AM 205: final project organization

- Final project worth 30% of grade
- Due on Wednesday December 10th at 5 PM in iSites dropbox, along with associated code
- Completed in teams of two or three. (Single-person projects will be allowed with instructor permission.) All team members receive the same grade.
- Piazza is best place to find teammates

Very rough length guidelines

Team members	Pages
1	9
2	14
3	18

- Precise length of write-up is not important. Scientific content is more important.
- Optional: submit a poster to the CS poster session on December 9th, 12 PM–2 PM in Maxwell–Dworkin lobby. IACS will cover poster cost. Posters must be completed by December 2nd. Roughly count as 25% reduction in write-up length.

AM 205: final project topic

- Find an application area of interest and apply methods from the course to it.
- Project must involve some coding. No purely theoretical projects allowed.
- Fine to take problems directly from research, within reason. It should be an aspect of a project that is carried out for this course, as opposed to something already ongoing

AM 205: plan for proposal

By November 20th at 6 PM complete at least one of the following:

- Submit a half-page summary of the project, as well as the numerical methods that you plan to use
- Arrange a half-hour meeting with Chris, Kevin, or Dustin to discuss project idea and direction

Four points automatically awarded for doing this.

Total grade for project: 60 points. A detailed breakdown will be posted on the website.

Hyperbolic PDEs: Numerical Approximation

Note that CFL is only a necessary condition for convergence

Its great value is its simplicity: CFL allows us to easily reject F.D. schemes for hyperbolic problems with very little investigation

For example, for $u_t + cu_x = 0$, the scheme

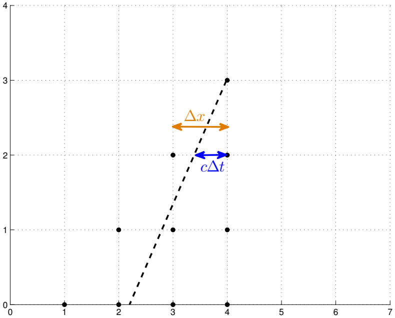
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_j^n - U_{j-1}^n}{\Delta x} = 0 \qquad (*)$$

cannot be convergent if $c < 0$

Question: What small change to $(*)$ would give a better method when $c < 0$?

Hyperbolic PDEs: Numerical Approximation

If $c > 0$, then we require $\nu \equiv \frac{c\Delta t}{\Delta x} \leq 1$ in $(*)$ for CFL to be satisfied



Hyperbolic PDEs: Upwind method

As foreshadowed earlier, we should pick our method to reflect the direction of propagation of information

This motivates the upwind scheme for $u_t + cu_x = 0$

$$U_j^{n+1} = \begin{cases} U_j^n - c\frac{\Delta t}{\Delta x}(U_j^n - U_{j-1}^n), & \text{if } c > 0 \\ U_j^n - c\frac{\Delta t}{\Delta x}(U_{j+1}^n - U_j^n), & \text{if } c < 0 \end{cases}$$

The upwind scheme satisfies CFL condition if $|\nu| \equiv |c\Delta t/\Delta x| \leq 1$

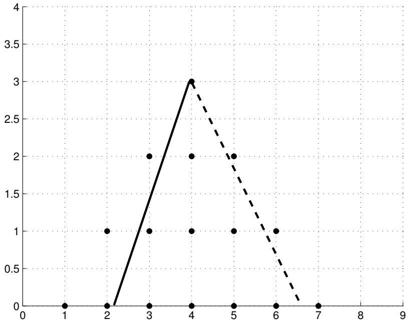
ν is often called the CFL number

Hyperbolic PDEs: Central difference method

Another method that seems appealing is the central difference method:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} = 0$$

This satisfies CFL for $|\nu| \equiv |c\Delta t/\Delta x| \leq 1$, regardless of sign$(c)$



We shall see shortly, however, that this is a bad method!

Hyperbolic PDEs: Accuracy

Recall that truncation error is "what is left over when we substitute exact solution into the numerical approximation"

Truncation error is analogous for PDEs, *e.g.* for the $(c > 0)$ upwind method, truncation error is:

$$T_j^n \equiv \frac{u(t^{n+1}, x_j) - u(t^n, x_j)}{\Delta t} + c\frac{u(t^n, x_j) - u(t^n, x_{j-1})}{\Delta x}$$

The order of accuracy is then the largest p such that

$$T_j^n = O((\Delta x)^p + (\Delta t)^p)$$

Hyperbolic PDEs: Accuracy

See Lecture: For the upwind method, we have

$$T_j^n = \frac{1}{2}\left[\Delta t\, u_{tt}(t^n, x_j) - c\Delta x\, u_{xx}(t^n, x_j)\right] + \text{H.O.T.}$$

