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I am submitting herewith a dissertation written by William Joseph Harrod entitled "Rank Modification Method for Certain Singular Systems of Linear Equations." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.

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RANK MODIFICATION METHOD
FOR CERTAIN SINGULAR SYSTEMS
OF LINEAR EQUATIONS

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ABSTRACT

This dissertation is mainly concerned with a general purpose algorithm for computing a solution to the consistent system of linear equations

$$Aw = f$$

where A is a real matrix of order n , with rank $n - 1$, and f is a real n -dimensional vector. The algorithm, called the Rank Modification Method, is based upon the transformation of A into a nonsingular matrix by a rank one modification, followed by the solution of an associated nonsingular system of linear equations. When the Rank Modification Method is applied to the consistent system of linear equations $Aw = f$, it results in a solution w such that $v^T w = \tau$, where v is an n -dimensional vector and τ is a real number. The vector v is any vector such that $y^T v \neq 0$, where y is a right null vector of A . The value of τ may be specified arbitrarily. Therefore the proposed method can be used to compute a solution to the constrained system of linear equations $Aw = f$ such that $v^T w = \tau$, if a solution exists.

The primary application of this research is the computation of a solution w to the homogeneous system of linear equations $Aw = 0$, where A is a singular irreducible M-matrix. This vector w is unique up to scalar multiples and it is important in many areas of the mathematical sciences, including queueing networks, input-output economic models, and in compartmental analysis tracer models.

The Rank Modification Method is developed and a complete error analysis is also given. Also developed is a special algorithm, called

the Partition Factorization Method, which involves a simple direct LU-decomposition of an $n - 1$ dimensional submatrix of A . It is shown that the Partition Factorization Method can be considered a variation of the Rank Modification Method. A simple updating method is developed for the Partition Factorization Method. Also investigated are tridiagonal irreducible M -matrices.

These methods are applied to the problem of computing the stationary distribution vector p of an ergodic finite Markov chain C with associated rate transition matrix Q . Computational results for several test problems are reported, they show that the Partition Factorization Method should be considered the preferred direct method for computing p .

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CHAPTER I

INTRODUCTION

This dissertation is concerned with a method for computing a solution to the consistent system of linear equations

$$Aw = f \tag{1.1}$$

where A is a real matrix of order n , with rank $n - 1$, and f is a real n -dimensional vector.

The computation of a vector w satisfying (1.1) is important in many areas of the mathematical sciences, including queueing networks (e.g., Kaufman [1982]), input-output economic models (e.g., Berman and Plemmons [1979], Chapter 9), compartmental analysis tracer models (e.g., Funderlic and Mankin [1981]), and in the discrete Neumann problem (e.g., Plemmons [1976a]).

The proposed method is based upon the transformation of A into a nonsingular matrix by a rank one modification followed by the solution of an associated nonsingular system of linear equations. This method is an extension of methods proposed in two recent papers.

In a paper by Hunter [1982], a method was proposed for computing the stationary distribution vector w of an ergodic finite Markov chain with rate transition matrix Q . Here Q is an irreducible nonnegative matrix. The vector w is a probability vector that satisfies the following equation

$$(I - Q^T)w = 0$$

where "T" denotes the transpose. This method is based upon the transformation of $I - Q^T$ into a nonsingular matrix. In a paper by Kemeny [1981], a similar method was proposed for solving the nonhomogeneous system of linear equations $Aw = f$, where A is a matrix of order n , with rank $n - 1$. This method requires the use of the right null vector associated with the zero eigenvalue of A . The method that is proposed in this dissertation does not explicitly use this right null vector.

It should be noted that in most applications of the stated problem, one usually requires a solution with minimal norm. When the proposed method is applied to the consistent system of linear equations $Aw = f$, it results in a solution w such that $v^T w = \tau$, where v is an n -dimensional vector and τ is a real number. The vector v is any vector such that $y^T v \neq 0$, where y is a right null vector of A . The value of τ may be specified arbitrarily. Therefore the proposed method will compute a solution to the constrained system of linear equations $Aw = f$ such that $v^T w = \tau$, if it exists.

The primary concern of this dissertation is the computation of the solution to the homogeneous system of linear equations $Aw = 0$, where A is a singular irreducible M-matrix.

Definition 1.1. A real matrix $A = (a_{ij})$ of order n , with $a_{ij} \leq 0$ for all $i \neq j$, and whose eigenvalues all have nonnegative real parts, is called an M-matrix.

M-matrices can be characterized in a large variety of ways (see Berman and Plemmons, Chapter 6). It is well known that if A is a singular irreducible M-matrix, then A has rank $n - 1$.

The proposed method can involve the theory of generalized inverses.

Definition 1.2. A (1)-inverse of the matrix A is any matrix A^- such that

$$AA^-A = A.$$

It is well known that any real matrix has a (1)-inverse. (e.g., Ben-Israel and Greville [1974], p. 10). The (1)-inverse of a matrix is not unique unless the matrix is nonsingular. The set of all (1)-inverses of the matrix A will be denoted by $A\{1\}$.

Definition 1.3. Let A be a matrix of order n . Then the group inverse of A , if it exists, is defined to be the unique matrix $A^\#$ such that

$$\begin{aligned} (1) \quad AA^\#A &= A, \\ (2) \quad A^\#AA^\# &= A^\#, \\ (3) \quad AA^\# &= A^\#A. \end{aligned}$$

Clearly, the group inverse of a matrix $A^\#$, is a (1)-inverse for A .

Definition 1.4. Let A be a matrix of order n . The smallest non-negative integer k such that the rank of A^k is equal to the rank of A^{k+1} , is called the index of A and is denoted by $\text{Ind}(A)$.

The following theorem provides a necessary and sufficient condition for the existence of the group inverse of a matrix.

Theorem 1.1. (e.g., Campbell and Meyer [1979], p. 124). Let A be a matrix of order n . Then the group inverse of A exists if and only if $\text{Ind}(A) \leq 1$.

If A is a singular irreducible M -matrix, then the group inverse of A exists (see Plemmons [1976b]).

Definition 1.5. Let A be a matrix of order n . The LU-decomposition of A is the factorization of A into triangular factors such that $A = LU$, where L is a lower triangular matrix with unit diagonal and U is an upper triangular matrix.

In general, the LU-decomposition of a matrix may not exist, but for any matrix A there exists a permutation matrix P such that PA has an LU-decomposition. It is well known that if A is a nonsingular M -matrix, then A has an LU-decomposition (see Fiedler and Pták [1962]). Singular M -matrices in general do not possess LU-decompositions. Recently Funderlic and Plemmons [1981] established the following condition for an M -matrix to possess an LU-decomposition.

Theorem 1.2. Let A be an M -matrix of order n . If there exists a vector x with all positive entries such that $x^T A \geq 0$, then A has an LU-decomposition where L and U are M -matrices.

In a recent paper by Varga and Cai [1981] the converse was proved.

