Chapter 1

Boundary value problem for ordinary differential equations

Nonlinear boundary value problems for ordinary differential equations often appear in chemical engineering. Examples being all models based on diffusion or heat conduction with exothermic chemical reaction, adsorption, ion exchange etc. Another important nonlinear boundary value problems are models including radiation.

The entire field of nonlinear boundary value problems is very large, often special properties of particular cases must be utilized. This chapter cannot cover all the cases, we try to show some typical approaches that can be used for a large number of boundary value problems. More interested readers can find detailed information in specialized literature.

Methods for nonlinear boundary value problems split into two main groups: difference methods and shooting methods. Besides, there are hybrid methods, e.g. multiple shooting method, collocation method, spline method etc.

1.1 Difference methods

We begin with a 2-point boundary value problem for one differential equation of the 2.nd order

$$y'' = f(x, y, y') \tag{1.1}$$

with linear boundary conditions

$$\alpha_0 \; y(a) + \beta_0 \; y'(a) = \gamma_0 \, , \tag{1.2}$$
$$\alpha_1 \; y(b) + \beta_1 \; y'(b) = \gamma_1 \, . \tag{1.3}$$

We divide the interval $[a, b]$ by an equidistant grid of points (nodes) $x_0 = a,\ x_1, \ldots, x_N = b,\ x_i = a + i\,h,\ h = (b-a)/N$. The values of the wanted solution $y(x)$ will be approximated by the values $y_i \sim y(x_i)$ in the nodes x_i. The differential equation (1.1) is replaced by the difference formula in x_i

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} = f\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \qquad i = 1, 2, \ldots, N-1. \tag{1.4}$$

Figure 1.1: Appearance of unknowns in (1.4), (1.5), (1.6)

	y_0	y_1	y_2		$\dots$		y_{N-1}	y_N
(1.5)	x	x						
(1.4), $i = 1$	x	x	x					
(1.4), $i = 2$		x	x	x				
$\vdots$			$\ddots$	$\ddots$	$\ddots$			
$\vdots$				$\ddots$	$\ddots$	$\ddots$		
$\vdots$					$\ddots$	$\ddots$	$\ddots$	
(1.4), $i = N - 1$						x	x	x
(1.6)							x	x

Difference formulas with the error $\mathcal{O}(h^2)$ were used for both derivatives. Finally we must replace the boundary conditions (1.2), (1.3). We start with the simplest approximation

$$\alpha_0 y_0 + \beta_0 \frac{y_1 - y_0}{h} = \gamma_0\,, \tag{1.5}$$

$$\alpha_1 y_N + \beta_1 \frac{y_N - y_{N-1}}{h} = \gamma_1\,, \tag{1.6}$$

with the approximation error $\mathcal{O}(h)$. The equations (1.4), (1.5), (1.6) form a system of $N+1$ nonlinear algebraic equations for $N+1$ unknowns $y_0, y_1, \dots, y_N$. This system can be solved using some method from chapter **??**, usually using the Newton's method. To get more precise results we choose the step-size h small, but then the number of equations $N + 1$ is large. Fortunately not all equations contain all unknowns, the scheme of their appearance is 3-diagonal and thus also the Jacobi matrix used in the Newton's method is 3-diagonal, i.e. it has zeroes besides 3 diagonals, see Fig. 1.1. A modified Gauss elimination is used to solved the system of linear algebraic equations in each step of the Newton's method. This modified Gauss elimination uses only the nonzero elements on the three diagonals, the zero elements are not considered, they do not even have to be stored in memory. This method is called factorization.

If boundary conditions (1.2), (1.3) contain derivatives, i.e. $\beta_0 \neq 0$ or $\beta_1 \neq 0$, then approximations (1.5), (1.6) with the error $\mathcal{O}(h)$ spoil the order of approximation (1.4) with the error $\mathcal{O}(h^2)$. When we use differential formula with the error $\mathcal{O}(h^2)$ for boundary conditions too, we have

$$\alpha_0 y_0 + \beta_0 \frac{-3y_0 + 4y_1 - y_2}{2h} = \gamma_0\,, \quad \alpha_1 y_N + \beta_1 \frac{3y_N - 4y_{N-1} + y_{N-2}}{2h} = \gamma_1\,. \tag{1.7}$$

This approximation, however, changes the 3-diagonal scheme by two new appearances, one in the first row, the other in the last one. The corresponding matrix (in the Newton's method) can still be transformed to a 3-diagonal matrix by adding an appropriate multiple of the 2-nd row to the 1.st row and similarly by adding an appropriate multiple of the N-the row to the $N + 1$-st row.

