Numerical Solution of Partial Differential Equations

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2025

Lecture 8

Finite difference approximation of parabolic equations

As a simple but representative model problem we focus on the unsteady diffusion equation (heat equation) in one space dimension:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \tag{1}$$

which we shall consider for $x \in (-\infty, \infty)$ and $t \geq 0$, subject to the initial condition

$$u(x, 0) = u_0(x), \qquad x \in (-\infty, \infty),$$

where u_0 is a given function.

The solution of this initial-value problem can be expressed explicitly in terms of the initial datum u_0.

We summarize here the derivation of this expression.

We recall that the Fourier transform of a function v is defined by

$$\hat{v}(\xi) = F[v](\xi) = \int_{-\infty}^{\infty} v(x)\, \mathrm{e}^{-\imath x \xi}\, \mathrm{d}x.$$

We shall assume henceforth that the functions under consideration are sufficiently smooth and that they decay to 0 as $x \to \pm\infty$ sufficiently fast in order to ensure that our manipulations make sense.

By Fourier-transforming the PDE (1) we obtain

$$\int_{-\infty}^{\infty} \frac{\partial u}{\partial t}(x,t)\, \mathrm{e}^{-\imath x \xi}\, \mathrm{d}x = \int_{-\infty}^{\infty} \frac{\partial^2 u}{\partial x^2}(x,t)\, \mathrm{e}^{-\imath x \xi}\, \mathrm{d}x.$$

After (formal) integration by parts on the right-hand side and ignoring 'boundary terms' at $\pm\infty$, we obtain

$$\frac{\partial}{\partial t}\hat{u}(\xi, t) = (\imath\xi)^2 \hat{u}(\xi, t),$$

whereby

$$\hat{u}(\xi, t) = \mathrm{e}^{-t\xi^2}\hat{u}(\xi, 0),$$

and therefore

$$u(x, t) = F^{-1}\left(\mathrm{e}^{-t\xi^2}\hat{u}_0\right).$$

The inverse Fourier transform of a function is defined by

$$v(x) = F^{-1}[\hat{v}](x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{v}(\xi)\, \mathrm{e}^{\imath x \xi}\, \mathrm{d}\xi.$$

After some lengthy calculations, which we omit, we find that

$$u(x,t) = F^{-1}\left(\mathrm{e}^{-t\xi^2} \hat{u}_0(\xi)\right) = \int_{-\infty}^{\infty} w(x-y,t) u_0(y)\, \mathrm{d}y,$$

where the function w, defined by

$$w(x,t) = \frac{1}{\sqrt{4\pi t}}\, \mathrm{e}^{-x^2/(4t)},$$

is called the heat kernel. So, finally,

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \mathrm{e}^{-(x-y)^2/(4t)} u_0(y)\, \mathrm{d}y, \quad x \in (-\infty, \infty), \quad t > 0. \tag{2}$$

Boundedness in the L_∞ norm

This formula gives an explicit expression of the solution of the heat equation (1) in terms of the initial datum u_0. Because $w(x,t) > 0$ for all $x \in (-\infty, \infty)$ and all $t > 0$, and

$$\int_{-\infty}^{\infty} w(y,t)\,\mathrm{d}y = 1 \qquad \text{for all } t > 0,$$

we deduce from (2) that if u_0 is a bounded continuous function, then

$$\sup_{x\in(-\infty,+\infty)}|u(x,t)| \le \sup_{x\in(-\infty,\infty)}|u_0(x)|, \qquad t > 0. \tag{3}$$

In other words, the 'largest' and 'smallest' values of $u(\cdot,t)$ at $t > 0$ cannot exceed those of $u_0(\cdot)$.

Boundedness in the L_2 norm

We need the following important technical result.

Lemma (Parseval's identity)

Suppose that $u \in L_2((-\infty, \infty))$. Then, $\hat{u} \in L_2((-\infty, \infty))$, and the following equality holds:

$$\|u\|_{L_2((-\infty,\infty))} = \frac{1}{\sqrt{2\pi}} \|\hat{u}\|_{L^2((-\infty,\infty))},$$

where

$$\|u\|_{L_2((-\infty,\infty))} = \left(\int_{-\infty}^{\infty} |u(x)|^2 \, \mathrm{d}x \right)^{1/2}.$$