The proposed method will be developed in Chapter II and a complete error analysis will be given, including a backward error analysis. In Chapter III the problem of computing a right null vector of a

singular irreducible M-matrix will be investigated. Chapter IV contains an application of the proposed method to computing the stationary distribution vector of an ergodic finite Markov chain.

Throughout the dissertation the following notation will be used:

$\mathbb{R}^n$ denotes the n-dimensional real space.

I denotes the identity matrix of order n.

e denotes the n-dimensional vector whose entries are all equal to one.

e_j denotes the n-dimensional j^{th} unit vector.

For $x \in \mathbb{R}^n$, $x = (x_k)$,

$\|x\|_1$ denotes the norm of x defined by

$$\|x\|_1 = \sum_{k=1}^n |x_k|,$$

$\|x\|_2$ denotes the norm of x defined by

$$\|x\|_2 = \left(\sum_{k=1}^n x_k^2 \right)^{\frac{1}{2}},$$

$\|x\|_\infty$ denotes the norm of x defined by

$$\|x\|_\infty = \max_k |x_k|,$$

$x \geq 0$ means $x_i \geq 0$ for each i,

$x > 0$ means $x \geq 0$ and $x_i \neq 0$ for some i,

$x \gg 0$ means $x_i > 0$ for each i, and

$\langle x \rangle$ means the set of scalar multiples of x.

If A is a matrix of order n, $A = (a_{ij})$, $a_{ij} \in \mathbb{R}$,

A^T denotes the transpose of A,

$R(A)$ denotes the range of A,

$N(A)$ denotes the null space of A ,

$\text{adj}(A)$ denotes the adjoint of A ,

$\sigma(A)$ denotes the set of all eigenvalues of A ,

$\rho(A)$ denotes the absolute value of the eigenvalue of

A with maximum modulus,

$\det(A)$ denotes the determinant of A ,

$\|A\|_1$ denotes the norm of A , defined by

$$\|A\|_1 = \max_j \sum_{k=1}^n |a_{kj}|,$$

$\|A\|_2$ denotes the norm of A , defined by

$$\|A\|_2 = \rho(A^T A)^{\frac{1}{2}},$$

$(A)_{i,j}$ denotes the entry in the i,j position of A , and

$\text{Ind}(A)$ denotes the index of A ,

$\text{rank}(A)$ denotes the rank of A .

It will be assumed throughout this dissertation that all matrices and vectors have real components.

CHAPTER II

RANK MODIFICATION METHOD FOR CERTAIN MATRICES

1. Introduction

Let A be a real matrix of order n , such that the rank of A is $n - 1$. This chapter concerns the computation of a solution to the following consistent linear system of equations

$$Aw = f.$$

The proposed method is an extension of an algorithm that was presented in a recent paper by Kemeny [1981]. The method is based upon the transformation of A into a nonsingular matrix by a rank one modification, followed by the solution of an associated nonsingular system of linear equations.

Let x and y denote nonzero n -dimensional vectors such that $x^T A = 0$ and $Ay = 0$. It follows from the fact that A has rank $n - 1$, that the vectors x and y are unique up to scalar multiples. Also, x and y can be chosen so that $y^T x = 1$, if zero is a simple eigenvalue of A . Unless otherwise stated the letters x and y will denote the left and right null vectors of A corresponding to the zero eigenvalue of A , and w will denote any solution to the consistent system of linear equations $Aw = f$.

The following theorem states necessary and sufficient conditions for the system of linear equations $Aw = f$ to be consistent.

Theorem 2.1. (e.g., Stewart 1973, p. 66). Let A be a matrix of order n . The equation $Aw = f$ has a solution if and only if $z^T A = 0$ implies that $z^T f = 0$, where z is an n -dimensional vector.

If $z^T A = 0$, then there exists a scalar α such that $z = \alpha x$.

Therefore the equation $Aw = f$, where A has rank $n - 1$, is consistent if and only if $x^T f = 0$.

If the equation $Aw = f$ is consistent, then the set of all solutions, S , is precisely the following set

$$S = \{A^-f + (I - A^-A)h \mid h \in \mathbb{R}^n\}$$

where A^- is any matrix in $A\{1\}$. (see, Penrose [1955]).

If A has rank $n - 1$, then $I - A^-A$ has rank one. Using the definition of A^- , it follows that $I - A^-A = yb^T$, for some n -dimensional vector b . Hence, if h is an n -dimensional vector, then $(I - A^-A)h = (b^T h)y$. Using this fact the following lemma is obvious.

Lemma 2.1. Let A be a matrix of order n , with rank $n - 1$. If the system of linear equations $Aw = f$ is consistent, then the solution set S can be characterized as follows

$$S = \{A^-f + \alpha y \mid \alpha \in \mathbb{R}\},$$

where A^- is any matrix in $A\{1\}$, and y is a right null vector of A .

The proposed method will be called the Rank Modification Method. The Rank Modification Method and the Kemeny Method will be developed in Section 2 and a complete error analysis is given in Section 3. Finally, the special case when $f = 0$, will be investigated in Section 4.

2. Rank Modification Method

In this section the Rank Modification Method and the Kemeny Method are developed. Some problems associated with these methods are discussed in this section.

Theorem 2.2. Let A be a square matrix and let x and y be left and right null vectors of A . If $x^T u \neq 0$ and $y^T v \neq 0$, then

$$\text{rank } (A + uv^T) = \text{rank } (A) + 1.$$

Proof: Let $r = \frac{1}{x^T u} x$ and $s = \frac{1}{v^T y} y$. Then $(A + uv^T)s = u$, $r^T(A + uv^T) = v^T$, and $r^T(A + uv^T)s = 1$. Thus, by applying the Wedderburn-Householder Theorem (see, Householder [1964], p. 33, Ex. 34), it follows that $\text{rank } (A + uv^T) = \text{rank } (A) + 1$. ■

The converse of the previous theorem does not necessarily hold true as the following example illustrates.

Example 2.1.

Let

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

Clearly, the rank of A is equal to 1. Let

$$v = (1, 0, 0)^T,$$

and

$$u = (1, 0, 0)^T.$$

Then it follows that

$$A + uv^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

So that $\text{rank } (A + uv^T) = 2$ and hence

$$\text{rank } (A + uv^T) = \text{rank } (A) + 1.$$

If $x = e_3$ and $y = e_2$, then $x^T A = 0$ and $Ay = 0$. Clearly, it follows that $x^T u = 0$ and $y^T v = 0$.

The following corollary provides a necessary and sufficient condition for a matrix with rank $n - 1$, to be transformed into a non-singular matrix by a certain rank one modification.

Corollary 2.1. Let A be a matrix of order n , with rank $n - 1$.

Assume that x and y are left and right null vectors of A . Then

$x^T u \neq 0$ and $y^T v \neq 0$ if and only if $G = (A + uv^T)^{-1}$.

Proof: If $x^T u \neq 0$ and $y^T v \neq 0$, then, by applying Theorem 2.2, it follows that $(A + uv^T)^{-1}$ exists.

