The Numerov Method

The Numerov method is applicable to linear ordinary differential equations (such as the Schrödinger equation) that do not contain a y' term. A fairly general form of such an equation is

$$y'' + g(x)y = s(x), \quad a \leq x \leq b,$$

with appropriate boundary conditions at a and b, as discussed previously. Let's recast the derivation of the basic matrix method in a slightly different way.

We are interested in differencing the function $y(x)$, discretized on a grid (x_n, y_n) in a way that allows us to relate y_n to its neighboring values. Given that $y = y_n$ at $x = x_n$, we can write, for $y_{n+1} = y(x_{n+1}) = y(x_n + h)$:

$$y_{n+1} = y_n + hy'_n + \tfrac{1}{2}h^2y'' + \tfrac{1}{6}h^3y''' + \tfrac{1}{24}h^4y'''' + \tfrac{1}{120}h^5y''''' + O(h^6).$$

Similarly, for y_{n-1} (i.e. replacing h by $-h$),

$$y_{n-1} = y_n - hy'_n + \tfrac{1}{2}h^2y''_n - \tfrac{1}{6}h^3y'''_n + \tfrac{1}{24}h^4y''''_n - \tfrac{1}{120}h^5y'''''_n + O(h^6).$$

Adding these equations gives

$$y_{n+1} - 2y_n + y_{n-1} = h^2y''_n + \tfrac{1}{12}h^4y''''_n + O(h^6).$$

The left-hand side confirms our earlier second-order formula for the difference approximation to y''_n:

$$y''_n = \frac{y_{n_1} - 2y_n + y_{n-1}}{h^2} + O(h^2). \qquad (1)$$

but now we see that the next term in the expansion, i.e. the error we are making in the earlier differencing, is $\frac{1}{12}h^4y''''_n$. We can also view this formula as a general method for making a second-order accurate approximation to any second derivative.

The trick that Numerov invented is to determine the fourth derivative by differentiating the original differential equation:

$$\begin{aligned} y'' &= -g(x)y + s(x) \\ y'''' &= \frac{d^2}{dx^2}\left[-g(x)y + s(x)\right]. \end{aligned}$$

We can estimate the second derivative using the same formula as before:

$$y''''_n = \frac{-g_{n+1}y_{n+1} + 2g_ny_n - g_{n-1}y_{n-1} + s_{n+1} - 2s_n + s_{n-1}}{h^2} + O(h^2),$$

where $g_n = g(x_n)$, etc. Thus the next term in the Taylor series for y is

$$\tfrac{1}{12}h^4y''''_n = \tfrac{1}{12}h^2\left(-g_{n+1}y_{n+1} + 2g_ny_n - g_{n-1}y_{n-1} + s_{n+1} - 2s_n + s_{n-1}\right) + O(h^6).$$

Substituting this into equation (1) to obtain a new expression for y''_n

$$h^2y''_n = \left(1 + \tfrac{1}{12}h^2g_{n+1}\right)y_{n+1} - 2\left(1 + \tfrac{1}{12}h^2g_n\right)y_n + \left(1 + \tfrac{1}{12}h^2g_{n-1}\right)y_{n-1} - \tfrac{1}{12}h^2\left(s_{n+1} - 2s_n + s_{n-1}\right),$$

and the original ODE then becomes

$$\left(1+\tfrac{1}{12}h^2 g_{n+1}\right) y_{n+1} - 2\left(1-\tfrac{5}{12}h^2 g_n\right) y_n + \left(1+\tfrac{1}{12}h^2 g_{n-1}\right) y_{n-1} = \tfrac{1}{12}h^2 \left(s_{n+1}+10s_n+s_{n-1}\right).$$

We can now solve the (inhomogeneous) boundary value problem as a matrix equation just as before. Note that, once again, the boundary values y_0 and y_N enter the problem through the $n = 1$ and $n = N-1$ rows.

For eigenvalue problems, such as

$$y'' + g(x)y = -zy,$$

the differencing of the left side of the equation is as above, but now the right side becomes

$$-\tfrac{1}{12}h^2 z\left(y_{n+1}+10y_n+y_{n-1}\right),$$

so the matrix equation to solve is

$$\mathbf{A}\mathbf{y} = -\tfrac{1}{12}h^2 z\,\mathbf{B}\mathbf{y},$$

where $\mathbf{y}$ is the $N-1$ dimensional column vector $(y_1, y_2, \ldots, y_{N-1})^T$, and the matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$\mathbf{A} = \begin{pmatrix} \beta_1 & \alpha_1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \gamma_2 & \beta_2 & \alpha_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & \gamma_3 & \beta_3 & \alpha_3 & 0 & \cdots & 0 & 0 & 0 \\ . & & & & & & & & \\ . & & & & & & & & \\ . & & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \gamma_{N-1} & \beta_{N-1} \end{pmatrix},$$

where $\alpha_n = 1+\frac{1}{12}h^2 g_{n+1}$, $\beta_n = 2\left(1-\frac{5}{12}h^2 g_n\right)$, $\gamma_n = 1+\frac{1}{12}h^2 g_{n-1}$, for $n = 1, \ldots, N-1$, and

$$\mathbf{B} = \begin{pmatrix} 10 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 10 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 10 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 10 & 1 & \cdots & 0 & 0 & 0 \\ . & & & & & & & & \\ . & & & & & & & & \\ . & & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 10 \end{pmatrix}.$$

The solution to the problem then reduces to finding the eigenvectors and eigenvalues of the matrix $\mathbf{B}^{-1}\mathbf{A}$.