SF2520 — Applied numerical methods

Lecture 10

Parabolic equations

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2023-10-09

Today's lecture

- Parabolic equations, intro
- Numerical methods
  - Semi-discretizations
  - Stability, CFL conditions

Parabolic PDEs

We consider the 1D model parabolic equation (heat or diffusion equation) for $u = u(x,t)$

$$\begin{aligned} u_t - u_{xx} &= 0, && x \in (a,b), \quad t > 0, \\ u(x,0) &= g(x), && x \in (a,b), \\ u(a,t) = \alpha(t), &\quad u(b,t) = \beta(t), && t > 0. \end{aligned}$$

- General classification of

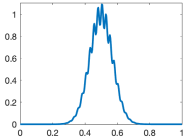
$$au_{xx} + 2bu_{xy} + cu_{yy} = 0$$

  gives $a = -1$, $b = c = 0$ and $b^2 - ac = 0$, i.e. parabolic.
- Two dimensional version, for $u = u(x,y,t)$,

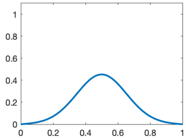
$$\begin{aligned} u_t - \Delta u &= 0, && (x,y) \in \Omega, \quad t > 0, \\ u(x,y,0) &= g(x,y), && (x,y) \in \Omega, \\ u &= h(x,y), && (x,y) \in \partial\Omega, \quad t > 0. \end{aligned}$$

Parabolic equations, examples

Parabolic equations describe diffusion, "smearing", in time.



t = 0



t = 0.01

- Heat flow in a rod.

$$u_t - \alpha u_{xx} = 0,$$

$$u(x,0) = 20, \qquad u(0,t) = \beta(t), \qquad u_x(1,t) = 0.$$

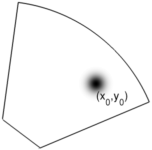
u — temperature　　　α — thermal diffusivity

20 — initial temperature　　　$\beta(t)$ — temperature at left end

- Coffee drop on a Melitta filter

$$u_t - \alpha \Delta u = f, \quad u(\boldsymbol{x},0) = 0,$$

$$\frac{\partial u}{\partial n}(\boldsymbol{x},t) = 0, \quad x \in \partial\Omega.$$



u — coffee concentration　　　f — coffee source

α — diffusion coefficient

Parabolic equations, examples

- Option prices (Black &Scholes eq.)

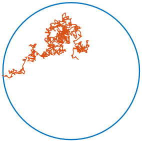
$$u_t - \frac{1}{2}\sigma^2 x^2 u_{xx} - rxu_x + ru = 0, \qquad u(x,0) = \max(x-K,0)$$

$$u(0,t) = 0, \qquad \lim_{x\to\infty} u(x,t) - (x-K) = 0.$$

$u(x,t)$ — option price
x — share price
t — time to maturity
σ — volatility
r — risk free interest rate
K — strike price

- Brownian motion statistics (Fokker-Planck)

$$u_t - \frac{1}{2}\Delta u = 0, \quad u(\boldsymbol{x},0) = \delta(\boldsymbol{x}-\boldsymbol{x}_0),$$
$$\frac{\partial u}{\partial n}(\boldsymbol{x},t) = 0, \quad x \in \partial\Omega.$$



u — probability distribution of position for Brownian motion starting in $\boldsymbol{x}_0$

Parabolic PDEs, smearing property

Consider the 1D model parabolic equation

$$\begin{aligned} u_t - u_{xx} &= 0, && x \in (0,\pi), \quad t > 0, \\ u(x,0) &= g(x), && x \in (0,\pi), \\ u(0,t) = u(\pi,t) &= 0, && t > 0. \end{aligned}$$

- Exact solution can be expressed by Fourier series. Write u as

$$u(x,t) = \sum_{k=1}^{\infty} \hat{u}_k(t)\sin(kx), \qquad \hat{u}_k(0) = \hat{g}_k \quad \left(\text{where } g(x) = \sum_{k=1}^{\infty} \hat{g}_k \sin(kx).\right)$$

(Boundary conditions $u(0) = u(\pi) = 0$ and initial condition $u(x,0) = g(x)$ satisfied.)