If $\text{rank}(A + uv^T) = n$, then by applying the Wedderburn-Householder Theorem (see, Householder [1964], p. 33, Ex. 34) it follows that there exist vectors r and s , such $(A + uv^T)s = u$, $r^T(A + uv^T) = v^T$, and $r^T(A + uv^T)s = 1$. Then $s^T v = 1$ and $u^T r = 1$, hence $As = 0$ and $r^T A = 0$. Since $\text{rank}(A) = n - 1$, there exists a real number α such that $s = \alpha y$, thus $v^T y \neq 0$. Similarly it can be shown that $u^T x \neq 0$. ■

Unless otherwise stated, the letter G will denote the inverse of $A + uv^T$ throughout this dissertation. Also u and v will denote two arbitrary vectors such that $x^T u \neq 0$ and $y^T v \neq 0$.

Definition 2.1. Let A be a matrix of order n , with rank $n - 1$.

Let x and y be left and right null vectors of A . Define

$$G = \{G \in \mathbb{R}^{n \times n} \mid G = (A + uv^T)^{-1}, \text{ where } u, v \in \mathbb{R}^n, \\ x^T u \neq 0 \text{ and } y^T v \neq 0\}.$$

Since the vectors x and y are unique up to scalar multiples, it follows that the conditions $x^T u \neq 0$ and $y^T v \neq 0$, are independent of which null vectors are used. Therefore the set G is well defined.

Assume that $G \in G$. Then since $(A + uv^T)G = I$, it follows that

$$AG + u(v^T G) = I \quad (2.1)$$

Multiplying equation (2.1) on the left by x^T leads to the equation

$$x^T AG + (x^T u)(v^T G) = x^T I.$$

Using the fact that $x^T A = 0$, one obtains

$$v^T G = \frac{1}{x^T u} x^T I. \quad (2.2)$$

Solving equation (2.1) for $I - AG$ yields the equation

$$I - AG = u(v^T G). \quad (2.3)$$

Substituting (2.2) into (2.3) it follows that

$$I - AG = \frac{1}{x^T u} ux^T. \quad (2.4)$$

Using the same approach, it follows that

$$Gu = \frac{1}{v^T y} y, \quad (2.5)$$

and

$$I - GA = \frac{1}{v^T y} yv^T. \quad (2.6)$$

Equations (2.2), (2.4), (2.5), and (2.6) will be used throughout Chapter II. The following theorem which follows from Rao and Mitra [1971, p. 31] will be used to derive the Rank Modification Method.

Theorem 2.3. Let A be a matrix of order n , with rank $n - 1$. Then $G \in A\{1\}$.

The following lemma provides an alternate characterization for the set $A\{1\}$.

Lemma 2.2. (e.g., Campbell and Meyer [1979], p. 97) Let A be a matrix of order n . Then the set $A\{1\}$ can be written as

$$A\{1\} = \{A^- + E(I - AA^-) + (I - A^-A)F \mid E, F \in \mathbb{R}^{n \times n}\}$$

where A^- is any $\{1\}$ -inverse of A .

The next theorem provides a more useful characterization of $A\{1\}$, when A has rank $n - 1$.

Theorem 2.4. Let A be a matrix of order n , with rank $n - 1$. Then

$$A\{1\} = \{G + yr^T + sx^T \mid r, s \in \mathbb{R}^n\},$$

where x and y are left and right null vectors of A , and $G \in G$.

Proof. Let $H = \{G + yr^T + sx^T \mid r, s \in \mathbb{R}^n\}$.

Assume that $G_1 \in H$. Then $G_1 = G + yr^T + sx^T$ for some $r, s \in \mathbb{R}^n$.

Hence

$$AG_1A = A(G + yr^T + sx^T)A$$

or

$$AG_1A = AGA + (Ay)r^TA + As(x^TA).$$

Using the facts that $x^TA = 0$, $Ay = 0$, and $AGA = A$ it follows that

$AG_1A = A$. So $G_1 \in A\{1\}$.

Assume that $G_1 \in A\{1\}$. Then using Lemma 2.2, there exist matrices $E, F \in \mathbb{R}^{n \times n}$ such that $G_1 = G + (I - AG)E + F(I - GA)$. Substituting equations (2.4) and (2.6) into this equation for G_1 leads to the following equation

$$G_1 = G + y \left(\frac{1}{v^T y} v^T E \right) + \left(\frac{1}{u^T x} Fu \right) x^T.$$

Setting $r^T = \frac{1}{v^T y} v^T E$ and $s = \frac{1}{u^T x} Fu$ leads to the following equation

$$G_1 = G + yr^T + sx^T,$$

hence $G_1 \in H$.

Therefore, it follows that $H = A\{1\}$. ■

The following theorem provides an alternate characterization for the solution set of a consistent system of linear equations $Aw = f$.

Theorem 2.5. Let A be a matrix of order n with rank $n - 1$. Assume that the system of linear equations $Aw = f$ is consistent. Then the set of all solutions S can be written as

$$S = \{Gf + \tau Gu \mid \tau \in \mathbb{R}\}$$

where $G \in G$ with $G = (A + uv^T)^{-1}$. Furthermore if $w = Gf + \tau Gu$, then $v^T w = \tau$.

Proof. Let $R = \{Gf + \tau Gu \mid \tau \in \mathbb{R}\}$.

Assume that w is a solution to $Aw = f$. Then using the definition of the solution set it follows that

$$w = A^-f + (I - A^-A)h$$

where $h \in \mathbb{R}^n$. Let $A^- = G$, where $G \in G$. Thus

$$w = Gf + (I - GA)h.$$

Substituting equation (2.6) into the above equation leads to

$$w = Gf + (v^T h) \left(\frac{1}{v^T y} y \right). \quad (2.7)$$

Next, substituting equation (2.5) into (2.7) yields

$$w = Gf + (v^T h)Gu. \quad (2.8)$$

The vector h was arbitrary, so the term $v^T h$ can be replaced in equation (2.8) by the term τ , where τ is any real number. Hence

$$w = Gf + \tau Gu,$$

and thus $w \in R$.

Assume that $w \in R$. Then

$$w = Gf + \tau Gu \quad (2.9)$$

where τ is any real number.

Multiplying equation (2.9) on the left by A yields

$$Aw = AGf + \tau AGu. \quad (2.10)$$

Using equation (2.4) it follows that $AG = I - \frac{1}{x^T u} ux^T$. Substituting this equation into (2.10) it follows that

$$Aw = \left(I - \frac{1}{x^T u} ux^T\right)f + \tau \left(I - \frac{1}{x^T u} ux^T\right)u$$

or

$$Aw = f - \begin{pmatrix} \frac{x^T f}{x^T u} \\ \frac{x^T f}{x^T u} \end{pmatrix} u + \tau \left(u - \begin{pmatrix} \frac{x^T u}{x^T u} \\ \frac{x^T u}{x^T u} \end{pmatrix} u \right).$$

Thus $Aw = f$ and hence $w \in S$.

Therefore, it follows that $S = \{Gf + \tau Gu \mid \tau \in \mathbb{R}\}$.

