Finite difference method for Dirichlet boundary problem with variable coefficients

Let us consider the following boundary value problem

$$\begin{cases} -(\lambda(x)u')' + \gamma(x)u = f(x), & x \in (a,\, b), \\ u(a) = d_0, \quad u(b) = d_1, \end{cases} \tag{1}$$

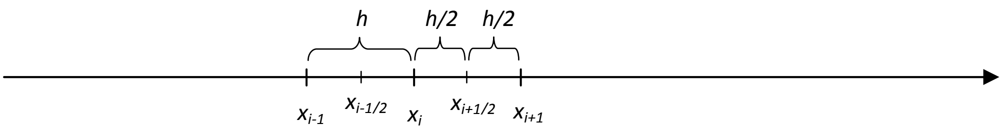
where $d_0,\, d_1 \in \mathbb{R}$ are given constants, functions $\lambda,\, \gamma,\, f : [a,\, b] \to \mathbb{R}$ are also given and continuous (α is moreover continuously differentiable). The task is to find a function $u : [a,\, b] \to \mathbb{R}$ twice differentiable which satisfies the equation and attains prescribed values $d_0,\, d_1$ at the boundary.

The problem (1) may be viewed as a one-dimensional stationary case of some process with the flux given by $J = -\lambda(x)\nabla u,$ which in one dimension is just $J = -\lambda(x)u'.$

For the approximation we introduce on the interval $[a,\, b]$ the main grid $\{x_i\}_{i=0}^{n+1}$ such that

$$x_i = a + i / h, \quad i = 0, 1, \ldots, n+1, \tag{2}$$

where $x_{n+1} = b,$ so $h = (b-a)/(n+1).$ This is of course a uniform grid with $x_{i+1} = x_i + h.$ To carry out the proper discretization of the term $-(\lambda(x)u')'$ it is also convenient to introduce the additional midpoints $x_{i+1/2} = (x_i + x_{i+1})/2$ of the intervals $[x_i,\, x_{i+1}]$ for $i = 0, 1, \ldots, n.$ This arrangement is presented on the picture below:



Let us denote the approximation of the unknown function $u = u(x)$ at $x = x_i$ by $u_i,$ i.e. $u_i \approx u(x_i).$ Now using the centered difference for a derivative $-(\lambda(x)u')'|_{x=x_i}$ we can write

$$\left(\lambda(x_i)u'(x_i)\right)' \approx \frac{\lambda(x_{i+1/2})u'(x_{i+1/2}) - \lambda(x_{i-1/2})u'(x_{i-1/2})}{h} \quad \text{for } i = 1, 2, \ldots, n.$$

so the equation from the problem (1) is

$$-\frac{\lambda(x_{i+1/2})u'(x_{i+1/2}) - \lambda(x_{i-1/2})u'(x_{i-1/2})}{h} + \gamma(x_i)u_i \approx f(x_i) \quad \text{for } i = 1, 2, \ldots, n.$$

Derivatives $u'(x_{i+1/2})$ and $u'(x_{i-1/2})$ are discretized also by the centered differences

$$u'(x_{i+1/2}) \approx \frac{u_{i+1} - u_i}{h}, \quad u'(x_{i-1/2}) \approx \frac{u_i - u_{i-1}}{h}.$$

Combining above expression we get

$$-\frac{\lambda(x_{i+1/2})\dfrac{u_{i+1}-u_i}{h}-\lambda(x_{i-1/2})\dfrac{u_i-u_{i-1}}{h}}{h}+\gamma(x_i)u_i \approx f(x_i) \quad \text{for } i=1,2,\ldots,n.$$

what can be written as

$$-\lambda_{i-1/2}u_{i-1}+(\lambda_{i-1/2}+\lambda_{i+1/2}+h^2\gamma_i)u_i-\lambda_{i+1/2}u_{i+1}=h^2 f_i \qquad \text{for } i=1,2,\ldots,n, \tag{3}$$

where notation $\lambda_{i\pm1/2}=\lambda(x_{i\pm1/2})$, $\gamma_i=\gamma(x_i)$, and $f_i=f(x_i)$ has been used.

Taking into account the boundary condition $u_0=d_0$ and $u_{n+1}=d_1$ we arrive finally at the following tridiagonal system of $n-1$ equations

$$\begin{cases} (\lambda_{1/2}+\lambda_{3/2}+h^2\gamma_1)u_1-\lambda_{3/2}u_2=h^2 f_1+\lambda_{1/2}d_0, & (i=1) \\ \ldots & \\ -\lambda_{i-1/2}u_{i-1}+(\lambda_{i-1/2}+\lambda_{i+1/2}+h^2\gamma_i)u_i-\lambda_{i+1/2}u_{i+1}=h^2 f_i, & (2\le i\le n-1), \\ \ldots & \\ -\lambda_{n-3/2}u_{n-2}+(\lambda_{n-3/2}+\lambda_{n-1/2}+h^2\gamma_{n-1})u_{n-1}=h^2 f_{n-1}+\lambda_{n-1/2}d_1 & (i=n-1), \end{cases} \tag{4}$$

for unknown values $U=(u_1,\ldots,u_{n-1})\in\mathbb{R}^{n-1}$.