- Compute derivatives:

$$u_t(x,t) = \sum_{k=1}^{\infty} \hat{u}_k'(t)\sin(kx), \qquad u_{xx}(x,t) = \sum_{k=1}^{\infty} -k^2\hat{u}_k(t)\sin(kx).$$

$$u_t - u_{xx} = 0 \quad \Rightarrow \quad \hat{u}_k'(t) + k^2\hat{u}_k(t) = 0 \quad \Rightarrow \quad \hat{u}_k(t) = \hat{u}_k(0)e^{-k^2 t}.$$

- Solution is $u(x,t) = \sum_{k=1}^{\infty} \hat{g}_k e^{-k^2 t}\sin(kx)$.
  High frequencies are damped fast $\Rightarrow$ "smearing" of rough solution.

Numerical methods

Want to construct numerical methods for heat equation

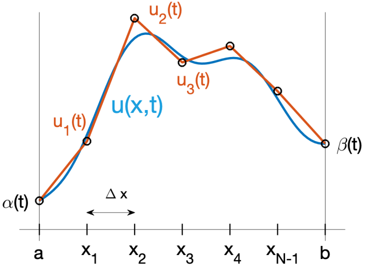
$$
\begin{aligned}
u_t - u_{xx} &= f, && x \in (a,b), \quad t > 0, \\
u(x,0) &= g(x), && x \in (a,b), \\
u(a,t) = \alpha(t), &\quad u(b,t) = \beta(t), && t > 0.
\end{aligned}
$$

- Simplest approach: semi-discretization, "method of lines" (MoL)
  - Just discretize in space $\Rightarrow$ system of ODEs
  - Solve ODEs with standard ODE method
- As in boundary value problem, discretize

$$x_j = a + j\Delta x, \qquad \Delta x = \frac{b-a}{N},$$

$$j = 0, \ldots, N,$$

and let $u_j(t) \approx u(x_j, t)$ be the unknowns.



Numerical methods

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$$\begin{aligned}
u_t - u_{xx} &= f, && x \in (a,b), \quad t > 0, \\
u(x,0) &= g(x), && x \in (a,b), \\
u(a,t) = \alpha(t), \quad u(b,t) &= \beta(t), && t > 0.
\end{aligned}$$

- Approximate u_{xx} with central differences,

$$\begin{aligned}
u_{xx}(x_j,t) &= \frac{u(x_{j+1},t) - 2u(x_j,t) + u(x_{j-1},t)}{\Delta x^2} + O(\Delta x^2) \\
&\approx \frac{u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)}{\Delta x^2}.
\end{aligned}$$

- Since $u_{xx}(x_j,t) + f(x_j,t) = u_t(x_j,t) \approx u_j'(t)$ we get ODEs

$$\frac{du_j(t)}{dt} = \frac{u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)}{\Delta x^2} + f(x_j,t), \qquad j = 1, \ldots, N-1.$$

Numerical methods

- Adding boundary and initial conditions:

$$
\begin{aligned}
\frac{du_1(t)}{dt} &= \frac{u_2(t) - 2u_1(t) + \alpha(t)}{\Delta x^2} + f(x_1, t), \\
\frac{du_j(t)}{dt} &= \frac{u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)}{\Delta x^2} + f(x_j, t), \qquad j = 2, \ldots, N-2, \\
\frac{du_{N-1}(t)}{dt} &= \frac{\beta(t) - 2u_{N-1}(t) + u_{N-2}(t)}{\Delta x^2} + f(x_{N-1}, t), \\
u_j(0) &= g(x_j).
\end{aligned}
$$

