Chapter 3
Boundary Value Problem

A boundary value problem (BVP) is a problem, typically an ODE or a PDE, which has values assigned on the physical boundary of the domain in which the problem is specified. Let us consider a genearal ODE of the form

$$\mathbf{x}^{(n)} = f(t, \mathbf{x}, \mathbf{x}', \mathbf{x}'', \cdots, \mathbf{x}^{(n-1)}), \qquad t \in [a, b] \tag{3.1}$$

At $t = a$ and $t = b$ the solution is supposed to satisfy

$$\begin{aligned} r_1(\mathbf{x}(a)\,\mathbf{x}'(a), \cdots, \mathbf{x}^{(n-1)}(a), \mathbf{x}(b)\,\mathbf{x}'(b), \cdots, \mathbf{x}^{(n-1)}(b)) &= 0\,, \\ &\vdots \\ r_n(\mathbf{x}(a)\,\mathbf{x}'(a), \cdots, \mathbf{x}^{(n-1)}(a), \mathbf{x}(b)\,\mathbf{x}'(b), \cdots, \mathbf{x}^{(n-1)}(b)) &= 0\,. \end{aligned} \tag{3.2}$$

The resulting problem (3.1)–(3.2) is called a *two point boundary value problem* [8]. In order to be useful in applications, a BVP (3.1)–(3.2) should be *well posed*. This means that given the input to the problem there exists a unique solution, which depends continuously on the input. However, questions of existence and uniqueness for BVPs are much more difficult than for IVPs and there is no general theory.

3.1 Single shooting methods

3.1.1 Linear shooting method

Consider a linear two-point second-order BVP of the form

$$x''(t) = p(t)\,x'(t) + q(t)\,x(t) + r(t)\,, \qquad t \in [a, b] \tag{3.3}$$

with

$$x(a) = \alpha\,, \qquad x(b) = \beta\,.$$

The main idea of the method is to reduce the solution of the BVP (3.3) to the solution of an initial value problem [10, 6]. Namely, let us consider two special IVPs for two functions $u(t)$ and $v(t)$. Suppose that $u(t)$ is a solution of the IVP

$$u''(t) = p(t)\,u'(t) + q(t)\,u(t) + r(t)\,, \qquad u(a) = \alpha\,, \qquad u'(a) = 0$$

and $v(t)$ is the unique solution to the IVP

$$v''(t) = p(t)\,v'(t) + q(t)\,v(t)\,, \qquad v(a) = 0\,, \qquad v'(a) = 1\,.$$

Then the linear combination

$$x(t) = u(t) + c\,v(t)\,, \qquad c = \text{const}\,. \tag{3.4}$$

is a solution to BVP (3.3). The unknown constant c can be found from the boundary condition on the right end of the time interval, i.e.,

$$x(b) = u(b) + c\,v(b) = \beta \;\Rightarrow c = \frac{\beta - u(b)}{v(b)}\,.$$

That is, if $v(b) \neq 0$ the unique solution of (3.3) reads

$$x(t) = u(t) + \frac{\beta - u(b)}{v(b)}\,v(t)\,.$$

Example 1

Let us solve a BVP [6]

$$\begin{aligned} x''(t) &= \frac{2t}{1+t^2}\,x'(t) - \frac{2}{1+t^2}\,x(t) + 1\,, \\ x(0) &= 1.25, \qquad x(1) = -0.95\,. \end{aligned} \tag{3.5}$$

over the time interval $t \in [0, 4]$ using the linear shooting method (3.4).
According to Eq. (3.4) the solution of this equation has the form

$$x(t) = u(t) - \frac{0.95 + u(4)}{v(4)}\,v(t)\,,$$

where $u(t)$ and $v(t)$ are solutions of two IVPs

$$u''(t) = \frac{2t}{1+t^2}\,u'(t) + \frac{2}{1+t^2}\,u(t) + 1\,, \qquad u(0) = 1.25\,, \qquad u'(0) = 0$$

and

$$v''(t) = \frac{2t}{1+t^2}\,v'(t) + \frac{2}{1+t^2}\,v(t)\,, \qquad v(0) = 0\,, \qquad v'(0) = 1\,.$$

