Lecture 22-23

Finite Difference Methods for IBVP

MA 322: Scientific Computing

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1 Finite Difference for Parabolic Equation

We consider following simple initial boundary value problem (IBVP)

$$u_t(x,t) - u_{xx}(x,t) = 0, \;\; (x,t) \in (a,b) \times (0,T], \; T < \infty, \tag{1}$$

with boundary conditions

$$u(a,t) = 0 \;\text{ and }\; u(b,t) = 0 \;\forall t > 0 \tag{2}$$

and initial condition

$$u(x,0) = g(x) \;\; x \in [a,b]. \tag{3}$$

As a first step towards numerical approximation, we now divide the computational domain $[a,b] \times [0,T]$ by the following points

$$(x_i,t_j), \;\; x_0 = a, \; x_{i+1} = x_i + h, \; \ldots, x_N = x_{N-1} + h = b \;\;\&\;\; t_0 = 0, \; t_{j+1} = t_j + k, \;\; t_M = T,$$

with mesh parameters

$$h = \frac{b-a}{n} \;\;\&\;\; k = \frac{T}{M}.$$

Now, at (x_i,t_j), we have

$$u_t(x_i,t_j) - u_{xx}(x_i,t_j) = 0. \tag{4}$$

In operator notation, we obtain

$$(T(u))(x_i,t_j) = 0, \;\; T(u) = u_t - u_{xx}. \tag{5}$$

2 Forward Scheme for Parabolic Problem

The forward scheme for the equation (4) is given by

$$\frac{u(x_i,t_{j+1}) - u(x_i,t_j)}{k} - \frac{u(x_{i+1},t_j) - 2u(x_i,t_j) + u(x_{i-1},t_j)}{h^2} = 0. \tag{6}$$

In operator notation, we write

$$(T_{h,k}(u))(x_i,t_j) = 0, \;\; (T_{h,k}(u))(x_i,t_j) = \frac{u(x_i,t_{j+1}) - u(x_i,t_j)}{k} - \frac{u(x_{i+1},t_j) - 2u(x_i,t_j) + u(x_{i-1},t_j)}{h^2}. \tag{7}$$

For the consistency, we observe that

$$((T - T_{h,k})(u))(x_i,t_j) = (T(u))(x_i,t_j) - (T_{h,k}(u))(x_i,t_j) = \mathrm{O}(k) + \mathrm{O}(h^2),$$

which tends to zero as $h \to 0$ and $k \to 0$. Therefore, forward scheme is consistent.
Remark:

- Forward scheme is of first order in time and second order in space. In fact, we can expect second order by increasing the computation along time direction setting $k = \mathrm{O}(h^2)$.

Since we can not expect to calculate the value $u(x_i,t_j)$ exactly, rather we look for approximation of $u(x_i,t_j)$. Let

$$u(x_i,t_j) \approx u_{i,j}$$

and subsequently, the scheme (6) is approximated as

$$\frac{u_{i,j+1} - u_{i,j}}{k} - \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} = 0, \tag{8}$$

which gives

$$u_{i,j+1} - u_{i,j} - r(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) = 0, \quad r = \frac{k}{h^2}. \tag{9}$$

Above equation involves two time levels $t = t_j$ and $t = t_{j+1}$. Let us separate both levels

$$u_{i,j+1} = ru_{i-1,j} + (1-2r)u_{i,j} + ru_{i+1,j}, \quad r = \frac{k}{h^2}. \tag{10}$$

At $t = t_{j+1}$ level, unknown grid points are

$$(x_1, t_{j+1}),\ (x_2, t_{j+1}), \dots, (x_{N-1}, t_{j+1}).$$

Thus, we have following $N-1$ unknowns

$$u_{1,j+1},\ u_{2,j+1}, \dots, u_{N-1,j+1}.$$

We calculate following unknowns by setting $1 \le i \le N-1$. For $i = 1$, we have

$$\begin{aligned} u_{1,j+1} &= ru_{0,j} + (1-2r)u_{1,j} + ru_{2,j}, \quad r = \frac{k}{h^2} \\ &= (1-2r)u_{1,j} + ru_{2,j}, \quad u_{0,j} = 0. \end{aligned} \tag{11}$$

