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Abstract

Several algorithms are presented for solving block tridiagonal systems of linear algebraic equations when the matrices on the diagonal are equal to each other and the matrices on the subdiagonals are all equal to each other. It is shown that these matrices arise from the finite difference approximation to certain elliptic partial differential equations on rectangular regions. Generalizations are derived for higher order equations and non-rectangular regions.

1. Introduction

In many physical applications, it is necessary to solve an $N \times N$ system of linear algebraic equations

$$\underline{M}\underline{x} = \underline{y} \quad (1.1)$$

where M arises from a finite difference approximation to an elliptic partial differential equation. For this reason, the matrix M is sparse and the non-zero elements occur in a very regular manner. As an example of this, let

$$M = \begin{pmatrix} I & F \\ F^T & I \end{pmatrix} \quad (1.2)$$

and we partition \underline{x} and \underline{y} to conform with M . If it is possible to interchange the rows and interchange the columns of a matrix so that it has the form of $(M-I)$, then the matrix is said to be 2-cyclic (cf. [10]). Expanding (1.1), we have

$$\begin{aligned} \underline{x}_1 + \underline{F}\underline{x}_2 &= \underline{y}_1 \\ F^T \underline{x}_1 + \underline{x}_2 &= \underline{y}_2 \end{aligned}$$

Multiplying the first equation by $-F^T$ and adding we have

$$(I - F^T F) \underline{x}_2 = \underline{y}_2 - F^T \underline{y}_1. \quad (1.3)$$

Thus by this simple device, we have reduced the number of equations. If $(I - F^T F)$ is also 2-cyclic then we can again eliminate a number of the variables, and we can continue until the resulting matrix is no longer 2-cyclic.

Based on the suggestion of one of the authors, Hockney[6] has used this device extensively and effectively. Recently Buneman [2] has devised a method for easily solving the reduced system of equations. The technique is particularly attractive since in theory it yields the exact solution to the difference equation whereas commonly used methods seek to approximate the solution by iterative procedures (cf. Varga [10]). An extensive list of references is given in the excellent survey of direct methods by Fred W. Dorr [4]. The method of odd/even reduction and factorization described in this paper is similar to that of Buneman. In addition, a generalization of Hockney's direct method using Fourier analysis is given. Extensive numerical computations will be reported later.

2. Matrix decompositions

Consider the system of equations

$$\underline{M}\underline{x} = \underline{y} \quad (2.1)$$

where M is an $N \times N$ real symmetric matrix which has the block tridiagonal form

$$M = \begin{bmatrix} A & T & & & \\ & T & A & & \\ & & \ddots & \ddots & \\ 0 & & & T & A \\ & & & T & A \end{bmatrix} \quad (2.2)$$

The matrices A and T are $p \times p$ symmetric matrices, and we assume that

$$AT = TA.$$

Such a situation arises for those problems which can be handled by the classical separation of variables technique. Indeed, the methods discussed here amount to an efficient computer implementation of the idea of separation of variables carried out on a discretized model of the elliptic differential equation. Since A and T commute and are symmetric it is well known (cf. [1]) that there exists an orthogonal matrix Q such that

$$Q^T A Q = \Lambda, \quad Q^T T Q = \Omega \quad (2.3)$$

and Λ and Ω are real diagonal matrices. The matrix Q is the set of eigenvectors of A and T , and Λ and Ω are the diagonal matrices of eigenvalues of A and T , respectively.

In order to conform with the matrix M , we write the vector \underline{x} and \underline{y} in partitioned form

$$\tilde{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_q \end{bmatrix}, \quad \tilde{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_q \end{bmatrix}$$

Furthermore, it will be quite natural to write

$$\tilde{x}_j = \begin{bmatrix} x_{1j} \\ x_{2j} \\ \vdots \\ x_{pj} \end{bmatrix}, \quad \tilde{y}_j = \begin{bmatrix} y_{1j} \\ x_{2j} \\ \vdots \\ y_{pj} \end{bmatrix} \quad (2.4)$$

The system (2.2) may be written

$$A\tilde{x}_1 + T\tilde{x}_2 = \tilde{y}_1, \quad (2.5a)$$

$$T\tilde{x}_{j-1} + A\tilde{x}_j + T\tilde{x}_{j+1} = \tilde{y}_j, \quad j = 2, 3, \dots, q-1 \quad (2.5b)$$

$$T\tilde{x}_{q-1} + A\tilde{x}_q = \tilde{y}_q. \quad (2.5c)$$

Using (2.3), this becomes

$$\left. \begin{aligned} \Lambda\bar{x}_1 + \Omega\bar{x}_2 &= \bar{y}_1 \\ \Omega\bar{x}_{j-1} + \Lambda\bar{x}_j + \Omega\bar{x}_{j+1} &= \bar{y}_j, \quad (j = 2, 3, \dots, q-1) \\ \Omega\bar{x}_{q-1} + \Lambda\bar{x}_q &= \bar{y}_q \end{aligned} \right\} \quad (2.6)$$

where

$$\tilde{x}_j = Q^T x_j, \quad \tilde{y}_j = Q^T y_j, \quad j = 1, 2, \dots, q.$$

The components of \tilde{x}_j and \tilde{y}_j are labeled as in (2.4). Then equation (2.6) may be rewritten for $i = 1, 2, \dots, p$

$$\begin{aligned} \lambda_i \bar{x}_{i1} + \omega_i \bar{x}_{i2} &= \bar{y}_{i1}, \\ \omega_i \bar{x}_{ij-1} + \lambda_i \bar{x}_{ij} + \omega_i \bar{x}_{ij+1} &= \bar{y}_{ij} \quad (j = 2, \dots, q-1), \\ \omega_i \bar{x}_{iq-1} + \lambda_i \bar{x}_{iq} &= \bar{y}_{iq}. \end{aligned} \quad (2.7)$$

Now let us write

$$\Gamma_i = \begin{bmatrix} \lambda_i & \omega_i & & & \\ & \omega_i & \lambda_i & & \\ & & & \ddots & \\ 0 & & & & \omega_i & \lambda_i \\ & & & & & \omega_i & \lambda_i \end{bmatrix}_{q \times q}, \quad \hat{\tilde{x}}_i = \begin{bmatrix} \bar{x}_{i1} \\ \bar{x}_{i2} \\ \vdots \\ \bar{x}_{iq} \end{bmatrix}, \quad \hat{\tilde{y}}_i = \begin{bmatrix} \bar{y}_{i1} \\ \bar{y}_{i2} \\ \vdots \\ \bar{y}_{iq} \end{bmatrix}$$

so that (2.7) is equivalent to the system of equations

$$\boxed{\Gamma_i \hat{\tilde{x}}_i = \hat{\tilde{y}}_i} \quad (2.8)$$

Thus the vector $\hat{\tilde{x}}_i$ satisfies a symmetric tridiagonal system of equations which has a constant diagonal element and a constant super and sub-diagonal element. In [6], a fast and accurate algorithm is given for solving such a system of equations. After (2.8) has been solved, it is possible to solve for $\tilde{x}_j = Q \tilde{x}_j$.