Hence the upwind scheme is first order accurate

Hyperbolic PDEs: Accuracy

Just like with ODEs, truncation error is related to convergence in the limit $\Delta t, \Delta x \to 0$

Note that to let $\Delta t, \Delta x \to 0$, we generally need to decide on a relationship between Δt and Δx

e.g. to let $\Delta t, \Delta x \to 0$ for the upwind scheme, we would set $\frac{c\Delta t}{\Delta x} = \nu \in (0, 1]$; this ensures CFL is satisfied for all $\Delta x, \Delta t$

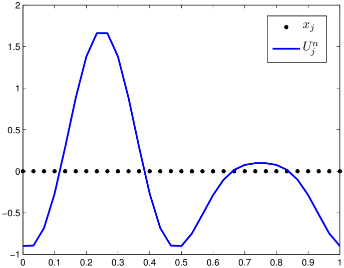
Hyperbolic PDEs: Accuracy

In general, convergence of a finite difference method for a PDE is related to both its truncation error and its stability

We'll discuss this in more detail shortly, but first we consider how to analyze stability via Fourier stability analysis

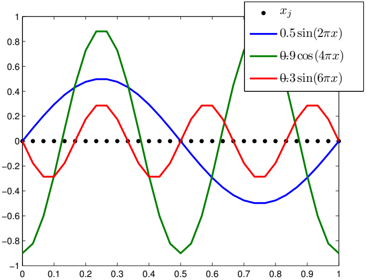
Hyperbolic PDEs: Stability

Let's suppose that U_j^n is periodic on the grid $x_1, x_2, \dots, x_n$



Hyperbolic PDEs: Stability

Then we can represent U_j^n as a linear combination of sin and cos functions, i.e. Fourier modes



Or, equivalently, as a linear combination of complex exponentials, since $e^{ikx} = \cos(kx) + i\sin(kx)$ so that

$$\sin(x) = \frac{1}{2i}(e^{ix} - e^{-ix}), \qquad \cos(x) = \frac{1}{2}(e^{ix} + e^{-ix})$$

Hyperbolic PDEs: Stability

For simplicity, let's just focus on only one of the Fourier modes

In particular, we consider the ansatz $U_j^n(k) \equiv \lambda(k)^n e^{ikx_j}$, where k is the wave number and $\lambda(k) \in \mathbb{C}$

Key idea: Suppose that $U_j^n(k)$ satisfies our finite difference equation, then this will allow us to solve[1] for $\lambda(k)$

The value of $|\lambda(k)|$ indicates whether the Fourier mode e^{ikx_j} is amplified or damped

If $|\lambda(k)| \leq 1$ for all k then the scheme does not amplify any Fourier modes $\implies$ stable!

[1] In general a solution for $\lambda(k)$ exists, which justifies our choice of ansatz

Hyperbolic PDEs: Stability

We now perform Fourier stability analysis for the ($c > 0$) upwind scheme (recall that $\nu = \frac{c\Delta t}{\Delta x}$):

$$U_j^{n+1} = U_j^n - \nu(U_j^n - U_{j-1}^n)$$

Substituting in $U_j^n(k) = \lambda(k)^n e^{ik(j\Delta x)}$ gives

$$\begin{aligned} \lambda(k)e^{ik(j\Delta x)} &= e^{ik(j\Delta x)} - \nu(e^{ik(j\Delta x)} - e^{ik((j-1)\Delta x)}) \\ &= e^{ik(j\Delta x)} - \nu e^{ik(j\Delta x)}(1 - e^{-ik\Delta x}) \end{aligned}$$

Hence

$$\lambda(k) = 1 - \nu(1 - e^{-ik\Delta x}) = 1 - \nu(1 - \cos(k\Delta x) + i\sin(k\Delta x))$$

Hyperbolic PDEs: Stability

It follows that

$$
\begin{aligned}
|\lambda(k)|^2 &= [(1-\nu) + \nu\cos(k\Delta x)]^2 + [\nu\sin(k\Delta x)]^2 \\
&= (1-\nu)^2 + \nu^2 + 2\nu(1-\nu)\cos(k\Delta x) \\
&= 1 - 2\nu(1-\nu)(1-\cos(k\Delta x))
\end{aligned}
$$

and from the trig. identity $(1-\cos(\theta)) = 2\sin^2(\frac{\theta}{2})$, we have

$$
|\lambda(k)|^2 = 1 - 4\nu(1-\nu)\sin^2\left(\frac{1}{2}k\Delta x\right)
$$

Due to the CFL condition, we first suppose that $0 \leq \nu \leq 1$

It then follows that $0 \leq 4\nu(1-\nu)\sin^2\left(\frac{1}{2}k\Delta x\right) \leq 1$, and hence $|\lambda(k)| \leq 1$

