Lecture 42: Special Boundary Value Problems

The Lecture Contains:

Previous Next

Finite Difference Method:

For the direct numerical solution of a boundary value problem of class M, we introduce the points $x_n = a + n\,h\,(n = 0, 1, \ldots, N)$, where $h = (b-a)/N$ and N is an appropriate integer. A scheme is then designed for the determination of numbers y_n which approximate the values $y\,(x_n)$ of the true solution at the point x_n.

The natural way to obtain such a scheme is to demand that the y_n satisfy at each interior mesh point x_n a difference equation

$$\alpha_K\, y_{n+K} + \alpha_{K-1}\, y_{n+K-1} + \cdots + \alpha_0\, y_n - h^{\,2}\,\{\beta_K\, f_{n+K} + \cdots + \beta_0\, f_n\} = 0 \quad (10.22)$$

Again the coefficients are chosen in such a way that the associated difference operator is small for a solution of $y'' = f\,(x,y)$. One difficulty arises here in the difference scheme. As in any algebraic problem, we need as many equations for the determination of the unknowns as there are unknowns. Since y_0 and y_N are determined by the boundary condition, the unknowns in our case are $y_1, \ldots, y_{N-1}$. If the step number of the difference equation $> 2\;(\mathrm{i\,.e}\ldots K > 2)$, new unknown values such as y_{-1} or y_{N+1} are introduced for which there is no equation.

This difficulty can be circumvented by suitably modifying the difference equations near the boundary points; it does not arise at all if $K = 2$, the smallest possible value. If $K = 2$ in (10.22) and if the associated–difference operator has order p, the difference equation is necessarily proportional to an equation of the form

$$-y_{n-1} + 2y_n - y_{n+1} + h^2\,\{\beta_0\, f_{n-1} + \beta_1 f_n + \beta_2\, f_{n-1}\} = 0 \qquad (10.23)$$

where $\beta_0 + \beta_1 + \beta_2 = 1$. The difference equations most frequently used for boundary value problems are.

$$-y_{n-1} + 2y_n - y_{n+1} + h^2\, f_n = 0 \qquad (p = 2) \qquad (10.24)$$

and

$$-y_{n-1} + 2y_n - y_{n+1} + \frac{1}{12}\, h^2\,(f_{n-1} + 10\, f_n + f_{n+1}) = 0 \qquad (p = 4) \quad (10.25)$$

Previous Next

Boundary conditions of the second and third kind:

In addition to the boundary conditions in (10.16), which are called conditions of the first kind, there occur in practice also conditions of the form

$$\alpha\, y\,(a) + \beta\, y'(a) = A$$

$$\gamma\, y\,(b) + \delta\, y'(b) = B \qquad (10.26)$$

where $\alpha, \beta, \gamma,$ and δ are constants, $\beta^2 + \delta^2 > 0$. Conditions (10.26) are said to be of the second or third kind according to whether $\alpha^2 + \gamma^2 = 0 \text{ or} > 0$. It is easy to extend the above scheme to these cases. An additional equation for y_0 is obtained by writing (10.23) for $n = 0$ and eliminating y_{-1} by means of the first equation of (10.26) where $y\,(a) = y_0$ and $y'(a) = (y_1 - y_{-1})/2h$. A similar procedure can be adopted in order to obtain an equation for y_N.

Previous Next

Solution of the difference scheme: Linear case

We introduce the vectors

$$Y=\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \end{bmatrix}, \quad f(y)=\begin{bmatrix} f(x_1,y_1) \\ f(x_2,y_2) \\ \vdots \\ f(x_{N-1},y_{N-1}) \end{bmatrix}$$

$$a=\begin{bmatrix} A_1-\beta_0 h^2 f(x_0,A_1) \\ 0 \\ \vdots \\ 0 \\ \beta_1-\beta_2 h^2 f(x_N,B_1) \end{bmatrix}$$

and the matrices

$$J=\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

$$B=\begin{bmatrix} \beta_1 & \beta_2 & & & & \\ \beta_0 & \beta_1 & \beta_2 & & & \\ & \beta_0 & \beta_1 & \beta_2 & & \\ & & \beta_0 & \beta_1 & \beta_2 & \\ & & & \beta_0 & \beta_1 & \beta_2 \end{bmatrix}$$

(in which all elements not on the main diagonal or on the diagonal adjacent to it are zero), the system of equations arising from demanding that (10.22) hold for $n=1,\ldots,N-1$ can be written compactly in the form

$$J\,y+h^2\,B\,f(y)=a \qquad (10.27)$$

Previous Next

We first of all derive a method for solving this system when the given differential equation is linear,

i.e.

