PDE - Lecture 2, 9/10/2013

Today's focus: several ways of representing/approximating/thinking about solns of $u_t - \Delta u = 0$ (+ related eqns) in a bounded domain $\Omega \subset \mathbb{R}^n$ (with suitable bdry cond). We'll discuss mainly

A) separation of variables (eg Fourier series)

B) finite differences (cont's in time, discrete in space)

C) implicit-in-time discretization (cont's in space, discrete in time)

Recurrent themes:

1) linear heat eqn is, essentially, an "infinite-dimensional ODE" (indeed, a rather special one, similar to $\dot{x} = Ax$ where $x \in \mathbb{R}^n$ + A is an $n \times n$ pos def symmetric matrix)

2) different viewpts have different strengths (eg with regard to what's easy to see, + what types of generalizations are possible).

Separation of variables

Consider $u_t - \Delta u = 0$ in $\Omega \subset \mathbb{R}^n$

$$u = 0 \text{ at } \partial\Omega$$

$$u = u_0(x) \text{ at } t = 0$$

with Ω = bounded domain. Key fact: the (normalized) eigenfunctions of the Laplacian (with Dir bc)

$$-\Delta \varphi_n = \lambda_n \varphi_n \quad \text{in } \Omega$$
$$\varphi_n = 0 \quad \text{at } \partial\Omega$$

form a complete orthonormal set (i.e they span $L^2(\Omega)$). So we can write

$$u_0 = \sum a_n \varphi_n(x)$$

with $a_n = \langle u_0, \varphi_n \rangle = \int_\Omega u_0(x)\varphi_n(x)\,dx$ (I use here the normalization $\int_\Omega \varphi_n^2(x)\,dx = \|\varphi_n\|^2 = 1$) and soln to our pbm is

$$(*) \qquad u(x,t) = \sum_{n=1}^{\infty} a_n e^{-\lambda_n t} \varphi_n(x)$$

Notes:

(1) In 1D, with $\Omega = [0, L]$, $\varphi_n(x) = \sin\left(\frac{n\pi}{L}x\right)$ and $\lambda_n = n^2\pi^2/L^2$, $n = 1, 2, \ldots$

Eigenvalues are simple in this case.

In 2D, if $\Omega = [0,L] \times [0,L]$, eigenfns are $\sin\left(\frac{k\pi}{L}x\right)\sin\left(\frac{l\pi}{L}y\right)$ with assoc eigenvalue $(k^2+l^2)\pi^2/L^2$. Eigenvalues are not always simple in this case! (We naturally order them s.t. $\lambda_1 \le \lambda_2 \le \lambda_3 \le \ldots$)

In general we can't expect to write a formula for the eigenfns + eigenvalues, but (*) is still a good repn of the soln

(2) We see from (*) that u decays exp to 0 (since $\lambda_1 > 0$), and that higher modes decay faster.

(3) We also see from (*) that solving heat equation backward in time is ill-posed; put differently: eqn of $v_t + \Delta v = 0$ for $t > 0$ is exquisitely sensitive to small changes of initial data, since if $v(x,0) = v_0(x)$ then $v = \sum a_n e^{+\lambda_n t}\varphi_n(x)$, $a_n = \langle v_0, \varphi_n \rangle$

and higher modes (large n, so large λ_n) grow faster. So it is not true that $\|v_0 - \tilde{v}_0\|$ small at time $0 \Rightarrow v - \tilde{v}$ small later on. Such an est is true when we solve the "right way" in time, eg $u_t - \Delta u = 0$ for $t > 0$.

(4) Situation is very much like ODE

$$\dot{x} = Ax \quad \text{in } \mathbb{R}^N$$

where A is a symm, pos def $N \times N$ matrix (which we can diagonalize by using a basis of eigenvectors).

In fact, $u \to \Delta u$ is a self-adjoint linear map on the class of (smooth enough) fns u with $u|_{\partial\Omega} = 0$, using the L^2 inner product, since if $u|_{\partial\Omega} = 0$ + $v|_{\partial\Omega} = 0$ then

$$\langle u, \Delta v \rangle = \int_\Omega u \Delta v = -\int_\Omega (\nabla u, \nabla v)$$

$$= \int_\Omega \Delta u \cdot v$$

$$= \langle \Delta u, v \rangle$$

We also see from this that $-\Delta$ is positive:

$$\langle u, -\Delta u \rangle = \int_\Omega |\nabla u|^2 > 0 \quad (\text{unless } u \equiv 0)$$

so the eigenvalues of the (Dirichlet) Laplacian are strictly pos.