Thus the algorithm proceeds as follows:

- 1) Compute or determine the eigenvectors of A and the eigenvalues of A and T .
- 2) Compute $\bar{y}_j = Q^T y_j$ ($j = 1, 2, \dots, q$).
- 3) Solve $\Gamma_i \hat{x}_i = \hat{y}_i$ ($i = 1, 2, \dots, p$).
- 4) Compute $\bar{x}_j = Q \bar{y}_j$ ($j = 1, 2, \dots, q$).

Hockney[6] has carefully analyzed this algorithm for solving Poisson's equation in a square. He has taken advantage of the fact that in this case the matrix Q is known and that one can take advantage of the fast Fourier transform (cf. [3]). Shintani [9] has given methods for solving for the eigenvalues and eigenvectors in a number of special cases.

It is not necessary that A and T commute. Assume that T is positive definite and symmetric. It is well known (cf. [1]) that there exists a matrix P such that

$$T = P P^T, \quad A = P \Delta P^T \quad (2.9)$$

where Δ is the diagonal matrix of eigenvalues of $T^{-1}A$ and P^{-T} is the matrix of eigenvectors of $T^{-1}A$. Thus using (2.9), we make the following modifications in the algorithm.

- 1) Compute or determine the eigenvalues and eigenvectors of $T^{-1}A$.
- 2) Compute $\bar{y}_j = P^{-1} y_j$.
- 3) Solve $\Gamma_i \hat{x}_i = \hat{y}_i$ where

$$\Gamma_i = \begin{bmatrix} \delta_i & 1 & & 0 \\ 1 & \delta_i & \cdot & \\ & \cdot & \cdot & 1 \\ \bigcirc & & \cdot & 1 & \delta_i \end{bmatrix}$$

4) Compute $\tilde{x}_j = P^{-T} \bar{x}_j$.

Of course, one should avoid computing $T^{-1}A$ since this would destroy the sparseness of the matrices. In [5] an algorithm has been proposed for solving $A\tilde{u} = \delta T\tilde{u}$ when A and T are sparse.

3. Block cyclic reduction

In the previous section, we gave a method for which it was necessary to know the eigenvalues and eigenvectors of some matrix. In this section, we shall give a more direct method for solving the system of equations (2.1).

We assume again that A and T are symmetric, and that A and T commute. Furthermore we assume that $q = m-1$ and

$$m = 2^{k+1}$$

where k is some positive integer. Let us rewrite (2.5b) as follows:

$$Tx_{j-2} + Ax_{j-1} + Tx_j = y_{j-1}$$

$$Tx_{j-1} + Ax_j + Tx_{j+1} = y_j$$

$$Tx_j + Ax_{j+1} + Tx_{j+2} = y_{j+1}.$$

Multiplying the first and third equation by T , the second equation by $-A$, and adding we have

$$T^2 x_{j-2} + (2T^2 - A^2) x_j + T^2 x_{j+2} = Ty_{j-1} - Ay_j + Ty_{j+1}.$$

Thus if j is even, the new system of equations involves x_j 's with even indices. Similar equations hold for x_2 and x_{M-2} . This process of-reducing the equations in this fashion is known as cyclic reduction.

Then the equations (2.1) may be written as the following equivalent system:

$$\begin{bmatrix}
(2T^2 - A^2) & T^2 & & & \\
T^2 & (2T^2 - A^2) & T^2 & & \\
& & & & 0 \\
& & & & T^2 \\
0 & & T^2 & (2T^2 - A^2) &
\end{bmatrix}
\begin{bmatrix}
\tilde{x}_2 \\
\tilde{x}_4 \\
\vdots \\
\tilde{x}_{m-2}
\end{bmatrix}
=
\begin{bmatrix}
T\tilde{y}_1 + T\tilde{y}_3 - A\tilde{y}_2 \\
T\tilde{y}_3 + T\tilde{y}_5 - A\tilde{y}_4 \\
\vdots \\
T\tilde{y}_{m-1} + T\tilde{y}_{m-3} - A\tilde{y}_{m-2}
\end{bmatrix}, \quad (3.1)$$

and

$$\begin{bmatrix}
A & 0 & & & \\
0 & A & & & \\
& & & & 0 \\
& & & & 0 \\
0 & & & & A
\end{bmatrix}
\begin{bmatrix}
\tilde{x}_1 \\
\tilde{x}_3 \\
\vdots \\
\tilde{x}_{m-1}
\end{bmatrix}
=
\begin{bmatrix}
\tilde{y}_1 - T\tilde{x}_2 \\
\tilde{y}_3 - T\tilde{x}_2 - T\tilde{x}_4 \\
\vdots \\
\tilde{y}_m - T\tilde{x}_{m-2}
\end{bmatrix}. \quad (3.2)$$

Since $m = 2^{k+1}$ and the new system of equations (3.1) involves \tilde{x}_j 's with even indices, the block dimension of the new system of equations is 2^k . Note once (3.1) is solved, it is a simple task to solve for the \tilde{x}_j 's with odd indices as evidenced by (3.2). We shall refer to the system of equations (3.2) as the eliminated equations.