Remarks on the existence of solution to the 1D Dirichlet boundary problem and properties of the tridiagonal matrix

The final linear system (4), which is expected to approximate the solution of the original problem (1), has $n-1$ unknowns. These correspond to the internal nodes $x_1,\ldots,x_n$ as the values at x_0 and x_{n+1} are directly known due to the nature of Dirichlet boundary conditions. In other types of boundary conditions, which employ values of the derivatives of the unknown function on the boundary this must be handled separately. But, usually this will affect only the form of the first and last equations of the linear system.

The tridiagonal system is simple and easy to solve by the reduced version of the Gaussian elimination, but still there is a valid question of the existence and uniqueness to this system. Even tridiagonal system with nonzero elements on diagonals may be singular as is evidenced by the example

$$AU=\begin{bmatrix}1&1&0&0&0\\1&1&1&0&0\\0&1&1&1&0\\0&0&1&1&1\\0&0&0&1&1\end{bmatrix}\begin{bmatrix}u_1\\u_2\\u_3\\u_4\\u_5\end{bmatrix}=\begin{bmatrix}b_1\\b_2\\b_3\\b_4\\b_5\end{bmatrix},$$

in which the matrix is not invertible ($\det A=0$).

The question of the solvability of the tridiagonal system (4) is related to the same question for the original problem for ODE (1) – the issue which we have not addressed so far: *does the boundary value problem (1) have unique solution for any given functions* $\lambda(x), \gamma(x), f(x)$ *and values* $d_0, d_1 \in \mathbb{R}$?

The answer is *no*, even for "nice" functions λ, γ. Here is an example of non-existence.

Example. Consider the problem on the interval $[0, 2\pi]$ with $\lambda(x) = -1, \ \gamma(x) = -1, \ f(x) = 0,$ and $g_0 = 0, \ g_1 = 1.$ The equation of the problem (1) reads now as $-(-u')' - u = 0,$ so the boundary problem to solve is

$$\begin{cases} u'' + u = 0, \\ u(0) = 0, \ u(2\pi) = 1. \end{cases} \tag{5}$$

The general solution to $u'' + u = 0$ is $u(x) = C_1 \sin x + C_2 \cos x.$ Inserting the left boundary condition we have $u(0) = 0 = C_1 \sin 0 + C_2 \cos 0 = C_2,$ thus $u(x) = C_1 \sin x.$ The value at the right boundary requires, however, $u(2\pi) = 1,$ but $u(2\pi) = C_1 \sin 2\pi = C_1 \cdot 0 = 0,$ thus we have clear contradiction. This proves that the problem (5) does not admit any solution.

On the other hand the discretized form of the problem (5) has the matrix form

$$\begin{bmatrix} -2-h^2 & 1 & 0 & \dots & 0 \\ 1 & -2-h^2 & 1 & & \vdots \\ 0 & 1 & -2-h^2 & 1 & 0 \\ \vdots & & \ddots & \ddots & \\ 0 & \dots & 0 & 1 & -2-h^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ -h^2 \end{bmatrix}, \tag{6}$$

and it can be show that the matrix is non-singular is for every $h > 0$ and size. This means that the approximation to the problem (5), which has no solution, will produce some approximate solution. This example shows that we must be cautious with numerical methods.

Coming back to the general problem (1) we state here the conditions for the functions λ, γ which guarantee the existence and uniqueness to this problem:

$$\gamma(x) \geq 0 \ \text{ and } \ \lambda(x) \geq m > 0 \quad \text{for} \ \ x \in [a, b], \tag{7}$$

where $m > 0$ is some constant. As we can see no constraint is imposed on the function f (save for the continuity requirement on the interval $[a, b]$).

Diagonal dominant matrices

One way to check whether a matrix is nonsingular is to see if its elements on the main diagonal dominate the off-diagonal ones in each row. In the case of tridiagonal matrix this condition reads as follows: a tridiagonal matrix

$$
\begin{bmatrix}
d_1 & c_1 & 0 & 0 & \dots & 0 \\
a_2 & d_2 & c_2 & 0 & \dots & 0 \\
0 & a_3 & d_3 & c_3 & \ddots & \vdots \\
0 & 0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \vdots & \ddots & a_{n-1} & d_{n-1} & c_{n-1} \\
0 & 0 & \dots & 0 & a_n & d_n
\end{bmatrix}, \tag{8}
$$

is said to be *diagonal dominant* if

$$
\begin{aligned}
&|d_1| > |c_1|, \\
&|d_i| \geq |b_i| + |c_i|, \quad \text{for } i = 2, \dots, n.
\end{aligned} \tag{9}
$$

It can be shown that when the tridiagonal matrix is diagonal dominant and $d_i \neq 0$ for $i = 1, \dots, n,$ then the matrix is nonsingular and the standard algorithm for solving the tridiagonal system of linear equations (presented in the lab 1 notes) finds the solution (no division by zero will be encountered).

