A NUMERICAL METHOD OF SOLVING SECOND-ORDER LINEAR DIFFERENTIAL EQUATIONS WITH TWO-POINT BOUNDARY CONDITIONS

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ABSTRACT. A direct method of integrating the equation $y'' + g(x)\, y = h(x)$, with the two-point linear boundary conditions $y'(a) + \alpha y(a) = A$, $y'(b) + \beta y(b) = B$, is based on the factorization of the equation into two first-order linear equations $v' - sv = h$ and $y' + sy = v$, where s is a solution of the Riccati equation $s' - s^2 = g$. The first-order equations for v and y are integrated in succession, one in the direction of x increasing, and one in the direction of x decreasing, one boundary condition being used in each of these integrations. The appropriate solution of the Riccati equation is determined by the boundary condition at the end of the range from which the integration of the equation for v is started. The process is compared with the matrix factorization method of Thomas and Fox, and its stability discussed.

1. *Introduction.* There are essentially two approaches to the numerical solution of a second-order linear differential equation with two-point boundary conditions:

(i) *Methods in which step-by-step integrations of the second-order equation are started from one boundary.* Since only one condition is given at each boundary, a second condition is needed to start the integration. In one method the second condition is estimated and corrected by trial until the condition given at the other boundary is satisfied. In another method, an arbitrary condition is chosen to start the numerical integration. The complementary function satisfying the homogeneous form of the condition given at the first boundary is also calculated. The condition at the second boundary is then satisfied by adding a suitable multiple of the complementary function to the particular integral. Both these methods are described by Hartree ((3), pp. 125, 143). Although satisfactory in some cases, they give trouble when the complementary function increases rapidly over the range of integration. The values of the functions obtained at the second boundary are not then well defined by the conditions chosen at the first boundary. In such cases it may be advantageous to use modifications of these methods in which integrations of the second-order equation are carried from both boundaries and matched at some internal point of the range.

(ii) *Methods in which both boundary conditions are used from the outset.* These tend to be more satisfactory since in physical examples the numerical approach is closely linked with the situation which the equations describe. They include Southwell's relaxation method as developed by Fox (1). Here the differential equation is replaced by a set of difference equations; and a trial function which satisfies the boundary conditions but does not satisfy the difference equations is made to approximate more and more closely to the required solution. Another method in which the differential equation is replaced by a set of difference equations has been developed by Thomas (4) and Fox ((2), p. 141). The equations are written in matrix form and are then solved by factorizing

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the square matrix. Corrections for higher differences are obtained by iteration. The method to be described below is direct and involves the factorization of the differential equation itself. It will be shown that the process is closely allied to the matrix factorization method and has similar advantages.

2. *The factorization process.* Our considerations will be restricted to linear differential equations of the second order with the first derivative absent, as in

$$y'' + g(x)\,y = h(x). \tag{1}$$

Suppose that we wish to integrate this equation numerically between the limits $x = a$ and $x = b$, with the two-point boundary conditions

$$\left.\begin{aligned} \frac{dy}{dx} + \alpha y = A \quad \text{at} \quad x = a, \\ \frac{dy}{dx} + \beta y = B \quad \text{at} \quad x = b. \end{aligned}\right\} \tag{2}$$

Using the differential operator notation, (1) may be written

$$[D^2 + g(x)]\,y = h(x). \tag{3}$$

We now 'factorize' the operator on the left-hand side of (3) into a product of two first-order linear terms,

$$[D + r(x)]\,[D + s(x)]\,y = h(x). \tag{4}$$

Expanding (4) and equating each term to the corresponding term in (3), we find that

$$r(x) + s(x) = 0 \tag{5}$$

and

$$Ds(x) + r(x)\,s(x) = g(x). \tag{6}$$

Now let

$$(D + s)\,y = v. \tag{7}$$

Substitution in (4) gives

$$(D + r)\,v = h. \tag{8}$$

From (5) to (8), we have

$$\frac{ds}{dx} - s^2 = g, \tag{9}$$

$$\frac{dv}{dx} - sv = h \tag{10}$$

and

$$\frac{dy}{dx} + sy = v. \tag{11}$$

We have thus replaced the second-order linear differential equation (1) by three first-order equations. Two of these, (10) and (11), are linear. The third, (9), is non-linear and is the Riccati equation equivalent to the homogeneous equation

