Finite Difference Method

Anh Ha LE

University of Sciences

October 31, 2015

Heat Equation

We now begin to study finite difference methods for time-dependent partial differential equations (PDEs), where variations in space are related to variations in time. We begin with the heat equation (or diffusion equation)

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \qquad \forall (x, t) \in [0, 1] \times [0, T]. \tag{1}$$

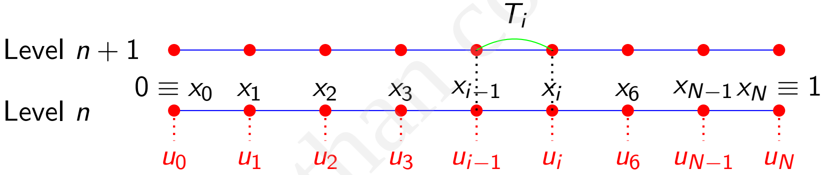
Along with this equation we need initial conditions at time 0

$$u(x, 0) = u_0(x), \tag{2}$$

and also boundary conditions if we are working on a bounded domain, e.g., the Dirichlet conditions

$$\begin{aligned} u(t, 0) &= g1(t), \\ u(t, 1) &= g2(t). \end{aligned} \tag{3}$$

Mesh



Let us consider a uniform partion with $N_x + 1$ points x_i for all $i = 0, 1, 2, \cdots, N_x$ (see figure), we have space step is $h = \frac{1}{N_x}$. We divide the interval [0, T] into $N_t - 1$ sub-intervals of constant length $k = \frac{T}{N_t}$. Then

$$x_i = ih \text{ and } t_n = nk \tag{4}$$

Let $U_i^n = u(x_i, t_n)$ represent the numerical approximation at grid point (x_i, t_n).

Scheme

As an example, one natural discretization of (1) would be

$$\frac{U_i^{n+1} - U_i^n}{k} = \kappa \frac{U_{i-1}^n - 2U_i^n + U_{i+1}^n}{h^2} \tag{5}$$

This uses our standard centered difference in space and a forward difference in time. This is an explicit method since we can compute each U_i^{n+1} explicitly in terms of the previous data:

$$U_i^{n+1} = U_i^n + \frac{\kappa k}{h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n) \tag{6}$$

Figure 1(a) shows the stencil of this method.

Scheme

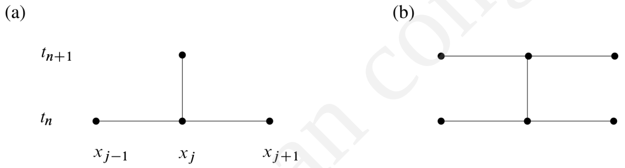


Figure: Stencil of the method (6) and ()

Another method, which is much more useful in practice, as we will see below, is the "θ method",

$$\frac{U_i^{n+1} - U_i^n}{k} = \kappa((1-\theta)D_2 U_i^n + \theta D_2 U_i^{n+1}) \tag{7}$$

where

$$D_2 U_i^n = \frac{U_{i-1}^n - 2U_i^n + U_{i+1}^n}{h^2}, \quad D_2 U_i^{n+1} = \frac{U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}}{h^2}$$

Scheme

We can rewrite that

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{\kappa}{h^2}((1-\theta)(U_{i-1}^n - 2U_i^n + U_{i+1}^n) + \theta(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1})) \tag{8}$$

Or

$$U_i^{n+1} = U_i^n + \frac{\kappa k}{h^2}((1-\theta)(U_{i-1}^n - 2U_i^n + U_{i+1}^n) + \theta(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}))$$

Scheme

We get the scheme of 'θ method'

$$
\begin{aligned}
&- r\theta U_{i-1}^{n+1} + (1 + 2 * r\theta)U_i^{n+1} + r\theta U_{i+1}^{n+1} \\
&= r(1-\theta)U_{i-1}^{n} + (1 - 2 * r(1-\theta))U_i^{n} + r(1-\theta)U_{i+1}^{n}
\end{aligned}
\tag{9}
$$

where $r = \frac{\kappa k}{h^2}$ This includes some common methods

1. $\theta = 0, \Rightarrow$ Explicit method (Forward Euler)
2. $\theta = 1, \Rightarrow$ Implicit method (Backward Euler)
3. $\theta = 1/2, \Rightarrow$ Implicit method (Crank-Nicolson)