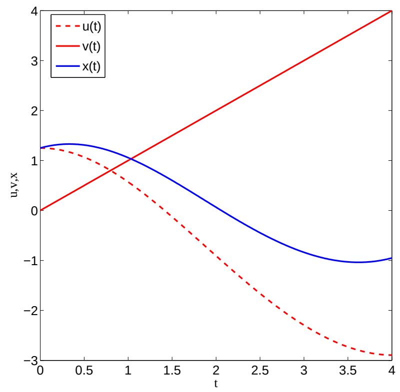

Fig. 3.1 Numerical solution of Eq. (3.5) over the interval $[0,4]$ by the linear shooting method (3.4).

Numerical solution of the problem 3.5 as well as both dunctions $u(t)$ and $v(t)$ are presented on Fig. 3.1

3.1.2 Single shooting for general BVP

For a general BVP for a second-order ODE, the simple shooting method is stated as follows: Let

$$\begin{aligned} x''(t) &= f(t, x(t), x'(t)), \qquad t \in [a, b] \\ x(a) &= \alpha, \qquad x(b) = \beta\,. \end{aligned} \tag{3.6}$$

be the BVP in question and let $x(t,s)$ denote the solution of the IVP

$$\begin{aligned} x''(t) &= f(t, x(t), x'(t)), \qquad t \in [a, b] \\ x(a) &= \alpha, \qquad x'(a) = s\,, \end{aligned} \tag{3.7}$$

where s is a parameter that can be varied. The IVP (3.7) is solved with different values of s with, e.g., RK4 method till the boundary condition on the right side $x(b) = \beta$ becomes fulfilled. As mentioned above, the solution $x(t,s)$ of (3.7) depends on the parameter s. Let us define a function

$$F(s) := x(b,s) - \beta\,.$$

If the BVP (3.6) has a solution, then the function $F(s)$ has a root, which is just the value of the slope $x'(a)$ giving the solution $x(t)$ of the BVP in question. The zeros of $F(s)$ can be found with, e.g., *Newton's method* [7].
The Newton's method is probably the best known method for finding numerical approximations to the zeroes of a real-valued function. The idea of the method is

to use the first few terms of the Taylor series of a function $F(s)$ in the vicinity of a suspected root, i.e.,

$$F(s_n+h) = F(s_n) + F'(s_n)\,h + \mathscr{O}(h^2)\,.$$

where s_n is a n'th approximation of the root. Now if one inserts $h = s - s_n$, one obtains

$$F(s) = F(s_n) + F'(s_n)\,(s - s_n)\,.$$

As the next approximation s_{n+1} to the root we choose the zero of this function, i.e.,

$$F(s_{n+1}) = F(s_n) + F'(s_n)\,(s_{n+1} - s_n) = 0 \Rightarrow s_{n+1} = s_n - \frac{F(s_n)}{F'(s_n)}\,. \tag{3.8}$$

The derivative $F'(s_n)$ can be calculated using the forward difference formula

$$F'(s_n) = \frac{F(s_n + \delta s) - F(s_n)}{\delta s}$$

where δs is small. Notice that this procedure can be unstable near a horizontal asymptote or a local extremum.

Example 1

Consider a simple nonlinear BVP [10]

$$\begin{aligned} x''(t) &= \frac{3}{2}x(t)^2, \\ x(0) &= 4, \qquad x(1) = 1 \end{aligned} \tag{3.9}$$

over the interval $t \in [0, 1]$ and let us solve it numerically with the single shooting method discussed above. First of all we define a corresponding IVP

$$x''(t) = \frac{3}{2}x(t)^2 \qquad x(0) = 4\,, \quad x'(0) = s$$

over $t \in [0, 1]$ and solve it for different values of s, e.g., $s \in [-100, 0]$ with the classical RK4 method. The result of calculation is presented on Fig. 3.2 (a). One can see, that the function $F(s) = x(t, s) - 1$ admits two zeros, depicted on Fig. 3.2 (a) as green points. In order to find them we use the Newton's method, discussed above. The method gives an approximation to both zeros of the function $F(s)$: $s = \{-35.8, -8.0\}$, which give the right slope $x'(0)$. Both solutions, corresponding to two different values of s are presented on Fig. 3.2 (b).