Also, note that the algorithm of Section 2 may be applied to the system (3.1). Since A and T commute, the matrix $(2T^2 - A^2)$ has the same set of eigenvectors as A and T. Also if

$$\begin{aligned} h(A) &= \lambda_i, & h(T) &= \omega_i & \text{for } i = 1, 2, \dots, m-1 \\ \lambda(2T^2 - A^2) &= 2\omega_i^2 - \lambda_i^2. \end{aligned}$$

This procedure has been advocated by Hockney [6].

Since the system (3.1) is block tridiagonal and of the form (2.2), we can apply the reduction repeatedly until we have one block. However, as noted above we can stop the process after any step and use the methods of Section 2 to solve the resulting equations.

To define the procedure recursively, let

$$A^{(0)} = A, \quad T^{(0)} = T, \quad \underline{y}_j^{(0)} = \underline{y}_j, \quad (j = 1, 2, \dots, m-1).$$

Then for $r = 0, 1, \dots, k$,

$$\left. \begin{aligned} A^{(r+1)} &= 2(T^{(r)})^2 - (A^{(r)})^2 \\ T^{(r+1)} &= (T^{(r)})^2 \\ \underline{y}_j^{(r+1)} &= T^{(r)}(\underline{y}_{j-2}^{(r)} + \underline{y}_{j+2}^{(r)}) - A^{(r)} \underline{y}_j^{(r)}. \end{aligned} \right\} \quad (3.3)$$

At each stage, we have a new system of equations to solve:

$$M^{(r)} \underline{z}^{(r)} = \underline{f}^{(r)} \quad (3.4)$$

-where

$$M^{(r)} = \begin{bmatrix} A^{(r)} & T^{(r)} & & & \\ T^{(r)} & A^{(r)} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & T^{(r)} \\ & & & & & T^{(r)} & A^{(r)} \end{bmatrix}$$

$$\tilde{z}^{(r)} = \begin{bmatrix} \tilde{x}_{2^r} \\ \tilde{x}_{2^{r+1}} \\ \vdots \\ \tilde{x}_{j \cdot 2^r} \end{bmatrix}, \quad \tilde{f}^{(r)} = \begin{bmatrix} \tilde{y}_{2^r}^{(r)} \\ \tilde{y}_{2^{r+1}}^{(r)} \\ \vdots \\ \tilde{y}_{j \cdot 2^r}^{(r)} \end{bmatrix}$$

The eliminated equations are the solution of the block diagonal system

$$N^{(r)} \tilde{w}^{(r)} = \tilde{g}^{(r)} \quad (3.5)$$

where

$$N^{(r)} = \begin{bmatrix} A^{(r-1)} & 0 & & & \\ 0 & A^{(r-1)} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & 0 \\ & & & & & 0 & A^{(r-1)} \end{bmatrix},$$

$$\tilde{w}^{(r)} = \begin{bmatrix} \tilde{x}_{2^r-2^{r-1}} \\ \tilde{x}_{2^{r+1}-2^{r-1}} \\ \vdots \\ \tilde{x}_{j2^r-2^{r-1}} \\ \vdots \end{bmatrix}, \quad \tilde{g}^{(r)} = \begin{bmatrix} \tilde{y}_{2^r-2^{r-1}}^{(r-1)} - T \tilde{x}_{2^r}^{(r-1)} \\ \tilde{y}_{2^{r+1}-2^{r-1}}^{(r-1)} - T (\tilde{x}_{2^{r+1}}^{(r-1)} + \tilde{x}_{2^r}^{(r-1)}) \\ \vdots \\ \tilde{y}_{j2^r-2^{r-1}}^{(r-1)} - T (\tilde{x}_{j2^r}^{(r-1)} + \tilde{x}_{(j-1)2^r}^{(r-1)}) \\ \vdots \end{bmatrix}$$

Either we can use the methods of Section 2 to solve the system $M^{(r)} \tilde{z}^{(r)} = \tilde{f}^{(r)}$ or we can proceed to compute $M^{(r+1)}$ and eliminate half of the unknowns. After k steps, we must solve the system of equations

$$A^{(k)} \tilde{x}_{2^k} = \tilde{y}_{2^k}^{(k)}. \quad (3.6)$$

In either case, we must solve (3.5) to find the eliminated unknowns just as in (3.2). This can be accomplished by any of the following methods:

- a) direct solution,
- b) eigenvalue-eigenvector factorization,
- c) polynomial factorization.

The direct solution is especially convenient when k is small.

One can form the powers of A and T quite easily and solve the resulting equations by Gaussian elimination. Thus if $k = 1$ and A and T are tridiagonal matrices, $A^{(1)}$ is a five diagonal matrix and for such band matrices it is easy to solve the resulting system of equations.

It is possible to compute the eigenvalue - eigenvector decomposition of $A^{(r)}$ and $T^{(r)}$. Since $A^{(0)} = Q A Q^T$ and $T^{(0)} = Q \Omega Q^T$, we may write

$$A^{(r)} = Q \Lambda^{(r)} Q^T \quad \text{and} \quad T^{(r)} = Q \Omega^{(r)} Q^T.$$

From (3.3), it follows that

$$\begin{aligned} \Lambda^{(r+1)} &= 2(\Omega^{(r)})^2 - (\Lambda^{(r)})^2 \\ \Omega^{(r+1)} &= (\Omega^{(r)})^2. \end{aligned}$$

Thus the eigenvalues of $A^{(r)}$ and $T^{(r)}$ can be generated by the simple rule

$$\begin{aligned} \lambda_i^{(r+1)} &= 2(\omega_i^{(r)})^2 - (\lambda_i^{(r)})^2, \quad \lambda_i^{(0)} = \lambda_i, \\ \omega_i^{(r+1)} &= 2(\omega_i^{(r)})^2, \quad \omega_i^{(0)} = \omega_i, \quad i = 1, 2, \dots, m-1. \end{aligned}$$

Hence the methods of Section 2 can easily be applied to solving the system $M^{(r)} \underline{z}^{(r)} = \underline{f}^{(r)}$ and $N^{(r)} \underline{w}^{(r)} = \underline{g}^{(r)}$. Hockney [7] has described this algorithm as the FACR(l) algorithm where l refers to the number of cyclic reductions performed. He has shown that under some circumstances for solving Poisson's equation, it is best to choose $l = 2$.

