Lecture 20-21

Finite Difference Methods for BVP

MA 322: Scientific Computing

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1 Finite Difference for ODE

We consider following second order linear ODE

$$y''(x) + P(x)y'(x) + Qy(x) = R(x), \quad x \in (a,b), \tag{1}$$

with boundary conditions

$$y(a) = \alpha \text{ and } y(b) = \beta. \tag{2}$$

Above boundary conditions are known as Dirichlet boundary conditions. For the existence and unique solution of the above BVP, we assume given data P, Q & $R \in C[a,b]$. In that case there exist an unique solution $y \in C^2[a,b]$ satisfying equation (1) at $x \in [a,b]$ and the conditions (2). In general, it might not be possible to evaluate the solution for the BVP (1)-(2) manually, so we rely on some numerical schemes. Finite Difference Method (FDM) is an another class of numerical method for such problems. The objective of this lecture is to develop finite difference tool kits for the equation (1) along with different boundary conditions.

As a first step towards numerical approximation, we now divide the interval $[a,b]$ into n equal parts by the following points

$$x_0 = a,\ x_1 = x_0 + h,\ \ldots, x_{i+1} = x_i + h,\ \ldots, x_n = x_{n-1} + h = b, \quad h = \frac{b-a}{n}.$$

Now, at $x = x_i$, we obtain

$$y''(x_i) + P(x_i)y'(x_i) + Q(x_i)y(x_i) = R(x_i). \tag{3}$$

Since, our objective is to find $y(x_i)$, we try to get rid of the derivatives $y''(x_i)$ and $y'(x_i)$. This is done by using Taylor's series expansion

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \ldots + \frac{h^n}{n!}y^{(n)}(x) + \mathrm{O}h^{n+1} \tag{4}$$

for $y \in C^{n+1}[a,b]$. Thus, we have following relations

$$\begin{aligned} y(x_{i+1}) &= y(x_i + h) = y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(x_i) + \ldots \\ y(x_{i-1}) &= y(x_i - h) = y(x_i) - hy'(x_i) + \frac{h^2}{2}y''(x_i) - \ldots \end{aligned}$$

so that

$$\begin{aligned} y'(x_i) &= \frac{y(x_{i+1}) - y(x_i)}{h} + \mathrm{O}(h), \\ y'(x_i) &= \frac{y(x_i) - y(x_{i-1})}{h} + \mathrm{O}(h), \\ y'(x_i) &= \frac{y(x_{i+1}) - y(x_{i-1})}{2h} + \mathrm{O}(h^2), \\ y''(x_i) &= \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + \mathrm{O}(h^2), \end{aligned}$$

which yields

$$\begin{aligned} y'(x_i) &\approx \frac{y(x_{i+1}) - y(x_i)}{h}, \text{ with T. E. } \mathrm{O}(h), \text{ known as forward approximation} \\ y'(x_i) &\approx \frac{y(x_i) - y(x_{i-1})}{h}, \text{ with T. E. } \mathrm{O}(h), \text{ known as backward approximation} \\ y'(x_i) &\approx \frac{y(x_{i+1}) - y(x_{i-1})}{2h}, \text{ with T. E. } \mathrm{O}(h^2), \text{ known as central approximation} \\ y''(x_i) &\approx \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2}, \text{ with T. E. } \mathrm{O}(h^2), \text{ known as symmetric approximation.} \end{aligned}$$

Therefore, at $x = x_i$, equation (1) can be approximated by following second order scheme

$$\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + P(x_i)\frac{y(x_{i+1}) - y(x_{i-1})}{2h} + Q(x_i)y(x_i) = R(x_i)$$

Now, collecting the coefficients of $y(x_{i+1}),\ y(x_i)$ and $y(x_{i-1})$, we arrive at

$$y(x_{i+1})\Big(1 + \frac{hP(x_i)}{2}\Big) + y(x_i)\big(-2 + h^2Q(x_i)\big) + y(x_{i-1})\Big(1 - \frac{hP(x_i)}{2}\Big) = h^2R(x_i). \tag{5}$$

For the discretization, our unknowns are

$$y(x_1),\ y(x_2),\ \ldots, y(x_{n-1}).$$

Therefore, we need $n-1$ equations. For which, we substitute $1 \leq i \leq n-1$ in (5). For $i = 1$, we we obtain

$$y(x_2)\Big(1 + \frac{hP(x_1)}{2}\Big) + y(x_1)\big(-2 + h^2Q(x_1)\big) + y(x_0)\Big(1 - \frac{hP(x_1)}{2}\Big) = h^2R(x_1).$$