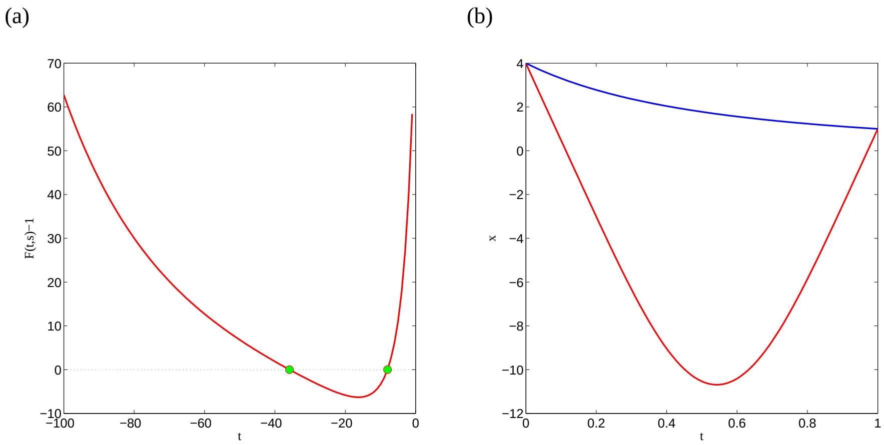

Fig. 3.2 Numerical solution of BVP (3.9) with single shooting method. (a) The Function $F(s) = x(t,s) - 1$ is presented. Green points depict two zeros of this function, which can be found with Newton's method. (b) Two solutions of (3.9) corresponding to two different values of parameter s (the red line corresponds to $s = -35.8$, whereas the blue one – to $s = -8.0$).

Example 2

Let us consider a linear eigenvalue problem of the form

$$x'' + \lambda x = 0\,, \qquad x(0) = x(1) = 0\,, \quad x'(0) = 1 \tag{3.10}$$

over $t \in [0,1]$ with the simple shooting method. The exact solution is

$$\lambda = n^2\pi^2\,, \quad n \in \mathbb{N}\,.$$

In order to apply the simple shooting method we consider a corresponding IVP of the first order with additional equation for the unknown function $\lambda(t)$:

$$x' = y\,, \qquad y' = -\lambda x\,, \quad \lambda' = 0$$

with

$$x(0) = 0\,, \quad x'(0) = 1\,, \quad \lambda(0) = s\,.$$

where s is a free shooting parameter. Here we choose $s = \{0.5, 50, 100\}$. Results of the shooting with these initial parameters are shown on Fig. 3.3. One can see, that numerical solutions correspond to first three eigenvalues $\lambda = \{\pi^2, (2\pi)^2, (3\pi)^2\}$.

Example 3

Consider a nonlinear BVP of the fourth order [8]

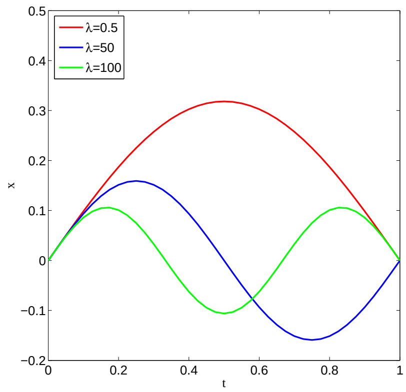

Fig. 3.3 Numerical solutions of Eq. (3.10) over the interval $[0,1]$ by single shooting method. First three eigenfunctions, corresponding to eigenvalues $\lambda = \{\pi^2, (2\pi)^2, (3\pi)^2\}$ are presented.