Let $w = Gf + \tau Gu$. Then $v^T w = v^T Gf + \tau v^T Gu$. When equations (2.2) and (2.5) are substituted into this equation for $v^T w$, this leads to the equation $v^T w = \tau$. ■

If $w = Gf + \tau Gu$, then $(A + uv^T)w = f + \tau u$. This system of linear equations suggests the following method for computing a solution of the consistent system of linear equations $Aw = f$.

Rank Modification Method

Let A be a matrix of order n , with rank $n - 1$. The following method can be used to compute a solution w to the consistent system of linear equations $Aw = f$.

- 1) Find nonzero vectors u and v such that $x^T u \neq 0$ and $y^T v \neq 0$, where x and y are left and right null vectors of A , respectively.
- 2) Apply Gaussian elimination with row pivoting to produce the following factorization

$$P(A + uv^T) = LU$$

where P is the permutation matrix that results from row pivoting.

- 3) Solve $Lz = P(f + \tau u)$ using forward substitution
- 4) Solve $Uw = z$ using back substitution.

When this method is applied to the consistent system of linear equations $Aw = f$ it results in a solution w such that $v^T w = \tau$.

Suppose that the constraint $b^T w = \alpha$, where b is an n -dimensional vector, and α is a real number, is added to the problem, i.e. one wishes to compute the solution to the system of linear equations $Aw = f$, such that $b^T w = \alpha$, if it exists. Then the Rank Modification Method can be applied to this problem by setting $v = b$ and $\tau = \alpha$. If the system of linear equations $Aw = f$ is consistent, then this does not imply that the constrained system of linear equations admits a solution. If $y^T b \neq 0$, then by applying Theorem 2.5 it follows that the solution to the constrained linear system exists. If $y^T b = 0$, then the solution to the constrained linear system may not exist. It was proven in Theorem 2.5 that

$$S = \{Gf + \tau Gu \mid \tau \in \mathbb{R}\}$$

where $G \in G$ and $G = (A + uv^T)^{-1}$. Using equation (2.5) it follows that

$$Gf + \tau Gu = Gf + \frac{1}{y^T v} y,$$

where y is a right null vector of A . Thus the following theorem holds.

Theorem 2.6. (Kemeny [1981]). Let A be a matrix of order n , with rank $n - 1$. Assume that the system of linear equations $Aw = f$ is consistent. Then the solution set S can be written as

$$S = \{Gf + \gamma y \mid \gamma \in \mathbb{R}\}$$

where $G \in G$, and y is a right null vector of A .

Let $w \in S$. Then $w = Gf + \gamma y$. If $y^T b = 0$ then $b^T w = b^T Gf$. So, if $\alpha = b^T Gf$, then the solution to the constrained linear system will exist, otherwise it will not. The following example illustrates the second case.

Example 2.2.

$$\text{Let } A = \begin{pmatrix} 1 & -1 \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}, b = (1, -1)^T, \text{ and } f = (-2, 1)^T.$$

Suppose one wishes to compute the vector w , such that $Aw = f$ and $b^T w = 1$.

If $x = (1, 2)^T$ and $y = (1, 1)^T$, then $x^T A = 0$ and $Ay = 0$. Clearly $x^T f = 0$, hence the equation $Aw = f$ is consistent.

Let $u = v = e$. Then $x^T u \neq 0$ and $y^T v \neq 0$. So the inverse $G = (A + uv^T)^{-1}$ exists.

$$\begin{aligned} A + uv^T &= \begin{pmatrix} 1 & -1 \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 2 & 0 \\ \frac{1}{2} & 3/2 \end{pmatrix}. \end{aligned}$$

If $G = (A + uv^T)^{-1}$, then

$$G = 1/3 \begin{pmatrix} 3/2 & 0 \\ -\frac{1}{2} & 2 \end{pmatrix}.$$

Let $w \in S$. Then

$$w = 1/3 \begin{pmatrix} 3/2 & 0 \\ -\frac{1}{2} & 2 \end{pmatrix} \begin{pmatrix} -2 \\ 1 \end{pmatrix} + \gamma \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

where $\gamma \in \mathbb{R}$.

Hence, it follows that

$$w = \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \gamma \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

and

$$b^T w = -2.$$

Therefore there does not exist a $w \in S$ such that $b^T w = 1$.

Notice that the Rank Modification Method may actually require knowledge of the vectors x and y . However, if A is a singular irreducible M -matrix, then $x \gg 0$ (see Bermmman and Plemmons [1979], Ch. 6). Thus any nonzero n -dimensional vector u with all nonpositive entries or all nonnegative entries will satisfy the equation $x^T u \neq 0$. If the system of linear equations is constrained, then one only has to find a vector u such that $x^T u \neq 0$.

To see that this method produces the unique solution to the system of linear equations $Aw = f$, such that $v^T w = \tau$, assume that $w_1, w_2 \in S$. Then there exists real numbers τ_1 and τ_2 such that

$$w_1 = Gf + \tau_1 y,$$

and

$$w_2 = Gf + \tau_2 y,$$

where $G \in G$. If $v^T w_1 = v^T w_2$, then

$$v^T Gf + \tau_1 v^T y = v^T Gf + \tau_2 v^T y.$$

Hence $\tau_1 = \tau_2$, as long as $v^T y \neq 0$, so that $w_1 = w_2$.

Suppose that u and v are arbitrary n -dimensional vectors such that $P(A + uv^T)$ has an LU-decomposition, where P is a permutation matrix. If L and U are nonsingular matrices, then A is a nonsingular matrix. Thus, one technique for verifying that $u^T x \neq 0$ and $v^T y \neq 0$, is to perform Gaussian elimination with row pivoting on the system of linear equations $A + uv^T$ and examine the diagonal entries of the factor U .

The following example illustrates the computations involved in the Rank Modification Method.

Example 2.3.

Let

$$A = \begin{pmatrix} 2 & 0 & 2 \\ -4 & -2 & -3 \\ 4 & -2 & 5 \end{pmatrix} \text{ and } f = (0, 1, 1)^T.$$

Suppose one wishes to compute the solution to the constrained system of linear equations $Aw = f$, such that $b^T w = 1$, where $b = (1, 1, 0)^T$.

1) Let $u = (-1, 1, 1)^T$ and $v = b$. Then

$$\begin{aligned} A + uv^T &= \begin{pmatrix} 2 & 0 & 2 \\ -4 & -2 & -3 \\ 4 & -2 & 5 \end{pmatrix} + \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix} (1, 1, 0) \\ &= \begin{pmatrix} 1 & -1 & 2 \\ -3 & -1 & 3 \\ 5 & -1 & 5 \end{pmatrix}. \end{aligned}$$

The matrix $A + uv^T$ has the following LU-decomposition

$$A + uv^T = \begin{pmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 5 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 & 2 \\ 0 & -4 & 3 \\ 0 & 0 & -2 \end{pmatrix}.$$

Both factors L and U , of the LU-decomposition of $A + uv^T$, are nonsingular. Hence the matrix $A + uv^T$ is nonsingular. Therefore $x^T u \neq 0$ and $y^T v \neq 0$.