We can check that conditions (7), which guarantee the solvability of the differential problem (1), will also guarantee the solvability of the discretized system (4). It is because now $\lambda_{i\pm 1/2} > 0,\ \gamma_i \geq 0$ so

$$
\begin{aligned}
&d_1 = \lambda_{1/2} + \lambda_{3/2} + h^2\gamma_1 > 0,\ c_1 = -\lambda_{3/2}, \\
&d_i = \lambda_{i-1/2} + \lambda_{i+1/2} + h^2\gamma_i > 0,\ a_i = -\lambda_{i-1/2},\ c_i = -\lambda_{i+1/2} \quad i = 2, \dots,
\end{aligned}
$$

and now we see that conditions (9) are obviously met.

Nuemann boundary conditions

In some application the physical model requires that the values of the gradient at the boundary – or its part – must be set. Generally, if u describes density of some quantity, this means that some form of flux through the boundary is controlled. Let us analyze the following problem

$$
\begin{cases}
-u'' = f(x), \quad x \in (a, b), \\
u'(a) = g_0,\ u(b) = d_1,
\end{cases} \tag{10}
$$

where $f : [a, b] \to \mathbb{R}$ is given function, and $g_0, d_1 \in \mathbb{R}$ given constants. This boundary value problem is called mixed (Nuemann at the left, Dirichlet at the right part of the boundary).[1]

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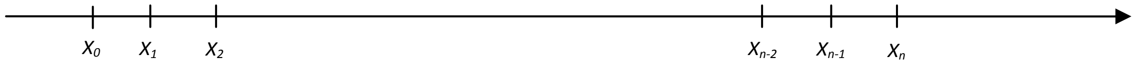
[1] We do not consider "full" Neumann boundary condition, say $u'(a) = g_0,\ u'(b) = g_1,$ because there are troubles with uniqueness. For example, the problem

$$
\begin{cases}
-u'' = f(x), \\
u'(0) = 0,\ u'(1) = 0,
\end{cases}
$$

obviously lacks uniqueness, because if u is some solution to this problem, then $u + c,$ where $c \in \mathbb{R}$ is any constant, is also a solution.

Discretization on the uniform grid $\{x_i\}_{i=0}^{n}$ for the internal nodes $x_1, \dots, x_{n-1}$ and for the last node $x_n = b$ is the same as in the Dirichlet boundary conditions. But for the first node $x_0 = a$ it must be different, as now we are not given the value of the function but its first derivative $u'(x_0) = g_0$ so $u_0 \approx u(x_0)$ is unknown.



The first choice could be

$$u_0' \approx \frac{u_1 - u_0}{h} = g_0,$$

which is a valid approximation of the first derivative. But the problem is that this approximation is of the first order in h, which means

$$\left| \frac{u_1 - u_0}{h} - g_0 \right| \le const \cdot h, \tag{11}$$

and centered finite difference for the second derivative u_i'' is of second order

$$\left| \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - u_i'' \right| \le const \cdot h^2. \tag{12}$$

By using both schemes (11) and (12) in the same set of discretized equations we would mixed up two orders of accuracy what would effectively produce the method of the lower order. Thus we would lose any advantage that might be expected from using the second order approximation (12). To remedy this disparity we look for a finite difference for u_0' that is of second order. Basically two approaches can be adopted: (i) *ghost point* method (ii) *three points one sided* finite difference.

Ghost point method. Let us introduce the auxiliary point $x_{-1} = x_0 - h$, which lies beyond the domain of the function $u : [x_0, x_n] \to \mathbb{R}$, and introduce an auxiliary unknown u_{-1}. It may look suspicious as the function u is not defined at $x = a - h$, but nevertheless this procedure leads to some final expression that depends only on the values belonging the interval $[a, b]$. Now we employ the centered difference at $x = x_0$, so

$$u_0' = \frac{u_1 - u_{-1}}{2h} = g_0. \tag{13}$$

To get rid of u_{-1} we will also discretize the equation (10) at the point $x = x_0$, thus

$$-\frac{u_1 - 2u_0 + u_{-1}}{h^2} = f_0. \tag{14}$$

Eliminating u_{-1} from (13) and (14) gives the following expression

$$u_0 - u_1 = \frac{1}{2}h^2 f_0 - hg_0. \qquad (15)$$

Three-points one sided finite difference. A derivative u' at any point x can also be approximated with second order error by values which are on one side of this point. Namely we have

$$u'(x) = \frac{-3u(x) + 4u(x+h) - u(x+2h)}{2h} + O(h^2). \qquad (16)$$

Applying this formula at the point $x = x_0$ and using the boundary condition $u'(x_0) = g_0$ we get the following expression

$$3u_0 - 4u_1 + u_2 = -2hg_0. \qquad (17)$$