1D Parabolic PDEs: Finite Difference Methods

M.Sc. in Mathematical Modelling & Scientific Computing,
Practical Numerical Analysis

Michaelmas Term 2019, Lecture 7

1D Heat Equation

First we consider the simplest parabolic PDE in the form of the heat equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} ,$$

for $t > 0$ and $x \in [a, b]$ with an initial condition

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

for $x \in [a, b]$. We begin by considering Dirichlet boundary conditions

$$\begin{aligned} u(a, t) &= u_a(t) , \\ u(b, t) &= u_b(t) , \end{aligned}$$

for $t > 0$.

The Mesh

We define a sequence of uniform timesteps by

$$t_m \quad = \quad m\Delta t$$

for $m = 0, 1, 2, \ldots$ where $\Delta t > 0$ is the constant timestep size.

We also define a set of uniform mesh points by

$$x_j \quad = \quad a + j\Delta x \ ,$$

for $j = 0, 1, \ldots, N$ and with the meshsize $\Delta x = (b - a)/N$.

We write $u(x_j, t_m) = u_j^m$ and seek to approximate u_j^m by U_j^m for $j = 0, 1, \ldots, N$ and $m = 0, 1, 2, \ldots$.

Finite Difference Schemes

As was the case for 1D boundary value problems we may write a central difference

$$\frac{\partial^2 u}{\partial x^2}(x_j, t) \quad = \quad \frac{u(x_{j+1}, t) - 2u(x_j, t) + u(x_{j-1}, t)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \; .$$

Similarly, as was the case for ODEs we may write a forward difference

$$\frac{\partial u}{\partial t}(x, t_m) \quad = \quad \frac{u(x, t_{m+1}) - u(x, t_m)}{\Delta t} + \mathcal{O}(\Delta t) \; ,$$

or a backward difference

$$\frac{\partial u}{\partial t}(x, t_{m+1}) \quad = \quad \frac{u(x, t_{m+1}) - u(x, t_m)}{\Delta t} + \mathcal{O}(\Delta t) \; .$$

Finite Difference Schemes

Alternatively we may combine these to get a θ-method of the form

$$(1-\theta)\frac{\partial u}{\partial t}(x,t_m)+\theta\frac{\partial u}{\partial t}(x,t_{m+1}) = \frac{u(x,t_{m+1})-u(x,t_m)}{\Delta t}+\mathcal{O}(\Delta t)$$

for $\theta \neq 1/2$ or, when $\theta = 1/2$,

$$\frac{1}{2}\frac{\partial u}{\partial t}(x,t_m)+\frac{1}{2}\frac{\partial u}{\partial t}(x,t_{m+1}) = \frac{u(x,t_{m+1})-u(x,t_m)}{\Delta t}+\mathcal{O}(\Delta t^2)\,.$$

Finite Difference Schemes

Such equalities lead to finite difference schemes of the form

- Forward Euler (or Explicit Euler)

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}$$

- Backward Euler (or Implicit Euler)

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2}$$

- θ-Method (Crank Nicolson when $\theta = 1/2$)

$$\begin{aligned}\frac{U_j^{m+1} - U_j^m}{\Delta t} &= \theta \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2} \\ &\quad + (1-\theta)\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}\end{aligned}$$

Finite Difference Schemes

All these finite difference schemes hold for $j = 1, \dots, N-1$ and $m = 0, 1, \dots$.

We must also discretise the initial and boundary conditions as

$$\begin{aligned} U_j^0 &= u_0(x_j)\,, \quad j = 0, 1, \dots, N \\ U_0^m &= u_a(t_m)\,, \quad m = 1, 2, \dots \\ U_N^m &= u_b(t_m)\,, \quad m = 1, 2, \dots \end{aligned}$$

Finite Differences — Implementation

We saw for ODEs that the forward Euler scheme was very simple to implement, whereas the θ-method for $\theta > 0$ required a nonlinear solve. Similar ideas hold for the heat equation but the nonlinear solve is replaced by the solution of a linear system.