From (3.1), we note that $A^{(1)}$ is a polynomial of degree 2 in A and T . By induction, it is easy to show that $A^{(r)}$ is a polynomial of degree 2^r in the matrices A and T so that

$$A^{(r)} = \sum_{j=0}^{2^r-1} c_{2^j}^{(r)} A^{2^j} T^{2^r-2^j} \equiv P_{2^r}(A, T).$$

We shall proceed to determine the linear factors of $P_{2^r}(A, T)$.

Let

$$p_{2^r}(a, t) = \sum_{j=0}^{2^r-1} c_{2^j}^{(r)} a^{2^j} t^{2^r-2^j}, \quad c_{2^r}^{(r)} = -1.$$

For $t \neq 0$, we make the substitution

$$a/t = -2 \cos \theta \quad (3.7)$$

From (3.3), we note that

$$p_{2^{r+1}}(a, t) = 2t^{2^{r+1}} - (p_{2^r}(a, t))^2 \quad (3.8)$$

It is easy to verify then, using (3.7) and (3.8), that

$$p_{2^r}(a, t) = -2t^{2^r} \cos 2^r \theta,$$

and consequently

$$p_{2^r}(a, t) = 0 \quad \text{when} \quad a/2t = -\cos \left(\frac{j-1}{2^{r+1}} \pi \right) \quad \text{for } j = 1, 2, \dots, 2^r.$$

Thus we may write

$$p_{2^r}(a, t) = - \prod_{j=1}^{2^r} (a + 2t \cos \frac{(j-1)\pi}{2^{r+1}}),$$

and hence

$$A^{(r)} = - \prod_{j=1}^{2^r} (A + 2 \cos \theta_j^{(r)}) T \quad (r > 0)$$

where $\theta_j^{(r)} = (2j-1)\pi/2^{r+1}$.

Let us write

$$G_j^{(k)} = A + 2 \cos \theta_j^{(k)} T.$$

Then in order to solve (3.6), we set $z_1 = z_2^{(k)}$ and solve repeatedly

$$G_j^{(k)} z_{j+1} = z_j \quad \text{for } j = 1, 2, \dots, 2^k. \quad (3.9)$$

Thus

$$\boxed{z_{2^k+1} = z_{2^k}}.$$

If A and T are of band structure it is simple to solve (3.9) although under some circumstances the equations may be "ill-conditioned". In order to determine the solution to the eliminated equations (3.5) a similar algorithm may be used with

$$A^{(r)} = - \prod_{j=1}^{2^r} G_j^{(1)} . \quad (3.10)$$

The factorization for $A^{(r)}$ may also be used to compute $y_j^{(r+1)}$ in (3.3). It is possible, however, to take advantage of the recursive nature of the polynomials $p_{2^r}(a, t)$. Let

$$p_s(a, t) = -2t^s \cos s\theta$$

where again for $t \neq 0$, $a/t = -2 \cos \theta$.

Then a short manipulation shows

$$p_s(a, t) = -ap_{s-1}(a, t) - t^2 p_{s-2}(a, t) , \quad s \geq 2 ,$$

$$p_0(a, t) = -2 , \quad p_1(a, t) = a .$$

Therefore to compute $A^{(r)} y_j^{(r)}$ as in (3.3), we compute the following sequence:

$$\begin{aligned} \eta_0 &= -2 \binom{r}{j} , & \eta_1 &= A y_j^{(r)} \\ \eta_s &= -A \eta_{s-1} - T^2 \eta_{s-2} & \text{for } s &= 2, 3, \dots, 2^r . \end{aligned}$$

Thus

$$\eta_{2^r} = p_{2^r}(A, T) y_j^{(r)} \equiv A^{(r)} y_j^{(r)} .$$

The factorization (3.10) must be used with care. Numerical experiments have indicated for $r \geq 5$, the roundoff error may become a significant problem. Buneman [2], however, has reorganized the calculation in a stable fashion; see [7] for details. We denote this method as the Cyclic Odd/Even Reduction and Factorization (CORF) algorithm.

4. Poisson's equation with Dirichlet boundary conditions

It is instructive to apply the results of Section 3 to the solution of the finite difference approximation to Poisson's equation on a rectangle R with specified boundary values. Consider the equation

$$\begin{aligned} u_{xx} + u_{yy} &= f(x,y) \quad \text{for } (x,y) \in R, \\ u(x,y) &= g(x,y) \quad \text{for } (x,y) \in \partial R. \end{aligned} \quad (4.1)$$

(Here ∂R indicates the boundary of R .) It is assumed that the reader has some familiarity with the general technique of imposing a mesh of discrete points onto R and approximating (4.1). The equation $u_{xx} + u_{yy} = f(x,y)$ is approximated at (x_i, y_j) by

$$\frac{v_{i-1,j} - 2v_{i,j} + v_{i+1,j}}{(\Delta x)^2} + \frac{v_{i,j-1} - 2v_{i,j} + v_{i,j+1}}{(\Delta y)^2} = f_{i,j}$$

$$(1 \leq i \leq n-1, \quad 1 \leq j \leq m-1),$$

with

$$v_{0,j} = g_{0,j}, \quad v_{m,j} = g_{m,j} \quad (1 \leq j \leq m-1)$$

and

$$v_{i,0} = g_{i,0}, \quad v_{i,m} = g_{i,m} \quad (1 \leq i \leq n-1).$$

Then v_{ij} is an approximation to $u(x_i, y_j)$ and $f_{i,j} = f(x_i, y_j)$, $g_{i,j} = g(x_i, y_j)$. From here-on-in we assume $m = 2^{k+1}$.

When $u(x,y)$ is specified on the boundary, we have the Dirichlet boundary condition. For simplicity, we shall assume hereafter that $\Delta x = \Delta y$. This leads to the system of equations

$$M_D \underline{v} = \underline{y}$$

where M_D is of the form (2.1) with

$$A = \begin{bmatrix} -4 & 1 & & 0 \\ 1 & -4 & 1 & \\ & \cdot & \cdot & \cdot \\ 0 & & \cdot & \cdot & 1 \\ & & & 1 & -4 \end{bmatrix}_{(n-1) \times (n-1)}, \text{ and } T = I_{n-1}.$$

The matrix I_{n-1} indicates the identity matrix of order $(n-1)$. A and T are symmetric and commute, and thus the results of Section 3 are applicable. In addition, since A is tridiagonal the solution of the resulting system of equations is greatly simplified (cf. [6]). In fact any tridiagonal matrix of the form (2.2) where A and T are scalars may be solved by either cyclic reduction or CORF. If the factorization is not used then $p_{2^r}(a, t)$ is computed recursively by (3.8).