$$x^{(4)}(t) - (1+t^2)x''(t)^2 + 5x(t)^2 = 0\,, \qquad t \in [0,1] \tag{3.11}$$

with

$$x(0) = 1\,, \quad x'(0) = 0\,, \quad x''(1) = -2\,, \quad x'''(1) = -3\,.$$

Our goal is to solve this equation with the simple shooting method. To this end, first we rewrite the equation as a system of four ODE's of the first order:

$$\begin{aligned}
x_1' &= x_2\,, \\
x_2' &= x_3\,, \qquad && x_1(0) = 1\,, \qquad && x_3(1) = -2\,, \\
x_3' &= x_4\,, && x_2(0) = 0\,, && x_4(1) = -3\,, \\
x_4' &= (1+t^2)x_3^2 - 5x_1^2\,.
\end{aligned}$$

As the second step we consider correspondig IVP

$$\begin{aligned}
x_1' &= x_2\,, \\
x_2' &= x_3\,, \qquad && x_1(0) = 1\,, \qquad && x_3(1) = p\,, \\
x_3' &= x_4\,, && x_2(0) = 0\,, && x_4(1) = q\,, \\
x_4' &= (1+t^2)x_3^2 - 5x_1^2
\end{aligned}$$

with two free shooting parameters p and q. The solution of this IVP fulfilles following two requirements:

$$\begin{aligned}
F_1(p,q) &:= x_3(1,p,q) + 2 = 0\,, \\
F_2(p,q) &:= x_4(1,p,q) + 3 = 0\,.
\end{aligned}$$

That is, a system of nonlinear algebraic equations should be solved to find (p,q). The zeros of the system can be found with the Newton's method (3.8). In this case the iteration step reads

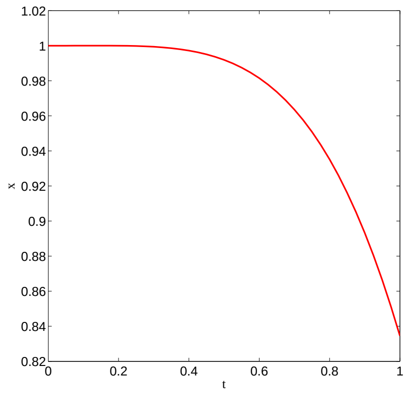

Fig. 3.4 Numerical solutions of (3.11) over the interval $[0,1]$ by single shooting method. Parameters are: $\Delta p = \Delta q = 0.05$, the time step $h = 0.025$, initial shooting parameters $(p_0, q_0) = (0,0)$.

$$s_{i+1} = s_i - \frac{F(s_i)}{DF(s_i)}$$

where $s = (p,q)^T$, $F = (F_1, F_2)^T$ and

$$DF(s_i) = \begin{pmatrix} \frac{\partial F_1}{\partial p} & \frac{\partial F_1}{\partial q} \\ \frac{\partial F_2}{\partial p} & \frac{\partial F_2}{\partial q} \end{pmatrix}$$

is a Jacobian of the system and

$$\frac{\partial F_i}{\partial p} = \frac{F_i(p+\Delta p, q) - F_i(p,q)}{\Delta p},$$
$$\frac{\partial F_i}{\partial q} = \frac{F_i(p, q+\Delta q) - F_i(p,q)}{\Delta q},$$

where $i = 1,2$ and Δp, Δq are given values. Numerical solution of the problem in question is presented on Fig. 3.4.

3.2 Finite difference Method

One way to solve a given BVP over the time interval $t \in [a,b]$ numerically is to approximate the problem in question by *finite differences* [8, 10, 6]. We form a partition of the domain $[a,b]$ using *mesh points* $a = t_0, t_1, \ldots, t_N = b$, where

$$t_i = a + ih, \qquad h = \frac{b-a}{N}, \qquad i = 0,1,\ldots N.$$

Difference quotient approximations for derivatives can be used to solve BVP in question [10, 6]. In particular, using a Taylor expansion in the vicinity of the point