Forward Euler Scheme

Recall the forward Euler scheme is

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}$$

for $j = 1, \ldots, N-1$ and $m = 0, 1, \ldots$. Writing $\mu = \Delta t / \Delta x^2$, we may re-arrange the scheme to get

$$U_j^{m+1} = U_j^m + \mu(U_{j+1}^m - 2U_j^m + U_{j-1}^m) \qquad (1)$$

for $j = 1, \ldots, N-1$ and $m = 0, 1, \ldots$.

Thus, once we have used the initial and boundary conditions to assign values to U_j^0 for $j = 0, 1, \ldots, N$ and U_0^m and U_N^m for $m = 1, 2, \ldots$, it is simple to set $m = 0$ in Equation (1) and compute all the U_j^1 etc.

θ-Method

The θ-method is

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \theta \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2} + (1-\theta)\frac{U_{j+1}^{m} - 2U_j^{m} + U_{j-1}^{m}}{\Delta x^2} .$$

(Recall this includes the backward Euler scheme if we take $\theta = 1$.)

Again we may write $\mu = \Delta t / \Delta x^2$ and re-arrange the scheme to get

$$\begin{aligned} & -\mu\theta U_{j+1}^{m+1} + (1+2\mu\theta)U_j^{m+1} - \mu\theta U_{j-1}^{m+1} \\ = \; & U_j^m + \mu(1-\theta)(U_{j+1}^m - 2U_j^m + U_{j-1}^m) \end{aligned} \qquad (2)$$

for $j = 1, \ldots, N-1$ and $m = 0, 1, \ldots$.

This time, once we have used the initial and boundary conditions to assign values to U_j^0 for $j = 0, 1, \ldots, N$ and U_0^m and U_N^m for $m = 1, 2, \ldots$, if we set $m = 0$ in Equation (2) then we have a linear system to solve in order to compute all the U_j^1.

θ-Method — Linear System

Let $A \in \mathbb{R}^{(N+1)\times(N+1)}$ be the tridiagonal matrix given by

$$A \;=\; \begin{pmatrix} 0 & 0 & 0 & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & 0 & 0 & 0 \end{pmatrix} .$$

Then we may write

$$(I - \mu\theta A)\mathbf{U}^{m+1} \;=\; (I' + \mu(1-\theta)A)\mathbf{U}^{m} + \mathbf{g}^{m+1} .$$

Here, $\mathbf{U}^m = (U_0^m, U_1^m, \ldots, U_N^m)^T$, I is the $(N+1)\times(N+1)$ identity matrix, I' is the $(N+1)\times(N+1)$ identity matrix but with the $(1,1)$ and $(N+1,N+1)$ entries being zero, and $\mathbf{g}^{m+1} = (u_a(t_{m+1}), 0, \ldots, 0, u_b(t_{m+1}))^T$.

θ-Method — Linear System

Since the linear system is tridiagonal it can be solved easily in Matlab using backslash, or it can be solved using the Thomas Algorithm. Either method is fast, but not as fast as using Equation (1) for the forward Euler scheme.

Truncation Error

The truncation error for the θ-method is given by

$$T_j^m = \frac{u_j^{m+1} - u_j^m}{\Delta t} - \theta \frac{u_{j+1}^{m+1} - 2u_j^{m+1} + u_{j-1}^{m+1}}{\Delta x^2} - (1-\theta)\frac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{\Delta x^2} \, .$$

It is standard to perform Taylor series approximations about the point $(x_j, t_{m+1/2})$. This gives

$$T_j^m = \left(\frac{1}{2} - \theta\right)\Delta t u_{xxt} - \frac{1}{12}\Delta t^2 u_{ttt} - \frac{1}{12}\Delta x^2 u_{xxxx} \, .$$

Thus for θ independent of Δt and Δx:

- in general, the θ-method is first order in Δt and second order in Δx;
- for the particular case $\theta = 1/2$, the Crank Nicolson method is second order in both Δt and Δx.

