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 Poisson operator
– how to solve the Possion equation
– the accuracy and convergence of the aforementioned methods

This quarter, we'll be tackling:

– time dependent problems such as

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

– mixed equations

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

– non-linear equations such as

$$u_t + u u_x = 0 \quad \text{OR} \quad u_t + u u_x = \epsilon u_{xx} \qquad \text{Burger's equation}$$

The latter non-linear example of Burger's equation is also an example of a singular perturbation.

– 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 $u_t = c^2 \Delta u$ is hyperbolic, let

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

which gives

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

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 this operator 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

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

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/weak form of the conservation law. Because x_1 and x_2 are arbitrary and ρ is smooth enough, we also get the differential form of the conservation law

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

Examples:

1) Let u be the concentration of a chemical

$$\implies u_t + (F(u))_x = 0$$

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

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

3) 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)):

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

Advection vs Diffusion

Compare the solutions of

$$u_t + a u_{xx} \text{ and } u_t = D u_x \text{ on } \mathbb{R}$$

We need an initial condition $u(x,0) = u_0(x)$. The solution to the advection equation is

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

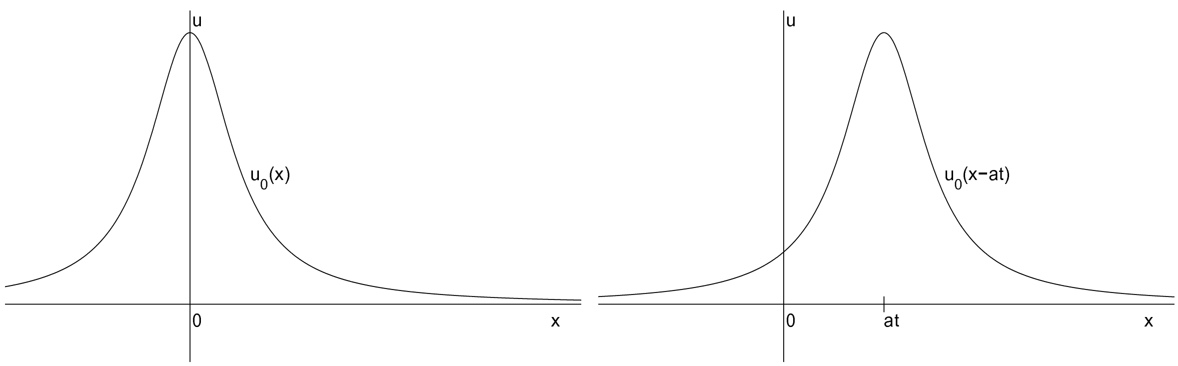

Figure 1: Behavior of a the solution to the advection equation.

For the heat equation (diffusion equation), $u_t = D u_{xx}$, 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 $u(x,t) = e^{-D\xi^2 t} e^{i\xi x} \implies |u(x,t)| = e^{-D\xi^2 t}$.

The amplitude decays and high wave numbers ξ decay more rapidly than low ξ, which gives us smoother solutions as time evolves.

In fact, if the initial data is discontinuous, the solution is still C^∞ for all $t > 0$. In particular, if the initial data is in L^2, 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

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

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,

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

Special case: initial data Gaussian

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

The solution to the diffusion equation will be

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

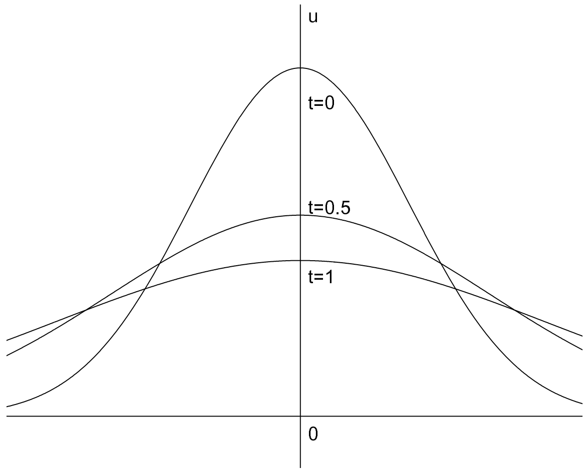

Figure 2: The plots of $u(x,t)$ with different t.

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

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

As $\beta \to 0$, the initial data gets narrower.

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 $u(x,0) = u_0(x)$,

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

Note that $u(x,t) \to u_0(x)$ pointwise as $t \to 0$.

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

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

which yields a system of the form

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

Now we discretize the space only and now solve the system of ODE: Method of lines.

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

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

[Bob's Pic here]

Choose a time step:

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

Forward euler discretization of advection equation

$$u_t + au_x = 0,$$

center 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

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

This scheme is always unstable for any Δt:

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

We know the solution should be bounded as $t \to \infty$.