As central difference formulas have lower error, a method of fictitious nodes is used for the approximation of the boundary condition. Then the boundary condition in $x = a$ is approximated by

$$\alpha_0 y_0 + \beta_0 \, \frac{y_1 - y_{-1}}{2h} \;=\; \gamma_0 \tag{1.8}$$

and the approximation (1.4) of the differential equation is considered also for $i = 0$. The new unknown y_{-1} can be expressed from (1.8) and the appearance scheme is again 3-diagonal.

If the equation (1.1) contains no first derivative, i.e. we have the equation

$$y'' = f(x, y) \tag{1.9}$$

and if the boundary conditions are

$$y(a) = \gamma_0 \,, \qquad y(b) = \gamma_1 \,, \tag{1.10}$$

we can use the 4-th order approximation instead of the 2-nd order approximation used above, namely

$$y_{i+1} - 2y_i + y_{i-1} = \frac{h^2}{12} \left(f_{i-1} + 10 f_i + f_{i+1} \right) . \tag{1.11}$$

Here $f_i = f(x_i, y_i)$. If we want to get the 4-th order approximation even for the equation containing the first derivative, we have to use a difference formula using more nodes. When we approximate the second derivative according to formula 10 in Table **??** and we approximate the first derivative according to formula 12 in Table **??**, we get

$$\frac{-2y_{i-2} + 32 y_{i-1} - 60 y_i + 32 y_{i+1} - 2 y_{i+2}}{24 h^2} \;=\; f\left(x_i, y_i, \frac{y_{i-2} - 8y_{i-1} + 8 y_{i+1} - y_{i+2}}{12h} \right) ,$$
$$i = 2, 3, \ldots, N-2 \,.$$

For $i = 1$ and $i = N-1$ we use the non-symmetric formulas and we approximate the boundary conditions by formulas of order high enough. The scheme of appearance is no more 3-diagonal and the computation time increases.

1.1.1 Difference approximation for systems of differential equations of the first order

Consider a system of differential equations of the first order

$$y_j' = f_j(x, y_1, \ldots, y_n) \,, \qquad j = 1, \ldots, n \tag{1.12}$$

with 2-point boundary condition

$$g_i(y_1(a), \ldots, y_n(a), y_1(b), \ldots, y_n(b)) = 0 \,, \quad i = 1, \ldots, n \,. \tag{1.13}$$

After approximating the equations (1.12) in the equidistant grid of nodes $x_0 = a$, $x_1, \ldots, x_N = b$ we get

$$\frac{y_j^{i+1} - y_j^i}{h} \;=\; f_j \left(\frac{x_{i+1} + x_i}{2}, \frac{y_1^{i+1} + y_1^i}{2}, \ldots, \frac{y_n^{i+1} - y_n^i}{2} \right) , \tag{1.14}$$
$$i = 0, 1, \ldots, N-1 \,; \quad j = 1, 2, \ldots, n \,;$$

and after approximating the boundary condition (1.13) we have

$$g_i(y_1^0, \dots, y_n^0, y_1^N, \dots, y_n^N) = 0\,, \quad i = 1, \dots, n\,. \tag{1.15}$$

Here we denote $y_j^i \sim y_j(x_i) = y_j(a + ih)$, $h = (b - a)/N$. We get the system of $n \cdot (N+1)$ nonlinear equations (1.14),(1.15) for $n \cdot (N+1)$ unknowns

$$(y_1^0, y_2^0, \dots, y_n^0, y_1^1, \dots y_n^1, \dots, y_1^N, \dots, y_n^N)\,. \tag{1.16}$$

The equations (1.14), (1.15) can be ordered as follows:

1) All the boundary conditions (1.15) depending on values in $x = a$ only, i.e. depending on $y_1^0, \dots, y_n^0$.

2) Equations (1.14) for $i = 0$, i.e. n equations for $j = 1, 2, \dots, n$.

3) Equation (1.14) for $i = 1$. (1.17)

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N+1) Equation (1.14) for $i = N - 1$.

N+2) Remaining boundary conditions (1.15), i.e. those depending on values in $x = b$, i.e. on $y_1^N, \dots, y_n^N$.

The scheme of appearance of such an ordered system of nonlinear equations (after ordering the unknowns according to (1.16)) has almost a multi-diagonal band structure, see Fig. 1.2. Boundary conditions (1.13) with no equations containing both $y(a)$ and $y(b)$ are called separated boundary conditions. The scheme of appearance has a multi-diagonal band structure, see Fig. 1.3.

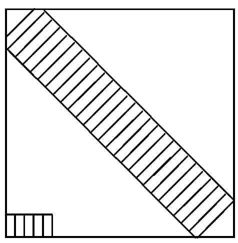

Figure 1.2: Scheme of appearance for (1.17)

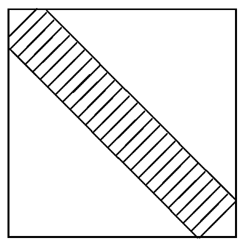

Figure 1.3: Scheme of appearance for separated boundary conditions