Explicit finite-difference method for the heat equation

Consider the heat (diffusion) equation

$$u_t = K\, u_{xx}, \quad 0 < x < L, \quad 0 < t < T, \tag{1}$$

subject to the boundary conditions

$$u(0, t) = u(L, t) = 0 \quad \text{for} \quad t \in (0, T), \tag{2}$$

and initial condition

$$u(x, 0) = u_0(x), \tag{3}$$

where $u_0(x)$ is a given function. In Eq. (1), $K > 0$.

Grid points (or mesh points)

Let $N, M \in \mathbb{N}$ and let

$$\tau = \frac{T}{M}, \quad h = \frac{L}{N}.$$

Then we define the grid points (x_k, t_j):

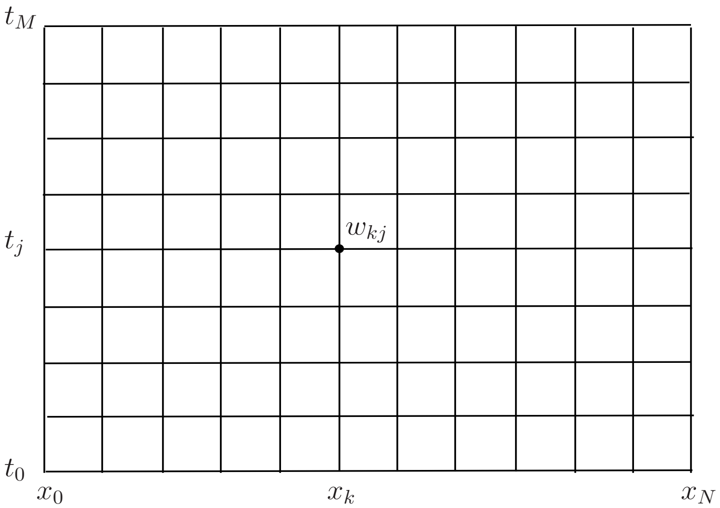
$$x_k = hk \quad \text{for} \quad k = 0, 1, \ldots, N;$$
$$t_j = \tau j \quad \text{for} \quad j = 0, 1, \ldots, M.$$

The problem is to find numbers w_{kj} such that w_{kj} approximates the value of the exact solution $u(x, t)$ at the grid point (x_k, t_j), i.e.

$$w_{kj} \approx u(x_k, t_j)$$

for $k = 0, 1, \ldots, N$ and $j = 0, 1, 2, \ldots$

Grid points



Approximations to partial derivatives

By definition,

$$u_t(x_k, t_j) = \lim_{\tau \to 0} \frac{u(x_k, t_j + \tau) - u(x_k, t_j)}{\tau}.$$

It is natural to expect that

$$u_t(x_k, t_j) \approx \frac{u(x_k, t_j + \tau) - u(x_k, t_j)}{\tau}$$

for sufficiently small τ.

What is the error of this formula?

Truncation error

The first Taylor polynomial for $u(x_k, t_j + \tau)$:

$$u(x_k, t_j + \tau) = u(x_k, t_j) + \tau \frac{\partial u}{\partial t}(x_k, t_j) + \frac{\tau^2}{2} \frac{\partial^2 u}{\partial t^2}(x_k, \xi)$$

where ξ is between t_j and $t_j + \tau$. Therefore,

$$\tau_{kj} = \frac{\partial u}{\partial t}(x_k, t_j) - \frac{u(x_k, t_j + \tau) - u(x_k, t_j)}{\tau} = -\frac{\tau}{2} \frac{\partial^2 u}{\partial t^2}(x_k, \xi).$$

τ_{kj} is called the *truncation error* .