(5) If eqn has nonzero RHS, no problem: write it in the eigenfunction basis, then solve each scalar ODE separately.

For example: consider

$$u_t - \Delta u = f(x) \quad \text{in } \Omega$$
$$u = u_0 \quad \text{at } t=0.$$
$$u = 0 \quad \text{at } \partial\Omega.$$

If $f(x) = \sum c_n \varphi_n(x)$ then

$$u = \sum u_n(t)\, \varphi_n(x)$$

where $u_n(t) \in \mathbb{R}$ solves

$$\dot{u}_n + \lambda_n u_n = c_n \quad \text{for } t>0$$
$$u_n(0) = \langle u_0, \varphi_n \rangle$$

(this ODE is easy to solve explicitly,

since we assumed f was indep of time so C_n is a constant; but the viewpt works even if $f = f(x,t)$ depends on t as well as x).

Less coordinate-bound version: recall from ODE that soln of

$$\dot{z} = Az + \xi(t), \quad z(0) = z_0$$

is
$$z(t) = e^{At} z_0 + \int_0^t e^{(t-s)A} \xi(s)\, ds$$

(pf: mult eqn by e^{-At} to get $(e^{-At} z)_t = e^{-At} \xi(t)$ then integrate). Analogous formula for

$$\begin{aligned} u_t - \Delta u &= f & t > 0 \\ u &= 0 & \text{at } \partial\Omega \\ u &= u_0 & \text{at } t = 0 \end{aligned}$$

is
$$u(\cdot, t) = e^{t\Delta} u_0(\cdot) + \int_0^t e^{(t-s)\Delta} f(\cdot, s)\, ds$$

where $e^{t\Delta} v$ means "the solution of the linear heat eqn for time t, with Dir b.c., and initial data v"

Note that using eigenfunctions of Δ we get a convenient rep'n for $e^{t\Delta} v$.

(6) What about nonzero (Dir-type) bc? Use linear character of problem! Example: let's solve

$$u_t - \Delta u = 0 \quad \text{for } t > 0$$
$$u = u_0 \quad \text{at } t = 0$$
$$u = 1 \quad \text{at } \partial\Omega .$$

Answer: let $\tilde{u} = u - 1$. Solve

$$\tilde{u}_t - \Delta\tilde{u} = 0 \quad \text{for } t > 0$$
$$\tilde{u} = u_0 - 1 \quad \text{at } t = 0 .$$
$$\tilde{u} = 0 \quad \text{at } \partial\Omega .$$

Then add 1. Evidently

$$u(x,t) = 1 + \sum_{n=1}^{\infty} \langle u_0 - 1, \varphi_n \rangle e^{-\lambda_n t}$$

L^2 inner product

(Generalization of this: for $u_t - \Delta u = 0$ with bc $u = g$ at $\partial\Omega$, consider $\tilde{u} = u - U$ where $\Delta U = 0$ in Ω and $U = g$ at $\partial\Omega$.)

(7) Almost everything done above works equally well for the Neumann bc $\partial u/\partial n = 0$ at $\partial\Omega$

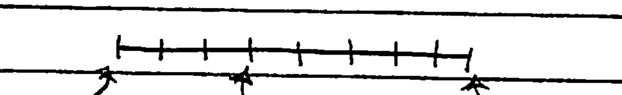
But: in that case you must use the <u>Neumann</u> eigenfunctions + eigenvalues

$$-\Delta\psi_n = \lambda_n \psi_n \quad \text{in } \Omega$$
$$\partial\psi_n/\partial n = 0 \quad \text{at } \partial\Omega.$$

One difference: 1^{st} eigenvalue is zero, with $\psi_1 = \text{const}$ as eigenfn. So soln doesn't decay to 0, but rather to a constant (namely: the average value of $u_0(x)$).

(8) The "separation of variables" (eigenfunction expansion) viewpt uses very strongly the <u>linear</u> character of the pde.

Now a different perspective: <u>finite difference approximation</u>. For simplicity let's do it in 1D (domain $\Omega = [0, L]$). Extnsn to square in 2D is obvious (but extnsn to domain with curved bdry is much more subtle).