$f(x,y)$ is of the form

$$f(x,y) = g(x)\, y + K(x)$$

where $g(x)$ and $K(x)$ are given functions. Defining the diagonal matrix

$$G = \begin{bmatrix} g(x_1) & & \\ & g(x_2) & \\ & & g(x_{N-1}) \end{bmatrix}$$

and the vector

$$K = \begin{bmatrix} K(x_1) \\ K(x_2) \\ \vdots \\ K(x_{N-1}) \end{bmatrix}$$

we may write

$$f(y) = G\, y + K$$

The system (10.27) now reduces to the system of linear equations,

$$A\, y = b \qquad (10.28)$$

where

$$A = J + h^2\, B\, G$$

$$b = a - h^2\, B\, K \qquad (10.29)$$

Previous Next

Although the order of the linear system (10.28) may be large (indeed, the order tends to infinity as $h \to 0$), its numerical solution is relatively easy owing to the fact that the matrix A shares with the matrices J and B the property of having non zero elements only on the main diagonal and the two diagonals adjacent to It. Matrices of this kind are called tri diagonal. In fact, if $A = \left(a_{n,m}\right)$, we have by virtue of (10.29)

$$a_{n,n} = 2 + h^2 \beta_1 g_n$$

$$a_{n,n-1} = -1 + h^2 \beta_0 g_{n-1}$$

$$a_{n,n+1} = -1 + h^2 \beta_2 g_{n+1}\,; \qquad n = 1, 2, \ldots, N-1$$

and $a_{n,m} = 0$ for $|n-m| > 1$

Linear systems involving non-singular tri diagonal matrices are most easily solved by an adaptation of the Gaussian algorithm which may conveniently be summarized as follows. Assume we have succeeded in determining two nonsingular matrices $L = \left(l_{m,n}\right)$ and $U = \left(U_{m,n}\right)$ of the special form

$$L = \begin{bmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ & l_{23} & 1 & & \\ & & \ddots & \ddots & \\ & & & & 1 \\ & & & & l_{n-1,\,n-2} \end{bmatrix}$$

$$\left(1_{m,m} = 1;\ 1_{m,n} = 0 \text{ for } n > m \text{ or } n < m-1\right)$$

$$U = \begin{bmatrix} u_{11} & u_{12} & & \\ & u_{22} & \ddots & \\ & & \ddots & u_{N-2,\,N-1} \\ & & & u_{N-1,\,N-1} \end{bmatrix}$$

having the property that

$$LU = A \tag{10.30}$$

Previous Next

In order to solve (10.28), we first determine the vector Z such that

$$LZ = b \qquad (10.31)$$

and then y such that

$$U\,y = Z \qquad (10.32)$$

Since $y = U^{-1}\ Z = U^{-1}\ L^{-1}\ b = A^{-1}b$, the vector y thus determined satisfies (10.28).

In order to carry out this method, we note that (10.30) is equivalent to the relations

$$u_{11} = a_{11} \qquad (10.33)$$

$$l_{n,n-1}\,u_{n-1,n-1} = a_{n,n-1} \qquad (10.34)$$

$$l_{n,n-1}\,u_{n-1,n} + u_{n,n} = a_{nn} \quad n = 2, 3, \ldots, N-1 \qquad (10.35)$$

$$u_{n,n+1} = a_{n,n+1} \quad n = 1, 2, \ldots, N-2 \qquad (10.36)$$

Relation (10.36) immediately yields $u_{n,n+1}$; relations (10.34) and (10.35) may be rearranged to yield $l_{n,n-1}$ and $u_{n\,n}$ recursively, as follows:

$$u_{11} = a_{11} \qquad (10.37)$$

$$l_{n,n-1} = \frac{a_{n,\ n-1}}{u_{n-1,\ n-1}} \qquad (10.38)$$

$$u_{nn} = a_{nn} - l_{n,n-1}u_{n-1,\ n} \qquad (10.39)$$

The algorithm (10.38) and (10.39) breaks down when $u_{n-1,n-1} = 0$. If this is the case, then, denoting by $\det A$ the determinant of the matrix A, we have $\det\ A = \det U \det L = u_{11}\ u_{22} \ldots u_{N-1,N-1} = 0$, and A is singular.