For $2 \le i \le N-2$, we have $N-3$ equations given by (10). For $i = N-1$, we arrive at

$$\begin{aligned} u_{N-1,j+1} &= ru_{N-2,j} + (1-2r)u_{N-1,j} + ru_{N,j} \\ &= ru_{N-2,j} + (1-2r)u_{N-1,j}, \quad u_{N,j} = 0. \end{aligned} \tag{12}$$

Collecting above equations, we have following system equations

$$\begin{pmatrix} u_{1,j+1} \\ u_{2,j+1} \\ u_{3,j+1} \\ \vdots \\ u_{N-1,j+1} \end{pmatrix} = \begin{pmatrix} 1-2r & r & 0 & \dots & 0 & 0 \\ r & 1-2r & r & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & r & 1-2r & r \\ \dots & \dots & \dots & \dots & r & 1-2r \end{pmatrix} \begin{pmatrix} u_{1,j} \\ u_{2,j} \\ u_{3,j} \\ \vdots \\ u_{N-1,j} \end{pmatrix}. \tag{13}$$

Let us set following notation

$$U^j = \begin{pmatrix} u_{x_1,t_j} \\ u_{x_2,t_j} \\ u_{x_3,t_j} \\ \vdots \\ u_{x_{N-1},t_j} \end{pmatrix} \approx \begin{pmatrix} u_{1,j} \\ u_{2,j} \\ u_{3,j} \\ \vdots \\ u_{N-1,j} \end{pmatrix} = V^j,$$

so that matrix U^j and V^j store the actual values of the solution at $t = t_j$ level and approximate values of the solution at $t = t_j$ level, respectively. Therefore, for the approximation at $j+1$ level, we solve following system of equations

$$V^{j+1} = LV^j, \quad L = \begin{pmatrix} 1-2r & r & 0 & \dots & 0 & 0 \\ r & 1-2r & r & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & r & 1-2r & r \\ \dots & \dots & \dots & \dots & r & 1-2r \end{pmatrix}, \quad j = 0, 1, \dots, M-1, \tag{14}$$

which is approximation of the theoretical system of equations

$$U^{j+1} = LU^j, \quad L = \begin{pmatrix} 1-2r & r & 0 & \dots & 0 & 0 \\ r & 1-2r & r & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & r & 1-2r & r \\ \dots & \dots & \dots & \dots & r & 1-2r \end{pmatrix}, \quad j = 0, 1, \dots, M-1. \tag{15}$$

Therefore, we call (14) as numerical scheme. Subsequently, $U^n - V^n \to 0$ as $h,\ k \to 0$, means convergence. Again due to Lax equivalence theorem, numerical scheme (14) is convergent if it is stable and consistent. Now, we need to check only the stability.

3 Matrix Norm

For $1 \le p \le \infty$, $\mathbb{R}^n$ is a normed linear space with respect to following norm

$$\|x\|_p = \begin{cases} \left(\sum_{i=1}^n |x_i|^p\right)^{\frac{1}{p}}, & \text{for } 1 \le p < \infty, \\ \max_{1\le i\le n} |x_i|, & \text{for } p = \infty. \end{cases}$$

Please see the properties of a norm.