In the next section, we shall generalize the CORF algorithm to situations where the matrix is not of the form (2.2).

5. Neumann boundary conditions

When the normal derivative, $\frac{\partial u}{\partial n}$, is specified on the boundary, we have the Neumann boundary condition. Assume

$$\frac{\partial u}{\partial n} = g(x,y) \quad \text{w h e n } (x,y) \in \partial R \quad .$$

We make the approximation

$$\frac{\partial u}{\partial x} \doteq \frac{u(x+\Delta x, y) - u(x-\Delta x, y)}{2\Delta x} \quad , \quad \frac{\partial u}{\partial y} \doteq \frac{u(x, y+\Delta y) - u(x, y-\Delta y)}{2\Delta y} \quad .$$

This approximation leads to the matrix equation

$$M_N \underline{v} = \underline{z}$$

where M_N is of the form

$$M_N = \begin{bmatrix} A & 2T & & & \\ T & A & T & & \\ & \cdot & \cdot & \cdot & \\ 0 & & & T & \cdot & T \\ & & & & 2T & A \end{bmatrix} \quad (5.1)$$

Here

$$A = \begin{bmatrix} -4 & 2 & & & \\ 1 & -4 & 1 & & \\ & \cdot & \cdot & \cdot & \\ 0 & & & 1 & -4 & 1 \\ & & & & 2 & -4 \end{bmatrix} \quad , \quad T = I_{n+1} \quad .$$

(n+1) x (n+1)

Again A and T commute but M_N no longer has the structure given by (2.2). Therefore it is necessary to modify the algorithm of Section 3.

From (5.1), we see that

$$\begin{aligned} A\tilde{v}_0 + 2T\tilde{v}_1 &= \tilde{y}_0 \\ T\tilde{v}_{j-1} + A\tilde{v}_j + T\tilde{v}_{j+1} &= \tilde{y}_j, \quad j = 1, 2, \dots, m-1, \\ 2T\tilde{v}_{m-1} + A\tilde{v}_m &= \tilde{y}_m. \end{aligned}$$

performing the cyclic reduction as in Section 3, we have

$$\left. \begin{aligned} (2T^2 - A^2)\tilde{v}_0 + 2T\tilde{v}_2 &= -A\tilde{y}_0 + 2T\tilde{y}_1 \\ T^2\tilde{v}_{j-2} + (2T^2 - A^2)\tilde{v}_j + T^2\tilde{v}_{j+2} &= T(\tilde{y}_{j-1} + \tilde{y}_{j+1}) - A\tilde{y}_j \\ j &= 2, 4, \dots, m-2, \\ 2T\tilde{v}_{m-2} + (2T^2 - A^2)\tilde{v}_m &= 2T\tilde{y}_{m-1} - A\tilde{y}_m. \end{aligned} \right\} \quad (5.2)$$

The similarity of (5.2) with (3.1) should now be evident. Since (5.2) is of block dimension $2^k + 1$, we have after k steps the system

$$\begin{bmatrix} A^{(k)} & 2T^{(k)} & 0 \\ T^{(k)} & A^{(k)} & T^{(k)} \\ 0 & 2T^{(k)} & A^{(k)} \end{bmatrix} \begin{bmatrix} \tilde{v}_0 \\ \tilde{v}_{2^k} \\ \tilde{v}_{2^{k+1}} \end{bmatrix} = \begin{bmatrix} \tilde{y}_0^{(k)} \\ \tilde{y}_{2^k}^{(k)} \\ \tilde{y}_{2^{k+1}}^{(k)} \end{bmatrix}; \quad (5.3)$$

and a final reduction yields

$$[4(T^{(k)})^2 - (A^{(k)})^2]\tilde{y}_{2^k}^{(k)} = T(\tilde{y}_0^{(k)} + \tilde{y}_{2^{k+1}}^{(k)}) - A\tilde{y}_{2^k}^{(k)} \quad (5.4)$$

Equation (5.4) is equivalent to writing

$$P_{2^{k+1}}^{(N)}(A, T) \underline{v}_{2^k} = \underline{y}_{2^k}^{(k+1)} \quad (5.5)$$

where $P_{2^{k+1}}^{(N)}(A, T)$ is again a polynomial of degree 2^{k+1} in A and T .
Note from (3.8)

$$P_{2^{r+1}}^{(N)}(a, t) = 2t^{2^{r+1}} - (P_{2^r}^{(N)}(a, t))^2, \quad r = 0, 1, \dots, k-1,$$

and from (5.4)

$$P_{2^{k+1}}^{(N)}(a, t) = 4t^{2^{k+1}} - (P_{2^k}^{(N)}(a, t))^2$$

Therefore since $P_{2^k}^{(N)}(a, t) = -2t^{2^k} \cos 2^k \theta$,

$$P_{2^{k+1}}^{(N)}(a, t) = [2t^{2^k} \sin 2^k \theta]^2$$

and thus

$$P_{2^{k+1}}^{(N)}(a, t) = 0 \quad \text{when} \quad a/2t = -\cos \frac{j\pi}{2^k} \quad \text{for } j = 1, 2, \dots, 2^{k+1}.$$

Consequently, we may rewrite (5.5) as

$$\prod_{j=1}^{2^{k+1}} [A + 2 \cos \theta_j^{(k+1)} T] \underline{v}_{2^k} = \underline{y}_{2^k}^{(k+1)} \quad (5.6)$$

where $\theta_j^{(k+1)} = j\pi/2^k$. Again \underline{v}_{2^k} is determined by solving 2^{k+1} tridiagonal systems. The other components of \underline{v} are solved for in the same manner as indicated in Section 3.

