Lecture 1

Introduction

Last quarter, we covered the following material:

- Poisson equation: $\Delta u = f$

In particular we used the Poisson equation as a model problem to learn

  - how to discretize the Laplacian operator
  - how to solve the Poisson equation
  - the accuracy and convergence of the aforementioned methods

This quarter, we'll be tackling:

- time dependent problems such as

$$\begin{array}{ll} u_t = D\Delta u & \text{diffusion/heat equation} \\ u_t + a u_x = 0 & \text{advection equation} \\ u_{tt} = c^2 \Delta u & \text{wave equation} \end{array}$$

- mixed equations

$$u_t + a u_x = D u_{xx} + R(u) \qquad \text{advection-diffusion-reaction equation}$$

- non-linear equations such as

$$u_t + u u_x = \epsilon u_{xx} \qquad \text{Burgers equation}$$

Solutions to the inviscid Burgers equation,

$$u_t + u u_x = 0,$$

can develop singularities in finite time from smooth initial data. This presents a challenge when solving nonlinear hyperbolic problems numerically.

- conservation laws

$$u_t + (f(u))_x = 0, \text{ where } f \text{ is the flux function}$$

Classification of PDEs

Recall that the Poisson equation is an elliptic equation. More generally, we can have $Lu = f$, where

$$L = \sum_{ij} a_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_j b_j(x) \frac{\partial}{\partial x_j} + c(x).$$

L is elliptic if the matrix a_{ij} is positive or negative definite. Moreover, if L is an elliptic operator, then $u_t = Lu + f$ is a parabolic equation.

Examples of hyperbolic equations are the advection and wave equations previously mentioned. Namely, the first order system $\underline{u}_t + A\underline{u}_x = 0$ is hyperbolic if A has real eigenvalues and is diagonalizable.

To see how $u_{tt} = c^2 \Delta u$ is hyperbolic, let

$$p = u_t \qquad \text{and} \qquad q = -u_x$$

which gives

$$p_t = u_{tt} = c^2 u_{xx} = -c^2 q_x \qquad \text{and} \qquad q_t = -u_{xt} = -u_{tx} = -p_x$$

Thus leaving us with

$$\begin{pmatrix} p \\ q \end{pmatrix}_t = \begin{pmatrix} 0 & -c^2 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix}_x \implies \begin{pmatrix} p \\ q \end{pmatrix}_t + \begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix}_x = 0$$

Note that the eigenvalues of the matrix A are $\pm c$, satisfying the criteria of a hyperbolic equation.

Conservation Laws

Let $\rho(x,t)$ be a density (e.g. $\frac{\text{mass}}{\text{length}}$ or $\frac{\text{moles}}{\text{length}}$).

Let F be a flux function (e.g. $\frac{\text{mass}}{\text{time}}$).

Suppose $F = F(\rho(x,t))$, or more generally $F = F(x, \rho, \rho_x)$.

Then the total amount of stuff in the interval $[x_1, x_2]$ is

$$M = \int_{x_1}^{x_2} \rho(x,t)dx \qquad \text{and} \qquad \frac{dM}{dt} = \frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t)dx = F(\rho(x_1,t)) - F(\rho(x_2,t))$$

Invoking the Fundamental Theorem of Calculus gives us

$$\frac{dM}{dt} = \frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t)dx = \int_{x_1}^{x_2} -(F(\rho(x,t)))_x dx \implies \int_{x_1}^{x_2} \rho_t + (F(\rho))_x dx = 0$$

The latter form is the integral form of the conservation law. Because x_1 and x_2 are arbitrary, assuming ρ is smooth enough so that these derivatives are defined, the integrand must be zero everywhere. This gives the differential form of the conservation law

$$\rho_t + (F(\rho))_x = 0$$

When dealing with discontinuous solutions the solutions are no longer unique, and we must use the integral form to determine which solution is the physical solutions.

Examples:
Let u be the concentration of a chemical

1) Assume $F = au$ (flux is proportional to the concentration)

$$\implies u_t + au_x = 0 \leftarrow \text{ advection equation}$$

2) Now assume $F = -Du_x$ (flux is proportional to the negative of the gradient)

$$\implies u_t + (-Du_x)_x = 0 \implies u_t = (Du_x)_x \leftarrow \text{ diffusion equation}$$

Near the end of the quarter we will study nonlinear hyperbolic conservation laws (e.g. Euler equation (gas dynamics)):

$$\begin{array}{ll} \rho_t + (v\rho)_x = 0 & \text{conservation of mass} \\ (\rho v)_t + (\rho v^2 + p)_x = 0 & \text{conservation of linear momentum} \\ E_t + (v(E+p))_x = 0 & \text{conservation of energy} \end{array}$$

Here ρ is density, p is pressure, v is velocity, and E is energy density.