$$\frac{d^2y}{dx^2} + g(x)\,y = 0. \tag{12}$$

Equation (9) may be obtained by making the substitution

$$\frac{1}{y}\frac{dy}{dx} = -s \tag{13}$$

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in (12) (Hartree (3), p. 148). It has a single infinity of solutions from which we can pick out one which enables the boundary conditions to be trivially satisfied. The boundary conditions (2) have the same form as equation (11). We can thus satisfy the boundary condition at $x = a$ if we take

$$s(a) = \alpha, \quad v(a) = A. \tag{14}$$

Using some standard step-by-step numerical procedure, we can then integrate (9) and (10) from $x = a$ to $x = b$. When $x = b$ is reached, $s(b)$ and $v(b)$ will be available. From (11) and the second of equations (2), it follows that

$$y(b) = [v(b) - B]/[s(b) - \beta]. \tag{15}$$

This gives the boundary condition for integrating (11) from $x = b$ to $x = a$ and, assuming the process to be stable, we have the required solution.

If the boundary conditions are of the form

$$\left.\begin{aligned} y &= y_a \quad \text{at} \quad x = a, \\ y &= y_b \quad \text{at} \quad x = b, \end{aligned}\right\} \tag{16}$$

a different treatment is necessary since for the appropriate solution of the Riccati equation the function s is unbounded at $x = a$. Let

$$s = 1/S, \quad v = V/S \quad \text{and} \quad y = SY + V. \tag{17}$$

Substitution in (9), (10) and (11) gives

$$\frac{dS}{dx} + gS^2 = -1, \tag{18}$$

$$\frac{dV}{dx} + SgV = Sh, \tag{19}$$

$$\frac{dY}{dx} - SgY = gV - h. \tag{20}$$

The boundary condition at $x = a$ will be satisfied if

$$S(a) = 0, \quad V(a) = y_a. \tag{21}$$

Equations (18) and (19) can now be integrated from $x = a$ to $x = b$. Then, knowing $V(b)$ and $S(b)$, $Y(b)$ is given by the last of equations (17),

$$Y(b) = [y_b - V(b)]/S(b). \tag{22}$$

This gives the boundary condition necessary to start the integration of (20) at $x = b$. Again, provided the process is stable, we have the required solution.

3. *A comparison of the matrix and factorization processes.* A matrix method of solving second-order linear differential equations with two-point boundary conditions has been developed by Thomas (4) and Fox ((2), p. 141) and has been described by Hartree ((3), p. 173). The differential equation (1) is replaced by a series of difference equations which in general take the form

$$y_{j-1} + [(\delta x)^2 g_j - 2] y_j + y_{j+1} = (\delta x)^2 h_j - C y_j, \tag{23}$$

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where δx is the integration interval and the equation is centred on x_j. The term Cy_j is a correction and includes differences of y of the fourth and higher orders. The first and last equations of the series are modified by the inclusion of the two-point boundary conditions.

In matrix form, the set of difference equations may be expressed

$$A\mathbf{y} = \mathbf{z}, \tag{24}$$

where, in general, a row of elements in the square matrix A is given by

$$\left.\begin{aligned} A_{j,j-1} &= 1, \\ A_{j,j} &= p_j = -[2-(\delta x)^2 g_j], \\ A_{j,j+1} &= 1 \end{aligned}\right\} \tag{25}$$

and all other elements are zero. A general element of the vector $\mathbf{z}$ is

$$z_j = (\delta x)^2 h_j - Cy_j. \tag{26}$$

As a first approximation, the difference corrections Cy_j are neglected and (24) solved by Choleski's method (see Hartree (3), p. 164). This resolves the matrix A into the product of a lower triangular matrix L and an upper triangular matrix U. We thus have

$$LU = A. \tag{27}$$

Substitution in (24) gives

$$LU\mathbf{y} = \mathbf{z}. \tag{28}$$

If we now let

$$U\mathbf{y} = \mathbf{w}, \tag{29}$$

then

$$L\mathbf{w} = \mathbf{z}. \tag{30}$$

The elements of L and U are found by solving a series of equations which in general take the form

$$l_j = 1/(p_j - l_{j-1}). \tag{31}$$

Either l_0 or l_1 is given by the boundary condition at $x = a$ and values of the l_j's may be obtained successively in order of increasing j. The matrix equation (30) represents a series of equations of the type

$$w_j = z_j - l_{j-1} w_{j-1}. \tag{32}$$

Again either w_0 or w_1 is given by the boundary condition at $x = a$ and the w_j's can be obtained successively in order of increasing j. Finally, the matrix equation (29) gives a series of equations which in general take the form

$$y_j = l_j(w_j - y_{j+1}). \tag{33}$$

Either y_n or y_{n-1} is given by the boundary condition at $x = b$ and the y_j's can be calculated successively in order of decreasing j.

