Chapter 8
Numerics of Ordinary Differential Equations: Boundary Value Problems

8.1 Introduction

It is the aim of this chapter to introduce some of the basics methods developed to solve boundary value problems. Since a treatment of all available concepts is far too extensive, we will concentrate on two approaches, namely the finite difference approach and shooting methods [1–5]. Furthermore, we will strictly focus on *linear boundary value problems* defined on a finite interval $[a, b] \subset \mathbb{R}$. A boundary value problem is referred to as linear if both the differential equation and the boundary conditions are linear. Such a problem of order n is of the form

$$\begin{cases} L[y] = f(x), & x \in [a, b] , \\ U_\nu[y] = \lambda_\nu, & \nu = 1, \dots, n . \end{cases} \tag{8.1}$$

Here, $L[y]$ is a linear operator

$$L[y] = \sum_{k=0}^{n} a_k(x) y^{(k)}(x) , \tag{8.2}$$

where $y^{(k)}(x)$ denotes the k-th spatial derivative of $y(x)$, i.e. $y^{(k)} \equiv \mathrm{d}^k y(x)/\mathrm{d}x^k$ and $f(x)$ as well as the $a_k(x)$ are given functions which we assume to be continuous. Accordingly, linear boundary conditions $U_\nu[y]$ can be formulated as

$$U_\nu[y] = \sum_{k=0}^{n-1} \left[\alpha_{\nu k} y^{(k)}(a) + \beta_{\nu k} y^{(k)}(b) \right] = \lambda_\nu , \tag{8.3}$$

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where the $\alpha_{\nu k}$, $\beta_{\nu k}$ and λ_ν are given constants. The question in which cases a solution to the boundary value problem (8.1) exists and whether or not this solution will be unique [6], will not be discussed here.

Let us introduce some further conventions: The differential equation in the first line of Eq. (8.1) is referred to as *homogeneous* if the function $f(x) = 0$ for all $x \in [a, b]$. In analogy, the boundary conditions are referred to as *homogeneous* if the constants $\lambda_\nu = 0$ for all $\nu = 1, \ldots, n$. Finally, the boundary value problem (8.1) is referred to as *homogeneous* if the differential equation is homogeneous and the boundary conditions are homogeneous as well. In all other cases it is referred to as *inhomogeneous*. Moreover, the boundary conditions are said to be *decoupled* if the function values at the two different boundaries do not mix.

One of the most important types of boundary value problems in physics are linear second order boundary value problems with decoupled boundary conditions. They are of the form:

$$a_2(x)y''(x) + a_1(x)y'(x) + a_0(x)y(x) = f(x) , \quad x \in [a, b] , \tag{8.4a}$$

$$\alpha_0 y(a) + \alpha_1 y'(a) = \lambda_1, \quad |\alpha_0| + |\alpha_1| \neq 0 , \tag{8.4b}$$

$$\beta_0 y(b) + \beta_1 y'(b) = \lambda_2, \quad |\beta_0| + |\beta_1| \neq 0 . \tag{8.4c}$$

This chapter focuses mainly on problems of this kind.

In particular, for second order differential equations, boundary conditions of the form

$$y(a) = \alpha , \qquad y(b) = \beta , \tag{8.5}$$

are referred to as *boundary conditions of the first kind* or DIRICHLET *boundary conditions*. On the other hand, boundary conditions of the form

$$y'(a) = \alpha , \qquad y'(b) = \beta , \tag{8.6}$$

are referred to as *boundary conditions of the second kind* or NEUMANN *boundary conditions* and boundary conditions of the form (8.4) are referred to as *boundary conditions of the third kind* or STURM *boundary conditions*.

We note, that the particular case of decoupled boundary conditions does not include problems like

$$y(a) = y(b) \neq 0 . \tag{8.7}$$

We encountered such a condition in Sect. 7.3 where we introduced boundary conditions of this form as periodic boundary conditions.