Advection vs Diffusion

We want to compare the solutions of

$$u_t + au_x = 0 \text{ and } u_t = Du_{xx} \text{ on } \mathbb{R}$$

Time dependent problems require an initial condition $u(x,0) = u_0(x)$. The solution to the advection equation is

$$\begin{array}{l} u(x,t) = u_0(x-at) \leftarrow \text{ initial data translates at a constant speed} \\ u_t(x,t) = u_0(x-at)(-a) = -au_x \end{array}$$

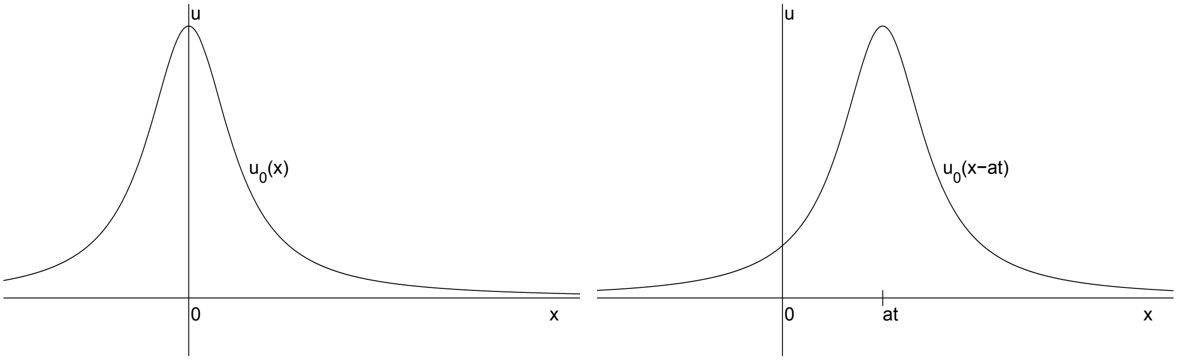

Figure 1: Behavior of a the solution to the advection equation for positive a.

For the heat equation (diffusion equation), $u_t = Du_{xx}$, we look at a special case:

$$u_0(x) = e^{i\xi x} \text{ for which we make the guess for the solution of the form } u(x,t) = g(t)e^{i\xi x}$$

giving us

$$g'(t)e^{i\xi x} = -D\xi^2 g(t)e^{i\xi x} \implies g(t) = e^{-D\xi^2 t}$$

Thus our solution is $u(x,t) = e^{-D\xi^2 t}e^{i\xi x} \implies |u(x,t)| = e^{-D\xi^2 t}$.

We see the amplitude decays for all ξ, and high wave numbers, ξ, decay more rapidly than low ξ, which gives us smoother solutions as time evolves.

In fact, even if the initial data is discontinuous, the solution is still C^∞ for all $t > 0$. Very singular initial data leads to smooth solutions in time. If the initial data is in L^p for $1 \le p \le \infty$, then the solution is in C^∞ for all $t > 0$.

Lecture 2

Fourier Transforms

We say $u \in L^2(\mathbb{R})$ if $\|u\|_2 = (\int_{\mathbb{R}} |u(x)|^2 \, dx)^{1/2} < \infty$. For $u \in L^2$, the Fourier transform $\hat{u}(\xi)$ is

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u(x) e^{-i\xi x} dx.$$

$\hat{u}(\xi)$ is also in L^2 and the inverse transform is

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x} d\xi.$$

Parseval's Relation: $\|u(x)\|_2 = \|\hat{u}(\xi)\|_2$. We will use a discrete version to analyze stability of numerical schemes.

Fourier Transforms of Derivatives

Start from

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x} d\xi$$

and take derivative w.r.t. x,

$$u_x(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} i\xi \hat{u}(\xi) e^{i\xi x} d\xi.$$

The Fourier transform of $u_x(x)$ is $i\xi\hat{u}(\xi)$. Similarly, the Fourier transform of $u_{xx}(x)$ is $-\xi^2\hat{u}(\xi)$.
Consider diffusion equation

$$\begin{cases} u_t = Du_{xx} \\ u(x,0) = u_0(x) \end{cases},$$

we take transform of this equation and it yields

$$\begin{cases} \hat{u}_t(\xi,t) = -\xi^2 D\hat{u}(\xi,t) \\ \hat{u}(\xi,0) = \hat{u}_0(\xi) \end{cases}.$$

The solution is

$$\hat{u}(\xi,t) = \hat{u}_0(\xi) e^{-D\xi^2 t}$$

From here, we observe that the higher frequency (large $|\xi|$) will be knocked out very quickly in time. Also,

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

Consider the special case of Gaussian initial data

$$u_0(x) = e^{-\beta x^2}, \quad \hat{u}_0(\xi) = \frac{1}{\sqrt{2\beta}} e^{-\xi^2/4\beta}.$$

The solution to the diffusion equation will be

$$u(x,t) = \frac{1}{(4\beta Dt + 1)^{1/2}} \exp\left(\frac{-x^2}{4Dt + \beta^{-1}}\right).$$