Scheme

We put

$$A = \begin{pmatrix} -2r & r & 0 & 0 & 0 & 0 \\ r & -2r & r & 0 & 0 & 0 \\ 0 & r & -2r & r & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & r & -2r & r \\ 0 & 0 & 0 & 0 & r & -2r \end{pmatrix}$$

The 'θ' method becomes

$$(I - \theta A)U^{n+1} = (I + (1-\theta)A)U^n \tag{10}$$

Scheme

We can see that

1. Forward Euler method:

$$U^{n+1} = U^n + AU^n \tag{11}$$

2. Backward Euler method:

$$U^{n+1} = U^n + AU^{n+1} \tag{12}$$

3. Crank-Nicolson:

$$U^{n+1} - U^n = \frac{1}{2}(AU^n + AU^{n+1}) \tag{13}$$

Scheme

These linear finite difference equations can be solved formally as

$$U^{n+1} = GU^n \tag{14}$$

where

1. Forward Euler method: $G = I + A$
2. Backward Euler method: $G = (I - A)^{-1}$
3. Crank-Nicolson: $G = (I - \frac{1}{2}A)^{-1}(I + \frac{1}{2}A)$

One can show the time step restriction

$$r \leq \begin{cases} \frac{1}{2(1-2\theta)} & \text{if } \theta < 1/2 \\ \infty & \text{if } 1/2 \leq \theta \leq 1 \text{ (unconditionally stable)} \end{cases}$$

Local truncation errors and order of accuracy

We can define the local truncation error as usual, we insert the exact solution $u(x,t)$ of the PDE into the finite difference equation and determine by how much it fails to satisfy the discrete equation. The local truncation error of the Forward Euler method is based on the form: τ_i^n

$$\tau_i^n = \frac{u(x_i, t^{n+1}) - u(x_i, t^n)}{k} - \kappa \frac{u(x_{i-1}, t^n) - 2u(x_i, t^n) + u(x_{i+1}, t^n)}{h^2}$$

Again we should be careful to use the form that directly models the differential equation in order to get powers of k and h that agree with what we hope to see in the global error. Although we dont know $u(x,t)$ in general, if we assume it is smooth and use Taylor series expansions about $u(x,t)$, we find that

Local truncation errors and order of accuracy

$$\tau_i^n = (u_t(x_i,t_n) + \frac{k}{2}u_{tt}(x_i,t_n) + O(k^2)) - \kappa(u_{xx}(x_i,t_n) + \frac{h^2}{12}u_{xxxx}(x_i,t_n) + O(h^4))$$

Since $u_t(x_i,t_n) = u_{xx}(x_i,t_n)$, the $O(h)$ terms drop out. By differentiating $u_t(x_i,t_n) = u_{xx}(x_i,t_n)$, we find that $u_{tt}(x_i,t_n) = u_{txx}(x_i,t_n) = u_{xxxx}(x_i,t_n)$ and so

$$\tau_i^n = (\frac{k}{2} - \frac{\kappa h^2}{12})u_{xxxx} + O(k^2 + h^4)$$

This method is said to be second order accurate in space and first order accurate in time since the truncation error is $O(h^2 + k)$.

Stability and Convergence for the Forward Euler method

Theorem (Lax equivalence theorem)

The approximate numerical solution to a well-posed linear problem converges to the solution of the continuous equation if and only if the numerical scheme is linear,consistent and stable.

Our goal is to show under what condition can U_i^n converges to $u(x_i, t_n)$ as the mesh sizes $h, k \to 0$.
To see this, we first see the local error a true solution can produce. Plug a true solution $u(x, t)$ into (6). We get

$$u_i^{n+1} - u_i^n = \frac{k\kappa}{h^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + k\tau_i^n \tag{15}$$

Let e_i^n denote for $u_i^n - U_i^n$. Then substract (6) from (15), we get

$$e_i^{n+1} - e_i^n = \frac{k\kappa}{h^2}(e_{i+1}^n - 2e_i^n + e_{i-1}^n) + k\tau_i^n \tag{16}$$