It is well known that the solution to Poisson's equation is not unique in this case. Therefore we would expect the finite difference approximation

to be singular. This is easy to verify by noting

$$M_N \underline{e} = 0$$

where $\underline{e}^T = (1, 1, \dots, 1)$. In addition, one of the systems of the tridiagonal matrices in (5.6) is also singular. It is easy to verify that the eigenvalues of $(A + 2 \cos \theta_j T)$ satisfy the equation

$$h(A + 2 \cos \theta_j T) = 4 - 2 \cos \left(\frac{l\pi}{n} \right) + 2 \cos \left(\frac{j\pi}{2^k} \right)$$

$$(l = 0, 1, 2, \dots, n; j = 1, 2, \dots, 2^{k+1}) .$$

Then $\lambda_0 = 0$ when $j = 2^k$. Normally the physics of the problem determines the coefficient of the homogeneous solution for the singular case.

6. Periodic boundary conditions

In this section, we shall consider the problem of solving the finite difference approximation to Poisson's equation over a rectangle when

$$u(x_0, y) = u(x_n, y) \quad (6.1)$$

$$u(x, y_0) = u(x, y_n)$$

The periodic boundary conditions (6.1) leads to the matrix equation

$$M_P \underline{y} = \underline{y} \quad (6.2)$$

where

$$M_P = \begin{bmatrix} A & T & 0 & \cdot & \cdot & 0 & T \\ T & A & T & & & & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & 0 & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & T & A & T \\ T & 0 & \cdot & \cdot & \cdot & 0 & T & A \end{bmatrix}$$

and

$$A = \begin{bmatrix} -4 & 1 & 0 & \cdot & \cdot & 0 & 1 \\ 1 & -4 & 1 & 0 & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & 1 & -4 & 1 \\ 1 & 0 & \cdot & \cdot & \cdot & 0 & 1 & -4 \end{bmatrix} \quad , \quad T = I_n$$

nxn

Note M_P is "almost" an m block tridiagonal system and similarly A is "almost" an $n \times n$ tridiagonal matrix. The cyclic reduction can again be performed on (6.2) and this leads to the reduced system

$$\begin{aligned}
 (2T^2 - A^2)\tilde{v}_2 + T^2\tilde{v}_4 + T^2\tilde{v}_m &= T(y_1 + y_3) - Ay_2 \\
 T^2\tilde{v}_{j-2} + (2T^2 - A^2)\tilde{v}_j + T^2\tilde{v}_{j+2} &= T(y_{j-1} + y_{j+1}) - Ay_j, \\
 j &= 2, 4, \dots, m-2, \\
 T^2\tilde{v}_2 + T^2\tilde{v}_{m-2} + (2T^2 - A^2)\tilde{v}_m &= T(y_1 + y_{m-1}) - Ay_m.
 \end{aligned} \tag{6.3}$$

The similarity with the previous cases is again evident. Equation (6.3) has block dimension 2^k . After $(k-1)$ reductions we have

$$M_P^{(k-1)} = \begin{bmatrix} A^{(k-1)} & T^{(k-1)} & 0 & T^{(k-1)} \\ T^{(k-1)} & A^{(k-1)} & T^{(k-1)} & 0 \\ 0 & T^{(k-1)} & A^{(k-1)} & T^{(k-1)} \\ T^{(k-1)} & 0 & T^{(k-1)} & A^{(k-1)} \end{bmatrix},$$

and finally after k reductions

$$\begin{bmatrix} A^{(k)} & 2T^{(k)} \\ 2T^{(k)} & A^{(k)} \end{bmatrix} \begin{bmatrix} \tilde{v}_{2^k} \\ \tilde{v}_{2^{k+1}} \end{bmatrix} = \begin{bmatrix} y_{2^k}^{(k)} \\ y_{2^{k+1}}^{(k)} \end{bmatrix}. \tag{6.4}$$

From (6.4) the final equation becomes

$$[(4T^{(k)})^2 - (A^{(k)})^2]\tilde{v}_{2^k} = y_{2^k}^{(k+1)}$$

which is equivalent to

$$P_{2^{k+1}}^{(P)}(A,T) \tilde{v}_{2^k} = \tilde{y}_{2^k}^{(k+1)}$$

The analysis of the factorization of $P_{2^{k+1}}^{(P)}(A,T)$ is identical to that of the Neumann case including the fact that one of the factors of the polynomial must be singular.

7. Higher dimensional problems

It is not difficult to extend the applications given in Sections 4, 5 and 6 to higher dimensional problems. We show this by a simple example. Consider Poisson's equation in 3 dimensions over the rectangle R :

$$u_{xx} + u_{yy} + u_{zz} = f(x,y,z) \quad (x,y,z) \in R \quad .$$

$$u(x,y,z) = g(x,y,z) \quad (x,y,z) \in \partial R \quad .$$

Again we assume the mesh is uniform in each direction so that

$$x_{i+1} = x_i + \Delta x \quad (i = 0, 1, \dots, n) \quad ,$$

$$y_{j+1} = y_j + \Delta y \quad (j = 0, 1, \dots, m) \quad ,$$

$$z_{l+1} = z_l + \Delta z \quad (l = 0, 1, \dots, p) \quad .$$

At the point (x_i, y_j, z_l) we approximate $u(x_i, y_j, z_l)$ by $v_{i,j,l}$. Let

$$\tilde{w}_l = \begin{pmatrix} v_{1,l} \\ v_{2,l} \\ \vdots \\ v_{m-1,l} \end{pmatrix} \quad \text{where} \quad \tilde{v}_{j,l} = \begin{pmatrix} v_{1,j,l} \\ v_{2,j,l} \\ \vdots \\ v_{n-1,j,l} \end{pmatrix}$$

Assume that the usual finite difference approximation is made to u_{zz} for fixed (x,y,z) , viz.

$$u_{zz}(x,y,z) \doteq \frac{u(x,y,z-\Delta z) - 2u(x,y,z) + u(x,y,z+\Delta z)}{(\Delta z)^2}$$

It is easy to verify then that for $l = 1, 2, \dots, p-1$,

$$\tilde{w}_{l-1} + H\tilde{w}_l + \tilde{w}_{l+1} = \underline{f}_l$$

where \tilde{w}_0 and \tilde{w}_p are prescribed by the initial conditions and \underline{f}_l is a function of the given data. Thus again we have a block tridiagonal matrix, and we are able to use the previous developed methods. Note, also, that H is a block tridiagonal matrix so that it is possible to solve any of the eliminated systems of equations by applying the CORF algorithm repeatedly. Other boundary conditions can be handled in the same manner as prescribed in Sections 5 and 6.