Stability

If we consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \, ,$$

for $t > 0$ and $x \in (-\infty, \infty)$ with an initial condition

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

for $x \in (-\infty, \infty)$, then it can be shown that

$$\|u(\cdot, t)\|_{L_2(-\infty,\infty)} \leq \|u_0\|_{L_2(-\infty,\infty)}$$

for all $t > 0$ (see NSDEI Lecture 12).

Stability

We would like the numerical scheme to mimic this, i.e. we would like

$$\|U^m\|_{\ell_2} \quad \leq \quad \|U^0\|_{\ell_2} \tag{3}$$

for $m = 1, 2, \ldots$, where

$$\|U^m\|_{\ell_2} \quad = \quad \left(\Delta x \sum_{j=-\infty}^{\infty} |U_j^m|^2 \right)^{1/2}$$

If Equation (3) holds, then the method is said to be practically stable.

Stability

Stability can be assessed by inserting the Fourier mode $U_j^m = [\lambda(k)]^m \, \mathrm{e}^{ikx_j}$ into the numerical scheme. It can be shown that the scheme is practically stable if $|\lambda(k)| \leq 1$ for all $k \in [-\pi/\Delta x, \pi/\Delta x]$.

Substituting such a Fourier mode into the θ-method (2) and simplifying gives

$$\begin{aligned}
\lambda(k) &= \frac{1 - 4\mu(1-\theta)\sin^2(k\Delta x/2)}{1 + 4\mu\theta\sin^2(k\Delta x/2)} \\
&= 1 - \frac{4\mu\sin^2(k\Delta x/2)}{1 + 4\mu\theta\sin^2(k\Delta x/2)} \\
&\leq 1
\end{aligned}$$

for $k \in [-\pi/\Delta x, \pi/\Delta x]$.

Stability

Thus we have $\lambda(k) \leq 1$ for all $k \in [-\pi/\Delta x, \pi/\Delta x]$. We also require $\lambda(k) \geq -1$.

We have

$$\lambda(k) = 1 - \frac{4\mu \sin^2(k\Delta x/2)}{1 + 4\mu\theta \sin^2(k\Delta x/2)}$$

and so $\lambda(k) \geq -1$ if

$$\frac{4\mu \sin^2(k\Delta x/2)}{1 + 4\mu\theta \sin^2(k\Delta x/2)} \leq 2\,.$$

Rearranging, we see that we require

$$2\mu \sin^2(k\Delta x/2)(1 - 2\theta) \leq 1\,.$$

This is clearly true for all $\theta \geq 1/2$, but for $\theta < 1/2$ this requires $\mu \leq 1/(2(1 - 2\theta))$.

Stability

Thus for the θ-method we have

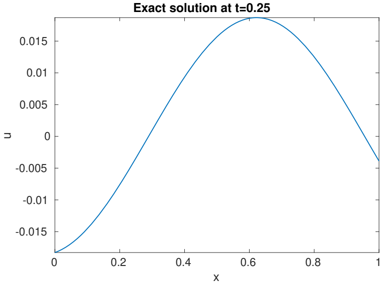
- If $\theta \geq 1/2$ the method is unconditionally stable. In particular this means that the backward Euler and Crank-Nicolson schemes are unconditionally stable.
- If $\theta < 1/2$ the method is only conditionally stable. The values of Δt and Δx must be chosen so that $\mu \leq 1/(2(1-2\theta))$, i.e. so that

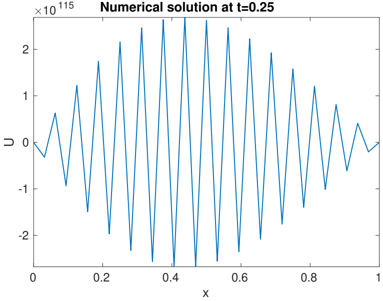
$$\Delta t \;\; \leq \;\; \frac{\Delta x^2}{2(1-2\theta)} \, .$$

 In particular this means that the forward Euler method is only conditionally stable and the condition for stability is that $\Delta t \leq \Delta x^2/2$.

Example of Instability

Suppose we try to solve the heat equation with Dirichlet boundary conditions with the forward Euler scheme with $\Delta t = \Delta x^2$ (recall we need $\Delta t \leq \Delta x^2/2$ for stability). The solution is disastrous!