- This is a system of ODEs of the form

$$
\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{g}, \qquad \text{where } \boldsymbol{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix},
$$

$$
A = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}, \quad \boldsymbol{b}(t) = \begin{pmatrix} f(x_1, t) + \frac{\alpha(t)}{\Delta x^2} \\ f(x_2, t) \\ \vdots \\ f(x_{N-2}, t) \\ f(x_{N-1}, t) + \frac{\beta(t)}{\Delta x^2} \end{pmatrix}, \quad \boldsymbol{g} = \begin{pmatrix} g(x_1) \\ g(x_2) \\ \vdots \\ g(x_{N-2}) \\ g(x_{N-1}) \end{pmatrix}.
$$

Numerical methods

Semi-discretization thus gives:

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{g}.$$

- PDE turned into a large ODE system, where $\partial_{xx} \approx A$.
- Differences/similarities to boundary value problem:
  - Cannot multiply equation with Δx^2 to rescale
  - Boundary conditions must be inserted into inner equations. Cannot (easily) be kept as separate equations.
  - This considered, A and $\boldsymbol{b}$ are the same as in BVP, upto the sign.
- Called "method of lines" (MoL) since problem is solved along the lines $x =$constant and $t > 0$.
- Can be solved by standard ODE method, e.g. Explicit Euler:

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t(A\boldsymbol{u}^n + \boldsymbol{b}(t_n)), \qquad \boldsymbol{u}_0 = \boldsymbol{g},$$

where $\boldsymbol{u}^n \approx \boldsymbol{u}(t_n)$.

Numerical methods in 1D – Robin boundary conditions

Consider instead Robin conditions at $x = a$,

$$
\begin{aligned}
u_t - u_{xx} &= f, \\
u(x,0) &= g(x), \\
u_x(a,t) &= \alpha_0(t)u(a,t) + \alpha_1(t), \quad u(b,t) = \beta(t).
\end{aligned}
$$

- Add a ghost point at $x_{-1} = a - \Delta x$ outside domain and a new unknown u_{-1}. Keep equation for $j = 0$,

$$\frac{du_0(t)}{dt} = \frac{u_{-1}(t) - 2u_0(t) + u_1(t)}{\Delta x^2} + f(x_0, t)$$

- Approximate derivative with central difference and neglect $O(\Delta x^2)$,

$$\frac{u(x_1,t) - u(x_{-1},t)}{2\Delta x} = \alpha_0(t)u(a,t) + \alpha_1(t) + O(\Delta x^2)$$

$$\Rightarrow \quad u_{-1} = d_{-1} + d_0 u_0 + u_1, \quad d_{-1} = -2\Delta x \alpha_1(t), \quad d_0 = -2\Delta x \alpha_0(t).$$

- Inserting in equation $j = 0$ gives the change in matrix form

$$A = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \ \boldsymbol{b} = \begin{pmatrix} f_1 + \frac{\alpha}{\Delta x^2} \\ f_2 \\ \vdots \end{pmatrix} \quad \Rightarrow \quad \frac{1}{\Delta x^2}\begin{pmatrix} -2 + d_0 & 2 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \ \begin{pmatrix} f_0 + \frac{d_{-1}}{\Delta x^2} \\ f_1 \\ \vdots \end{pmatrix}.$$

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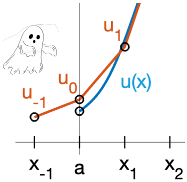

$$
\begin{aligned}
u_t - u_{xx} &= f, \\
u(x,0) &= g(x), \\
{\color{red} u_x(a,t) = \alpha_0(t)u(a,t) + \alpha_1(t),} \;\; & u(b,t) = \beta(t).
\end{aligned}
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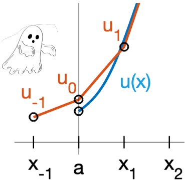

$$u_t - u_{xx} = f,$$
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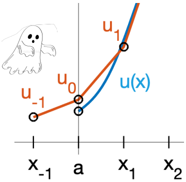

$$
\begin{aligned}
&u_t - u_{xx} = f,\\
&u(x,0) = g(x),\\
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- Add a ghost point at $x_{-1} = a - \Delta x$ outside domain and a new unknown u_{-1}. Keep equation for $j = 0$,

$$
\frac{du_0(t)}{dt} = \frac{u_{-1}(t) - 2u_0(t) + u_1(t)}{\Delta x^2} + f(x_0, t)
$$