8. Further applications

Consider the elliptic equation in self adjoint form

$$\begin{aligned} (\alpha(x)u_x)_x + (\beta(y)u_y)_y + u(x,y) &= q(x,y), \quad (x,y) \in R \\ u(x,y) &= g(x,y), \quad (x,y) \in \partial R \end{aligned} \quad (8.1)$$

Many equations can be transformed to this form. The usual five point difference equation when $\Delta x = \Delta y$ leads to the following equation:

$$\begin{aligned} -\alpha_{i+\frac{1}{2}} v_{i+1,j} - \alpha_{i-\frac{1}{2}} v_{i-1,j} - \beta_{j+\frac{1}{2}} v_{i,j+1} - \beta_{j-\frac{1}{2}} v_{i,j-1} \\ + (\alpha_{i+\frac{1}{2}} + \alpha_{i-\frac{1}{2}} + \beta_{j+\frac{1}{2}} + \beta_{j-\frac{1}{2}} - (\Delta x)^2) v_{i,j} = -(\Delta x)^2 q_{i,j} \end{aligned} \quad (8.2)$$

where

$$\alpha_{i \pm \frac{1}{2}} = \alpha(x_i \pm \frac{1}{2} \Delta x), \quad \beta_{j \pm \frac{1}{2}} = \beta(y_j \pm \frac{1}{2} \Delta y)$$

$$q_{i,j} = q(x_i, y_j)$$

If the equations are ordered with

$$\tilde{v} = \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_2 \\ \vdots \\ \tilde{v}_{m-1} \end{pmatrix}, \quad \tilde{v}_j = \begin{pmatrix} v_{1,j} \\ v_{2,j} \\ \vdots \\ v_{n-1,j} \end{pmatrix}$$

then the linear system of equations $M\tilde{v} = \tilde{d}$ will have the block form

$$\begin{bmatrix} A_1 & T_1 & & 0 \\ T_1 & A_2 & T_2 & \\ & & \ddots & \\ 0 & & & T_{m-2} & A_{m-1} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_{m-1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_{m-1} \end{bmatrix}$$

Here

$$A_j = [\beta_{j+\frac{1}{2}} + \beta_j \frac{1}{2} - (\Delta x)^2] I + \begin{bmatrix} \alpha_{1/2+\alpha_{3/2}} & -\alpha_{3/2} & & 0 \\ -\alpha_{3/2} & \alpha_{3/2+\alpha_{5/2}} & -\alpha_{5/2} & \\ & \ddots & \ddots & \ddots \\ 0 & & & -a_{n-\frac{3}{2}} & \alpha_{n-\frac{3}{2}+\alpha_{n-\frac{1}{2}}} \end{bmatrix}$$

$$\equiv \gamma_j I + C,$$

$$T_j = \beta_{j+\frac{1}{2}} I.$$

Now suppose we have the decomposition

$$Q^T C Q = \Phi$$

where $Q^T Q = I$ and $\text{diag}(\Phi) = (\varphi_1, \varphi_2, \dots, \varphi_{n-1})$. Thus

$$\lambda_i(A_j) = \gamma_j + \varphi_i, \quad (i = 1, 2, \dots, n-1),$$

$$\equiv \lambda_{i,j}.$$

As in Section 2, we define

$$\bar{v}_j = Q^T v_j, \quad \bar{d}_j = Q^T d_j$$

and after a suitable permutation we are led to the equations

$$\Gamma_i \hat{\bar{v}}_i = \hat{\bar{d}}_i \quad i = 1, 2, \dots, n-1,$$

where

$$\Gamma_i = \begin{bmatrix} \lambda_{i,1} & \beta_{3/2} & & & & \\ \beta_{3/2} & \lambda_{i,2} & \beta_{5/2} & & & \\ & & \cdot & \cdot & & \\ & & & \cdot & \cdot & \\ & & & & \cdot & \cdot \\ & & & & & \beta_{m-\frac{3}{2}} \\ & & & & & \beta_{m-\frac{3}{2}} & \lambda_{i,m-1} \end{bmatrix},$$

$$\hat{\bar{v}}_i = \begin{bmatrix} \bar{v}_{i1} \\ \bar{v}_{i2} \\ \vdots \\ \bar{v}_{i,m-1} \end{bmatrix}, \quad \hat{\bar{d}}_i = \begin{bmatrix} \bar{d}_{i1} \\ \bar{d}_{i2} \\ \vdots \\ \bar{d}_{i,m-1} \end{bmatrix}.$$

Thus the vector $\hat{\bar{v}}_i$ satisfies a symmetric tridiagonal system of equations. Again, once $\hat{\bar{v}}_i$ is computed for all i , it is possible to compute \bar{v} .

lynch et al[8] has considered a similar method but their algorithm requires more operations. Unfortunately, it does not seem possible to use the methods of Section 3 on (8.2) in this situation.

Now we may write the equivalent to Poisson's equation in two dimensions in cylindrical coordinates as follows:

$$(r u_r)_r + r^{-1} u_{\theta\theta} = s(r, \theta)$$

and

$$(r u_r)_r + r u_{zz} = t(r, z) .$$

The matrix A will still be tridiagonal and T will be a diagonal matrix with positive diagonal elements. We may make the transformation

$$\tilde{v}_j = T^{-8} v_j \quad \text{and are thus led to the equations}$$

$$\tilde{v}_{j-1} + T^{-8} A T^{-\frac{1}{2}} \tilde{v}_j + \tilde{v}_{j+1} = T^{-\frac{1}{2}} d_j .$$

Thus by ordering the equations correctly and by making a simple transformation it is possible to apply the cyclic reduction and the CORF algorithm to solve the finite difference approximation to Poisson's equation in cylindrical coordinates.

