Math 6620: Analysis of Numerical Methods, II
Finite difference methods for time-dependent problems, Part I

See LeVeque 2007, Chapter 9,
Langtangen and Linge 2017, Chapter 3,

Kreiss, Oliger, and Gustafsson 2013, Chapters 1, 3, 6

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Basics concepts for linear PDEs

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To contextualize what to expect from numerical approximations, we need some basic theory for linear PDEs.

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Consider a scalar PDE for $u = u(x, t)$ having the form,

$$u_t = p\left(\frac{\partial}{\partial x}\right) u,$$

with periodic boundary conditions on $x \in [0, 2\pi)$.
Above, p is a is an operator involving (possibly high-order) spatial derivatives of u.

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Example

The operator,

$$p\left(\frac{\partial}{\partial x}\right) = \frac{\partial^2}{\partial x^2}$$

corresponds to a prototypical *parabolic* equation, which we will our focus in these slides.

This is, in many senses, the "easiest" example.

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Example

The operator,

$$p\left(\frac{\partial}{\partial x}\right) = a(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial}{\partial x}\right) + r(x),$$

corresponds to a convection-reaction-diffusion problem with variable coefficients.

All of what follows applies for vector-valued problems in multiple space dimensions, as well.

Fourier transforms

Our main tool to understand basic PDEs will be Fourier transforms: Given a function $f(x)$ on $[0, 2\pi)$, the Fourier Transform of x is given by,

$$F(\omega) = \mathcal{F}[f] := \int_0^{2\pi} f(x)\overline{\phi(x,\omega)}\mathrm{d}x, \qquad \phi(x,\omega) := \frac{1}{\sqrt{2\pi}} e^{i\omega x},$$

where $\omega \in \mathbb{Z}$, and $\overline{\phi}$ is the complex conjugate with $i = \sqrt{-1}$ the imaginary unit.

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The Fourier transform is an isometry between $L^2([0, 2\pi]; \mathbb{C})$ and $\ell^2(\mathbb{Z}; \mathbb{C})$:

$$\int_0^{2\pi} |f(x)|^2 \,\mathrm{d}x = \sum_{\omega\in\mathbb{Z}} |F(\omega)|^2,$$

and in particular $\mathcal{F}$ and $\mathcal{F}^{-1}$ are well-defined operations,

$$f(x) \overset{L^2}{=} \mathcal{F}^{-1}[F(\omega)] = \sum_{\omega\in\mathbb{Z}} F(\omega)\phi(x,\omega).$$

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A particularly important property of Fourier transforms for us is the ω-representation of spatial derivatives:

$$\mathcal{F}\left(\frac{\mathrm{d}}{\mathrm{d}x} f\right) = i\omega F(\omega)$$

Fourier transforms allow us to "easily" identify solutions to PDEs:

Since $p\left(\frac{\partial}{\partial x}\right) u$ is a linear differential operator acting on u, then the Fourier transform of this expression is a polynomial in ω,

$$\mathcal{F}\left[p\left(\frac{\partial}{\partial x}\right) u(x,t)\right] = P(\omega)U(\omega,t),$$

where U is the Fourier transform of u.

The function $P(\omega)$ is called the symbol (of the operator $p(\frac{\partial}{\partial x})$).

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The symbol makes solving linear PDE's "easy":

$$u_t = p\left(\frac{\partial}{\partial x}\right) u, \qquad u(x,0) = u_0(x)$$

$$\Downarrow \mathcal{F}[\cdot] \qquad \Downarrow \mathcal{F}[\cdot]$$

$$\frac{\mathrm{d}}{\mathrm{d}t}U(\omega,t) = P(\omega)U, \qquad U(\omega,0) = U_0(\omega).$$

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The solution is

$$U(\omega,t) = U_0(\omega)e^{P(\omega)t} \implies u(x,t) = \sum_{\omega\in Z} U(\omega,t)\phi(x,\omega) = \frac{1}{\sqrt{2\pi}}\sum_{\omega=-\infty}^{\infty} U_0(\omega)e^{P(\omega)t}e^{i\omega x}.$$

$$u_t = p\left(\frac{\partial}{\partial x}\right) u, \qquad\qquad u(x,0) = u_0(x).$$

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \sum_{\omega \in \mathbb{Z}} U_0(\omega) e^{P(\omega)t} e^{i\omega x}$$

Although we obtained an explicit solution, there are some assumptions we need to ensure rigor of the arguments.

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Definition

The PDE above is **stable** if there exists $K, \alpha \in \mathbb{R}$ such that

$$\left| e^{P(\omega)t} \right| \leqslant K e^{\alpha t}, \qquad t \geqslant 0, \quad \omega \in \mathbb{Z}.$$

This notion of stability is a natural requirement for solvability of PDEs.

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Theorem (Well-posedness)

If the PDE above is stable, then the Fourier-based formula for $u(x,t)$ above is the unique solution, and is "smooth".

