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A Comparison of Newman's Numerical Technique and deBoor's Algorithm

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Newman's numerical technique (1-4) has been used extensively to solve two-point boundary value problems consisting of coupled, ordinary differential equations. Unfortunately, his method does not always yield a solution to a system of independent equations. Sometimes his algorithm (BAND) signals incorrectly that the coefficient matrix is singular (*e.g.*, DETERMINANT = 0 AT J = 2), and no solution is obtained to the system of equations. This problem sometimes occurs when one tries to use BAND to solve a two-point boundary value problem which consists of a set of mixed order ordinary differential equations. For example, the battery model equations presented recently by Evans and White (5) are representative of this type of equation set. This problem is referred to here as the "zero determinant problem." The cause of this problem with BAND is due to the way in which the algorithm in BAND is used to solve the system of equations. The problem can be avoided by using alternate difference expressions or coordinate systems, or by using algorithms by deBoor (6) or IMSL (7).

The boundary value problem tested here is given in Table I as Eq. [1]-[4]. The derivatives were written in finite difference form and programmed for solution using Newman's BAND computer code (2) and deBoor's computer code (6). Several subroutines were written to provide a means for using the BAND procedure with deBoor's method. These subroutines are available from the authors. In addition, a routine named LSLRG from the IMSL (7) library was used to verify the results obtained by deBoor's solver.

Results and Discussion

The zero determinant problem of Newman's BAND algorithm is due to the finite difference expression used for the gradient of y for a particular location of the origin of the coordinate system. The gradient of y, dy/dx, can be approximated with central, forward, or backward finite difference expressions as follows

Central difference (CD)

$$\frac{dy}{dx} = \frac{y_{j+1} - y_{j-1}}{2h} + O(h^2) \qquad [5]$$

Forward difference (FD)

$$\frac{dy}{dx} = \frac{y_{j+1} - y_j}{h} + O(h) \qquad [6]$$

Backward difference (BD)

$$\frac{dy}{dx} = \frac{y_j - y_{j-1}}{h} + O(h) \qquad [7]$$

where $h = 1/(N\text{-}1)$ and N is the total number of node points.

The governing equation shown in Table I can be solved in the x direction (coordinate system 1, CS1) or in the z direction (coordinate system 2, CS2). Several combinations of finite difference expressions and coordinate systems were used, together with Newman's BAND, deBoor's solver, and LSLRG to solve or attempt to solve the example problem. The end points without boundary conditions were treated by using backward difference (Eq. [7]) and forward difference (Eq. [6]) expressions for CS1 and CS2, respectively. A run was designated successful when the analytical solution was obtained, and a failure when the solver indicated that the numerical system was singular (*i.e.*, a zero determinant was indicated). The results are presented in Table II.

Table I. Boundary value problem

Coordinate system 1 (CS1):

$$\frac{dy}{dx} = 1 \qquad 0 < x \leq 1 \qquad [1]$$

boundary condition,

$$y = 1 \qquad \text{at } x = 0 \qquad [2]$$

Coordinate system 2 (CS2): $z = 1 - x$

$$\frac{dy}{dz} = -1 \qquad 0 \leq z < 1 \qquad [3]$$

boundary condition,

$$y = 1 \qquad \text{at } z = 1 \qquad [4]$$

As shown in Table II, all of the solvers fail for two of the cases; CS1 with FD and CS2 with BD. These results are correct because the matrix is singular. This can be seen, for example, by considering the last two rows of the coefficient matrix for CS1 with FD. Using the notation of (3), the matrix equation to be solved for this case is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{h} & \frac{1}{h} & 0 & 0 & 0 \\ 0 & 0 & \frac{-1}{h} & \frac{1}{h} & 0 & 0 \\ & & & \ddots & \ddots & \\ 0 & 0 & 0 & 0 & \frac{-1}{h} & \frac{1}{h} \\ 0 & 0 & 0 & 0 & \frac{-1}{h} & \frac{1}{h} \end{bmatrix} \begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ \vdots \\ C(N\text{-}1) \\ C(N) \end{bmatrix} = \begin{bmatrix} G(1) \\ G(2) \\ G(3) \\ \vdots \\ G(N\text{-}1) \\ G(N) \end{bmatrix} \qquad [8]$$