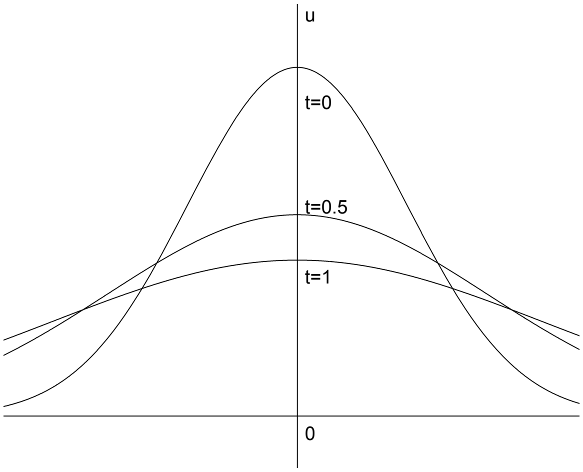

Figure 2: The plots of $u(x,t)$ with different t.

Now we rescale so that the initial data integrates to 1:

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt + \pi\beta^{-1}}} \exp\left(\frac{-x^2}{4Dt + \beta^{-1}}\right).$$

This is a normal distribution (i.e. the bell curve) with mean zero and variance $\sigma^2 = 2Dt + 1/(2\beta)$. The variance is growing linearly in time, which shows how the data becomes more spread out as time increases. As $\beta \to \infty$, the initial data gets narrower (the initial variance goes to zero) and the initial data approaches the Dirac delta function (which is a distribution, not a function).
The heat kernel

$$G(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)$$

is the solution to

$$\begin{cases} u_t = Du_{xx} \\ u(x,0) = \delta(x) \end{cases}$$

and for any initial data $u(x,0) = u_0(x)$, we can find u by convolving G with u_0

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{\mathbb{R}} \exp\left(\frac{-(x-y)^2}{4Dt}\right) u_0(y)dy, \quad t > 0$$

Note that $u(x,t) \to u_0(x)$ pointwise as $t \to 0$. Notice that information propagates infinitely fast. The initial data at a point affects the solution at all points for all $t > 0$.

Numerical Scheme

$$\begin{cases} u_t = Du_{xx} \text{ on } x \in [0,1] \\ u(0) = u(1) = 0 \\ u(x,0) = f(x) \end{cases}$$

We know how to discretize space and approximate $\frac{\partial^2}{\partial x^2}$ using finite differences.

Discretize space: $x_j = jh$, $h = \frac{1}{N+1}$. So $u_j(t) \approx u(x_j,t)$ and

$$\frac{du_j(t)}{dt} = \frac{D}{h^2}\left(u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\right),\ j = 1, 2, \ldots, N,$$

which yields a system of the form

$$\begin{cases} \dfrac{d\underline{u}(t)}{dt} = L\underline{u} \\ \underline{u}(0) = \underline{f} \end{cases}.$$

By discretizing in space, we obtain a system of N coupled ODEs. Numerically solving PDEs in this way is called the Method of Lines. Note that for 2 and 3 spatial dimensions, or fine grids in 1-D, the resulting system of ODEs is quite large and impractical to solve with a standard generic black box ODE solver (such as MATLAB's ode45 or ode23, etc.) A solver designed for the particular PDE will generally be much more efficient.

Numerical ODEs

The simplest method for solving ODEs numerically is forward Euler: discrete time $t_n = n\Delta t$, where Δt is the time step (in the textbook, $\Delta t = k$).
Apply forward Euler to this problem

$$\frac{dy}{dt} = f(y),$$

we have

$$y^{n+1} = y^n + \Delta t \cdot f(y^n), \quad \text{or} \quad \frac{y^{n+1} - y^n}{\Delta t} = f(y^n)$$

where $y^n \approx y(t_n) = y(n\Delta t)$.
Let $u_j^n \approx u(x_j, t_n) = u(jh, n\Delta t)$, Fourier Euler discretization of diffusion equation is

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{D}{h^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right)$$

See handout #1 for a demonstration of the numerical solution to the heat equation with two different time steps. For the smaller time step the solution behaves as expected, but for the larger time step high-frequency oscillations develop in time and appear to grow. When solving Poisson equation we could choose a space step based on considerations of accuracy and efficiency alone. When choosing a time step we also need to consider We need to choose a time step and space step based on considering:

1. accuracy,
2. efficiency,
3. stability.

Forward Euler discretization of advection equation

$$u_t + au_x = 0,$$

with center differencing in space:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{a}{2h}(u_{j+1}^n - u_{j-1}^n) = 0,$$

or equivalently

$$u_j^{n+1} = u_j - \frac{a\Delta t}{2h}(u_{j+1}^n - u_{j-1}^n).$$

For any time step Δt

$$\max_j \left|u_j^n\right| \to \infty \text{ as } n \to \infty.$$

and we know the solution is bounded as $t \to \infty$.