Maximum Principle

It can be shown that for the heat equation on $[a, b]$ and $t > 0$ with an initial condition $u(x, 0) = u_0(x)$ and boundary conditions at $x = a, b$, it holds that

$$u_{\min} \;\leq\; u(x,t) \;\leq u_{\max}$$

for all $x \in [a, b]$ and $t \geq 0$. Here we define

$$\begin{aligned} u_{\min} &= \min\left(\min_{x\in[a,b]} u_0(x), \min_{t>0} u(a,t), \min_{t>0} u(b,t)\right) \, , \\ u_{\max} &= \max\left(\max_{x\in[a,b]} u_0(x), \max_{t>0} u(a,t), \max_{t>0} u(b,t)\right) \, . \end{aligned}$$

Maximum Principle

It can be shown that, under certain conditions, the numerical solutions produced by the θ-method satisfy similar bounds. Define

$$\begin{aligned} U_{\min} &= \min\left(\min_{0\le j\le N} u_0(x_j), \min_{m>0} U_0^m, \min_{m>0} U_N^m\right) , \\ U_{\max} &= \max\left(\max_{0\le j\le N} u_0(x_j), \max_{m>0} U_0^m, \max_{m>0} U_N^m\right) . \end{aligned}$$

Then we have the discrete maximum principle

$$U_{\min} \le U_j^m \le U_{\max}$$

for $0 \le j \le N$ and $m \ge 0$, provided

$$\mu(1-\theta) \le \frac{1}{2} .$$

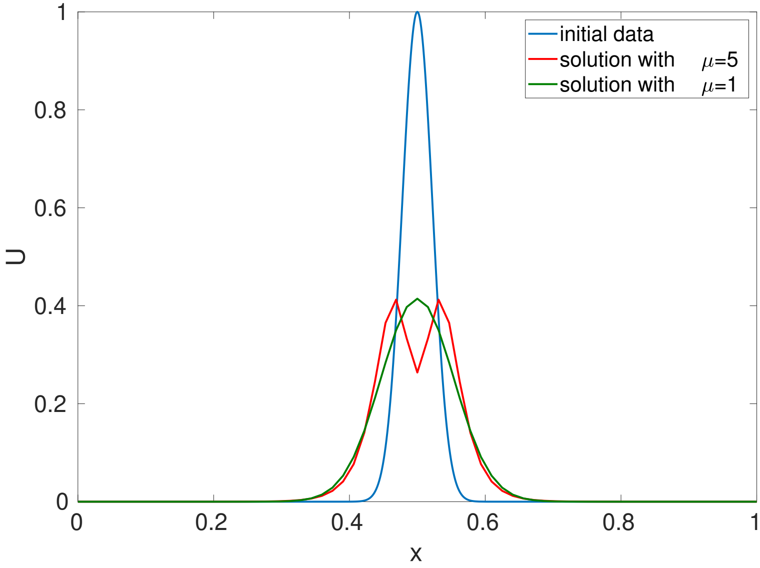
Maximum Principle

Note that, for $\theta \in (0, 1)$, this is a more restrictive condition than that for stability.

- For the implicit Euler scheme, with $\theta = 1$, the discrete maximum principle is automatically satisfied.
- For the θ-method with $\theta \neq 1$, the discrete maximum principle is satisfied whenever $\mu(1-\theta) \leq 1/2$, i.e. whenever

$$\Delta t \;\; \leq \;\; \frac{\Delta x^2}{2(1-\theta)} \; .$$

Maximum Principle: Example



More General Boundary Conditions

Instead of applying Dirichlet boundary conditions, we may wish to apply Neumann boundary conditions or mixed boundary conditions. Let us consider a mixed boundary condition

$$\alpha u(a,t) + \beta \frac{\partial u}{\partial x}(a,t) \;\; = \;\; \gamma$$

for α, β and γ non-zero constants. (What follows is easily extended to the case when α, β and γ are functions of time.)

