

On Solving $y'' = fy + g$ with a Boundary Condition at Infinity

By Charlotte Froese

Consider the class of differential equations

$$(1) \quad y'' = f(x)y + g(x)$$

for which

$$(i) \quad g(x) \rightarrow 0 \quad \text{as } x \rightarrow \infty$$

$$(ii) \quad f(x) > 0 \quad \text{and} \quad f(x) \rightarrow c \quad \text{as } x \rightarrow \infty,$$

together with the boundary conditions,

$$(iii) \quad y(a) = y_0 \quad \text{and} \quad y(\infty) = 0.$$

Suppose further that a numerical solution is required over the range (a, b) where b is such that $|y'(x)| \leq \tau$, for all $x \geq b$.

For large values of x , one solution of the equation tends to infinity whereas the other tends to zero; the latter is the desired solution. Because of round-off and truncation errors which are inherent in a numerical procedure, any outward integration will introduce some of the former solution into the calculation, so that the numerical solution will not tend to zero but eventually increase exponentially. This difficulty may be avoided by determining the solution at some large value of x from an asymptotic expansion, for example, and integrating inwards. It is avoided more simply by the procedure to be described, particularly when the inward integration cannot be started readily and the range (a, b) over which the solution extends is not known in advance.

Let

$$x_i = x_0 + ih, \quad x_0 = a,$$

and define y_i to be the computed approximation to $y(x_i)$; y_0 is known and y_1, y_2, \dots are to be determined.

It is well known that

$$(2) \quad \delta^2 y_i = h^2 \left(y_i'' + \frac{\delta^2}{12} y_i'' \right) + O(h^6).$$

Substituting for y'' from (1) and neglecting terms which are $O(h^6)$, we may rewrite (2) as a system of equations

$$\begin{pmatrix} -b_1 & a_2 & & & \\ a_1 & -b_2 & a_3 & & \\ & a_2 & -b_3 & a_4 & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} -a_0 y_0 + c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

where

$$a_i = 1 - \frac{h^2}{12} f_i$$

$$b_i = 2 + \frac{10}{12} h^2 f_i$$

and

$$c_i = \frac{h^2}{12} (g_{i+1} + 10g_i + g_{i-1}),$$

or, in matrix form, $AY = C$. The matrix A has a tridiagonal form so that the system of equations may readily be solved by the Gauss elimination method. An algorithm in this case is given by equations (3) and (4):

$$(3) \quad \begin{aligned} d_1 &= -b_1 & d_i &= -b_i - (a_{i-1}a_i/d_{i-1}) \\ z_1 &= c_1 - a_0y_0 & z_i &= c_i - (a_{i-1}z_{i-1}/d_{i-1}) \end{aligned}$$

and

$$(4) \quad y_i = (z_i - a_{i+1}y_{i+1})/d_i.$$

Unlike the standard case, the order N of the matrix is not known in advance but depends on the solution. For $f(x) > 0$ and h sufficiently small, it can be shown that $d_i \rightarrow -1 + 0(h)$ as i increases and obviously $a_i = 1 + 0(h^2)$. Thus, for i sufficiently large and h sufficiently small equation (4) becomes

$$y_{i+1} - y_i \sim z_i,$$

or

$$z_i \sim hy_i'.$$

Therefore, if we solve equations (3) for $i = 2, 3, \dots, N$ successively until $|z_N| < h\tau$ followed by (4) with $i = N, N - 1, \dots, 1$ we will have obtained a solution over the desired range. The solution of (4) when $i = N$ requires an approximation; the simplest is

$$(i) \quad y_{N+1} = 0.$$

A more accurate assumption is

$$(ii) \quad y_{N+1} = Cy_N,$$

where C is determined from an asymptotic expansion. Then

$$y_N = z_N/(d_N + a_{N+1}C).$$

The above boundary conditions are frequently associated with eigenvalue problems. An example is the Hartree-Fock equation for an electron,

$$P'' = \left(\epsilon - 2 \frac{Y(r)}{r} + \frac{l(l+1)}{r^2} \right) P = f(r)P.$$

Here ϵ is an eigenvalue and a solution of the problem may not exist for an arbitrary

choice of ϵ . The usual procedure is to divide the range of integration into two parts, integrate outwards for a solution satisfying one boundary condition, integrate inwards for a solution satisfying the other boundary condition, match the solutions at an intermediate point and adjust ϵ so that the derivatives also agree [1], [2]. The inward integration may be avoided with the procedure described earlier. A convenient way of dividing the range is according to the sign of $f(r)$. For some r , $f(r) < 0$ so that condition (ii) is not satisfied: the procedure described here is not always numerically stable when $f(r) < 0$ [3]; in fact, for some values of i , $|d_i| < 1$. Of a series of standard methods, the Numerov method,

$$(5) \quad y_{n+1} = \left(\left(2 + \frac{10}{12} h^2 f_n \right) y_n - \left(1 - \frac{h^2}{12} f_{n-1} \right) y_{n-1} + \frac{h^2}{12} (g_{n+1} + 10g_n + g_{n-1}) \right) / \left(1 - \frac{h^2}{12} f_{n+1} \right),$$

was found to be most accurate in this case, for a given number of evaluations of f for the outward integration. The procedure used successfully was to integrate outwards according to (5) until $f(r) > 0$, then, with the last value computed as a boundary condition, to solve for the "tail" of the wave function by the method described here. The energy adjustment will be the same as before.

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On the Inversion of Sparse Matrices

By A. L. Dulmage and N. S. Mendelsohn

1. Introduction. There are a number of problems in applied mathematics involving many equations in many unknowns, but for which each equation involves only a small fraction of the unknowns. If such problems are linear or are approximated by linearization, one is involved with a matrix, a large proportion of whose entries are zero. To invert such a matrix A it is sometimes advantageous to permute the rows and columns of A yielding PAQ where P and Q are permutation matrices. If

$$PAQ = \begin{vmatrix} A_1 & & 0 \\ & A_2 & \\ & & \ddots \\ * & & & A_r \end{vmatrix}$$

where A_1, A_2, \dots, A_r are square matrices, the problem of inverting PAQ is reduced

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