In the following section the method of finite differences will be applied to solve boundary value problems of the form (8.4). On the other hand, shooting methods, in particular the method developed by NUMEROV (see, for instance, [7] and references therein), will be the topic of the third section.

A common alternative in the case of constant coefficients is to solve the differential equation with the help of FOURIER transform techniques. A brief introduction to the numerical implementation of the FOURIER transform is given in Appendix D.

8.2 Finite Difference Approach

For illustrative purposes, we regard a boundary value problem of the form (8.4). The extension to more complex problems might be tedious but follows the same line of arguments. We discretize the interval $[a, b]$ according to the recipe introduced in Chap. 2: the positions x_k are given by $x_k = a + (k-1)h$, where the grid-spacing h is determined via the maximum number of grid-points N as $h = (b-a)/(N-1)$. Hence, we have $x_1 = a$ and $x_N = b$. Furthermore, we use the notation $y_k \equiv y(x_k)$ for all $k = 1, \ldots, N$. It will be used for all functions which appear in Eqs. (8.4).

Let us now employ the central difference derivative (2.10c) in order to approximate

$$y_k'' \equiv y''(x_k) \approx \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} \,, \tag{8.8}$$

for $k = 2, \ldots, N-1$ and

$$y_k' \equiv y'(x_k) \approx \frac{y_{k+1} - y_{k-1}}{2h} \,. \tag{8.9}$$

The boundary points x_1 and x_N will be treated in a separate step. In order to abbreviate the notation we will rewrite the differential equation (8.4) without the indices as

$$a(x)y''(x) + b(x)y'(x) + c(x)y(x) = f(x) \,. \tag{8.10}$$

Equations (8.8) and (8.9) are then applied and we arrive at the difference equation

$$a_k \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + b_k \frac{y_{k+1} - y_{k-1}}{2h} + c_k y_k = f_k \,, \tag{8.11}$$

where $k = 2, \ldots, N-1$. Sorting the y_k yields

$$\left(\frac{a_k}{h^2} - \frac{b_k}{2h}\right) y_{k-1} + \left(c_k - \frac{2a_k}{h^2}\right) y_k + \left(\frac{a_k}{h^2} + \frac{b_k}{2h}\right) y_{k+1} = f_k \,, \tag{8.12}$$

and this equation is only valid for $k = 2, \ldots, N-1$ because we defined N grid-points within the interval $[a, b]$.

A final step is necessary in which the boundary conditions are incorporated. This will then enable us to reduce the whole problem to a system of linear equations. Decoupled boundary conditions of a second order differential equation for the left-hand boundary (8.4b) are of the general form:

$$\alpha_0 y(a) + \alpha_1 y'(a) = \lambda_1, \quad |\alpha_0|, |\alpha_1| \neq 0 . \tag{8.13}$$

In analogy, we find for the right-hand boundary (8.4c):

$$\beta_0 y(b) + \beta_1 y'(b) = \lambda_2, \quad |\beta_0|, |\beta_1| \neq 0 . \tag{8.14}$$

We discretize $y'(a)$ as

$$y_1' \equiv y'(a) \approx \frac{y_2 - y_0}{2h} , \tag{8.15}$$

and set $y_1 = y(a)$. Note that the function value y_0 in Eq. (8.15) is unknown since the virtual point $x_0 = a - h$ is not within our interval $[a, b]$. Nevertheless, we use Eq. (8.15) in Eq. (8.13) and obtain:

$$\alpha_0 y_1 + \alpha_1 \frac{y_2 - y_0}{2h} = \lambda_1 . \tag{8.16}$$

We solve now Eq. (8.16) for y_0 under the premise that $\alpha_1 \neq 0$,

$$y_0 = y_2 - \frac{2h}{\alpha_1} (\lambda_1 - \alpha_0 y_1) , \tag{8.17}$$

rewrite Eq. (8.12) for $k = 1$,

$$\left(\frac{a_1}{h^2} - \frac{b_1}{2h} \right) y_0 + \left(c_1 - \frac{2a_1}{h^2} \right) y_1 + \left(\frac{a_1}{h^2} + \frac{b_1}{2h} \right) y_2 = f_1 , \tag{8.18}$$

