Boundary value problems: method of finite differences

We have seen how a boundary value problem such as

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

$$y(a) = \alpha, \qquad y(b) = \beta$$

can be solved numerically by the shooting method, which combines a time-stepping algorithm with a root-finding method.

An alternative approach to computing solutions of the boundary value problem is to approximate the derivatives y' and y'' in the differential equation by *finite differences*.

First, divide the interval $[a, b]$ into $N+1$ subintervals of equal length $\Delta x = \dfrac{b-a}{N+1}$, so that

$$\begin{aligned} &x_0 = a, \qquad x_{N+1} = b \\ &x_j = a + j\Delta x \quad \text{ for } j = 1, 2 \ldots, N \end{aligned}$$

The points x_j are called "nodes", "grid points" or "mesh points".
At each interior node x_j with $j = 1, 2 \ldots, N$, the equation

$$y''(x_j) = f\big(x_j,\, y(x_j),\, y'(x_j)\big)$$

must be satisfied. If we now replace $y''(x_j)$ and $y'(x_j)$ by their $O(\Delta x^2)$ centered difference approximations (the most common choice of finite difference formulas to use), we get

$$\frac{y(x_j + \Delta x) - 2y(x_j) + y(x_j - \Delta x)}{\Delta x^2} \approx f\left(x_j,\, y(x_j),\, \frac{y(x_j + \Delta x) - y(x_j - \Delta x)}{2\Delta x}\right)$$

or equivalently

$$\frac{y(x_{j+1}) - 2y(x_j) + y(x_{j-1})}{\Delta x^2} \approx f\left(x_j,\, y(x_j),\, \frac{y(x_{j+1}) - y(x_{j-1})}{2\Delta x}\right)$$

Let y_j denote the approximate value of $y(x_j)$ that we aim to compute. Then our task is to solve the system of equations

$$(\star) \qquad \frac{y_{j+1} - 2y_j + y_{j-1}}{\Delta x^2} = f\left(x_j,\, y_j,\, \frac{y_{j+1} - y_{j-1}}{2\Delta x}\right), \qquad j = 1, 2, \ldots, N$$

to find $y_1, y_2, \ldots, y_N$. At the endpoints, we apply the given boundary conditions and set

$$y_0 = y(x_0) = y(a) = \alpha, \qquad y_{N+1} = y(x_{N+1}) = y(b) = \beta$$

The system $(\star)$ can be difficult to solve if f is a nonlinear function of y and y'. But when f is linear in y and y', $(\star)$ becomes a linear algebraic system that can be solved easily with Matlab's backslash command (or one of the other methods for solving linear systems).

Linear boundary value problem

A general second-order linear ODE can be written in the form

$$y'' = p(x)y' + q(x)y + r(x)$$

This equation is also called the steady-state diffusion–convection–reaction equation, where y'' models diffusion, $p(x)y'$ models convection, $q(x)y$ models a reaction, and $r(x)$ represents a source term.
Here $f(x, y, y') = p(x)y' + q(x)y + r(x)$, and in this case the particular form of $(\star)$ is

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{\Delta x^2} = p(x_j)\,\frac{y_{j+1} - y_{j-1}}{2\Delta x} + q(x_j)y_j + r(x_j), \qquad j = 1, 2, \ldots, N$$

Collecting on the left-hand side all terms involving the unknown "y"s, we get

$$\left(\frac{1}{\Delta x^2} + \frac{p(x_j)}{2\Delta x}\right) y_{j-1} - \left(\frac{2}{\Delta x^2} + q(x_j)\right) y_j + \left(\frac{1}{\Delta x^2} - \frac{p(x_j)}{2\Delta x}\right) y_{j+1} = r(x_j), \qquad j = 1, 2, \ldots, N$$

Multiplying through by $-\Delta x^2$ gives

$$\left(-1 - \frac{p(x_j)}{2}\Delta x\right) y_{j-1} + \left(2 + q(x_j)\Delta x^2\right) y_j + \left(-1 + \frac{p(x_j)}{2}\Delta x\right) y_{j+1} = -r(x_j)\Delta x^2, \qquad j = 1, 2, \ldots, N$$

Note that for $j = 1$, the equation is

$$\left(-1 - \frac{p(x_1)}{2}\Delta x\right) y_0 + \left(2 + q(x_1)\Delta x^2\right) y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2$$

For $j = N$, the equation is

$$\left(-1 - \frac{p(x_N)}{2}\Delta x\right) y_{N-1} + \left(2 + q(x_N)\Delta x^2\right) y_N + \left(-1 + \frac{p(x_N)}{2}\Delta x\right) y_{N+1} = -r(x_N)\Delta x^2$$

The boundary conditions will be incorporated into these two equations.

Dirichlet boundary conditions

$$y(a) = \alpha, \qquad y(b) = \beta$$

i.e. values of y (not y') are specified at the boundary.
We know $y_0 = \alpha$, so moving the first term in the $j = 1$ equation to the right-hand side yields

$$\left(2 + q(x_1)\Delta x^2\right) y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2 + \left(1 + \frac{p(x_1)}{2}\Delta x\right) \alpha$$

Similarly, we know $y_{N+1} = \beta$, so moving the third term in the $j = N$ equation to the right-hand side yields

$$\left(-1 - \frac{p(x_N)}{2}\Delta x\right) y_{N-1} + \left(2 + q(x_N)\Delta x^2\right) y_N = -r(x_N)\Delta x^2 + \left(1 - \frac{p(x_N)}{2}\Delta x\right) \beta$$