More General Boundary Conditions

Since $x_0 = a$, we may write a forward difference

$$\frac{\partial u}{\partial x}(a,t) \;=\; \frac{\partial u}{\partial x}(x_0,t) \;\;=\;\; \frac{u(x_1,t) - u(x_0,t)}{\Delta x} + \mathcal{O}(\Delta x)\ .$$

This means we may approximate the mixed boundary condition using

$$\alpha U_0^{m+1} + \beta \frac{U_1^{m+1} - U_0^{m+1}}{\Delta x} \;\;=\;\; \gamma\ , \qquad (4)$$

for $m = 0, 1, \ldots$.

If we use this with the explicit Euler scheme then we have Equation (1) with $j = 1$,

$$U_1^{m+1} \;\;=\;\; U_1^m + \mu(U_2^m - 2U_1^m + U_0^m)$$

which couples with Equation (4) to give a 2×2 system for the unknowns U_0^{m+1} and U_1^{m+1}.

More General Boundary Conditions

If we use Equation (4) to approximate the mixed boundary condition with the θ-method then we need to adapt the system we had earlier, namely

$$B\mathbf{U}^{m+1} := (I - \mu\theta A)\mathbf{U}^{m+1} = (I' + \mu(1-\theta)A)\mathbf{U}^{m} + \mathbf{g}^{m+1}.$$

We now replace the first entry of $\mathbf{g}^{m+1}$ with $\gamma\Delta x$ and the first row of the matrix B is now $(\alpha\Delta x - \beta, \beta, 0, \ldots, 0)$.

This method applies the boundary condition using an $\mathcal{O}(\Delta x)$ approximation.

More General Boundary Conditions — Ficticious Node

An alternative method for applying the boundary conditions is to use a central difference

$$\frac{\partial u}{\partial x}(a,t) \;=\; \frac{\partial u}{\partial x}(x_0,t) \;=\; \frac{u(x_1,t)-u(x_{-1},t)}{2\Delta x} + \mathcal{O}(\Delta x^2)\;,$$

where $x_{-1} = a - \Delta x$ is a ficticious node to the left of the left-hand end of the interval. This means we may approximate the mixed boundary condition using

$$\alpha U_0^{m+1} + \beta \frac{U_1^{m+1} - U_{-1}^{m+1}}{2\Delta x} \;=\; \gamma\;, \tag{5}$$

for $m = 0, 1, \ldots$. To use this with the θ-method we use Equation (2) with $j = 0$, namely

$$\begin{aligned} -\mu\theta U_1^{m+1} + (1+2\mu\theta)U_0^{m+1} - \mu\theta U_{-1}^{m+1} \\ = \; U_0^m + \mu(1-\theta)(U_1^m - 2U_0^m + U_{-1}^m) \end{aligned}$$

More General Boundary Conditions — Ficticious Node

We use Equation (5) to replace U_{-1}^{m+1} and U_{-1}^{m} in this finite difference scheme to get

$$\begin{aligned} & -\mu\theta(1+\beta)U_1^{m+1} + (1+2\mu\theta(1-\alpha\Delta x))U_0^{m+1} \\ = \;& U_0^m + \mu(1-\theta)((1+\beta)U_1^m - 2(1-\alpha\Delta x)U_0^m) - 2\mu\gamma\Delta x\,. \end{aligned}$$

Again we can use this to replace the first line of the linear system.

This method applies the boundary condition using an $\mathcal{O}(\Delta x^2)$ approximation.

More General Boundary Conditions — Comparison

We solve the problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \,,$$

for $t > 0$ and $x \in [0, 1]$ with an initial condition

$$u(x, 0) = \sin\left(\frac{3\pi x}{2}\right) - \left(\frac{3\pi}{2}\right)\cos\left(\frac{3\pi x}{2}\right) \,,$$

for $x \in [0, 1]$. We use boundary conditions

$$\frac{\partial u}{\partial x}(0, t) + u(0, t) = 0 \,,$$
$$u(1, t) = \mathrm{e}^{-(3\pi/2)^2 t} \,,$$

for $t > 0$.

More General Boundary Conditions — Comparison