and insert (8.17) into (8.18):

$$\left[c_1 - \frac{2a_1}{h^2} + \frac{\alpha_0}{\alpha_1} \left(\frac{2a_1}{h} - b_1 \right) \right] y_1 + \frac{2a_1}{h^2} y_2 = f_1 - \frac{\lambda_1}{\alpha_1} \left(b_1 - \frac{2a_1}{h} \right) . \tag{8.19}$$

On the other hand, in the specific case of $\alpha_1 = 0$ we immediately obtain from Eq. (8.16):

$$y_1 = \frac{\lambda_1}{\alpha_0} . \tag{8.20}$$

The same strategy can be applied to incorporate the right-hand side boundary condition, Eq. (8.14): We discretize Eq. (8.14) by introducing the function value y_{N+1} at the virtual grid-point $x_{N+1} = N + h$ outside the interval $[a, b]$ via:

$$\beta_0 y_N + \beta_1 \frac{y_{N+1} - y_{N-1}}{2h} = \lambda_2 \; . \tag{8.21}$$

This equation is solved for y_{N+1} under the premise that $\beta_1 \neq 0$

$$y_{N+1} = y_{N-1} + \frac{2h}{\beta_1}\left(\lambda_2 - \beta_0 y_N\right) \; , \tag{8.22}$$

and insert this into Eq. (8.12) for $k = N$. This results in:

$$\frac{2a_N}{h^2} y_{N-1} + \left[c_N - \frac{2a_N}{h^2} - \frac{\beta_0}{\beta_1}\left(b_N + \frac{2a_N}{h}\right)\right] y_N = f_N - \frac{\lambda_2}{\beta_1}\left(b_N + \frac{2a_N}{h}\right) \; . \tag{8.23}$$

In the specific case $\beta_1 = 0$, the value y_N is fixed at the boundary and one obtains from Eq. (8.14):

$$y_N = \frac{\lambda_2}{\beta_0} \; . \tag{8.24}$$

All these manipulations reduced the boundary value problem to a system of inhomogeneous linear equations, namely Eqs. (8.12), (8.19), and (8.23). It can be written as

$$Ay = F \; , \tag{8.25}$$

where we introduced the vector $y = (y_1, y_2, \ldots, y_N)^T$, the vector F

$$F = \begin{pmatrix} f_1 - \frac{\lambda_1}{\alpha_1}\left(b_1 - \frac{2a_1}{h}\right) \\ f_2 \\ f_3 \\ \vdots \\ f_{N-1} \\ f_N - \frac{\lambda_2}{\beta_1}\left(b_N + \frac{2a_N}{h}\right) \end{pmatrix} \; , \tag{8.26}$$

and the tridiagonal matrix A:

$$A = \begin{pmatrix} B_1 & C_1 & 0 & & \cdots & 0 \\ A_2 & B_2 & C_2 & & \cdots & \vdots \\ 0 & \ddots & \ddots & \ddots & & \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ & & & A_{N-1} & B_{N-1} & C_{N-1} \\ 0 & \cdots & & 0 & A_N & B_N \end{pmatrix} . \tag{8.27}$$