Let $A = (a_{ij})_{n\times n},\ \ a_{ij} \in \mathbb{C}$, be a square matrix of order n. Then, the norm of A is defined by

$$\|A\| = \sup_{x\neq 0}\Big\{\frac{\|Ax\|}{\|x\|}\ :\ x \in \mathbb{R}^n\Big\}.$$

Using the p-norm of $\mathbb{R}^n$, we have

$$\|A\|_p = \sup_{x\neq 0}\Big\{\frac{\|Ax\|_p}{\|x\|_p}\ :\ x \in \mathbb{R}^n\Big\}. \tag{16}$$

From the above definition, we observe following

- For $p = 1$, we have

  $$\|A\|_1 = \sup_{x\neq 0}\Big\{\frac{\|Ax\|_1}{\|x\|_1}\ :\ x \in \mathbb{R}^n\Big\}.$$

  Above norm is simplified by the following equivalent definition

  $$\|A\|_1 = \max_j \sum_{i=1}^n |a_{ij}|.$$

  Similarly, for $p = \infty$, we have

  $$\|A\|_\infty = \sup_{x\neq 0}\Big\{\frac{\|Ax\|_\infty}{\|x\|_\infty}\ :\ x \in \mathbb{R}^n\Big\},$$

  which can be replaced by following equivalent definition

  $$\|A\|_\infty = \max_i \sum_{j=1}^n |a_{ij}|.$$

- For the square matrices A and B, we have

  $$\|AB\| \le \|A\|\|B\|.$$

  Proof. From the definition, we obtain

  $$\|Ax\| \le \|A\|\|x\|\ \ \forall x \in \mathbb{R}^n.$$

  Therefore,

  $$\|(AB)x\| = \|A(Bx)\| \le \|A\|\|Bx\| \le \|A\|\|B\|\|x\|.$$

For $x \neq 0$, we have

$$\frac{\|AB\|}{\|x\|} \leq \|A\|\|B\|, \; \forall x \neq 0,$$

so that

$$\|AB\| = \sup_{x \neq 0} \left\{ \frac{\|(AB)x\|}{\|x\|} \; : \; x \in \mathbb{R}^n \right\} \leq \|A\|\|B\|.$$

- As a consequence of the above result, we have

$$\|A^n\| \leq \|A\|^n, \;\; n \in \mathbb{N}.$$

- For an invertiable matrix A, we have

$$I = AA^{-1}, \;\; \text{so that} \;\; 1 = \|AA^{-1}\|.$$

Thus,

$$1 \leq \|A\|\|A^{-1}\| \;\; \text{and hence} \;\; \|A^{-1}\| \geq \|A\|^{-1}.$$

- Suppose $\rho(A)$ denotes the largest eigenvalue of matrix A in magnitude, then

$$\rho(A) \leq \|A\|.$$

Notation $\rho(A)$ is known as spectral radius of the matrix A.

Proof. Suppose $\lambda_i, \; 1 \leq i \leq n$, is an eigenvalue of the matrix A, then

$$Ax = \lambda_i x,$$

where $x \neq 0$ is an eigenvector of the matrix A. Hence, we have

$$\|Ax\| = \|\lambda_i x\| = |\lambda_i|\|x\|.$$

Thus, for any eigenvalue λ_i and corresponding eigenvector x, we arrive at

$$|\lambda_i| = \frac{\|Ax\|}{\|x\|} \leq \sup_{x \neq 0} \left\{ \frac{\|Ax\|}{\|x\|} \; : \; x \in \mathbb{R}^n \right\} = \|A\|.$$

Hence, $\rho(A) \leq \|A\|$.

- For a real symmetric matrix A, we spectral radius of a matrix A is a norm and it is equivalent to $\|\cdot\|_2$ norm. Now onwards, for real symmetric matrix A, we use following norm

$$\|A\|_2 = \rho(A).$$

Therefore

$$\|A\|_2 \leq \|A\|_1, \; \|A\|_\infty, \;\; \text{etc.}$$

4 Stability of Forward Scheme

Let us recall the forward scheme

$$V^{j+1} = LV^j, \;\; L = \begin{pmatrix} 1-2r & r & 0 & \dots & 0 & 0 \\ r & 1-2r & r & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & r & 1-2r & r \\ \dots & \dots & \dots & \dots & r & 1-2r \end{pmatrix}, \;\; j = 0, 1, \dots, M-1, \tag{17}$$