The heat equation

Our simplest example of a *parabolic* equation is,

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The symbol is rather easily computed here,

$$\mathcal{F}\left[\frac{\partial^2}{\partial x^2} u(x,t)\right] = -\omega^2 U(\omega,t) =: P(\omega) U(\omega,t).$$

Hence, the exact solution to this problem is,

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \sum_{\omega \in \mathbb{Z}} U_0(\omega) e^{-\omega^2 t} e^{i\omega x}.$$

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The main point here is that initial frequency components $U_0(\omega)$ are attentuated exponentially in time.

In particular, $|e^{P(\omega)t}| \leqslant 1$ for all t, ω, so the PDE is stable and the solution above is unique + smooth.

Parabolic equations, I

Equations that behave *essentially* like the heat equation are parabolic problems.

Let $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ be the standard $L^2([0, 2\pi])$ inner product and norm, respectively.

The signature behavior of the heat equation is energy dissipation according to the derivative (variation) of u:

$$u_t = u_{xx} \xrightarrow{\text{multiply by } u, \text{ integrate}} \frac{\mathrm{d}}{\mathrm{d}t} \|u\|^2 = -2\|u_x\|^2.$$

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Because of this, a linear PDE (defined by the operator p) is parabolic if

$$\langle u, pu \rangle + \langle pu, u \rangle \leqslant -\delta \|u_x\|^2,$$

for some $\delta > 0$.

Such an equation is "at least" as dissipative as $u_t = \delta u_{xx}$.

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for some $\delta > 0$.

Such an equation is "at least" as dissipative as $u_t = \delta u_{xx}$. For example,

$$u_t = \frac{\partial}{\partial x} \left(\kappa(x) u_x \right),$$

is parabolic if $\inf_x \kappa(x) = \delta > 0$.

A conceptually simple example of a PDE that is not stable (certainly not parabolic) is,

$$u_t = -u_{xx}, \qquad u(x,0) = u_0(x),$$

whose symbol is $P(\omega) = \omega^2$. In particular, there is no K, α such that,

$$|e^{\omega^2 t}| \leqslant K e^{\alpha t}$$

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When designing numerical methods, it's helpful to understand theoretical expectations for the scheme.

With an understanding of what is expected from parabolic problems, let's discretize the heat equation,

$$u_t = u_{xx}, \qquad u(x,0) = u_0(x), \qquad u(0,t) = u(2\pi, t),$$

for $x \in [0, 2\pi)$.

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for $x \in [0, 2\pi)$.

One strategy to dive right in:

- Equidistant discretization for x and t
- $x_j = \frac{j}{M2\pi}$, $j \in [M]$. Periodic BC's: we identify $x_M \leftrightarrow x_0$. $x_j = 2\pi\, j/M$
  $h = \Delta x = x_{j+1} - x_j$
- $t_n = nk$, $k > 0$ for $n = 0, 1, \ldots$
  $k = \Delta t = t_{k+1} - t_k$
- $u_j^n \approx u(x_j, t_n)$, $\boldsymbol{u}^n = (u_0^n, \ldots, u_{M-1}^n)^T$
- use our standard $D_- D_+$ discretization for u_{xx}
- use a Forward Euler discretization for u_t: $D^+ u_j^n := \frac{1}{k}(u_j^{n+1} - u_j^n)$

NB: The superscript n is a temporal index, *not* an exponent.

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The scheme is then:

$$D^+ u_j^n = D_- D_+ u_j^n, \qquad j \in [M], \qquad n \geqslant 0.$$

FD stencils

$$D^+ u_j^n = D_- D_+ u_j^n, \qquad j \in [M], \qquad n \geqslant 0.$$

This scheme, more explicity, is given by,

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

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To practice this notation: here is Crank-Nicolson for the same spatial discretization,

$$D^+ u_j^n = \frac{1}{2} D_- D_+ u_j^n + \frac{1}{2} D_- D_+ u_j^{n+1}, \qquad j \in [M], \qquad n \geqslant 0,$$

i.e.,

$$\begin{aligned} u_j^{n+1} = u_j^n + \frac{k}{2h^2}(&u_{j-1}^n - 2u_j^n + u_{j+1}^n \\ &u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}). \end{aligned}$$

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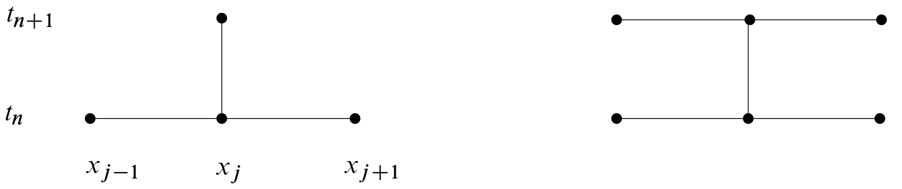

Figure: Finite difference stencils. LeVeque 2007, Figure 9.1

$$u_t = u_{xx}$$
$$D^+ u_j^n = D_+ D_- u_j^n.$$

This is our first finite difference scheme, but there are many questions we have yet to answer:

- Stability?
- Accuracy?
- Convergence?
- Other types of discretizations?

References I

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