PROOF. We begin by observing that

$$\begin{aligned}\int_{-\infty}^{\infty} \hat{u}(\xi)\, v(\xi)\, \mathrm{d}\xi &= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} u(x)\, \mathrm{e}^{-\imath x \xi}\, \mathrm{d}x \right) v(\xi)\, \mathrm{d}\xi \\ &= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} v(\xi)\, \mathrm{e}^{-\imath x \xi}\, \mathrm{d}\xi \right) u(x)\, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} u(x)\, \hat{v}(x)\, \mathrm{d}x.\end{aligned}$$

We then take

$$v(\xi) = \overline{\hat{u}(\xi)} = 2\pi F^{-1}[\bar{u}](\xi)$$

and substitute this into the identity above. ◇

Returning to equation (1), we thus have by Parseval's identity that

$$\|u(\cdot,t)\|_{L_2((-\infty,\infty))} = \frac{1}{\sqrt{2\pi}}\,\|\hat{u}(\cdot,t)\|_{L_2((-\infty,\infty))}, \qquad t > 0.$$

Therefore,

$$\begin{aligned} \|u(\cdot,t)\|_{L_2((-\infty,\infty))} &= \frac{1}{\sqrt{2\pi}}\,\|\mathrm{e}^{-t\xi^2}\hat{u}_0(\cdot)\|_{L_2((-\infty,\infty))} \\ &\leq \frac{1}{\sqrt{2\pi}}\,\|\hat{u}_0\|_{L_2((-\infty,\infty))} \\ &= \|u_0\|_{L_2((-\infty,\infty))}, \qquad t > 0. \end{aligned}$$

Thus we have shown that

$$\|u(\cdot,t)\|_{L_2((-\infty,\infty))} \leq \|u_0\|_{L_2((-\infty,\infty))} \qquad \text{for all } t > 0. \tag{4}$$

Stability with respect to perturbation of the data

Suppose that u_0 and $\tilde{u}_0$ are two functions contained in $L_2((-\infty,\infty))$ and denote by u and $\tilde{u}$ the solutions to (1) resulting from the initial data u_0 and $\tilde{u}_0$, respectively.

Then $u - \tilde{u}$ solves the heat equation with initial datum $u_0 - \tilde{u}_0$, and therefore, by (4), we have that

$$\|u(\cdot,t) - \tilde{u}(\cdot,t)\|_{L_2((-\infty,\infty))} \leq \|u_0 - \tilde{u}_0\|_{L_2((-\infty,\infty))} \qquad \text{for all } t > 0.$$

Analogously, from (3) we have that

$$\sup_{x\in(-\infty,\infty)} |u(x,t) - \tilde{u}(x,t)| \leq \sup_{x\in(-\infty,\infty)} |u_0(x) - \tilde{u}_0(x)| \qquad \text{for all } t > 0.$$

Finite difference approximation of the heat equation

We take our computational domain to be

$$\{(x, t) \in (-\infty, \infty) \times [0, T]\},$$

where $T > 0$ is a given final time.

We consider a finite difference mesh with spacing $\Delta x > 0$ in the x-direction and spacing $\Delta t = T/M$ in the t-direction, with $M \geq 1$, and we approximate the partial derivatives appearing in (1) using divided differences as follows.

Let $x_j = j\Delta x$ and $t_m = m\Delta t$, and note that

$$\frac{\partial u}{\partial t}(x_j, t_m) \approx \frac{u(x_j, t_{m+1}) - u(x_j, t_m)}{\Delta t}$$

and

$$\frac{\partial^2 u}{\partial x^2}(x_j, t_m) \approx \frac{u(x_{j+1}, t_m) - 2u(x_j, t_m) + u(x_{j-1}, t_m)}{(\Delta x)^2}.$$

This motivates us to approximate the heat equation at the point (x_j, t_m) by the following explicit Euler scheme:

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{(\Delta x)^2}, \quad j = 0, \pm 1, \pm 2, \ldots$$

$$U_j^0 = u_0(x_j), \qquad j = 0, \pm 1, \pm 2, \ldots$$

Equivalently, we can write this as

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

$$U_j^0 = u_0(x_j), \qquad j = 0, \pm 1, \pm 2, \ldots$$

where $\mu = \frac{\Delta t}{(\Delta x)^2}$.

Thus, U_j^{m+1} can be explicitly calculated, for all $j = 0, \pm 1, \pm 2, \ldots$, from the values U_{j+1}^m, U_j^m, and U_{j-1}^m from the previous time level.

Alternatively, if instead of time level m the expression on the right-hand side of the explicit Euler scheme is evaluated on the time level $m+1$, we arrive at the implicit Euler scheme:

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{(\Delta x)^2}, \quad j = 0, \pm 1, \pm 2, \ldots$$

$$U_j^0 = u_0(x_j), \qquad j = 0, \pm 1, \pm 2, \ldots.$$

The explicit and implicit Euler schemes are special cases of a more general one-parameter family of numerical methods for the heat equation, called the θ-method, with a parameter $\theta \in [0, 1]$.