If $u_{tt}(x, t)$ is bounded, then

$$\tau_{kj} = O(\tau) \quad \text{as} \quad \tau \to 0.$$

Forward- and backward-difference formulae

Formula

$$u_t(x_k, t_j) \approx \frac{u(x_k, t_j + \tau) - u(x_k, t_j)}{\tau}$$

for $\tau > 0$ is called the **forward-difference formula.**

If we replace τ by $-\tau$, we obtain the **backward-difference formula**:

$$u_t(x_k, t_j) \approx \frac{u(x_k, t_j) - u(x_k, t_j - \tau)}{\tau}.$$

Finite difference formula for u_{xx}

From Taylor's theorem,

$$\begin{aligned} u(x_k+h,t_j) &= u(x_k,t_j) + h u_x(x_k,t_j) + \frac{h^2}{2} u_{xx}(x_k,t_j) \\ &\quad + \frac{h^3}{6} u_{xxx}(x_k,t_j) + \frac{h^4}{24} u_{xxxx}(\xi_1,t_j), \\ u(x_k-h,t_j) &= u(x_k,t_j) - h u_x(x_k,t_j) + \frac{h^2}{2} u_{xx}(x_k,t_j) \\ &\quad - \frac{h^3}{6} u_{xxx}(x_k,t_j) + \frac{h^4}{24} u_{xxxx}(\xi_2,t_j) \end{aligned}$$

for some ξ_1 between x_k and x_k+h and some ξ_2 between x_k-h and x_k.

Now take the sum of these.

The sum of these yields

$$\begin{aligned} u(x_k + h, t_j) + u(x_k - h, t_j) &= 2u(x_k, t_j) + h^2 u_{xx}(x_k, t_j) \\ &\quad + \frac{h^4}{24}\left[u_{xxxx}(\xi_1, t_j) + u_{xxxx}(\xi_2, t_j)\right]. \end{aligned}$$

The number

$$\frac{1}{2}\left[u_{xxxx}(\xi_1, t_j) + u_{xxxx}(\xi_2, t_j)\right]$$

is between

$$u_{xxxx}(\xi_1, t_j) \quad \text{and} \quad u_{xxxx}(\xi_2, t_j).$$

If u_{xxxx} is continuous, then by the intermediate value theorem,

$$\frac{1}{2}\left[u_{xxxx}(\xi_1, t_j) + u_{xxxx}(\xi_2, t_j)\right] = u_{xxxx}(\xi, t_j).$$

for some ξ between ξ_1 and ξ_2.

Hence,

$$u_{xx}(x_k, t_j) = \frac{u(x_{k+1}, t_j) - 2u(x_k, t_j) + u(x_{k-1}, t_j)}{h^2} - \frac{h^2}{12} u_{xxxx}(\xi, t_j),$$

where $\xi \in (x_{k-1}, x_{k+1})$.
This is called the **central difference formula** for u_{xx}. If u_{xxxx} is bounded, the truncation error is $O(h^2)$

Forward-difference method for the heat eqn.

Let

$$w_{kj} \approx u(x_k, t_j).$$

Then

$$\frac{w_{k,j+1} - w_{kj}}{\tau} - K\frac{w_{k+1,j} - 2w_{kj} + w_{k-1,j}}{h^2} = 0,$$

for each interior grid point. Local truncation error is $O(\tau)+O(h^2)$.

Boundary conditions:

$$w_{0,j} = w_{N,j} = 0 \quad \text{for each} \;\; j = 1, \ldots, M.$$

Initial conditions:

$$w_{k,0} = u_0(x_k) \quad \text{for each} \;\; k = 0, 1, \ldots, N.$$

Matrix form

The equivalent difference equation

$$w_{k,j+1} = (1 - 2\gamma)\, w_{kj} + \gamma \left(w_{k+1,j} + w_{k-1,j} \right), \quad \gamma \equiv \frac{K\tau}{h^2}.$$

can be written as

$$\mathbf{w}^{(j)} = A\mathbf{w}^{(j-1)} \quad \text{for} \quad j = 1, 2, \ldots,$$

where

$$A = \begin{bmatrix} 1-2\gamma & \gamma & 0 & \ldots & \ldots & 0 \\ \gamma & 1-2\gamma & \gamma & \ddots & & \vdots \\ 0 & \gamma & 1-2\gamma & \gamma & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \gamma \\ 0 & \ldots & \ldots & 0 & \gamma & 1-2\gamma \end{bmatrix}, \quad \mathbf{w}^{(j)} = \begin{bmatrix} w_{1,j} \\ w_{2,j} \\ \vdots \\ \vdots \\ \vdots \\ w_{N-1,j} \end{bmatrix}.$$

The forward-difference method is an example of an **explicit finite-difference method**.