Stability and Convergence for the Forward Euler method

This can be expressed as

$$e_i^{n+1} = G(e_{i-1}^n, e_i^n, e_{i+1}^n) + k\tau_i^n \tag{17}$$

or in operator form:

$$e^{n+1} = Ge^n + k\tau^n \tag{18}$$

Suppose G satisfies

$$\|GU\| \leq \|U\| \tag{19}$$

under certain norm $\|\cdot\|$, we can accumulate the local truncation errors in time to get the global error as the follows.

$$\begin{aligned}
\|e^n\| &\leq \|Ge^{n-1}\| + k\|\tau^{n-1}\| \\
&\leq \|e^{n-1}\| + k\|\tau^{n-1}\| \\
&\leq \|e^{n-2}\| + k(\|\tau^{n-1}\| + \|\tau^{n-2}\|) \\
&\leq \|e^0\| + k(\|\tau^{n-1}\| + \cdots + \|\tau^0\|)
\end{aligned}$$

Stability and Convergence for the Forward Euler method

The local truncation error has the estimate

$$\max_n \|\tau^n\| = O(h^2) + O(k)$$

and the initial error e^0 satisfies

$$\|e^0\| = O(h^2)$$

then so does the global true error e^n for all n.

Stability and Convergence for the Forward Euler method

The above analysis leads to the following definitions.

Definition

A finite difference method is called consistent if its local truncation error satisfies:

$$\|\tau_i^n\| \to 0 \text{ when } h, k \to 0$$

Definition

A finite difference scheme $U^{n+1} = G(U^n)$ is called stable under the norm $\|\cdot\|$ in a region $(h, k) \in \mathbf{R}$ if

$$\|G(U)\| \leq \|U\|$$

Stability

Method 1: Matrix stability analysis
Consider the heat equation

$$u_t = \kappa u_{xx}$$

subject to a Dirichlet boundary condition.
After discretization by forward Euler scheme we obtain

$$U^{n+1} = (I + A)U^n$$

Let $r = \frac{\kappa k}{h^2}$ and $G = I + A$. For regular grid the matrix G has the

$$G = \begin{pmatrix} 1-2r & r & 0 & 0 & 0 & 0 \\ r & 1-2r & r & 0 & 0 & 0 \\ 0 & r & 1-2r & r & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & r & 1-2r & r \\ 0 & 0 & 0 & 0 & r & 1-2r \end{pmatrix}$$

Stability

Iteration of the scheme will converge to a solution only if all the eigenvalues of G do not exceed 1 in magnitude. Indeed, if any of these eigenvalues exceeds 1 (say, $\lambda > 1$), then $U^n = G^n U^0$ will grow as λ^n .

Proposition

Let Q be an $N \times N$ matrix of the form

$$Q = \begin{pmatrix} b & c & 0 & 0 & 0 & 0 \\ a & b & c & 0 & 0 & 0 \\ 0 & a & b & c & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & a & b & c \\ 0 & 0 & 0 & 0 & a & b \end{pmatrix}$$

Stability

The eigenvalues and the corresponding eigenvectors of G are

$$\lambda_j = b + 2\sqrt{ac}\cos\frac{\pi j}{N+1}, \quad env_j = \sqrt{\frac{a}{c}}\sin\frac{\pi j}{N+1}$$

We can immediately deduce that the eigenvalues of G are

$$\lambda_j = 1 - 2r + 2r\cos\frac{\pi j}{N_x}$$

and hence

$$\lambda_{min} = \lambda_{N_x-1} = 1 - 2r + 2r\cos\frac{\pi(N_x-1)}{N_x}$$
$$\lambda_{max} = \lambda_1 = 1 - 2r + 2r\cos\frac{\pi}{N_x}$$

Stability

If $\pi/N_x << 1$ the preceding expressions reduce to

$$\lambda_{min} = \lambda_{N_x-1} = 1 - 4r + r(\pi/N_x)^2$$
$$\lambda_{max} = \lambda_1 = 1 - r(\pi/N_x)^2$$

The condition for convergence for λ_{min} yields

$$r \leq \frac{2}{4 - (\pi/N_x)^2} \approx 1/2 \qquad (20)$$

With this condition, all the round-off errors will eventually decay, and the scheme is stable.