$x_0 = 0$ $\quad x_j = j\Delta x$ $\quad x_N = 1$ $\quad \Delta x = \frac{1}{N}$

Obvious discretization (in space only) of $u_t = u_{xx}$

is the system of ODE's for $u_j(t) = u(j\Delta x, t)$

$$\dot{u}_j = \frac{u_{j-1} + u_{j+1} - 2u_j}{(\Delta x)^2}$$

[Recall: if $f(x)$ is smooth enough then

$$f(x+\Delta x) = f(x) + \Delta x \cdot f'(x) + \tfrac{1}{2}(\Delta x)^2 f''(x) + \tfrac{1}{6}(\Delta x)^3 f'''(x) + O(|\Delta x|^4).$$

$$f(x-\Delta x) = f(x) - \Delta x \cdot f'(x) + \tfrac{1}{2}(\Delta x)^2 f''(x) - \tfrac{1}{6}(\Delta x)^3 f'''(x) + O(|\Delta x|^4).$$

so $\left| \dfrac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{(\Delta x)^2} - f''(x) \right| \le C|\Delta x|^2$.].

Bdry conds?

- if we have Dir bc ($u_0(t)$ + $u_N(t)$ are given) then no problem: just solve for $u_1(t), \dots, u_{N-1}(t)$.

- if we have homogeneous Neumann bc ($u_x = 0$ at $x = 0, 1$) then look for a soln that's <u>even</u> about endpts, ie view $u_{-1}(t) = u_1(t)$ + $u_{N+1}(t) = u_{N-1}(t)$; then we solve for $u_0(t)$ + $u_N(t)$ as well as $u_j(t)$ $(1 \le j \le N-1)$ but we have enough eqns:

$$\dot{u}_N = \frac{2u_{N-1} - 2u_N}{(\Delta x)^2}, \quad \dot{u}_0(t) = \frac{2u_1 - 2u_0}{(\Delta x)^2}$$

How accurate is it? Let's focus on case of Dir bc, and let's assume the exact soln is C^4 (HW 2 will include a problem about that). Let

$$z_j = u_j - u_j^{exact}$$

where u_j^{exact} = exact soln at $x_j = j\Delta x$. Then

$z_j = 0$ initially; $z_0(t) = 0$ + $z_N(t) = 0$ for all time; and

$$\dot{z}_j - \frac{z_{j+1} + z_{j-1} - 2z_j}{(\Delta x)^2} = O(|\Delta x|^2)$$

See HW2 for how this implies the error est $|z_j(t)| \le C(\Delta x)^2 t$

Note that this viewpt is not so linear. For example: if pde were $u_t = u_{xx} + f(u)$ we could do something very similar.

What if we discretize both space + time? The simplest ("explicit Euler") scheme is

$$\frac{u_j(t_{n+1}) - u_j(t_n)}{\Delta t} = \frac{u_{j-1}(t_n) + u_{j+1}(t_n) - 2u_j(t_n)}{(\Delta x)^2}$$

with $t_n = n\Delta t$. Reorganizing, we get

$$u_j(t_{n+1}) = \alpha u_{j-1}(t_n) + \alpha u_{j+1}(t_n) + (1-2\alpha)\, u_j(t_n)$$

with $\alpha = \frac{\Delta t}{(\Delta x)^2}$. View this as

$$u_j(t_{n+1}) = \text{weighted avg of } u_{j-1},\ u_j,\ u_{j+1} \text{ at time } t_n$$

It is crucially important that $\boxed{\alpha \le 1/2}$, ie that $\Delta t \le \frac{1}{2}(\Delta x)^2$. Then the weights are all nonneg, + we get a discrete max principle

$$\max_j |u_j(t_{n+1})| \le \max_j |u_j(t_n)|$$

If $\alpha > 1/2$ the weight $1-2\alpha$ is neg; the discrete max prin fails, and the scheme is unstable (eg small initial data can grow exponentially).

Now a third viewpt, that of "<u>steepest descent</u>".