Now, substitute $y(a) = \alpha = y(x_0)$ to have

$$y(x_1)\big(-2 + h^2Q(x_1)\big) + y(x_2)\Big(1 + \frac{hP(x_1)}{2}\Big) = h^2R(x_1) - \alpha\Big(1 - \frac{hP(x_1)}{2}\Big). \tag{6}$$

For $2 \leq i \leq n-2$, we have

$$\begin{aligned}&0 \times y(x_1) + \ldots + 0 \times y(x_{i-2}) + y(x_{i-1})\Big(1 - \frac{hP(x_i)}{2}\Big) + y(x_i)\big(-2 + h^2Q(x_i)\big) \\ &+ y(x_{i+1})\Big(1 + \frac{hP(x_i)}{2}\Big) + 0 \times y(x_{i+2}) + \ldots + 0 \times y(x_{n-1}) = h^2R(x_i).\end{aligned} \tag{7}$$

Similarly, for $i = n-1$, we obtain

$$y(x_{n-2})\Big(1 - \frac{hP(x_{n-1})}{2}\Big) + y(x_{n-1})\big(-2 + h^2Q(x_{n-1})\big) = h^2R(x_{n-1}) - \beta\Big(1 + \frac{hP(x_{n-1})}{2}\Big). \tag{8}$$

Now, we set

$$\begin{aligned}A(i) &= 1 - \frac{hP(x_i)}{2}, \ \text{ coefficient of } y(x_{i-1}), \ \ 2 \leq i \leq n-1 \\ B(i) &= -2 + h^2Q(x_i), \ \text{ coefficient of } y(x_i), \ \ 1 \leq i \leq n-1 \\ C(i) &= 1 + \frac{hP(x_i)}{2}, \ \text{ coefficient of } y(x_{i+1}) \ \ 1 \leq i \leq n-2.\end{aligned}$$

Therefore, we have following system of equations

$$\begin{pmatrix} B(1) & C(1) & 0 & \ldots & 0 & 0 \\ A(2) & B(2) & C(2) & 0 & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & A(n-2) & B(n-2) & C(n-2) \\ \ldots & \ldots & \ldots & \ldots & A(n-1) & B(n-1) \end{pmatrix} \begin{pmatrix} y(x_1) \\ y(x_2) \\ y(x_3) \\ \vdots \\ y(x_{n-1}) \end{pmatrix}$$

$$= \begin{pmatrix} h^2R(x_1) - \alpha\Big(1 - \frac{hP(x_1)}{2}\Big) \\ h^2R(x_2) \\ \vdots \\ h^2R(x_{n-2}) \\ h^2R(x_{n-1}) - \beta\Big(1 + \frac{hP(x_{n-1})}{2}\Big) \end{pmatrix} \quad \text{Or} \ \ LU = F. \tag{9}$$

Remark: Now, we need to justify the invertibility of the coefficient matrix L. This can be verified by checking the eigenvalues of the tridiagonal matrix L. Regarding eigenvalues of a tridiagonal matrix, we have following result.

Theorem 1.1 The eigenvalues of the order n tridiagonal matrix

$$\begin{pmatrix} a & b & 0 & \dots & 0 & 0 \\ c & a & b & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & c & a & b \\ \dots & \dots & \dots & \dots & c & a \end{pmatrix}$$

are

$$\lambda_s = a + 2\sqrt{bc}\cos\left(\frac{s\pi}{n+1}\right), \quad 1 \leq 2 \leq s \leq n,$$

where a, b and c may be real or complex.

2 Influence of Truncation Error

At $x = x_i$, we have following equation

$$y''(x_i) + P(x_i)y'(x_i) + Q(x_i)y(x_i) = R(x_i). \tag{10}$$

In operator notation, above equation is expressed as

$$(T(y))(x_i) = R(x_i), \;\; T(y) = y'' + Py' + Qy. \tag{11}$$

Again, approximation of (10) is given by

$$\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + P(x_i)\frac{y(x_{i+1}) - y(x_{i-1})}{2h} + Q(x_i)y(x_i) = R(x_i). \tag{12}$$

In operator notation, we write

$$(T_h(y))(x_i) = R(x_i), \;\; (T_h(y))(x_i) = \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + P(x_i)\frac{y(x_{i+1}) - y(x_{i-1})}{2h} + Q(x_i)y(x_i).$$

At the grid point x_i, the truncation error is given by

$$\begin{aligned} ((T - T_h)(y))(x_i) &= \Big(y''(x_i) - \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2}\Big) \\ &\quad + P(x_i)\Big(y'(x_i) - \frac{y(x_{i+1}) - y(x_{i-1})}{2h}\Big) = \mathrm{O}(h^2). \end{aligned}$$

As the T.E. tends to zero as $h \to 0$, our approximation (12) to (10) is consistent.