L^2 Stability-Von Neumann Analysis

We use two methods, one is the energy method, the other is the Fourier method, that is the von Neumann analysis. We describe the Von Neumann analysis below.
Given $\{U_j\}_{j\in\mathbb{Z}}$, we define

$$\widehat{U}(\xi) = \frac{1}{2\pi}\sum_j U_j e^{ij\xi}$$

The advantages of Fourier method for analyzing finite difference scheme are

1. the shift operator is transformed to a multiplier:

$$\widehat{TU}(\xi) = e^{i\xi}\widehat{U}(\xi)$$

where $T(U)_j = U_{j+1}$

L^2 Stability-Von Neumann Analysis

1. The Parseval equality

$$\|U\|^2 = \|\widehat{U}\|^2 = \int_{-\pi}^{\pi} |\widehat{U}(\xi)|^2 d\xi$$

If a finite difference scheme is expressed as

$$U_j^{n+1} = (GU^n)_j = \sum_{k=-l}^{m} a_k (T^k U^n)_j$$

Then

$$\widehat{U^{n+1}}(\xi) = \sum_{k=-l}^{n} a_k \widehat{T^k U^n}(\xi) = \sum_{k=-l}^{n} a_k e^{ik\xi} \widehat{U^n}(\xi)$$

Putting $\widehat{G}(\xi) = \sum_{k=-l}^{m} a_k e^{ik\xi}$, we have $\widehat{U^{n+1}}(\xi) = \widehat{G}(\xi)\widehat{U^n}(\xi)$.

L^2 Stability-Von Neumann Analysis

From the Parseval equality,

$$\|U^{n+1}\|^2 = \|\widehat{U^{n+1}}\|^2 = \int_{-\pi}^{\pi} |\widehat{U^{n+1}}(\xi)|^2 d\xi = \int_{-\pi}^{\pi} |\widehat{G}(\xi)\widehat{U^n}(\xi)|^2 d\xi$$

$$\leq \max_{\xi} |\widehat{G}(\xi)|^2 \int_{-\pi}^{\pi} |\widehat{U}^n(\xi)|^2 d\xi = |\widehat{G}|_\infty^2 \|\widehat{U}^n\|^2 = |\widehat{G}|_\infty^2 \|U^n\|^2$$

Thus a sufficient condition for stability is

$$|\widehat{G}|_\infty \leq 1 + \alpha k$$

Conversely, suppose $|\widehat{G}(\xi_0)| > 1$, from $\widehat{G}$ being a smooth function in ξ, we can find and σ such that

$$\widehat{G}(\xi) > 1 + \varepsilon \text{ for all } |\xi - \xi_0| < \sigma$$

L^2 Stability-Von Neumann Analysis

Let us choose an initial data U_0 in L^2 such that $\widehat{U}_0(\xi) = 1$ for $|\xi - \xi_0| < \sigma$

$$\begin{aligned}
\|U^n\|^2 &= \int_{-\pi}^{\pi} |\widehat{G}|^{2n}(\xi)|\widehat{U_0}|^2(\xi)d\xi \\
&\geq \int_{|\xi-\xi_0|<\sigma} |\widehat{G}|^{2n}(\xi)|\widehat{U_0}|^2(\xi)d\xi \\
&\geq (1+\varepsilon)^{2n}\sigma \to \infty \text{ as } n \to \infty
\end{aligned}$$

Thus, the scheme can not be stable. We conclude the above discussion by the following theorem.
Exercises: Compute the G for the schemes: Forward Euler, Backward Euler, and Crank- Nicolson and find the stable condition for each method

Existence and Uniqueness of the solution

We get the backward scheme for heat equation at level $n+1$

$$U_i^{n+1} = U_i^n + \frac{\kappa k}{h^2}(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1})$$

We only need to prove the uniqueness of the solution. For a given $n \in \{1, \cdots, N_t + 1\}$, set $U_i^n = 0$. Multiplying this equation by U_i^{n+1} and summing over $i \in \{1, \cdots, N_x - 1\}$ gives

$$\sum_{i=1}^{N_x-1} h(U_i^{n+1})^2 = \frac{\kappa k}{h} \sum_{i=1}^{N_x-1} ((U_{i+1}^{n+1} - U_i^{n+1})U_i^{n+1} - (U_i^{n+1} - U_{i-1}^{n+1})U_i^{n+1})$$

Or

$$\|U^{n+1}\|_{2,h}^2 + \kappa k |||U^{n+1}|||_{1,h} = 0$$

It yields that $U_i^{n+1} = 0$ for all $i = 0, \cdots, N_x$.