Previous Next

The vector Z can be determined simultaneously with L from the relations

$$Z_1 = b_1,$$

$$l_{n,n-1} \; Z_{n-1} + Z_n = b_n \qquad n = 2, \dots, N-1$$

which may be recursively arranged in the from

$$Z_1 = b_1 \tag{10.40}$$

$$Z_n = b_n - l_{n,n-1} \; Z_{n-1} \qquad n = 2, \dots, N-1 \tag{10.41}$$

If (10.32) is written out in components, we find

$$u_{N-1,N-1} \; y_{N-1} = Z_{n-1}$$

$$u_{n\,n} \; y_{n-1} + u_{n,n+1} \, y_{n+1} = Z_n \qquad n = 1, 2, \dots, N-2$$

These relations can be arranged so as to furnish the components of y, starting with the last component. One finds

$$y_{N-1} = \frac{Z_{N-1}}{u_{N-1,N-1}} \tag{10.42}$$

$$y_n = \frac{Z_{n-} a_{n,n+1} \, y_{n+1}}{y_{n\,n}} \qquad n = N-2, \dots, 1 \tag{10.43}$$

Previous Next

The complete procedure may be summarized as follows:

1. Calculate $u_{n\,n}$ and Z_n, starting with $n = 1$, from the relations :

$u_{11} = a_{11} \qquad Z_1 = b_1$

$l_{n,n-1} = \frac{a_{n,n-1}}{u_{n-1,n-1}}$

$u_{n\,n} = a_{n\,n} - l_{n\,,n-1}\, u_{n\,-1,n}$

$Z_n = b_n - l_{n,n-1}\; Z_{n-1} \qquad\qquad n = 2,\ 3, \dots, N-1$

The quantities a_{nn} need not be saved, unless the same system is solved repeatedly for different non–homogeneous terms. The quantities a_{nn} and b_n are not used after $u_{n\,n}$ and Z_n have been computed.

2. Calculate y_n, stating with $n = N - 1$, form the relations:

$y_{N-1} = \frac{Z_{N-1}}{U_{N-1\,,N-1}}$

$y_n = \frac{Z_{n-}\,a_{n,n+1}\,y_{n+1}}{u_{nn}} \qquad n = N - 2, \dots, 1$

The whole process requires approximately $3\,N$ additions, $3\,N$ multiplications and $2\,N$ divisions. This compares very favorably to the $\frac{N^3}{3}$ multiplications alone that have to be performed in the solution of a system with a matrix of order N that has no zero elements.

Solution of the difference scheme: nonlinear case.

If the function $f(x\,,y)$ is not linear in y, one can not hope to solve the system (10.27) by algebraic methods. Some iterative procedure must be resorted to. The method which is recommended for this purpose is generalization of the Newton-Raphson method to systems of transcendental equations.

In the case of a single equation, the Newton-Raphson method consists of linearizing the given function $f(x) = 0$ by replacing $f\,(x) - f\left(x^{(0)}\right)$ by its differential at a point $x^{(0)}$ believed to be close to the actual solution, and solving the linearized equation $f\left(x^{(0)}\right) + f'\left(x^{(0)}\right) \Delta\, x = 0$. The value $x^{(1)} = x^{(0)} + \Delta\, x$ is then accepted as a better approximation, and the process is continued if necessary. Quite analogously if $y^{(0)}$ is a vector believed to be close to the actual solution of the equation

$$J\, y + h^2\, B\, f(y) - a = 0 \qquad (10.44)$$

so that the residual vector

$$r\left(y^{(0)}\right) = J\, y^{(0)} + h^2\, B\, f\left(y^{(0)}\right) - a \qquad (10.45)$$

is small, we replace the increments of the function by their differentials at the point