- Approximate derivative with central difference and neglect $O(\Delta x^2)$,

$$
\frac{u(x_1,t) - u(x_{-1},t)}{2\Delta x} = \alpha_0(t)u(a,t) + \alpha_1(t) + O(\Delta x^2) \quad \Rightarrow \quad \frac{u_1 - u_{-1}}{2\Delta x} = \alpha_0 u_0 + \alpha_1,
$$
$$
\Rightarrow \quad u_{-1} = d_{-1} + d_0 u_0 + u_1, \quad d_{-1} = -2\Delta x \alpha_1(t), \quad d_0 = -2\Delta x \alpha_0(t).
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$$

Generalizations

Method of lines can be generalized straightforwardly to

- General 1D case,

$$u_t = \partial_x \kappa(x) \partial_x u + p(x) u_x + q(x) u + f(x).$$

- 2D case,

$$u_t = \Delta u.$$

  Use same spatial discretization of right hand side as for elliptic case, see e.g. Edsberg 6.4.

Stability

Let

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad A \in \mathbb{R}^{(N-1)\times(N-1)}, \quad \boldsymbol{u}(t), \boldsymbol{b}(t) \in \mathbb{R}^{N-1},$$

be a semi-discretization of the heat equation.

- Suppose we solve this with an ODE method. A necessary condition is then that the method is absolutely stable, i.e.

  $$\Delta t \lambda_k \in \mathcal{S}, \qquad k = 1, \ldots, N-1,$$

  where

  λ_k are the eigenvalues of A,
  $\mathcal{S}$ is the stability region of the ODE method.

- What does this mean for Δt?
  Note: A depends on Δx $\Rightarrow$ stability limit for Δt depends on Δx!

Stability (Explicit Euler)

For the central difference approximation used above (see Edsberg A.2)

$$A = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \end{pmatrix}, \qquad \lambda_k = -\frac{4}{\Delta x^2} \sin^2\left(\frac{k\pi}{2N}\right).$$

- Eigenvalues λ_k are real and for $k = 1, \ldots, N-1$ they lie in interval

$$\lambda_k \in \left(\frac{-4}{\Delta x^2}, \quad 0\right).$$

- For Explicit Euler we need $-2 < \Delta t \lambda_k < 0$ for all k, meaning that

$$-2 < \frac{-4\Delta t}{\Delta x^2} < 0 \quad \Rightarrow \quad \Delta t < \frac{1}{2}\Delta x^2.$$

  This is a necessary condition!
- A severe restriction on Δt! Note that Δx is already small, and $\Delta t \sim \Delta x^2$ is much smaller. For instance, we cannot take $\Delta t \sim \Delta x$.

Stability (Explicit Euler)

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad A \in \mathbb{R}^{(N-1)\times(N-1)}, \quad \boldsymbol{u}(t), \boldsymbol{b}(t) \in \mathbb{R}^{N-1},$$

is a semi-discretization of the heat equation $u_t - u_{xx} = f(t)$, where

$$A = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & & \end{pmatrix}, \qquad \lambda_k = -\frac{4}{\Delta x^2}\sin^2\left(\frac{k\pi}{2N}\right).$$

- If we add a diffusion coefficient α such that the heat equation is $u_t - \alpha u_{xx} = f(t)$, we get

$$A = \frac{\alpha}{\Delta x^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & & \end{pmatrix}, \qquad \lambda_k = -\frac{4\alpha}{\Delta x^2}\sin^2\left(\frac{k\pi}{2N}\right).$$