3 Influence of Roundoff Error

Consider following BVP

$$y'' + y = \pi, \;\; y(0) = 0 \;\; \& \;\; y(1) = 0.$$

For the discretization

$$x_0 = 0, \; x_1 = x_0 + h, \; \dots, x_{i+1} = x_i + h, \; \dots, x_n = x_{n-1} + h = 1, \;\; h = \frac{1}{n},$$

we need to solve a $(n-1) \times (n-1)$ system of equations $LU = F$ with

$$L = \begin{pmatrix} -2+h^2 & 1 & 0 & \dots & 0 & 0 \\ 1 & -2+h^2 & 1 & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 1 & -2+h^2 & 1 \\ \dots & \dots & \dots & \dots & 1 & -2+h^2 \end{pmatrix} \;\; \text{and} \;\; F = \begin{pmatrix} h^2\pi \\ h^2\pi \\ \vdots \\ h^2\pi \\ h^2\pi \end{pmatrix}.$$

Note: In practice, the data π will be rounded as

$$\pi \approx 3.14 \text{ or } \pi \approx 3.146, \text{ and so on.}$$

More precisely, π will be perturbed to another data π_ϵ due to roundoff error and subsequently the matrix F will be perturbed to F_ϵ. Similarly, matrix L will be perturbed to another data L_ϵ. Hence, during computation, we are solving a perturbed system of equation

$$L_\epsilon U_\epsilon = F_\epsilon.$$

Now, we expect $U_\epsilon \to U$ as $\epsilon \to 0$ when perturbation is small. This is exactly known as **stability** of a numerical scheme. For our present case stability means

$$U_\epsilon \to U \text{ as } \epsilon \to 0 \text{ when } L_\epsilon \to L \ \& \ F_\epsilon \to F \text{ as } \epsilon \to 0$$

that is

$$(L_\epsilon \to L \ \& \ F_\epsilon \to F \text{ as } \epsilon \to 0) \Rightarrow U_\epsilon \to U \text{ as } \epsilon \to 0.$$

4 Numerical Scheme

Apart from roundoff error, we may encounter some other errors also. Therefore, we can not expect to solve U from the $LU = F$. Note that matrix U store the actual value $y(x_i)$ of the true solution at $x = x_i$. For the approximation of U, we use matrix Y. That is

$$U = \begin{pmatrix} y(x_1) \\ y(x_2) \\ y(x_3) \\ \vdots \\ y(x_{n-1}) \end{pmatrix} \approx \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-1} \end{pmatrix} = Y, \quad y(x_i) \approx y_i.$$

In fact, using the notation $y(x_i) \approx y_i$, we have following notation

$$\begin{aligned} y'(x_i) &\approx \frac{y(x_{i+1}) - y(x_i)}{h} \approx \frac{y_{i+1} - y_i}{h}, \\ y'(x_i) &\approx \frac{y(x_i) - y(x_{i-1})}{h} \approx \frac{y_i - y_{i-1}}{h}, \\ y'(x_i) &\approx \frac{y(x_{i+1}) - y(x_{i-1})}{2h} \approx \frac{y_{i+1} - y_{i-1}}{2h}, \\ y''(x_i) &\approx \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}. \end{aligned}$$

Using above notation in (3), we arrive at following system

$$\begin{pmatrix} B(1) & C(1) & 0 & \dots & 0 & 0 \\ A(2) & B(2) & C(2) & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & A(n-2) & B(n-2) & C(n-2) \\ \dots & \dots & \dots & \dots & A(n-1) & B(n-1) \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-1} \end{pmatrix}$$

$$= \begin{pmatrix} h^2 R(x_1) - \alpha\left(1 - \frac{hP(x_1)}{2}\right) \\ h^2 R(x_2) \\ \vdots \\ h^2 R(x_{n-2}) \\ h^2 R(x_{n-1}) - \beta\left(1 + \frac{hP(x_{n-1})}{2}\right) \end{pmatrix} \quad \text{Or } LV = F. \tag{13}$$

as an approximation of the original system (9). Therefore, we call original system (9) as theoretical scheme and (13) as numerical scheme. If the approximated solution V tends to actual solution U, we call the scheme is convergent.

Remark: Why consistency and stability of a numerical approximation are important? It is illustrated in the next result.

Theorem 4.1 Lax Equivalence Theorem: A numerical scheme for a linear problem is convergent if and only if the scheme is consistent.

Example 4.1 Try to implement a second order scheme for the following mixed BVP

$$y'' + Py' + Qy = R, \;\; y'(a) = \alpha, \;\; y(b) = \beta.$$