This matrix process is closely related to the factorization method described in § 2. Let us consider the homogeneous matrix problem corresponding to (24). The vector $\mathbf{z}$ is then zero. From (30), we see that $\mathbf{w}$ is also zero. Equation (33) then becomes

$$y_j = -l_j y_{j+1}. \tag{34}$$

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It follows that the l_j's are nearly -1 except in the neighbourhood of a node of the solution of the homogeneous problem. Let us write to the first order

$$l_j = -[1 + \delta x \eta_j]. \tag{35}$$

Substituting (25) and (35) in (31),

$$[(\eta_j - \eta_{j-1})/\delta x] - \eta_j \eta_{j-1} = g_j + \delta x g_j \eta_j. \tag{36}$$

Similarly, if we let

$$w_j = \nu_j \delta x \tag{37}$$

and substitute (37), (35) and (26) in (32), we find that

$$[(\nu_j - \nu_{j-1})/\delta x] - \eta_{j-1} \nu_{j-1} = h_j - C y_j/(\delta x)^2. \tag{38}$$

A similar substitution in (33) gives

$$[(y_{j+1} - y_j)/\delta x] + \eta_j y_{j+1} = \nu_j + \nu_j \eta_j \delta x. \tag{39}$$

If now δx tends to zero, (36), (38) and (39) become

$$\frac{d\eta}{dx} - \eta^2 = g, \tag{40}$$

$$\frac{d\nu}{dx} - \eta\nu = h, \tag{41}$$

$$\frac{dy}{dx} + \eta y = \nu. \tag{42}$$

These are the equations (9)–(11) obtained above by factorization of the differential equation. There is thus a close parallel between the two processes.

4. *The accuracy of the factorization process.* Thomas (4) has discussed the stability of the matrix factorization method. He shows that the accuracy of the process may be related to the behaviour of the corresponding homogeneous problem. There is complete stability only when the homogeneous solution is numerically increasing.

As might be expected, there are similar conditions for stability of the factorization method. Inspection of equations (9)–(11) shows that the numerical integrations are completely stable only if s is negative throughout the range. The Riccati equation (9) and the equation (10) for v are then stable for integration in the direction of increasing x. Equation (11) for y must be integrated in the direction of decreasing x and this, too, is then stable. This condition upon s may be related to the behaviour of the solution of the corresponding homogeneous problem for which h and v in (10) are everywhere zero. Equation (11) then becomes

$$\frac{dy}{dx} + sy = 0. \tag{43}$$

We see that when s is negative, the solution is numerically increasing. For s positive, the solution is numerically decreasing. Thus, as in the matrix method, there is complete stability only when the solution of the corresponding homogeneous problem is numerically increasing. By retaining extra figures we may expect to be able to carry the solution through short regions of instability.

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A node of the homogeneous solutions requires a modification of procedure. From (43) it is clear that s becomes infinite. This may be overcome by changing to the variables S, V and Y defined by (17) and using equations (18)–(20) to pass through the node. It would not be possible to use these variables at stationary values of the homogeneous solution since S then becomes infinite. A convenient procedure is to change from one set of variables to the other as the need arises.

When equations (18)–(20) are used for the integrations, errors die out when gS is positive and accumulate when it is negative. Two situations arise:

(i) If g is negative, the solution of the homogeneous problem is exponential in character and the process will be completely stable only in regions where this solution is numerically increasing.

(ii) If g is positive, the solution of the homogeneous problem is oscillatory and the situation is reversed. Errors die out in regions where the solution is numerically decreasing, with increasing x.

5. *Conclusion.* A method of solving second-order linear differential equations with two-point boundary conditions by factorizing the differential equation has been described. It has been shown that the method is closely allied to the matrix factorization method of Fox and Thomas and has similar stability conditions. Although the description given above is for the sake of simplicity restricted to equations in which the first derivative is absent, the process is easily generalized to cover equations which have a first derivative term. The Riccati equation (9) is then replaced by a generalized Riccati equation (Watson (5), p. 92).

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