Example

Let's employ the forward-difference method to solve the heat equation

$$u_t = u_{xx} \quad \text{for} \quad 0 < x < 1 \quad \text{and} \quad 0 < t < 0.1$$

subject to zero boundary conditions

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

and the initial condition

$$u(x,0) = 2\sin(2\pi x).$$

Note that the **exact** solution is given by

$$u(x,t) = 2e^{-4\pi^2 t}\sin(2\pi x).$$

Stability

Let $\mathbf{w}^{(j)}$ be the solution generated by the formula

$$\mathbf{w}^{(j)} = A\mathbf{w}^{(j-1)}$$

from the initial data $\mathbf{w}^{(0)}$.

Let $\tilde{\mathbf{w}}^{(j)}$ be the solution generated by the same formula from slightly different initial data

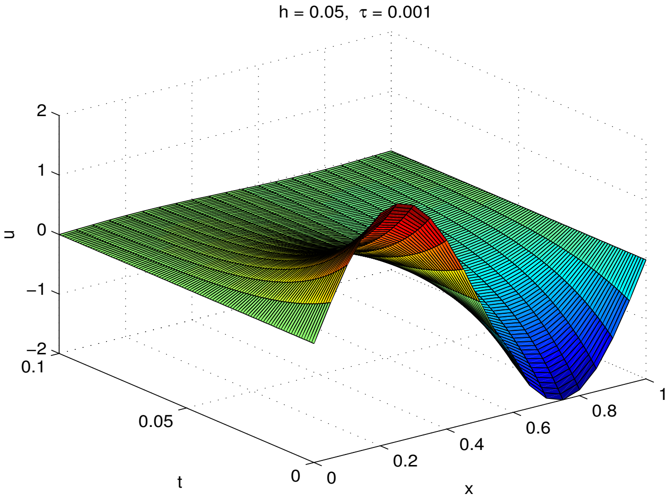
$$\tilde{\mathbf{w}}^{(0)} = \mathbf{w}^{(0)} + \mathbf{z}^{(0)}$$

where $\mathbf{z}^{(0)}$ is the initial error (perturbation).

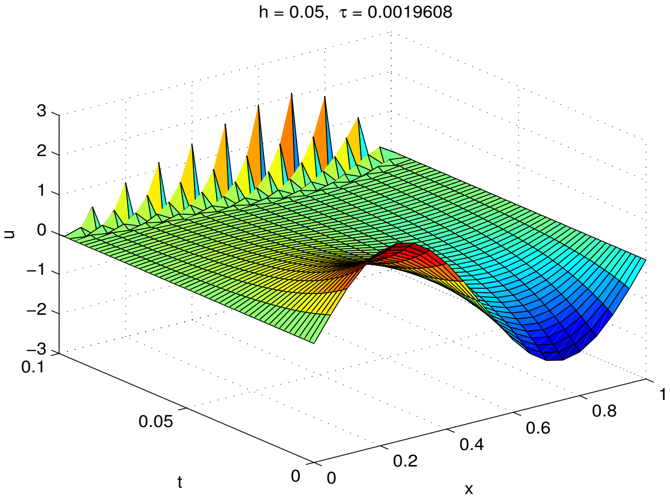
If the errors grow with each time step, then the difference method in ***unstable****. If they do not grow, it is stable.*

How to find out whether the forward-difference method is stable?

Example: stable scheme



Example: unstable scheme



Stability

Matrix method.

