

Numerical methods for parabolic partial differential equations

Let's consider the linear parabolic equation with constant coefficients

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}. \quad (1)$$

A more general equation (describing heat conduction or mass diffusion)

$$\frac{\partial u}{\partial \tau} = \sigma \frac{\partial^2 u}{\partial x^2} \quad (2)$$

can be converted to (1) by the substitution $t = \sigma \tau$.

The solution of equation (1) is often defined on a rectangle $D = [0, 1] \times [0, T]$. The solution $u(x, t)$ satisfy the initial condition (the function $\varphi(x)$ is given)

$$u(x, 0) = \varphi(x), \quad 0 < x < 1, \quad (3)$$

and a boundary condition

$$u(0, t) = u(1, t) = 0. \quad (4)$$

1 Simple explicit formula

Let us divide the interval $[0, 1]$ in x into n subintervals by equidistant grid points

$$x_0 = 0, x_1 = h, x_2 = 2h, \dots, x_{n-1} = 1 - h, x_n = 1,$$

where $h = 1/n$ and $x_i = ih, i = 0, 1, \dots, n$. Similarly the interval $[0, T]$ in t is divided into r equal parts by the grid points

$$t_0 = 0, t_1 = k, \dots, t_r = T,$$

where the time step is $k = T/r$ and $t_j = jk, j = 0, 1, \dots, r$. The set of nodes - the intersections of the lines $x = ih, i = 0, 1, \dots, n$, and the lines $t = jk, j = 0, 1, \dots, r$, forms a rectangular grid denoted by $D^{(h)}$. On this grid we can approximate the derivatives of the function u by the difference formulas for $i = 1, \dots, n - 1, j = 0, \dots, r - 1$:

$$\left. \frac{\partial u}{\partial t} \right|_{(x_i, t_j)} = \frac{u_i^{j+1} - u_i^j}{k} + \mathcal{O}(k), \quad (5)$$

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_{(x_i, t_j)} = \frac{u_{i-1}^j - 2u_i^j + u_{i+1}^j}{h^2} + \mathcal{O}(h^2), \quad (6)$$

where we denote $u(ih, jk) = u(x_i, t_j) \doteq u_i^j$.

Consider the equation (1) in one node $(x_i, t_j) \in D^{(h)}$ and the approximation using (5) and (6):

$$\frac{u_i^{j+1} - u_i^j}{k} = \frac{u_{i-1}^j - 2u_i^j + u_{i+1}^j}{h^2} + \mathcal{O}(k + h^2). \quad (7)$$

Neglecting $\mathcal{O}(k + h^2) = \mathcal{O}(k) + \mathcal{O}(h^2)$, which is called the approximation error and using the initial condition (3) and the boundary conditions (4) we get the following difference problem:

$$u_i^{j+1} = \frac{k}{h^2} (u_{i-1}^j + u_{i+1}^j) + \left(1 - \frac{2k}{h^2}\right) u_i^j, \quad \begin{array}{l} i = 1, 2, \dots, n-1 \\ j = 0, 1, \dots, r-1, \end{array} \quad (8)$$

$$u_i^0 = \varphi(ih), \quad i = 1, 2, \dots, n-1, \quad (9)$$

$$u_0^j = 0, \quad u_n^j = 0, \quad j = 0, 1, \dots, r. \quad (10)$$

It is easy to rewrite (8), (9) and (10) using profiles as

$$\begin{aligned} \mathbf{u}^{j+1} &= \mathbf{A}_1 \mathbf{u}^j, \\ \mathbf{u}^0 &= [0, \varphi(h), \varphi(2h), \dots, \varphi((n-1)h), 0]^T, \end{aligned} \quad (11)$$

where the matrix \mathbf{A}_1 is three-diagonal

$$\mathbf{A}_1 = \begin{pmatrix} 0 & 0 & & & & & & & \\ \alpha & (1-2\alpha) & \alpha & & & & & & \\ & \alpha & (1-2\alpha) & \alpha & & & & & 0 \\ & & \ddots & \ddots & \ddots & & & & \\ & 0 & & \alpha & (1-2\alpha) & \alpha & & & \\ & & & & \alpha & (1-2\alpha) & \alpha & & \\ & & & & & & 0 & 0 & 0 \end{pmatrix}, \quad (12)$$

where

$$\alpha = \frac{k}{h^2}. \quad (13)$$

If $\alpha \leq \frac{1}{2}$ then the method (11) is stable.