Hyperbolic PDEs: Stability

In contrast, consider stability of the central difference approx.:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} = 0$$

Recall that this also satisfies the CFL condition as long as $|\nu| \leq 1$

But Fourier stability analysis yields

$$\lambda(k) = 1 - \nu i \sin(k\Delta x) \implies |\lambda(k)|^2 = 1 + \nu^2 \sin^2(k\Delta x)$$

and hence $|\lambda(k)| > 1$ (unless $\sin(k\Delta x) = 0$), i.e. unstable!

Consistency

We say that a numerical scheme is consistent with a PDE if its truncation error tends to zero as $\Delta x, \Delta t \to 0$

For example, any first (or higher) order scheme is consistent

Lax Equivalence Theorem

Then a fundamental theorem in Scientific Computing is the Lax[2] Equivalence Theorem:

> For a consistent finite difference approx. to a linear evolutionary problem, the stability of the scheme is necessary and sufficient for convergence

This theorem refers to linear evolutionary problems, *e.g.* linear hyperbolic or parabolic PDEs

[2]Peter Lax, Courant Institute, NYU

Lax Equivalence Theorem

We know how to check consistency: Derive the truncation error

We know how to check stability: Fourier stability analysis

Hence, from Lax, we have a general approach for verifying convergence

Also, as with ODEs, convergence rate is determined by truncation error

Lax Equivalence Theorem

Note that strictly speaking Fourier stability analysis only applies for periodic problems

However, it can be shown that conclusions of Fourier stability analysis hold true more generally

Hence Fourier stability analysis is the standard tool for examining stability of finite difference methods for PDEs

Hyperbolic PDEs: Semi-discretization

So far, we have developed full discretizations (both space and time) of the advection equation, and considered accuracy and stability

However, it can be helpful to consider semi-discretizations, where we discretize only in space, or only in time

For example, discretizing $u_t + c(t,x)u_x = 0$ in space[3] using a backward difference formula gives

$$\frac{\partial U_j(t)}{\partial t} + c_j(t)\frac{U_j(t) - U_{j-1}(t)}{\Delta x} = 0, \qquad j = 1, \ldots, n$$

[3]Here we show an example where c is not constant

Hyperbolic PDEs: Semi-discretization

This gives a system of ODEs, $U_t = f(t, U(t))$, where $U(t) \in \mathbb{R}^n$ and

$$f(t, U(t)) \equiv -c_j(t) \frac{U_j(t) - U_{j-1}(t)}{\Delta x}$$

We could approximate this ODE using forward Euler (to get our Upwind scheme):

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

Or backward Euler:

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

Hyperbolic PDEs: Method of Lines

Or we could use a "black box" ODE solver, such as `ode45`, to solve the system of ODEs

This "black box" approach is called the method of lines

The name "lines" is because we solve each $U_j(t)$ for a fixed x_j, i.e. a line in the xt-plane

With method of lines we let the ODE solver to choose step sizes Δt to obtain a stable and accurate scheme

The Wave Equation

We now briefly return to the wave equation:

$$u_{tt} - c^2 u_{xx} = 0$$

In one spatial dimension, this models, say, vibrations in a taut string

The Wave Equation

Many schemes have been proposed for the wave equation

One good option is to use central difference approximations[4] for both u_{tt} and u_{xx}:

$$\frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{\Delta t^2} - c^2 \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2} = 0$$

Key points:

- Truncation error analysis $\implies$ second-order accurate
- Fourier stability analysis $\implies$ stable for $0 \leq c\Delta t/\Delta x \leq 1$
- Two-step method in time, need a one-step method to "get started"

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[4]Can arrive at the same result by discretizing the equivalent first order system

Parabolic PDEs

The Heat Equation

The canonical parabolic equation is the heat equation

$$u_t - \alpha u_{xx} = f(t, x),$$

where α models thermal diffusivity

In this section, we shall omit α for convenience

Note that this is an Initial-Boundary Value Problem:

- We impose an initial condition $u(0, x) = u_0(x)$
- We impose boundary conditions on both sides of the domain

The Heat Equation

A natural idea would be to discretize u_{xx} with a central difference, and employ the Euler method in time:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{\Delta x^2} = 0$$