Examination of Eq. [8] reveals that the last two rows of the coefficient matrix are the same, which yields a singular matrix. This is due to the forward difference formulation of the N-1th equation and the backward difference formulation of the Nth equation. This numerical singularity can be avoided by using a central or backward difference formulation for dy/dx for the middle nodes. Table II also shows that deBoor's solver and LSLRG work for one case where Newman's technique does not: CS1 and CD. Newman's technique signals incorrectly that the coefficient matrix is singular. This problem occurs because Newman's algorithm is based on solving the block system of equations sequentially (3) and does not utilize the entire system of equations at any given point, as does deBoor's method. This problem with BAND for this case becomes clear by stepping through Newman's algorithm using the test problem given in Table I. Using the notation of (3), the matrix equation

$$\begin{bmatrix} B(1) & D(1) & X(1) & 0 & 0 \\ A(2) & B(2) & D(2) & 0 & 0 \\ 0 & A(3) & B(3) & D(3) & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & 0 & A(N\text{-}1) & B(N\text{-}1) & D(N\text{-}1) \\ 0 & 0 & Y(N) & A(N) & B(N) \end{bmatrix} \begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ \vdots \\ C(N\text{-}1) \\ C(N) \end{bmatrix} = \begin{bmatrix} G(1) \\ G(2) \\ G(3) \\ \vdots \\ G(N\text{-}1) \\ G(N) \end{bmatrix} \qquad [9]$$

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Table II. Comparison of the performance of BAND, deBoor's solver, and LSLRG (IMSL)

(F-failure, R-successful run)

Method	Coordinate system	BD	CD	FD
Newman's BAND	CS1	R	F	F
	CS2	F	R	R
deBoor's solver	CS1	R	R	F
	CS2	F	R	R
LSLRG (IMSL)	CS1	R	R	F
	CS2	F	R	R

can be written as

$$MT = Z \quad [10]$$

Equation [10] can be solved by decomposing the coefficient matrix, M, into lower and upper triangular matrices

$$M = LU \quad [11]$$

as explained in (3). In this case

$$B(1) = 1 \text{ and } D(1) = 0 \quad [12]$$

$$A(2) = -D(2) = \frac{-1}{2h} \text{ and } B(2) = 0 \quad [13]$$

Using Eq. [16]-[19] of (3), some of the values for elements of L and U ($b(1)$, $a(2)$, and $b(2)$) can be obtained

$$b(1) = B(1) = 1.0 \quad [14]$$

$$E(1) = \frac{-D(1)}{b(1)} = 0 \quad [15]$$

$$a(2) = A(2) = \frac{-1}{2h} \quad [16]$$

$$b(2) = B(2) + a(2)E(1) = 0 \quad [17]$$

Consideration of Eq. [14]-[17] reveals that a singularity is developed; in particular, Eq. [17] shows that $b(2)$, a diagonal element of L, is zero which results in a singular condition. The analogous case for multiple equations would be one in which zeros would be in one column or row of the block that lies on the diagonal, again resulting in a singular condition. This failure could be avoided by using partial pivoting for the entire coefficient matrix, as is done in deBoor's method. Unfortunately, this is not done in BAND. It may be possible to modify BAND to use partial pivoting of the entire block coefficient matrix; however, the additional storage requirements for this would detract from the benefits of BAND.

Equations [14]-[17] can also be used to show why Newman's algorithm works for CS2 with CD. In this case, $D(1)$ is not zero because the derivative boundary equation is approximated by using a forward difference expression. Therefore, $E(1)$ is not zero and $b(2)$ is non-zero.

Conclusion

Newman's algorithm fails for the CS1 with CD case because the coefficient matrix contains a zero on the diagonal, as shown by Eq. [17], which is not removed by partial pivoting. The solver presented by deBoor for block matrix equations does not have this limitation and can be used to solve this case. Since cases like this one may occur during mathematical modeling of electrochemical systems, one may want to use deBoor's method instead of BAND to avoid this problem.

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LIST OF SYMBOLS

- $a(j)$ element of U in j^{th} row
- $A(j)$ partial derivative of the governing equation with respect to $C(j-1)$
- $b(j)$ element of L in j^{th} row
- $B(j)$ partial derivative of the governing equation with respect to $C(j)$
- $C(j)$ value of the unknown, y, at node j
- $D(j)$ partial derivative of the governing equation with respect to $C(j+1)$
- $E(j)$ element of U in j^{th} row
- $G(j)$ right-hand side of governing equation at node j
- h distance between successive nodes, dimensionless
- j j^{th} node
- L lower triangular matrix formed from decomposition of M
- M coefficient matrix for Newman's numerical technique
- N number of node points
- T vector of unknowns in Newman's numerical technique (cf. Eq. [9] and [10])
- U upper triangular matrix formed from decomposition of M
- x independent variable, dimensionless
- $X(j)$ partial derivative of the governing equation with respect to $C(j+2)$
- y dependent variable, dimensionless
- z transformation of coordinate system ($= 1 - x$), dimensionless
- Z right-hand side of equation in Newman's numerical technique (cf. Eq. [9] and [10])

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