Reminder from ODE: given a function $F: \mathbb{R}^N \to \mathbb{R}$, the assoc "steepest descent" ODE is

$$\dot{z} = -\nabla F(z).$$

Also, the meaning of $\nabla F(z)$ is that for any curve $z(\tau)$ (not solving any ode)

$$\frac{d}{d\tau} F(z(\tau)) = \langle \nabla F(z(\tau)), \dot{z}(\tau) \rangle$$

using the standard inner product on $\mathbb{R}^N$ on the RHS.

There are two "obvious" ways to discretize such an ODE in time:

$$\frac{z(t_{n+1}) - z(t_n)}{\Delta t} = -\nabla F(z(t_n)) \qquad \text{"explicit Euler"}$$

which is what we did above at top of pg 2.11; or

$$\frac{z(t_{n+1}) - z(t_n)}{\Delta t} = -\nabla F(z(t_{n+1})) \qquad \text{"implicit Euler".}$$

The latter is less easy to implement (you have to solve a linear or nonlinear system for $z(t_{n+1})$) but it is always stable (no restr on Δt of the type we experienced above). Note that implicit time step is equiv to 1st order optimality condn for

$$y = z(t_{n+1}) \text{ solves } \min_y F(y) + \frac{|y - z(t_n)|^2}{2\Delta t}.$$

(1st order condn $\Leftrightarrow$ optimality if F is convex + $F \to \infty$ as $|y| \to \infty$).

Connection to heat eqn:

1st pass: our discrete-space, cont's time version of 1D heat eqn with Dir bc

$$\dot{u}_j(t) = \frac{u_{j-1} + u_{j+1} - 2u_j}{(\Delta x)^2}$$

$$u_0(t) = 0 \quad + \quad u_N(t) = 0 \quad \text{for all } t$$

$$u_j(0) = u_0(j\Delta x)$$

is the steepest-descent ODE for

$$F = \sum_{j=1}^{N} \frac{|u_j - u_{j-1}|^2}{(\Delta x)^2}$$

viewed as a fn of $u_1, \dots, u_{N-1}$, with the convention $u_0 = u_N = 0$.

This is, of course, a finite-difference version of $\int |\nabla u|^2 dx$.

2nd pass: for any bounded $\Omega \subset \mathbb{R}^n$, the heat eqn

$$\begin{aligned} u_t &= \Delta u \quad \text{in } \Omega \\ u &= 0 \quad \text{at } \partial\Omega \\ u &= u_0 \quad \text{at } t=0 \end{aligned}$$

is the "steepest-descent" ODE in function space for the "Dirichlet integral"

$$E[u] = \frac{1}{2}\int_\Omega |\nabla u|^2 dx$$

and bc $u=0$ at $\partial\Omega$, using the L^2 inner product.

Justification: if $v(\tau, x)$ is any (smooth) fn with $v=0$ at $\partial\Omega$,

$$\begin{aligned} \frac{d}{d\tau} E[v(\tau)] &= \int_\Omega (\nabla v, \nabla v_\tau)\, dx \\ &= -\int_\Omega \Delta v \cdot v_\tau \, dx \\ &= \langle -\Delta v, v_\tau \rangle_{L^2(\Omega)} \end{aligned}$$

so $\nabla E = -\Delta v$. Thus the steepest descent eqn $u_t = -\nabla E[u]$ says $u_t = \Delta u$.

From this perspective, we see that the natural "implicit" time step for solving the heat eqn is

$$\frac{u(x,t_{n+1}) - u(x,t_n)}{\Delta t} = \Delta u(x, t_{n+1}) \quad \text{in } \Omega.$$

Also that a convenient way to find u at time t_{n+1} is to solve

$$\min_{\substack{v=0 \\ \text{at } \partial\Omega}} \frac{1}{2}\int_\Omega |\nabla v|^2 + \int_\Omega \frac{|v - u(x,t_n)|^2}{2\Delta t}\,dx$$

then set $u(x,t_{n+1}) = v(x)$. (We'll talk abt such var'l problems when we get to the segment on Laplace's eqn + its cousins.)

The "steepest-descent" viewpt extends easily to many nonlinear problems; for example

$u_t = \Delta u + u^3$ is steepest descent for $\int_\Omega \frac{1}{2}|\nabla u|^2 - \frac{1}{4}u^4$

and

$u_t = \operatorname{div}(|\nabla u|^2 \nabla u)$ is steepest descent for $\int_\Omega \frac{1}{4}|\nabla u|^4$.