Or we could use backward Euler in time:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} = 0$$

The Heat Equation

Or we could do something "halfway in between":

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{1}{2}\frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} - \frac{1}{2}\frac{U_{j-1}^{n} - 2U_j^{n} + U_{j+1}^{n}}{\Delta x^2} = 0$$

This is called the Crank–Nicolson method[5]

In fact, it is common to consider a 1-parameter "family" of methods that include all of the above: the θ-method

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \theta\frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} - (1-\theta)\frac{U_{j-1}^{n} - 2U_j^{n} + U_{j+1}^{n}}{\Delta x^2} = 0$$

where $\theta \in [0, 1]$

[5]From a paper by Crank and Nicolson in 1947, note: "Nicolson" is not a typo!

The Heat Equation

With the θ-method:

- $\theta = 0 \implies$ Euler
- $\theta = \frac{1}{2} \implies$ Crank–Nicolson
- $\theta = 1 \implies$ backward Euler

For the θ-method, we can

1. perform Fourier stability analysis
2. calculate the truncation error

The θ-Method: Stability

Fourier stability analysis: Set $U_j^n(k) = \lambda(k)^n e^{ik(j\Delta x)}$ to get

$$\lambda(k) = \frac{1 - 4(1-\theta)\mu \sin^2\left(\frac{1}{2}k\Delta x\right)}{1 + 4\theta\mu \sin^2\left(\frac{1}{2}k\Delta x\right)}$$

where $\mu \equiv \Delta t/(\Delta x)^2$

Here we cannot get $\lambda(k) > 1$, hence only concern is $\lambda(k) < -1$

Let's find conditions for stability, i.e. we want $\lambda(k) \geq -1$:

$$1 - 4(1-\theta)\mu \sin^2\left(\frac{1}{2}k\Delta x\right) \geq -\left[1 + 4\theta\mu \sin^2\left(\frac{1}{2}k\Delta x\right)\right]$$

The θ-Method: Stability

Or equivalently:

$$4\mu(1-2\theta)\sin^2\left(\frac{1}{2}k\Delta x\right) \leq 2$$

For $\theta \in [0.5, 1]$ this inequality is always satisfied, hence the θ-method is unconditionally stable (i.e. stable independent of μ)

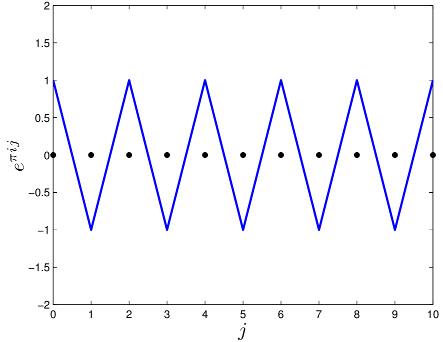
In the $\theta \in [0, 0.5)$ case, the "most unstable" Fourier mode is when $k = \pi/\Delta x$, since this maximizes the factor $\sin^2\left(\frac{1}{2}k\Delta x\right)$

The θ-Method: Stability

Note that this corresponds to the highest frequency mode that can be represented on our grid, since with $k = \pi/\Delta x$ we have

$$e^{ik(j\Delta x)} = e^{\pi ij} = (e^{\pi i})^j = (-1)^j$$

The $k = \pi/\Delta x$ mode:



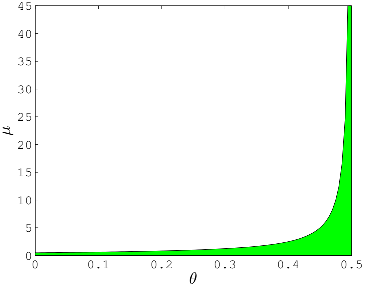
The θ-Method: Stability

This "sawtooth" mode is stable (and hence all modes are stable) if

$$4\mu(1-2\theta) \leq 2 \iff \mu \leq \frac{1}{2(1-2\theta)},$$

Hence for $\theta \in [0, 0.5)$, the θ-method is conditionally stable

The θ-Method: Stability



For $\theta \in [0, 0.5)$, θ-method is stable if μ is in the "green region," i.e. approaches unconditional stability as $\theta \to 0.5$

The θ-Method: Stability

Note that if we set θ to a value in $[0, 0.5)$, then stability time-step restriction is quite severe: $\Delta t \leq \frac{(\Delta x)^2}{2(1-2\theta)}$

Contrast this to the hyperbolic case where we had $\Delta t \leq \frac{\Delta x}{c}$

This is an indication that the system of ODEs that arise from spatially discretizing the heat equation are stiff