks may arise for nonlinear F, drive oscillation (Gibbs' phenomenon)
  - Oscillations drive further instabilities

DG and Modern Computers: Possible Advantages

DG on modern processor architectures: Why?

- On-chip parallelism
  - DG inherently parallel.
- Deepening Memory Hierarchy
  - The majority of DG is local.
- Compute Bandwidth $\gg$ Memory Bandwidth
  - DG is arithmetically intense.
- Processors favor dense data.
  - Local parts of the DG operator are dense.
- Penalty on scattered access.
  - DG's cell connectivity is sparser than CG's
  - and more regular.