The θ-method is defined as follows:

$$
\begin{aligned}
\frac{U_j^{m+1} - U_j^m}{\Delta t} &= (1-\theta)\,\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{(\Delta x)^2} + \theta\,\frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{(\Delta x)^2}, \\
U_j^0 &= u_0(x_j), \qquad j = 0, \pm 1, \pm 2, \dots,
\end{aligned}
$$

where $\theta \in [0, 1]$ is a parameter. Special cases:

$\theta = 0$: explicit Euler scheme
$\theta = 1$: implicit Euler scheme
$\theta = 1/2$: Crank–Nicolson scheme

Accuracy of the θ-method

In order to assess the accuracy of the θ-method for the heat equation we define its consistency error by

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

where

$$u_j^m \equiv u(x_j, t_m).$$

We shall explore the size of the consistency error by performing a Taylor series expansion about the point $(x_j, t_{m+1/2}) = (j\Delta x, (m + \frac{1}{2}\Delta t))$.

Note that

$$u_j^{m+1} = \left[u + \frac{1}{2}\Delta t\, u_t + \frac{1}{2}\left(\frac{1}{2}\Delta t\right)^2 u_{tt} + \frac{1}{6}\left(\frac{1}{2}\Delta t\right)^3 u_{ttt} + \cdots\right]_j^{m+1/2},$$

$$u_j^{m} = \left[u - \frac{1}{2}\Delta t\, u_t + \frac{1}{2}\left(\frac{1}{2}\Delta t\right)^2 u_{tt} - \frac{1}{6}\left(\frac{1}{2}\Delta t\right)^3 u_{ttt} + \cdots\right]_j^{m+1/2}.$$

Therefore,

$$\frac{u_j^{m+1} - u_j^m}{\Delta t} = \left[u_t + \frac{1}{24}(\Delta t)^2 u_{ttt} + \cdots\right]_j^{m+1/2}.$$

Similarly,

$$
\begin{aligned}
(1-\theta)\,\frac{u_{j+1}^{m}-2u_{j}^{m}+u_{j-1}^{m}}{(\Delta x)^2}+\theta\,\frac{u_{j+1}^{m+1}-2u_{j}^{m+1}+u_{j-1}^{m+1}}{(\Delta x)^2} \\
=\left[u_{xx}+\frac{1}{12}\left(\Delta x\right)^2 u_{xxxx}+\frac{2}{6!}\left(\Delta x\right)^4 u_{xxxxxx}+\cdots\right]_j^{m+1/2} \\
+\left(\theta-\frac{1}{2}\right)\Delta t\left[u_{xxt}+\frac{1}{12}\left(\Delta x\right)^2 u_{xxxxt}+\cdots\right]_j^{m+1/2} \\
+\frac{1}{8}\left(\Delta t\right)^2\left[u_{xxtt}+\cdots\right]_j^{m+1/2}.
\end{aligned}
$$

Combining these, we deduce that

$$
\begin{aligned}
T_j^m = & \boxed{[u_t - u_{xx}]_j^{m+1/2}} \\
& + \left[\left(\frac{1}{2} - \theta \right) \Delta t \, u_{xxt} - \frac{1}{12} (\Delta x)^2 \, u_{xxxx} \right]_j^{m+1/2} \\
& + \left[\frac{1}{24} (\Delta t)^2 \, u_{ttt} - \frac{1}{8} (\Delta t)^2 \, u_{xxtt} \right]_j^{m+1/2} \\
& + \left[\frac{1}{12} \left(\frac{1}{2} - \theta \right) \Delta t \, (\Delta x)^2 \, u_{xxxxt} - \frac{2}{6!} (\Delta x)^4 \, u_{xxxxxx} \right]_j^{m+1/2} + \cdots .
\end{aligned}
$$

Note however that the term contained in the box vanishes, as u is a solution to the heat equation $u_t = u_{xx}$. Hence,

$$
T_j^m = \begin{cases} \mathcal{O}\left((\Delta x)^2 + (\Delta t)^2 \right) & \text{for } \theta = 1/2 \quad \text{(Crack–Nicolson scheme)} \\ \mathcal{O}\left((\Delta x)^2 + \Delta t \right) & \text{for } \theta \neq 1/2 \quad \text{(e.g. Euler scheme(s)).} \end{cases}
$$