Numerical Solution of Partial Differential Equations

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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.

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We summarize here the derivation of this expression.

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

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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

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

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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

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is called the **heat kernel**. So, finally,

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

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

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

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

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

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We will show, using Parseval's identity, that the L^2 norm of the solution, at any time $t > 0$, is bounded by the L^2 norm of the initial datum.

We shall then try to mimic this when using various numerical approximations of the initial-value problem for the heat equation.

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

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

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We then take

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

and substitute this into the identity above. $\diamond$

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

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

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Therefore, because

$$\hat{u}(\xi,t) = \mathrm{e}^{-t\xi^2}\,\hat{u}_0(\xi),$$

it follows that

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

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

Thus we have shown that

$$\|u(\cdot,t)\|_{L^2(-\infty,\infty)} \leq \|u_0\|_{L^2(-\infty,\infty)} \qquad \text{for all } t > 0. \tag{4}$$

This is a useful result as it can be used to deduce stability of the solution of the equation (1) with respect to perturbations of the initial datum in a sense which we shall now explain.

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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 functions u_0 and $\tilde{u}_0$, respectively.

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

$$\|u(\cdot, t) - \tilde{u}(\cdot, t)\|_{L^2(-\infty,\infty)} \leq \|u_0 - \tilde{u}_0\|_{L^2(-\infty,\infty)} \qquad \text{for all } t > 0.$$

This inequality implies continuous dependence of the solution on the initial function: small perturbations in u_0 in the $L^2(-\infty, \infty)$ norm will result in small perturbations in the associated analytical solution $u(\cdot, t)$ in the $L^2(-\infty, \infty)$ norm for all $t > 0$.

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Analogously,

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

Model problem: heat equation in one space dimension

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

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where u_0 is a given function.

Finite difference approximation of the heat equation

We take our computational domain to be

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

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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.

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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**:

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

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Equivalently, we can write this as

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

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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**:

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

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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**, which is a convex combination of the two Euler schemes, with a parameter $\theta \in [0, 1]$.

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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}, \\
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where $\theta \in [0, 1]$ is a parameter.

For $\theta = 0$ it coincides with the explicit Euler scheme, for $\theta = 1$ it is the implicit Euler scheme, and for $\theta = 1/2$ it is the arithmetic average of these, and is called the **Crank–Nicolson scheme**.

Accuracy of the θ-method

In order to assess the accuracy of the θ-method for the Dirichlet initial-boundary-value problem 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 a suitable point.

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Note that

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

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

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Therefore,

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

Similarly,

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

Combining these, we deduce that

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

Note however that the term contained in the box vanishes, as u is a solution to the heat equation. Hence,

$$
T_j^m = \begin{cases} \mathcal{O}\left((\Delta x)^2 + (\Delta t)^2\right) & \text{for } \theta = 1/2, \\ \mathcal{O}\left((\Delta x)^2 + \Delta t\right) & \text{for } \theta \neq 1/2. \end{cases}
$$

Thus, in particular, the explicit and implicit Euler schemes have consistency error

$$T_j^m = \mathcal{O}\left((\Delta x)^2 + \Delta t\right),$$

while the Crank–Nicolson scheme has consistency error

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