At nth stage, we have

$$V^n = LV^{n-1} = L^2V^{n-2} = \ldots = L^nV^0. \tag{18}$$

Suppose due to roundoff error the initial data V^0 is perturbed to V^0_ϵ and coefficient matrix L is perturbed to L_ϵ. That is, during computation at nth stage, we are actually solving following perturbed system

$$V^n_\epsilon = L^n_\epsilon V^0_\epsilon. \tag{19}$$

Now stability means $V^n_\epsilon - V^n$ tends to zero as $\epsilon \to 0$ for all n, when

$$L_\epsilon - L \;\;\&\;\; V^0_\epsilon - V^0 \;\text{ tends to 0 as } \epsilon \to 0.$$

First note that

$$\begin{aligned} V^n_\epsilon - V^n = L^n_\epsilon V^0_\epsilon - L^nV^0 &= (L^n_\epsilon V^0_\epsilon - L^nV^0_\epsilon) + (L^nV^0_\epsilon - L^nV^0) \\ &= (L^n_\epsilon - L^n)V^0_\epsilon + L^n(V^0_\epsilon - V^0). \end{aligned}$$

Taking norm both sides, we obtain

$$\begin{aligned} \|V^n_\epsilon - V^n\| &\le \|(L^n_\epsilon - L^n)V^0_\epsilon\| + \|L^n(V^0_\epsilon - V^0)\| \\ &\le \|(L^n_\epsilon - L^n)V^0_\epsilon\| + \|L^n\|\|(V^0_\epsilon - V^0)\| \\ &\le \|(L^n_\epsilon - L^n)V^0_\epsilon\| + \|L\|^n\|(V^0_\epsilon - V^0)\|. \end{aligned}$$

Clearly, $L^n_\epsilon - L^n \to 0$ as $\epsilon \to 0$ yields

$$(L^n_\epsilon - L^n)x \to 0 \;\; \forall\, x \in \mathbb{R}^n.$$

Assuming $V^0_\epsilon - V^0 \to 0$ as $\epsilon \to 0$, we observe that $\|V^n_\epsilon - V^n\| \to 0$ at any stage n provided $\|L\| \le 1$.
Remark:

- For the stability, we need to find a matrix norm which yields $\|L\| \le 1$. In the present case, for the matrix L, we have

  $$\|L\|_1 = \|L\|_\infty = \max\{|r| + |1-2r|, 2|r| + |1-2r|\} = 2|r| + |1-2r| = 2r + |1-2r|.$$

  Clearly, $\|L\|_1 = \|L\|_\infty \le 1$ provided

  $$2r + |1-2r| \le 1 \;\text{ Or }\; |1-2r| \le 1-2r \;\text{ Or }\; -(1-2r) \le 1-2r,$$

  which gives

  $$r \le \frac{1}{2} \;\text{ Or }\; \frac{k}{h^2} \le \frac{1}{2}.$$

- Hence, forward scheme for parabolic equation is explicit and conditionally stable with truncation error

  $$\text{T. E.} = \text{O}(k) + \text{O}(h^2).$$

5 Backward Scheme

For the backward scheme to the IBVP (1)-(3), we consider following equation

$$u_t(x,t) - u_{xx}(x,t) = 0, \;\; (x,t) \in (a,b) \times (0,T], \; T < \infty, \tag{20}$$

at the grid point (x_i, t_{j+1}). That is

$$u_t(x_i, t_{j+1}) - u_{xx}(x_i, t_{j+1}) = 0. \tag{21}$$

In operator notation, we obtain

$$(T(u))(x_i,t_{j+1})=0,\ \ T(u)=u_t-u_{xx}. \tag{22}$$

The backward scheme for the equation (21) is given by

$$\frac{u(x_i,t_{j+1})-u(x_i,t_j)}{k}-\frac{u(x_{i+1},t_{j+1})-2u(x_i,t_{j+1})+u(x_{i-1},t_{j+1})}{h^2}=0. \tag{23}$$