- 2) The LU-decomposition was computed in step 1 above.
- 3) Solving the following system of linear equations

$$\begin{pmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 5 & -1 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \\ 2 \end{pmatrix}$$

results in the solution $z = (-1, -1, 6)^T$.

- 4) Solving the following system of linear equations

$$\begin{pmatrix} 1 & -1 & 2 \\ 0 & -4 & 3 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ 0 \end{pmatrix}$$

results in the solution $w = (3, -2, -3)^T$.

It can be easily shown that $Aw = f$ and that $b^T w = 1$.

To summarize, the Rank Modification Method is a simple direct method for computing a solution to the consistent system of linear equations $Aw = f$. One of the disadvantages of this method is that when the matrix A is transformed into a nonsingular matrix some useful properties of A might be lost. Also, if A is a sparse matrix, then the matrix $A + uv^T$ might be dense.

In a recent paper by Kemeny [1981], a method was proposed from solving the consistent system of linear equations $Aw = f$ that requires the use of a right null vector of A . This algorithm will be called the Kemeny Method, and it is based upon the characterization of the solution set provided by Theorem 2.6.

Kemeny Method

Let A be a matrix of order n , with rank $n - 1$. Assume that y is a right null vector of A . The following method can be used to compute a solution to the consistent system of linear equations $Aw = f$.

- 1) Find vectors u and v , such that $x^T u \neq 0$ and $y^T v \neq 0$, where x is a left null vector of A .
- 2) Apply Gaussian elimination with row pivoting to $A + uv^T$ to produce the following factorization

$$P(A + uv^T) = LU$$

where P is the permutation matrix that results from row pivoting.

- 3) Solve $Ly = Pf$ using forward substitution.
- 4) Solve $Uz = y$ using back substitution.
- 5) Set $w = z + \frac{\tau}{v^T y} y$.

When this method is applied to the consistent system of linear equations $Aw = f$, it results in a unique solution w such that $v^T w = \tau$. Notice that the Kemeny Method requires the use of a right null vector of A , where as the Rank Modification does not explicitly use the right null vector. The following example illustrates the computations involved in the Kemeny Method.

Example 2.4.

Let

$$A = \begin{pmatrix} 2 & 0 & 2 \\ -4 & -2 & -3 \\ 4 & -2 & 5 \end{pmatrix}, \quad y = (-2, 1, 2)^T,$$

and $f = (0, 1, 1)^T$.

Suppose one wishes to compute the solution to the constrained system of linear equations $Aw = f$ such that $b^T w = 1$, where $b = (0, 0, 1)^T$.

1) Let $u = (0, 0, 1)^T$ and $v = b$. Then

$$A + uv^T = \begin{pmatrix} 2 & 0 & 2 \\ -4 & -2 & -3 \\ 4 & -2 & 6 \end{pmatrix}.$$

The matrix $A + uv^T$ has the following LU-decomposition

$$A + uv^T = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 2 & 1 & 1 \end{pmatrix} \begin{pmatrix} 2 & 0 & 2 \\ 0 & -2 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Clearly $A + uv^T$ is a nonsingular matrix. Therefore $x^T u \neq 0$ and $y^T v \neq 0$.

2) The LU-decomposition was computed in step 1 above.

3) Solving the following system of linear equations

$$\begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 2 & 1 & 1 \end{pmatrix} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

results in the solution $s = (0, 1, 0)^T$.

4) Solving the following system of linear equations

$$\begin{pmatrix} 2 & 0 & 2 \\ 0 & -2 & 1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

results in the solution $z = (0, -\frac{1}{2}, 0)^T$.

5) If $w = z + \frac{1}{v^T y} y$, then

$$w = (-1, 0, 1)^T.$$

It can be easily shown that $Aw = f$ and that $b^T w = 1$.

It should be remarked that various results in this section and in the papers by Kemeny [1981] and Hunter [1982] could be improved upon by using the concepts developed in the papers by Cline and Funderlic [1979] and Marsaglia and Styon [1974].

3. Error Analysis for the Rank Modification Method

Assume that B is a matrix of order n with an LU-decomposition, $B = LU$. Let $B^{(1)} = B$ and let $B^{(k)}$ denote the result of the first $k - 1$ steps of Gaussian elimination applied to B .

If the Rank Modification Method is implemented on a finite precision computer, then instead of the computing the exact solution to the equation $Aw = f$, an approximation $\hat{w}$ is computed. This computed solution in general will not satisfy exactly the equation $Aw = f$. Assume that the Rank Modification Method is executed on a machine with unit roundoff error μ in floating point arithmetic. Then a simple backward error analysis, using Wilkinson [1965], p. 215 and Stewart [1973], p. 150, shows that the computed solution $\hat{w}$ satisfies a perturbed system of linear equations $(A + uv^T + E)\hat{w} = f + \tau u$.

Theorem 2.7. Let A be a matrix of order n , with rank $n - 1$.

Assume that the matrix $A + uv^T$ is nonsingular. Suppose that the system $(A + uv^T)w = f + \tau u$ is solved for the vector w by Gaussian elimination with row pivoting applied to $A + uv^T$, in floating point arithmetic with machine unit roundoff error μ . Then there exists a matrix $E = (e_{ij})$ such that the computed solution to $(A + uv^T)w = f + \tau u$ satisfies exactly the following system of linear equations

$$(A + uv^T + E)w = f + \tau u \quad (2.11)$$

such that for all $1 \leq i, j \leq n$,

$$|e_{ij}| \leq [3.03 + 2.02n + \mu(1.01)^2(n+1)^2] \mu n \max_{i,j,k} |\hat{b}_{ij}^{(k)}| \quad (2.12)$$

where $\hat{b}_{ij}^{(k)}$ is the entry in the i, j position of the floating point version of $(P(A + uv^T))^{(k)}$, and P is the permutation matrix that results from row pivoting

Proof. Consider the LU-decomposition of $A + uv^T$ by Gaussian elimination with row pivoting. From Wilkinson [1965], p. 215, there exists a matrix $F = (f_{ij})$ such that the computed factors $\hat{L}$ and $\hat{U}$ satisfy

$$P(A + uv^T) + F = \hat{L}\hat{U} \quad (2.13)$$

where P is the permutation matrix that results from row pivoting. Set $B = P(A + uv^T)$. Also, for all $1 \leq i, j \leq n$,

$$|f_{ij}| \leq \begin{cases} 2.01 \mu(i-1) \max_{i,j,k} |\hat{b}_{ij}^{(k)}| & \text{if } j \geq i, \\ 2.01 \mu j \max_{i,j,k} |\hat{b}_{ij}^{(k)}| & \text{if } j < i. \end{cases}$$