Another situation in which the methods of Sections 2 and 3 are applicable is when the nine point formula is used for solving the finite difference approximation to Poisson's equation in the rectangle. In this case when $\Delta x = \Delta y$,

$$A = \begin{bmatrix} & & & & \\ & -4 & -20 & & 0 \\ & 0 & & & \\ & & & & 4 \\ 4 & -20 & & & \end{bmatrix}_{(n-1) \times (n-1)} \quad T = \begin{bmatrix} 4 & 1 & & & 0 \\ 1 & 4 & & & \\ & & & & \\ 0 & & & & 1 \\ & & 1 & 4 & \end{bmatrix}_{(n-1) \times (n-1)}$$

It is easy to verify that $AT = TA$, and that the eigenvalues of A and T are

$$\lambda_i(A) = -20 + 8 \cos \frac{i\pi}{n} \quad (i = 1, 2, \dots, n-1)$$

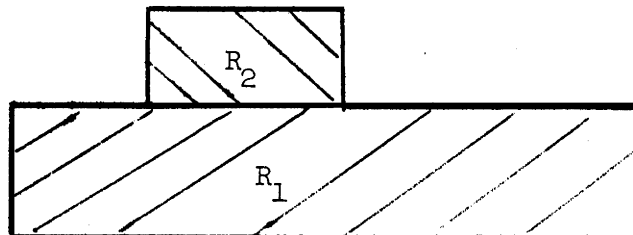
$$\lambda_i(T) = 4 + 2 \cos \frac{i\pi}{n} \quad (i = 1, 2, \dots, n-1)$$

Because of the structure of A and T the fast Fourier transform may be employed when using the methods of Section 2.

We leave as an exercise to the reader the application of the methods in Sections 2 and 3 to the biharmonic equation.

9. Non-rectangular regions

In many situations, one wishes to solve an elliptic equation over the region



We shall assume Dirichlet boundary conditions are given. When Δx is the same throughout the region, this leads to a matrix equation of the form

$$\begin{bmatrix} G & 0 \\ P^T & H \end{bmatrix} \begin{bmatrix} \tilde{x}^{(1)} \\ \tilde{x}^{(2)} \end{bmatrix} = \begin{bmatrix} \tilde{y}^{(1)} \\ \tilde{y}^{(2)} \end{bmatrix} \quad (9.1)$$

where

$$G = \begin{bmatrix} A & T & & 0 \\ T & A & & \\ & & \ddots & \\ 0 & & & T & A \end{bmatrix} \quad H = \begin{bmatrix} B & S & & 0 \\ S & B & & \\ & & \ddots & \\ 0 & & & S & B \end{bmatrix} \quad (9.2)$$

Also, we write

$$\tilde{x}^{(1)} = \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ \vdots \\ x_r^{(1)} \end{bmatrix} \quad \tilde{x}^{(2)} = \begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \\ \vdots \\ x_s^{(2)} \end{bmatrix} \quad (9.3)$$

We assume again that $AT = TA$ and $BS = SB$.

From (9.1), we see that

$$\tilde{x}^{(1)} = G^{-1} \tilde{y}^{(1)} - G^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ P \end{bmatrix} \tilde{x}_1^{(2)} \quad (9.4)$$

$$\tilde{x}^{(2)} = H^{-1} \tilde{y}^{(2)} - H^{-1} \begin{bmatrix} P^T \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tilde{x}_r^{(1)} \quad (9.5)$$

Now let us write

$$\tilde{G}\tilde{z}^{(1)} = \tilde{y}^{(1)} \quad , \quad \tilde{H}\tilde{z}^{(2)} = \tilde{y}^{(2)} \quad (9.6)$$

$$\tilde{G}\tilde{w}^{(1)} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ P \end{bmatrix} \quad , \quad \tilde{H}\tilde{w}^{(2)} = \begin{bmatrix} P^T \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (9.7)$$

Then partitioning the vectors $\tilde{z}^{(1)}$, $\tilde{z}^{(2)}$ and the matrices $W^{(1)}$ and $W^{(2)}$ as in (9.3), the equation (9.4) and (9.5) becomes

$$\left. \begin{aligned} \tilde{x}_j^{(1)} &= \tilde{z}_j^{(1)} - W_j^{(1)} \tilde{x}_1^{(2)} & (j = 1, 2, \dots, r) \\ \tilde{x}_j^{(2)} &= \tilde{z}_j^{(2)} - W_j^{(2)} \tilde{x}_r^{(1)} & (j = 1, 2, \dots, s) \end{aligned} \right\} \quad (9.8)$$

From (9.8), we have

$$\begin{bmatrix} I & W_r^{(1)} \\ W_1^{(2)} & I \end{bmatrix} \begin{bmatrix} \tilde{x}_r^{(1)} \\ \tilde{x}_1^{(2)} \end{bmatrix} = \begin{bmatrix} \tilde{z}_r^{(1)} \\ \tilde{z}_1^{(2)} \end{bmatrix}.$$

This system of equations is 2-cyclic and thus we may reduce the system to

$$(I - W_r^{(1)} W_1^{(2)}) \tilde{x}_r^{(1)} = \tilde{z}_r^{(1)} - W_r^{(1)} \tilde{z}_1^{(2)}. \quad (9.9)$$

This system of equations can most easily be solved using Gaussian elimination.

Once the 'L-cyclic system of equations (9.9) has been solved, all other

components may be computed using (9.8) or by solving the system

$$\begin{aligned} \tilde{Gx}^{(1)} &= \tilde{y}^{(1)} - \begin{bmatrix} 0 \\ 0 \\ \vdots \\ P \end{bmatrix} \tilde{x}_1^{(2)} \\ \tilde{Hx}^{(2)} &= \tilde{y}^{(2)} - \begin{bmatrix} P^T \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tilde{x}_r^{(1)} \end{aligned}$$

If the system (9.1) is to be solved for a number of different right hand sides, then it is best to save the LU decomposition of

$$(I - W_r^{(1)} W_1^{(2)}), \quad (9.10)$$

Thus the algorithm proceeds as follows:

- 1) Solve for $\tilde{z}_r^{(1)}$ and $\tilde{z}_1^{(2)}$ using the methods of Section 2 or Section 3.
- 2) Solve for $W_r^{(1)}$ and $W_1^{(2)}$ using the methods of Section 2 or Section 3.
- 3) Solve (9.9) using Gaussian elimination. Save the LU decomposition of (9.10).
- 4) Solve for the unknown components of $\tilde{x}^{(1)}$ and $\tilde{x}^{(2)}$.

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