- We have
$$\tilde{\mathbf{w}}^{(1)} = A\tilde{\mathbf{w}}^{(0)} = A\left(\mathbf{w}^{(0)} + \mathbf{z}^{(0)}\right) = A\mathbf{w}^{(0)} + A\mathbf{z}^{(0)},$$
i.e.
$$\mathbf{z}^{(1)} = \tilde{\mathbf{w}}^{(1)} - \mathbf{w}^{(1)} = A\mathbf{z}^{(0)}.$$
- At the *n*-th time step,
$$\mathbf{z}^{(n)} = \tilde{\mathbf{w}}^{(n)} - \mathbf{w}^{(n)} = A^n\mathbf{z}^{(0)}.$$
- The method is stable if for any initial error $\mathbf{z}^{(0)}$,
$$\|A\mathbf{z}^{(0)}\| \leq \|\mathbf{z}^{(0)}\|$$
Here $\|\cdot\|$ is any vector norm.
- This is equivalent to
$$|\lambda_i| \leq 1 \quad \text{for} \quad i = 1, 2, \ldots, N-1,$$
where the λ_i are the eigenvalues of matrix A.

Periodic boundary conditions

If we impose $u(x,0) = u(x,L)$ then $w_N = w_0$. We also define $w_{N+1} = w_1$ Then we can use forward difference equation

$$w_{k,j+1} = (1-2\gamma)\, w_{kj} + \gamma \left(w_{k+1,j} + w_{k-1,j} \right)$$

for $k = 1, \dots N$. Which can be written as $\mathbf{w}^{(j)} = A\mathbf{w}^{(j-1)}$ where now

$$A = \begin{bmatrix} 1-2\gamma & \gamma & 0 & \dots & 0 & \gamma \\ \gamma & 1-2\gamma & \gamma & \ddots & \vdots & 0 \\ 0 & \gamma & 1-2\gamma & \gamma & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & \ddots & \ddots & \gamma \\ \gamma & 0 & \dots & 0 & \gamma & 1-2\gamma \end{bmatrix}, \quad \mathbf{w}^{(j)} = \begin{bmatrix} w_{1,j} \\ w_{2,j} \\ \vdots \\ \vdots \\ \vdots \\ w_{N,j} \end{bmatrix}.$$

This is a circulant matrix and its eigenvectors are known.

Stability

Fourier method.

Let w_{kj} and $\tilde{w}_{kj}$ be two solutions of the difference equation

$$\frac{w_{k,j+1} - w_{k,j}}{\tau} - K\frac{w_{k+1,j} - 2w_{k,j} + w_{k-1,j}}{h^2} = 0,$$

corresponding to slightly different initial data. Then the error (perturbation) $z_{kj} = \tilde{w}_{kj} - w_{kj}$ satisfies the equation

$$\frac{z_{k,j+1} - z_{k,j}}{\tau} - K\frac{z_{k+1,j} - 2z_{k,j} + z_{k-1,j}}{h^2} = 0.$$

We seek a particular solution of this equation in the form

$$z_{k,j} = \rho_q^j e^{iqx_k}, \quad q \in \mathbb{R}.$$

The finite-difference method is stable, if all solutions having this form are such that

$$|\rho_q| \leq 1 \quad \text{for all} \quad q \in \mathbb{R}.$$

Stability

Substituting $z_{k,j} = \rho_q^j e^{iqx_k}$ gives

$$\frac{\rho_q^{j+1} e^{iqx_k} - \rho_q^j e^{iqx_k}}{\tau} - K \frac{\rho_q^j \left(e^{iqx_{k+1}} - 2e^{iqx_k} + e^{iqx_{k-1}} \right)}{h^2} = 0$$

or

$$\rho_q - 1 - \gamma \left(e^{iqh} - 2 + e^{-iqh} \right) = 0.$$

Since

$$e^{iqh} - 2 + e^{-iqh} = \left(e^{iqh/2} - e^{-iqh/2} \right)^2 = -4 \sin^2 \frac{qh}{2},$$

we obtain

$$\rho_q = 1 - 4\gamma \sin^2 \frac{qh}{2}.$$

The method is stable if

$$-1 \leq 1 - 4\gamma \sin^2 \frac{qh}{2} \leq 1.$$

Stability

The stability condition is equivalent to

$$0 \le \gamma \sin^2 \frac{qh}{2} \le \frac{1}{2},$$

for all q, which means that

$$0 \le \gamma \le \frac{1}{2} \quad \text{or equivalently} \quad 0 \le \tau \le \frac{h^2}{2K}.$$

A method which is stable only if a certain condition holds is called **conditionally stable.**

The forward-difference method for the heat equation is conditionally stable.