Here we defined

$$A_k = \begin{cases} \left(\dfrac{a_k}{h^2} - \dfrac{b_k}{2h} \right) & k = 2, \ldots, N-1 \ , \\ \dfrac{2a_N}{h^2} & k = N \ , \end{cases} \tag{8.28}$$

$$B_k = \begin{cases} \left[c_1 - \dfrac{2a_1}{h^2} + \dfrac{\alpha_0}{\alpha_1} \left(\dfrac{2a_1}{h} - b_1 \right) \right] & k = 1 \ , \\ \left(c_k - \dfrac{2a_k}{h^2} \right) & k = 2, \ldots N-1 \ , \\ \left[c_N - \dfrac{2a_N}{h^2} - \dfrac{\beta_0}{\beta_1} \left(b_N + \dfrac{2a_N}{h} \right) \right] & k = N \ , \end{cases} \tag{8.29}$$

and, finally,

$$C_k = \begin{cases} \dfrac{2a_1}{h^2} & k = 1 \ , \\ \left(\dfrac{a_k}{h^2} + \dfrac{b_k}{2h} \right) & k = 2, \ldots, N-1 \ . \end{cases} \tag{8.30}$$

The remaining task is now to solve this linear system of equations (8.25). (A brief introduction to the numerical treatment of linear systems of equations can be found in Appendix C.) Very effective methods exist for cases where the matrix A is tridiagonal [8] as it is the case here. Although we discussed the method of finite differences for the particular case of a second order differential equation with decoupled boundary conditions, the same strategy can be employed to derive similar methods for higher order boundary value problems. However, these methods will, in general, be more complex. Furthermore, we note that in cases where $\alpha_1 = \beta_1 = 0$ the function values at the boundaries y_1 and y_N are fixed and the corresponding system of linear equations reduces to $(N-2)$ equations.

Let us briefly investigate the differential equation which corresponds to the problem (8.4) together with periodic boundary conditions of the form (8.7). In this case we have to consider that

$$y_1 = y_N \,, \tag{8.31}$$

and, for a solution to exist, we have necessarily

$$a_1 = a_N, \quad b_1 = b_N, \quad \text{and} \quad c_1 = c_N \,. \tag{8.32}$$

The finite difference approximations (8.8) and (8.9) are again applied to derive Eqs. (8.12) for $k = 2, \ldots, N-1$. For $k = 2$ Eq. (8.12) becomes

$$\left(\frac{a_2}{h^2} - \frac{b_2}{2h}\right) y_1 + \left(c_2 - \frac{2a_2}{h^2}\right) y_2 + \left(\frac{a_2}{h^2} + \frac{b_2}{2h}\right) y_3 = f_2 \,, \tag{8.33}$$

and we have for $k = N-1$

$$\left(\frac{a_{N-1}}{h^2} - \frac{b_{N-1}}{2h}\right) y_{N-2} + \left(c_{N-1} - \frac{2a_{N-1}}{h^2}\right) y_{N-1} + \left(\frac{a_{N-1}}{h^2} + \frac{b_{N-1}}{2h}\right) y_N = f_{N-1} \,. \tag{8.34}$$

Since $y_1 = y_N$ this can be rewritten as

$$\left(\frac{a_{N-1}}{h^2} - \frac{b_{N-1}}{2h}\right) y_{N-2} + \left(c_{N-1} - \frac{2a_{N-1}}{h^2}\right) y_{N-1} + \left(\frac{a_{N-1}}{h^2} + \frac{b_{N-1}}{2h}\right) y_1 = f_{N-1} \,. \tag{8.35}$$

Finally, Eq. (8.12) results for $k = 1$ in

$$\left(\frac{a_1}{h^2} - \frac{b_1}{2h}\right) y_{N-1} + \left(c_1 - \frac{2a_1}{h^2}\right) y_1 + \left(\frac{a_1}{h^2} + \frac{b_1}{2h}\right) y_2 = f_1 \,, \tag{8.36}$$

where we identified $y_0 = y(x_1 - h) \equiv y(x_N - h) = y_{N-1}$. All this results in a closed system of $N-1$ equations, which is of the form (8.25)

$$Ay = F \,, \tag{8.37}$$

where $y = (y_1, y_2, \ldots, y_{N-1})^T$,

$$F = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N-1} \end{pmatrix} , \tag{8.38}$$

and the $(N-1) \times (N-1)$ matrix A is given by

$$A = \begin{pmatrix} B_1 & C_1 & 0 & \cdots & 0 & A_1 \\ A_2 & B_2 & C_2 & & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & & & A_{N-2} & B_{N-2} & C_{N-2} \\ C_{N-1} & 0 & \cdots & 0 & A_{N-1} & B_{N-1} \end{pmatrix} . \tag{8.39}$$