t_j, for the first derivative one obtains *a forward difference*

$$x'(t_i) = \frac{x(t_{i+1}) - x(t_i)}{h} + \mathscr{O}(h)\,. \tag{3.12}$$

In a similar way one gets *a backward difference*

$$x'(t_i) = \frac{x(t_i) - x(t_{i-1})}{h} + \mathscr{O}(h)\,. \tag{3.13}$$

We can combine these two approaches and derive *a central difference*, which yields a more accurate approximation:

$$x'(t_i) = \frac{x(t_{i+1}) - x(t_{i-1})}{2h} + \mathscr{O}(h^2)\,. \tag{3.14}$$

The second derivative $x''(t_i)$ can be found in the same way using the linear combination of different Taylor expansions. For example, a central difference reads

$$x''(t_i) = \frac{x(t_{i+1}) - 2\,x(t_i) + x(t_{i-1})}{h^2} + \mathscr{O}(h^2)\,. \tag{3.15}$$

3.2.1 Finite Difference for linear BVP

Let us consider a linear BVP of the second order (3.3)

$$x'' = p(t)\,x'(t) + q(t)\,x(t) + r(t)\,, \quad t \in [a, b]\,, \quad x(a) = \alpha\,, \quad x(b) = \beta\,.$$

and introduce the notation $x(t_i) = x_i$, $p(t_i) = p_i$, $q(t_i) = q_i$ and $r(t_i) = r_i$. Then, using Eq. (3.14) and Eq. (3.15) one can rewrite Eq. (3.3) as *a difference equation*

$$\begin{aligned} x_0 &= \alpha\,, \\ \frac{x_{i+1} - 2\,x_i + x_{i-1}}{h^2} &= p_i\,\frac{x_{i+1} - x_{i-1}}{2\,h} + q_i\,x_i + r_i\,, \qquad i = 1\,, \ldots, N-1\,, \\ x_N &= \beta\,. \end{aligned}$$

Now we can multiply both sides of the second equation with h^2 and collect terms, involving x_{i-1}, x_i and x_{i+1}. As result we get a system of linear equations

$$\left(1 + \frac{h}{2}\,p_i\right)x_{i-1} - (2 + h^2 q_i)x_i + \left(1 - \frac{h}{2}\,p_i\right)x_{i+1} = h^2\,r_i\,, \qquad i = 1, 2, \ldots N-1\,.$$

or, in matrix notation

$$A\,\mathbf{x} = b\,, \tag{3.16}$$

or, more precisely

$$
\begin{pmatrix}
-(2+h^2q_1) & 1-\frac{h}{2}p_1 & 0 & \dots & \dots & 0 \\
1+\frac{h}{2}p_2 & -(2+h^2q_2) & 1-\frac{h}{2}p_2 & 0 & \dots & 0 \\
0 & 1+\frac{h}{2}p_3 & -(2+h^2q_3) & 1-\frac{h}{2}p_3 & \dots & 0 \\
\dots & \dots & \dots & \dots & \dots & \dots \\
\dots & \dots & \dots & \dots & \dots & 1-\frac{h}{2}p_{N-2} \\
0 & \dots & \dots & 0 & 1+\frac{h}{2}p_{N-1} & -(2+h^2q_{N-1})
\end{pmatrix}
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ x_{N-1} \end{pmatrix}
=
\begin{pmatrix} h^2 r_1 - \gamma_1 \\ h^2 r_2 \\ h^2 r_3 \\ \cdot \\ \cdot \\ h^2 r_{N-1} - \gamma_N \end{pmatrix},
$$

where

$$
\gamma_1 = \alpha \left(\frac{h}{2} p_1 + 1 \right), \qquad \gamma_N = \beta \left(1 - \frac{h}{2} p_{N-1} \right).
$$

Our goal is to find unknown vector $\mathbf{x}$. To this end we should invert the matrix A. This matrix has a band structure and is *tridiagonal*. For matrices of this kind a tridiagonal matrix algorithm (TDMA), also known als *Thomas algorithm* can be used (see Appendix A for details).

