Numerical Solution of Differential Equations I

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2019

Lecture 13

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 the PDE 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**:

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

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

Equivalently, we can write this as

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

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

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

Thus, U_j^{m+1} can be explicitly calculated, for all $j = 0, \pm 1, \pm 2, \dots$, 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**:

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

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

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 $\theta \in [0, 1]$.

The θ-method is defined as follows:

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

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.

Note that

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

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

Therefore,

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

Similarly,

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

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. 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

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