Here, we defined

$$A_k = \left(\frac{a_k}{h^2} - \frac{b_k}{2h} \right) , \qquad k = 1, \ldots, N-1 , \tag{8.40}$$

$$B_k = \left(c_k - \frac{2a_k}{h^2} \right) , \qquad k = 1, \ldots, N-1 , \tag{8.41}$$

and

$$C_k = \left(\frac{a_k}{h^2} + \frac{b_k}{2h} \right) , \qquad k = 1, \ldots, N-1 . \tag{8.42}$$

In contrast to the matrix (8.27) the matrix (8.39) is not tridiagonal since the matrix elements $(A)_{1,N-1}$ and $(A)_{N-1,1}$ are non-zero. Nevertheless, it was possible to reduce the boundary value problem to a system of linear equations which can be solved iteratively.

8.3 Shooting Methods

For illustrative purposes, we restrict here the discussion to a second order boundary value problem with decoupled boundary conditions of the form (8.4). The essential idea of shooting methods is to treat the boundary value problem as an initial value problem. The resulting equations can then be solved with the help of methods discussed in Chap. 5. Of course, such an approach is ill-defined because no initial conditions but only boundary conditions are given. The trick is, that one modifies the initial conditions iteratively in such a way that in the end the boundary conditions are fulfilled. Let us put this train of thoughts into a mathematical form: We rewrite the second order differential equation (8.4a) as

$$y'' = f(y, y', x) , \tag{8.43}$$

which can be reduced to a set of first order differential equations as was demonstrated in Chap. 5. We note that Eq. (8.43) is not yet well posed since the initial conditions have not been defined. The boundary condition on the left-hand side reads:

$$\alpha_0 y(a) + \alpha_1 y'(a) = \lambda_1 \ . \tag{8.44}$$

We now *assume* that $y'(a) = z$, where z is some number. This gives the well posed initial value problem

$$\begin{cases} y'' = f(y, y', x) \ , \\ y(a) = \dfrac{\lambda_1}{\alpha_0} - \dfrac{\alpha_1}{\alpha_0} z \ , \\ y'(a) = z \ , \end{cases} \tag{8.45}$$

under the assumption that $\alpha_0 \neq 0$. The solution of this problem will be written as $y(x; z)$ in order to indicate its dependence on the particular choice $y'(a) = z$. We remember, that the boundary condition at the right-hand boundary is defined as:

$$\beta_0 y(b) + \beta_1 y'(b) = \lambda_2 \ . \tag{8.46}$$

Let us introduce the function:

$$F(z) = \beta_0 y(b; z) + \beta_1 y'(b; z) - \lambda_2 \ . \tag{8.47}$$

We observe that the solution of the equation

$$F(z) = 0 \ , \tag{8.48}$$

gives the desired solution to the boundary value problem (8.4), because in this case the second boundary condition (8.46) is fulfilled. In practice, one tries several values of z until relation (8.48) is fulfilled. However, from a numerical point of view this method is very inefficient since usually several initial value problems have to be solved until the correct value of z is found. Nevertheless, in some cases shooting methods proved to be very useful [7].