Example

Solve a linear BVP [8]

$$
\begin{aligned}
-x''(t) - (1+t^2)\,x(t) &= 1\,, \\
x(-1) = x(1) &= 0
\end{aligned} \tag{3.17}
$$

over $t \in [-1, 1]$ with finite difference method. First we introduce discrete set of nodes $t_i = -1 + i\,h$ with given time step h. According to notations used in previous section, $p(t) = 0$, $q(t) = -(1+t^2)$, $r(t) = -1$, $\alpha = \beta = 0$. Hence, the linear system (3.16) we are interested in reads

$$
\begin{pmatrix}
-(2+h^2q_1) & 1 & 0 & \dots & \dots & 0 \\
1 & -(2+h^2q_2) & 1 & 0 & \dots & 0 \\
0 & 1 & -(2+h^2q_3) & 1 & \dots & 0 \\
\dots & \dots & \dots & \dots & \dots & \dots \\
\dots & \dots & \dots & \dots & \dots & 1 \\
0 & \dots & \dots & 0 & 1 & -(2+h^2q_{N-1})
\end{pmatrix}
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ x_{N-1} \end{pmatrix}
= -
\begin{pmatrix} h^2 \\ h^2 \\ h^2 \\ \cdot \\ \cdot \\ h^2 \end{pmatrix}.
$$

The numerical solution of the problem in question is presented on Fig. 3.5.

3.2.2 Finite difference for linear eigenvalue problems

Consider a Sturm-Liouville problem of the form

$$
-x''(t) + q(t)\,x(t) = \lambda\, v(t)\,x(t)\,, \tag{3.18}
$$

over $t \in [a, b]$ with

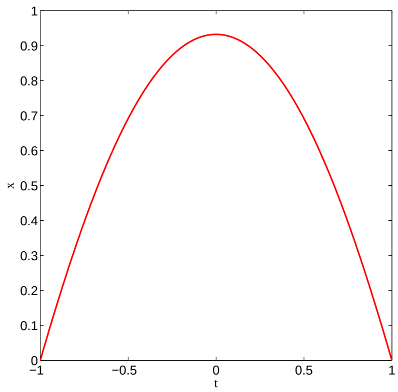

Fig. 3.5 Numerical solutions of (3.17) over the interval $[-1, 1]$ by finite difference method.

$$x(a) = 0\,, \qquad x(b) = 0\,.$$

Introducing notation $x_i := x(t_i)$, $q_i := q(t_i)$, $v_i := v(t_i)$, we can write down a difference equation for Eq. (3.18)

$$\begin{aligned} x_0 &= 0 \\ -\frac{x_{i+1} - 2x_i + x_{i-1}}{h^2} + q_i x_i - \lambda\, v_i x_i &= 0\,, \qquad i = 1, \ldots N-1\,, \\ x_N &= 0\,. \end{aligned}$$

If $v_i \neq 0$ for all i we can rewrite the difference equation above as an eigenvalue problem

$$(A - \lambda I)x = 0 \tag{3.19}$$

for a tridiagonal matrix A

$$A = \begin{pmatrix} \frac{2}{h^2 v_1} + \frac{q_1}{v_1} & \frac{-1}{h^2 v_1} & 0 & \ldots & \ldots & 0 \\ \frac{-1}{h^2 v_2} & \frac{2}{h^2 v_2} + \frac{q_2}{v_2} & \frac{-1}{h^2 v_2} & \ldots & \ldots & 0 \\ 0 & \frac{-1}{h^2 v_3} & \frac{2}{h^2 v_3} + \frac{q_3}{v_3} & \frac{-1}{h^2 v_3} & \ldots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \frac{-1}{h^2 v_{N-2}} \\ 0 & \ldots & \ldots & 0 & \frac{-1}{h^2 v_{N-1}} & \frac{2}{h^2 v_{N-1}} + \frac{q_3}{v_{N-1}} \end{pmatrix}$$

and a vector $x = (x_1, x_2, \ldots, x_{N-1})^T$.