In summary, we have the equations

$$\begin{aligned}
&\left(2 + q(x_1)\Delta x^2\right) y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2 + \left(1 + \frac{p(x_1)}{2}\Delta x\right) \alpha \\
&\left(-1 - \frac{p(x_j)}{2}\Delta x\right) y_{j-1} + \left(2 + q(x_j)\Delta x^2\right) y_j + \left(-1 + \frac{p(x_j)}{2}\Delta x\right) y_{j+1} = -r(x_j)\Delta x^2 \quad \text{for } j = 2, \ldots, N-1 \\
&\left(-1 - \frac{p(x_N)}{2}\Delta x\right) y_{N-1} + \left(2 + q(x_N)\Delta x^2\right) y_N = -r(x_N)\Delta x^2 + \left(1 - \frac{p(x_N)}{2}\Delta x\right) \beta
\end{aligned}$$

Neumann boundary conditions

$$y'(a) = \gamma_\ell, \qquad y'(b) = \gamma_r$$

i.e. values of the first derivative y' are specified at the boundary.
This will make the entries in the first and last rows of A and **rhs** more complicated.

Let's say we use an $\boxed{O(\Delta x) \text{ forward difference formula at the left end}}$; then $y'(a) \equiv y'(x_0)$ is approximated by the difference quotient $\dfrac{y_1 - y_0}{\Delta x}$, and the boundary condition becomes

$$\frac{y_1 - y_0}{\Delta x} = \gamma_\ell, \qquad \text{so that} \quad \boxed{y_0 = y_1 - \gamma_\ell \Delta x}$$

Substituting this into the $j = 1$ equation gives

$$\left(-1 - \frac{p(x_1)}{2}\Delta x\right)(y_1 - \gamma_\ell \Delta x) + \left(2 + q(x_1)\Delta x^2\right) y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2, \quad \text{or}$$

$$\left\{\left(-1 - \frac{p(x_1)}{2}\Delta x\right) + \left(2 + q(x_1)\Delta x^2\right)\right\} y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2 + \left(-1 - \frac{p(x_1)}{2}\Delta x\right)\gamma_\ell \Delta x$$

Thus, the $(1, 1)$ entry of A and the first entry of **rhs** may need to be modified.

If we use an $\boxed{O(\Delta x^2) \text{ forward difference formula at the left end}}$, then $y'(a) \equiv y'(x_0)$ is approximated by the difference quotient $\dfrac{-3y_0 + 4y_1 - y_2}{2\Delta x}$, and the boundary condition becomes

$$\frac{-3y_0 + 4y_1 - y_2}{2\Delta x} = \gamma_\ell, \qquad \text{so that} \quad \boxed{y_0 = \frac{4}{3}y_1 - \frac{1}{3}y_2 - \frac{2}{3}\gamma_\ell \Delta x}$$

Substituting this into the $j = 1$ equation gives

$$\left(-1 - \frac{p(x_1)}{2}\Delta x\right)\left(\frac{4}{3}y_1 - \frac{1}{3}y_2 - \frac{2}{3}\gamma_\ell \Delta x\right) + \left(2 + q(x_1)\Delta x^2\right) y_1 + \left(-1 + \frac{p(x_1)}{2}\Delta x\right) y_2 = -r(x_1)\Delta x^2,$$

$$\text{or} \quad \left\{\frac{4}{3}\left(-1 - \frac{p(x_1)}{2}\Delta x\right) + \left(2 + q(x_1)\Delta x^2\right)\right\} y_1 + \left\{-\frac{1}{3}\left(-1 - \frac{p(x_1)}{2}\Delta x\right) + \left(-1 + \frac{p(x_1)}{2}\Delta x\right)\right\} y_2$$
$$= -r(x_1)\Delta x^2 + \left(-1 - \frac{p(x_1)}{2}\Delta x\right)\frac{2}{3}\gamma_\ell \Delta x$$

Thus, the $(1, 1)$ and $(1, 2)$ entries of A and the first entry of **rhs** may need to be modified.

Similarly, using an $\boxed{O(\Delta x) \text{ backward difference formula at the right end}}$ gives $\dfrac{y_{N+1} - y_N}{\Delta x} = \gamma_r$ and hence $\boxed{y_{N+1} = y_N + \gamma_r \Delta x}$, which leads to the following modified $j = N$ equation:

$$\left(-1 + \frac{p(x_N)}{2}\Delta x\right) y_{N-1} + \left\{\left(-1 + \frac{p(x_N)}{2}\Delta x\right) + \left(2 + q(x_N)\Delta x^2\right)\right\} y_N$$
$$= -r(x_N)\Delta x^2 - \left(-1 + \frac{p(x_N)}{2}\Delta x\right)\gamma_r \Delta x$$

Thus, the (N, N) entry of A and the last entry of **rhs** may need to be modified.

Using an $\boxed{O(\Delta x^2) \text{ backward difference formula at the right end}}$ gives $\dfrac{3y_{N+1} - 4y_N + y_{N-1}}{2\Delta x} = \gamma_r$ and hence $\boxed{y_{N+1} = \frac{4}{3}y_N - \frac{1}{3}y_{N-1} + \frac{2}{3}\gamma_r \Delta x}$, which leads to the following modified $j = N$ equation:

$$\left\{-\frac{1}{3}\left(-1 + \frac{p(x_N)}{2}\Delta x\right) + \left(-1 - \frac{p(x_N)}{2}\Delta x\right)\right\} y_{N-1} + \left\{\frac{4}{3}\left(-1 + \frac{p(x_N)}{2}\Delta x\right) + \left(2 + q(x_N)\Delta x^2\right)\right\} y_N$$
$$= -r(x_N)\Delta x^2 - \left(-1 + \frac{p(x_N)}{2}\Delta x\right)\frac{2}{3}\gamma_r \Delta x$$

Thus, the $(N, N-1)$ and (N, N) entries of A and the last entry of **rhs** may need to be modified.