Thus by combining these inequalities in terms of i , it follows that

$$|f_{ij}| \leq 2.01 i \mu \max_{i,j,k} |\hat{b}_{ij}^{(k)}|. \quad (2.14)$$

Next, if $Lz = P(f + \tau u)$ is solved using $\hat{L}$ in the forward substitution step 3, then by Stewart [1973], p. 150, there exists a matrix $G = (g_{ij})$ such that the computed solution $\hat{z}$ to $\hat{L}z = P(f + \tau u)$ satisfies the system

$$(\hat{L} + G)\hat{z} = P(f + \tau u) \quad (2.15)$$

where for all $1 \leq i, j \leq n$,

$$|g_{ij}| \leq 1.01 \mu(n+1) \max_{i,j} |\hat{\ell}_{ij}|.$$

Because row pivoting was used, it follows that

$$\max_{i,j} |\hat{\ell}_{ij}| \leq 1. \quad (2.16)$$

Hence

$$|g_{ij}| \leq 1.01 \mu(n+1). \quad (2.17)$$

Next, if $Uw = z$ is solved using $\hat{U}$ and $\hat{z}$ in the back substitution step 4, then by Stewart [1973], p. 150, there exists a matrix $H = (h_{ij})$ such that the computed solution $\hat{w}$ to $\hat{U}\hat{w} = \hat{z}$ satisfies the system

$$(\hat{U} + H)\hat{w} = \hat{z} \quad (2.18)$$

where for all $1 \leq i, j \leq n$

$$|h_{ij}| \leq 1.01 \mu(n+1) \max_{i,j} |\hat{u}_{ij}|.$$

Applying the inequality $\max_{i,j} |\hat{u}_{ij}| \leq \max_{i,j,k} |\hat{b}_{ij}^{(k)}|$ it follows that

$$|h_{ij}| \leq 1.01 \mu(n+1) \max_{i,j,k} |\hat{b}_{ij}^{(k)}|. \quad (2.19)$$

Multiplying equation (2.18) on the left by $\hat{L} + G$ and applying equation (2.15) it follows that

$$(\hat{L} + G)(\hat{U} + H)\hat{w} = P(f + \tau u).$$

The above equation can be rewritten as

$$(\hat{L}\hat{U} + \hat{L}H + \hat{G}\hat{U} + GH)\hat{w} = P(f + \tau u).$$

Using equation (2.13) it follows that

$$[P(A + uv^T) + F + \hat{L}H + \hat{G}\hat{U} + GH]\hat{w} = P(f + \tau u). \quad (2.20)$$

Multiplying equation (2.20) on the left by P^T leads to the following equation

$$[A + uv^T + P^T(F + \hat{L}H + \hat{G}\hat{U} + GH)]\hat{w} = f + \tau u.$$

Let $E = P^T(F + \hat{L}H + G\hat{U} + GH)$. Then

$$(A + uv^T + E)\hat{w} = f + \tau u.$$

Also, using (2.14), (2.17), and (2.19) it follows that (2.12) holds. ■

An algorithm is often called stable when the computed solution is the actual solution to a problem close to the original problem. Thus the Rank Modification Method will be a stable algorithm for a problem when the order of the matrix is not excessively large and the entries $\hat{b}_{ij}^{(k)}$ do not grow excessively in the course of reduction.

Using Theorem 2.7, an explicit relationship between $\hat{w}$ and w can be derived.

Theorem 2.8. Let A be a matrix of order n , with rank $n - 1$. If w and $\hat{w}$ are n -dimensional vectors such that

$$(A + uv^T)w = f + \tau u$$

and

$$(A + uv^T + E)\hat{w} = f + \tau u$$

where $(A + uv^T)^{-1} \in G$, f is an n -dimensional vector, and τ is a real number, then

$$w = [I + (A + uv^T)^{-1}E]\hat{w}.$$

Proof. If $(A + uv^T)w = f + \tau u$ and $(A + uv^T + E)\hat{w} = f + \tau u$, then
 $(A + uv^T)w = (A + uv^T + E)\hat{w}$. Hence

$$w = (A + uv^T)^{-1} (A + uv^T + E)\hat{w},$$

and thus

$$w = [I + (A + uv^T)^{-1} E]\hat{w} \quad \blacksquare$$

Let $G = (A + uv^T)^{-1}$. Then the computed vector $\hat{w}$ satisfies the following equation

$$w = (I + GE)\hat{w}.$$

The exact solution w satisfies the equation $v^T w = \tau$; but $\hat{w}$ is an approximation to w , so in general, $v^T \hat{w}$ will not equal τ . The next lemma establishes a relationship between $v^T w$ and $v^T \hat{w}$.

Lemma 2.2. Assume that w and $\hat{w}$ satisfy the hypothesis of Theorem 2.8.

Then

$$v^T w - v^T \hat{w} = \frac{x^T E \hat{w}}{x^T u}.$$

Proof. Applying Theorem 2.8 it follows that

$$w = (I + GE)\hat{w}. \quad (2.21)$$

Multiplying equation (2.21) on the left by v^T yields

$$v^T w = v^T (I + GE)\hat{w}.$$

Using equation (2.2) leads to the following equation

$$v^T w = v^T \hat{w} + \frac{1}{x^T u} x^T E \hat{w}.$$

Therefore

$$v^T w - v^T \hat{w} = \frac{1}{x^T u} x^T E \hat{w}. \quad \blacksquare$$

Thus it would seem that the vector u should be chosen so that $1/x^T u$ is small.

Suppose that $v = x$. Then the following lemma gives a relationship between the eigenvalues of A and the eigenvalues of $A + ux^T$.

Lemma 2.3. (Brauer [1952]) Let A be a matrix of order n , with eigenvalues $0 = \lambda_1, \lambda_2, \dots, \lambda_n$ and having rank $n - 1$. Assume that $x^T A = 0$, then the eigenvalues of $A + ux^T$ are $x^T u, \lambda_2, \dots, \lambda_n$.

Therefore it can be shown that a good choice for u , when $v = x$, is a vector such that $1 \leq x^T u \leq \max \{1, \rho(A)\}$.

Theorem 2.9. Let A be a matrix of order n , with rank $n - 1$. If $\hat{w}$ is the computed solution that results when the Rank Modification Method is implemented on a computer in floating point arithmetic with machine unit roundoff error μ , then

$$(A + F)\hat{w} = f$$

where

$$F = \left(I - \frac{1}{x^T u} ux^T \right) E,$$

and the matrix E is given by Theorem 2.7.

Proof. From Theorem 2.7 it follows that $\hat{w}$ satisfies exactly the following system of linear equations

$$(A + uv^T + E)\hat{w} = f + \tau u. \quad (2.22)$$

Expanding equation (2.22) leads to

$$A\hat{w} + uv^T\hat{w} + E\hat{w} = f + \tau u,$$

so that

$$A\hat{w} + (v^T\hat{w})u + E\hat{w} = f + \tau u. \quad (2.23)$$

In Lemma 2.2 it was proved that

$$v^T w = v^T \hat{w} + \frac{x^T E \hat{w}}{x^T u}.$$

Applying this equation to (2.23), it follows that

$$A\hat{w} + \left(v^T w - \frac{x^T E \hat{w}}{x^T u} \right) u + E\hat{w} = f + \tau u. \quad (2.24)$$

Using the fact that $v^T w = \tau$, it follows that

$$A\hat{w} - \frac{x^T E \hat{w}}{x^T u} u + E\hat{w} = f$$

or

$$\left[A + \left(I - \frac{1}{x^T u} ux^T \right) E \right] \hat{w} = f.$$

Letting $F = \left(I - \frac{1}{x^T u} ux^T \right) E$, it follows that

$$(A + F)\hat{w} = f. \quad \blacksquare$$

Therefore, if the elements of the matrix F are relatively small, then the computed solution $\hat{w}$ will solve a problem close to the original problem.