It is easy to see that backward scheme has truncation error of order

$$\mathrm{O}(k)+\mathrm{O}(h^2).$$

Further, the numerical scheme corresponding to the theoretical scheme (23) is given by

$$\frac{u_{i,j+1}-u_{i,j}}{k}-\frac{u_{i+1,j+1}-2u_{i,j+1}+u_{i-1,j+1}}{h^2}=0, \tag{24}$$

which gives

$$u_{i,j+1}-u_{i,j}-r(u_{i+1,j+1}-2u_{i,j+1}+u_{i-1,j+1})=0,\ \ r=\frac{k}{h^2}. \tag{25}$$

Let us separate both time levels

$$-ru_{i-1,j+1}+(1+2r)u_{i,j+1}-ru_{i+1,j+1}=u_{i,j}. \tag{26}$$

At $t=t_{j+1}$ level, unknown grid points are

$$(x_1,t_{j+1}),\ (x_2,t_{j+1}),\ldots,(x_{N-1},t_{j+1}).$$

Thus, we have following $N-1$ unknowns

$$u_{1,j+1},\ u_{2,j+1},\ldots,u_{N-1,j+1}.$$

We calculate following unknowns by setting $1\le i\le N-1$. For $i=1$, we have

$$(1+2r)u_{1,j+1}-ru_{2,j+1}=u_{1,j}. \tag{27}$$

For $2\le i\le N-2$, we have $N-3$ equations given by (26). For $i=N-1$, we arrive at

$$-ru_{N-2,j+1}+(1+2r)u_{N-1,j+1}=u_{N-1,j}. \tag{28}$$

Collecting above equations, we have following system equations

$$\begin{pmatrix} 1+2r & -r & 0 & \ldots & 0 & 0\\ -r & 1+2r & r & 0 & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & -r & 1+2r & -r\\ \ldots & \ldots & \ldots & \ldots & -r & 1+2r \end{pmatrix}\begin{pmatrix} u_{1,j+1}\\ u_{2,j+1}\\ u_{3,j+1}\\ \vdots\\ u_{N-1,j+1}\end{pmatrix}=\begin{pmatrix} u_{1,j}\\ u_{2,j}\\ u_{3,j}\\ \vdots\\ u_{N-1,j}\end{pmatrix}. \tag{29}$$

Equivalently,

$$LV^{j+1}=V^j,\ \ L=\begin{pmatrix} 1+2r & -r & 0 & \ldots & 0 & 0\\ -r & 1+2r & r & 0 & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & -r & 1+2r & -r\\ \ldots & \ldots & \ldots & \ldots & -r & 1+2r \end{pmatrix}.$$

The unknown level depends on the invertibility of the matrix L. The eigenvalues of the matrix L is given by

$$\begin{aligned}\lambda_n &= 1 + 2r + 2r\cos\left(\frac{n\pi}{N}\right), \quad 1 \le n \le N \\ &= 1 + 2r(1 + \cos\theta), \quad \theta = \frac{n\pi}{N} \\ &= 1 + 4r\cos^2\left(\frac{\theta}{2}\right) \ge 1.\end{aligned}$$

Therefore L^{-1} exists and the unknown level is given by

$$V^{j+1} = L^{-1}V^j. \tag{30}$$

For the stability, like previous case, we need $\|L^{-1}\| \le 1$. Again apply the fact that

$$\text{eigenvalue of } L^{-1} = \frac{1}{\text{eigenvalue of } L} = \frac{1}{\lambda_n}$$

to arrive at

$$\|L^{-1}\|_2 = \rho(L^{-1}) \ \text{ so that } \ \|L^{-1}\|_2 \le 1 \ \text{ as } \ \lambda_n \ge 1.$$

Hence, backward scheme is unconditionally stable implicit scheme with

$$\text{T. E.} = \text{O}(k) + \text{O}(h^2).$$