$r(y)$ $y = y^{(0)}$

and solve the resulting linear system of equations for the increment of the vector y, which we shall call by Δy. Since the expression $J y$ is already linear in y, the differential of the vector $r(y)$ at $y = y_0$ is found to be $F\left(y^{(0)}\right)\Delta y$, where $F(y)$ denotes the diagonal matrix

$$F(y) = \begin{bmatrix} f_y(x_1, y_1) & & & \\ & f_y(x_2, y_2) & & \\ & & \ddots & \\ & & & f_y(x_{N-1}, y_{N-1}) \end{bmatrix} \quad (10.46)$$

Previous Next

The linearized system (10.44) thus reads

$$r\left(y^{(0)}\right)+\left(J+h^2\,B\,F\left(y^{(0)}\right)\right)\Delta\,y=0 \qquad (10.47)$$

and its solution is given by

$$\Delta\,y=\Delta\,y^{(0)}=\;-A\left(y^{(0)}\right)^{-1}r\left(y^{(0)}\right)$$

provided that the inverse of the matrix

$$A\,(y)=\;J+\;h^2\,B\,F\,(y)$$

exists for $y=y^{(0)}$. If all goes well, the vector $y^{(1)}\;=\;y^{(0)}+\Delta\,y^{(0)}$ will be a better approximation to the exact solution, the residual vector $r\,\left(y^{(1)}\right)$ will be smaller, and the process

can be repeated with $y^{(1)}$ taking the place of $y^{(0)}$, etc. until the convergence is achieved. Since for problems of class M, the system (10.44) has a unique solution y for sufficiently small values of h, and it is known that Newton's method produces a sequence of vectors $y^{(n)}, n=1,2,\ldots,$ which converges rapidly to y provided that the initial approximation $y^{(0)}$ is not too bad. Here we are mainly concerned with the question of computational technique. In this respect it should be noted that for the solution of (10.47) it is not necessary to calculate the inverse of the matrix $A\,\left(y^{(0)}\right)$. All that is required is the solution of the system of linear equations

$$A\,\left(y^{(0)}\right)\Delta\,y=\;-\,r\,\left(y^{(0)}\right)$$

For the components of $\Delta\,y$. This solution is greatly facilitated by the fact that the matrix $A\,\left(y^{(0)}\right)$ is again tri-diagonal. In fact, if $A\,\left(y^{(0)}\right)=\left(a_{m\,n}\right)$, we have

$$a_{n,n-1}=-1+h^2\beta_0\,f_y\left(x_{n-1},\,y_{n-1}^{(0)}\right), \qquad n=\;2,3,\ldots,N-1$$

$$a_{n,n}=-2+h^2\,\beta_1\,f_y\left(x_{n-1},\,y_n^{(0)}\right), \qquad n=1\,,2,\ldots,N-1$$

$$a_{n,n+1}=-1+h^2\,\beta_2\,f_y\left(x_{n+1},\,y_{n+1}^{(0)}\right), \qquad n=\;1,\ldots,N-2$$

and all other elements are zero.

The method described for the linear case thus is immediately applicable. The only work that is required for one step of Newton's method in addition to the work involved in the solution of a linear system is the evaluation of the residual vector $r\left(y^{(0)}\right)$ and of the partial derivative $f_y\left(x_n,\,y_n\right)$ (n = 1, 2, … , N -1).

Previous Next

Problems

1. Determine the Constant α (correct to two places) such that the problem

   $$Y'' = x\,y$$

   $$y(0) = \alpha, \;\; y'(0) = 1$$

   has a solution satisfying $y(1) = 1.2$

2. Solve the boundary value problem

   $$y'' = (1 + x^2)y, \qquad -1 < x < 1$$

   $$y(-1) = y(1) = 1$$

   using second and forth order difference methods with $h = 0.2$.

3. Solve the boundary value problem

   $$y'' = 6\,x + y^3 \qquad 0 < x < 1$$

   $$y(x) = y(1) = 0$$

   using a second order difference method with $h = 0.25$. Solve we nonlinear difference equation by Newton's method, using an initial approximation as the solution of the given problem after omitting the term y^3.

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Previous Next