- Stability limit is

$$\Delta t < \frac{\alpha}{2}\Delta x^2.$$

Stability, conclusions

- Computer example.
- Absolute stability depends on Δt and Δx. When Δx is reduced, the size of A increases and a different ODE system is solved.
- It is not enough to have $\Delta t \ll 1$ and $\Delta x \ll 1$ for stability (as one might infer from ODE theory). It is the ratio $\Delta t/\Delta x^2$ that must be small.
- The ratio $\Delta t/\Delta x^2$ is often called the Courant number (sometimes CFL number). A stability restriction like

$$\frac{\Delta t}{\Delta x^2} < C \quad \text{or} \quad \frac{\Delta t}{\Delta x} < C,$$

  often called a "CFL condition".
- For parabolic equations solved with explicit methods the condition

$$\frac{\Delta t}{\Delta x^2} < C \quad \text{is typical.}$$

Implicit methods for parabolic equations

- Severe CFL condition stems from the fact that semi-discretizations of parabolic PDEs lead to stiff ODE systems. Typically,

$$\lambda_k \in \left(-\frac{C}{\Delta x^2}, \quad -\delta\right], \qquad \delta > 0, \quad k = 1, \dots, n,$$

  and λ_k evenly distributed over the interval.

$$\Rightarrow \quad \text{stiffness ratio} = \frac{\max|\lambda_k|}{\min|\lambda_k|} \sim \frac{C}{\delta \Delta x^2} \gg 1.$$

- Implicit methods therefore preferred for parabolic problems.
- More expensive per time step, but fewer steps can be taken. Time step Δt can be chosen only based on accuracy requirements, not stability.

Implicit methods for parabolic equations

Example: Implicit Euler

System is:

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad A \in \mathbb{R}^{(N-1)\times(N-1)}, \quad \boldsymbol{u}(t), \boldsymbol{b}(t) \in \mathbb{R}^{N-1},$$

- Then Implicit Euler reads

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t(A\boldsymbol{u}^{n+1} + \boldsymbol{b}(t_{n+1}))$$

or

$$(I - \Delta tA)\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t\boldsymbol{b}(t_{n+1}). \underbrace{(I - \Delta tA)}_{\text{sparse}}\boldsymbol{u}^{n+1} = \underbrace{\boldsymbol{u}^n + \Delta t\boldsymbol{b}(t_{n+1})}_{\text{known}}.$$

- Need to solve one sparse linear system per time step (tridiagonal in 1D, block tridiagonal in 2D). LU factorization of $I - \Delta tA$ recommended.
- Only first order accurate, but stable for all Δt, independent of Δx.

Implicit methods for parabolic equations

Example: Crank–Nicolson

- = central difference approximation in space + trapzeoidal method in time
- For
$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u} + \boldsymbol{b}(t), \qquad A \in \mathbb{R}^{(N-1)\times(N-1)}, \quad \boldsymbol{u}(t), \boldsymbol{b}(t) \in \mathbb{R}^{N-1},$$
it reads
$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \frac{1}{2}\Delta t\Big(A\boldsymbol{u}^n + \boldsymbol{b}(t_n) + A\boldsymbol{u}^{n+1} + \boldsymbol{b}(t_{n+1})\Big)$$
or
$$\underbrace{\left(I - \frac{1}{2}\Delta t A\right)}_{\textit{sparse}} \boldsymbol{u}^{n+1} = \underbrace{\left(I + \frac{1}{2}\Delta t A\right)\boldsymbol{u}^n + \frac{1}{2}\Delta t\Big(\boldsymbol{b}(t_n) + \boldsymbol{b}(t_{n+1})\Big)}_{\textit{known}}.$$
- Again, need to solve one sparse linear system per time step (tridiagonal in 1D, block tridiagonal in 2D). LU factorization of $I - \frac{1}{2}\Delta t A$ recommended.
- Second order accurate. Stable for all Δt independent of Δx.
- Other common choices for parabolic PDEs are BDF multistep methods.