For instance, shooting methods are particularly effective if a solution to an eigenvalue problem of the form

$$a(x)y''(x) + b(x)y'(x) + c(x)y(x) = \lambda y(x) \ , \tag{8.49a}$$

in combination with homogeneous boundary conditions,

$$\alpha_0 y(a) + \alpha_1 y'(a) = 0 \ , \tag{8.49b}$$

and

$$\beta_0 y(b) + \beta_1 y'(b) = 0 \,, \tag{8.49c}$$

is to be found. We note that Eq. (8.49a) has the trivial solution $y(x) \equiv 0$ for all values of λ. However a non-trivial solution will only exist for particular values of λ. These particular values will be indexed by λ_n and are referred to as *eigenvalues* of Eq. (8.49a) [9]. The corresponding functions $y_n(x)$ are referred to as *eigenfunctions*. We note that the differential equation (8.49a) in combination with the boundary conditions (8.49b) and (8.49c) define a homogeneous boundary value problem. Such a problem is commonly referred to as an *eigenvalue problem* [9]. Furthermore, we note the following property of homogeneous boundary value problems: Suppose that $y(x)$ is a solution of the boundary value problem (8.49), then $\tilde{y}(x) = \gamma y(x)$, with $\gamma = \text{const}$ will also be a solution of (8.49). Hence, the solution of a homogeneous boundary value problem is not unique but invariant under multiplication by a constant γ. Typically, the multiplicative factor γ is fixed by some additional condition, such as a normalization condition of the form

$$\int_a^b \mathrm{d}x |y(x)|^2 = 1 \,. \tag{8.50}$$

We now employ this property and *choose* $y(a) = 1$. Inserting this choice into (8.49b) yields

$$y'(a) = -\frac{\alpha_0}{\alpha_1} \,. \tag{8.51}$$

Note that for $\alpha_0 = 0$ or $\alpha_1 = 0$, we are restricted to the choices $y'(a) = 0$ and $y(a)$ is arbitrary or $y(a) = 0$ and $y'(a)$ is arbitrary, respectively. If we assume that $a(x) \neq 0$ for all $x \in [a, b]$, we can solve the initial value problem

$$\begin{cases} y''(x) = -\dfrac{b(x)}{a(x)} y'(x) - \dfrac{c(x) - \lambda}{a(x)} y(x) \,, \\ y(a) = 1 \,, \\ y'(a) = -\dfrac{\alpha_0}{\alpha_1} \,. \end{cases} \tag{8.52}$$

The solutions are denoted by $y(x; \lambda)$ in order to emphasize that they will highly depend on the choice of the parameter λ. The strategy is to solve the initial value problem (8.52) for several values of λ and whenever one finds that

$$F(\lambda_n) = \beta_0 y(b; \lambda_n) + \beta_1 y'(b; \lambda_n) - \lambda_n = 0 \,, \tag{8.53}$$

is satisfied, an eigenvalue λ_n with the corresponding eigenfunction $y_n(x) = y(x; \lambda_n)$ of the eigenvalue problem (8.49) has been found.

However, this strategy is also very time consuming. The most common application of the shooting method is its combination with a very fast and accurate solution of initial value problems. This method is known as the NUMEROV method [7]. It is applicable whenever one is confronted with a differential equation of the form

$$y''(x) + k(x)y(x) = 0 \,, \tag{8.54}$$

in combination with homogeneous boundary conditions. Here $k(x)$ is some function. If we are particularly interested in eigenvalue problems then $k(x)$ has the form $k(x) = q(x) - \lambda$, where $q(x)$ is some function and λ is the eigenvalue [see the discussion after Eq. (8.49)]. For instance, consider the one-dimensional stationary SCHRÖDINGER equation [10–12],

$$\psi''(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \,, \tag{8.55}$$

where $\psi(x)$ is the wave-function, m is the mass, $\hbar$ denotes the reduced PLANCK constant, E is the energy, and $V(x)$ is some potential. In this case we identify

$$k(x) = \frac{2m}{\hbar^2}\left[E - V(x)\right] \,. \tag{8.56}$$

We note that Eq. (8.55) together with its boundary conditions defines an eigenvalue problem with eigenvalues E_n, the possible energies of the system. We remember from Chap. 2, Eq. (2.34), that

$$y_j'' = \frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} - \frac{h^2}{12}y_j^{(4)} - \ldots = -k_j y_j \,. \tag{8.57}$$