Using Theorem 2.8 an upper bound can be derived for the relative error term $\|w - \hat{w}\| / \|w\|$.

Theorem 2.10. Let A be a matrix of order n , with rank $n - 1$. Assume that $G \in G$, where $G = (A + uv^T)^{-1}$. Let w and $\hat{w}$ be n -dimensional vectors such that

$$(A + uv^T)w = f + \tau u,$$

and

$$(A + uv^T + E)\hat{w} = f + \tau u$$

where E is some matrix of order n , τ is a real number, and f is an n -dimensional vector.

If $\|G\| \|E\| < 1$, for some consistent matrix norm, then

$$\frac{\|w - \hat{w}\|}{\|w\|} \leq \frac{\|A\| \|G\|}{1 - \|G\| \|E\|} \cdot \frac{\|E\|}{\|A\|}.$$

Proof. Applying Theorem 2.8 it follows that

$$w = (I + GE)\hat{w}. \quad (2.25)$$

If $\|G\| \|E\| < 1$, then $(I + GE)^{-1}$ exists. Hence equation (2.25) can be written as

$$\hat{w} = (I + GE)^{-1}w.$$

Using the identity $(I + GE)^{-1} = I - (I + GE)^{-1} GE$ it follows that

$$\hat{w} = w - (I + GE)^{-1} GEw,$$

and thus

$$w - \hat{w} = (I + GE)^{-1} GEw. \quad (2.26)$$

Taking the norm of both sides of equation (2.26) yields

$$\|w - \hat{w}\| = \|(I + GE)^{-1} GEw\|.$$

Therefore

$$\frac{\|w - \hat{w}\|}{\|w\|} \leq \frac{\|A\| \|G\|}{1 - \|G\| \|E\|} \cdot \frac{\|E\|}{\|A\|}. \quad \blacksquare$$

The term $\|A\| \|G\|$ can be considered a condition number for the constrained system of linear equation $Aw = f$, such that $v^T w = \tau$. If $\|A\| \|G\|$ is very large, then the error term $\|E\| / \|A\|$ will be magnified. The following lemma proves that

$$K(A, G) = \|A\| \|G\| \quad (2.27)$$

has the usual lower bound of a condition number.

Lemma 2.4. Let A be a matrix of order n , with rank $n - 1$. If $G \in \mathcal{G}$ and $K(A, G) = \|A\| \|G\|$, then $1 \leq K(A, G)$, where $\|\cdot\|$ is any consistent matrix norm.

Proof. If $G \in \mathcal{G}$, then $G = (A + uv^T)^{-1}$ for some vectors u and v .

Using equation (2.3) it is obvious that AG is an idempotent matrix

and has rank $n - 1$. Thus $\rho(AG) = 1$. So using basic properties of consistent matrix norms, it follows that

$$\rho(AG) \leq \|A\| \|G\|.$$

Therefore $1 \leq K(A, G)$. ■

Assume that zero is a simple eigenvalue of A . Then $A^\#$ exists (e.g. Campbell and Meyer [1979], p. 133). In Chapter IV, problems will be considered where one wishes to compute the solution to the homogeneous system of linear equations $Aw = 0$, such that $x^T w = 1$, where x is a left null vector of A . Let $\hat{w}$ denote the computed solution to system of linear equations $Aw = f$, that results when the Rank Modification Method, with $v = x$, is implemented on a finite precision machine. Let $\hat{z} = \alpha \hat{w}$, where $\alpha = x^T w / x^T \hat{w}$, assuming that $x^T \hat{w} \neq 0$. Then $x^T \hat{z} = x^T w$, and $\hat{z}$ satisfies the following system of linear equations

$$(A + F)\hat{z} = \alpha f$$

where F is the matrix given by Theorem 2.9. The following theorem provides an explicit relationship between w and $\hat{z}$ in terms of $A^\#$.

Theorem 2.11. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Let x be a left null vector of A , f be an n -dimensional vector, F be a matrix of order n , and let α be any real number. If w and $\hat{z}$ are n -dimensional vectors such that,

$$\begin{aligned} Aw &= f, \\ (A + F)\hat{z} &= f, \end{aligned} \tag{2.28}$$

and

$$\mathbf{x}^T \mathbf{w} = \mathbf{x}^T \hat{\mathbf{z}},$$

then

$$\mathbf{w} = (\mathbf{I} + \mathbf{A}^\# \mathbf{F}) \hat{\mathbf{z}} + (1 - \alpha) \mathbf{A}^\# \mathbf{f}.$$

Proof. Let

$$\mathbf{s} = (\mathbf{I} + \mathbf{A}^\# \mathbf{F}) \hat{\mathbf{z}} + (1 - \alpha) \mathbf{A}^\# \mathbf{f}. \quad (2.29)$$

Using equation (2.28) it follows that $\mathbf{F}\hat{\mathbf{z}} = \alpha \mathbf{f} - \mathbf{A}\hat{\mathbf{z}}$. Substituting this equation into equation (2.29), it follows that

$$\mathbf{s} = \hat{\mathbf{z}} + \mathbf{A}^\# (\alpha \mathbf{f} - \mathbf{A}\hat{\mathbf{z}}) + (1 - \alpha) \mathbf{A}^\# \mathbf{f}.$$

So that

$$\mathbf{s} = \hat{\mathbf{z}} - \mathbf{A}^\# \mathbf{A} \hat{\mathbf{z}} + \mathbf{A}^\# \mathbf{f},$$

or

$$\mathbf{s} = (\mathbf{I} - \mathbf{A}^\# \mathbf{A}) \hat{\mathbf{z}} + \mathbf{A}^\# \mathbf{f}.$$

Multiplying the above equation on the left by $\mathbf{A}$ yields

$$\mathbf{A}\mathbf{s} = (\mathbf{A} - \mathbf{A}\mathbf{A}^\# \mathbf{A}) \hat{\mathbf{z}} + \mathbf{A}\mathbf{A}^\# \mathbf{f}.$$

The vector $\mathbf{f}$ is in the range of $\mathbf{A}$, thus, $\mathbf{A}\mathbf{A}^\# \mathbf{f} = \mathbf{f}$. Also, from the definition of $\mathbf{A}^\#$ it follows that $\mathbf{A} - \mathbf{A}\mathbf{A}^\# \mathbf{A} = \mathbf{0}$, hence

$$\mathbf{A}\mathbf{s} = \mathbf{f}.$$

Therefore s is a solution to the equation $Aw = f$. Since zero is a simple eigenvalue of A , $x^T y \neq 0$. Hence, if $x^T w = x^T s$, then $w = s$.