Here we made use of Eq. (8.54) and introduced $k_j \equiv k(x_j)$. Furthermore, we write the fourth derivative of $y(x)$ at point $x = x_j$ as

$$y_j^{(4)} \approx \frac{y_{j+1}'' - 2y_j'' + y_{j-1}''}{h^2} = \frac{-k_{j+1}y_{j+1} + 2k_j y_j - k_{j-1}y_{j-1}}{h^2} \,, \tag{8.58}$$

where we employed Eq. (8.54). Truncating (8.57) after the fourth order derivative $y_j^{(4)}$, inserting relation (8.58), and solving for y_{j+1} yields

$$y_{j+1} = \frac{2\left(1 - \frac{5h^2}{12}k_j\right)y_j - \left(1 + \frac{h^2}{12}k_{j-1}\right)y_{j-1}}{1 + \frac{h^2}{12}k_{j+1}} \,. \tag{8.59}$$

This gives a very fast algorithm to solve the differential equation (8.54) with some initial values of the form (8.52). The remaining strategy is the same as discussed above, i.e. one *screens* the parameter λ in order to find the eigenvalues λ_n and eigenfunctions $y_n(x)$. In case of the SCHRÖDINGER equation, one can screen the energy E in order to obtain the energy eigenvalues E_n which satisfy a condition of the form (8.53).

Before we present two illustrating examples in the next two chapters let us conclude this section with two important remarks on the NUMEROV method. We note from Eq. (8.59) that in order to compute y_3 one already needs the function values y_1 and y_2. Usually, one obtains these values from the boundary conditions in combination with some additional condition for the problem at hand. Such an additional condition might be, for instance, the normalization of the function $y(x)$, like Eq. (8.50). We also emphasized that one has to run the NUMEROV algorithm several times for different *trial values* of the parameter λ. In order to reduce the computational cost of the method it is in many cases advantageous to store the function values q_i, where $k_i = q_i - \lambda$, in an array which is then regarded as an input argument of the NUMEROV algorithm.

Summary

We focused on linear boundary value problems defined on a finite interval $[a, b] \subset \mathbb{R}$. Most important for physics are second order boundary value problems with decoupled boundary conditions, i.e. the boundary conditions at the two different boundaries do not mix. The numerical treatment of the second order differential equation together with its boundary conditions concentrated either on the application of finite differences or on shooting methods. In the finite difference approach the methods developed in Chap. 2 were applied and the boundary conditions were incorporated directly. This resulted in a set of linear algebraic equations which was to be solved for each grid-point of the discretisized interval $[a, b]$. The case of periodic boundary conditions was also discussed in detail.

The shooting methods, on the other hand, try to link the decoupled boundary value problem to an initial value problem. This allowed the application of the methods discussed in Chap. 5. The idea was to start with some initial value at one of the two boundaries, solve the differential equation numerically and to modify the initial value iteratively until it agreed with the original boundary condition within some predefined error. Such a procedure is rather time consuming. Nevertheless, shooting methods, in particular its NUMEROV variation, proved to be very useful in the numerical solution of eigenvalue problems. This was demonstrated using the homogeneous boundary value problem of the one-dimensional stationary SCHRÖDINGER equation as an example.

Problems

1. Solve the linear second order boundary value problem

$$y''(x) + y(x) = x,$$

for $x \in [0, \pi/2]$ with the boundary conditions $y(0) = 0$ and $y(\pi/2) = 1$ analytically and then numerically with the help of finite differences.

2. Solve the linear, second order boundary value problem

$$y''(x) - 2\cos(2x)y(x) = 0,$$

on the interval $[-\pi/2, \pi/2]$ and with the boundary conditions $y(\pm\pi/2) = 1$. Use the finite difference method.

Comment: The solution can be expressed analytically in terms of so-called MATHIEU functions [13, 14] which might be intrinsically available from your computing environment. If this happens to be the case, it might be a good idea to compare the numerical solution with the analytical result.

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