Multiplying equation (2.29) on the left by x^T leads to the following equation

$$x^T s = x^T \hat{z} + x^T A^\# F \hat{z} + (1 - \alpha) x^T A^\# f.$$

Using that fact that $N(A) = N(A^\#)$, it follows that $x^T s = x^T \hat{z}$, but this implies that $x^T s = x^T w$. Therefore $w = s$. ■

Using this relationship between w and $\hat{z}$, an upper bound can be derived for the relative error term $\|w - \hat{z}\| / \|w\|$.

Theorem 2.12. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Let x be a left null vector of A , f be an n -dimensional vector, F be a matrix of order n , and α any real number. Let w and $\hat{z}$ be n -dimensional vectors such that,

$$\begin{aligned} Aw &= f, \\ (A + F)\hat{z} &= \alpha f, \end{aligned}$$

and

$$x^T w = x^T \hat{z}.$$

If $\|A^\#\| \|F\| < 1$, for some consistent matrix norm $\|\cdot\|$, then

$$\frac{\|w - \hat{z}\|}{\|w\|} \leq \frac{\|A\| \|A^\#\|}{1 - \|A^\#\| \|F\|} \left(\frac{\|F\|}{\|A\|} + |1 - \alpha| \right).$$

Proof. Applying Theorem 2.11 it follows that

$$w = (I + A^{\#}F)\hat{z} + (1 - \alpha)A^{\#}f \quad (2.30)$$

If $\|A^{\#}\| \|F\| < 1$, then $(I + A^{\#}F)^{-1}$ exists. Multiplying equation (2.30) on the left by $(I + A^{\#}F)^{-1}$ leads to the following equation

$$\hat{z} = (I + A^{\#}F)^{-1}w - (1 - \alpha)(I + A^{\#}F)^{-1}A^{\#}f.$$

Applying the identity $(I + A^{\#}F)^{-1} = I - (I + A^{\#}F)^{-1}A^{\#}F$, only to the first occurrence of $(I + A^{\#}F)^{-1}$, it follows that

$$\hat{z} = [I - (I + A^{\#}F)^{-1}A^{\#}F]w - (1 - \alpha)(I + A^{\#}F)^{-1}A^{\#}f$$

or

$$w - \hat{z} = (I + A^{\#}F)^{-1}A^{\#}[Fw + (1 - \alpha)f].$$

Taking the norm of both sides and dividing by $\|w\|$ yields

$$\frac{\|w - \hat{z}\|}{\|w\|} = \frac{\|(I + A^{\#}F)^{-1}A^{\#}[Fw + (1 - \alpha)f]\|}{\|w\|}$$

Hence

$$\frac{\|w - \hat{z}\|}{\|w\|} \leq \|(I + A^{\#}F)^{-1}\| \|A^{\#}\| \frac{\|F\| \|w\| + |1 - \alpha| \|f\|}{\|w\|}.$$

If $Aw = f$, then $\|f\| / \|w\| \leq \|A\|$. Applying this inequality the result follows. $\blacksquare$

The term $\|A\| \|A^\# \|$ can be considered a condition number for the constrained system of linear equations $Aw = f$, such that $x^T w = \tau$, when the computed solution $\hat{z}$ is scaled so that $x^T \hat{z} = 1$. If $\|A\| \|A^\# \|$ is very large, then the error term $\|F\| / \|A\| + |1 - \alpha|$ will be magnified.

Lemma 2.5. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Then $I - A^\# A = yx^T$, where x and y are right and left null vectors of A , such that $x^T y = 1$.

Proof. If $\text{rank}(A) = n - 1$, then $\text{rank}(I - A^\# A) = 1$. Using the definition of $A^\#$ it follows that $A(I - A^\# A) = 0$ and $(I - A^\# A)A = 0$. Clearly $\dim N(A) = 1$ and $\dim N(A^T) = 1$. So each column of $I - A^\# A$ is scalar multiple of y and each row of $I - A^\# A$ is a scalar multiple of x . Hence there exists a $\gamma \in \mathbb{R}$ such that

$$I - A^\# A = \gamma yx^T.$$

The matrix $I - A^\# A$ is the projector onto $N(A)$ along $R(A)$ and since it has rank one it must have as its only nonzero eigenvalue the number one. Therefore

$$(I - A^\# A)y = (\gamma yx^T)y,$$

or

$$(I - A^\# A)y = \gamma y.$$

Hence $\gamma = 1$ and $I - A^\# A = yx^T$. ■

The following theorem provides a useful lower bound for $K(A)$.

Theorem 2.14. Let A be a matrix of order n , with rank $n - 1$.

Assume that zero is a simple eigenvalue of A . If $|\lambda_{n-1}|$ is the second smallest nonzero eigenvalue of A in modulus, and if $|\lambda_1| = \rho(A)$, then

$$\left| \frac{\lambda_1}{\lambda_{n-1}} \right| \leq K(A)$$

where $K(A) = \|A\| \|A^\# \|$, and $\|\cdot\|$ is any consistent matrix norm.

Proof. Clearly $|\lambda_1| \leq \|A\|$. If $\lambda \in \sigma(A)$, then $\lambda^{-1} \in \sigma(A^\#)$ if $\lambda \neq 0$, and $0 \in \sigma(A^\#)$ if $\lambda = 0$. (e.g., Campbell and Meyer [1979], p. 129). Thus $\rho(A^\#) = 1/|\lambda_{n-1}|$. So, it follows that $\frac{1}{|\lambda_{n-1}|} \leq \|A^\# \|$.

Therefore the result follows. ■

Clearly it follows that $K(A) \geq 1$. Finally it is shown that if A is a normal matrix, then $K_2(A) = \|A\|_2 \|A^\# \|_2$ has a simple representation.

Theorem 2.15. Let A be a matrix of order n , with rank $n - 1$.

Assume that zero is a simple eigenvalue of A and that A is a normal matrix. If $|\lambda_{n-1}|$ is the second smallest nonzero eigenvalue of A in modulus, and $|\lambda_1| = \rho(A)$, then $K_2(A) = |\lambda_1/\lambda_{n-1}|$.

Proof. If $\sigma(A) = \{\lambda_k\}_{k=1}^n$, where

$$|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_{n-1}| > |\lambda_n| = 0,$$

then there exists a unitary matrix U such that $A = UDU^*$, where

$D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{n-1}, 0)$. Hence $A^\# = UD^\#U^*$, where

$D^\# = \text{diag}(\lambda_1^{-1}, \lambda_2^{-1}, \dots, \lambda_{n-1}^{-1}, 0)$. Therefore

$$K_2(A) = \|A\|_2 \|A^\#\|_2 = \|UDU^*\|_2 \|UD^\#U^*\|_2$$

or

$$K_2(A) = \|D\|_2 \|D^\#\|_2 = \left| \frac{\lambda_1}{\lambda_{n-1}} \right|. \quad \blacksquare$$

If A is a normal matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, then the singular values of A are $|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|$. Thus $K_2(A)$ is equal to largest singular value of A divided by the smallest nonzero singular value of A . As shall be noted in the test results of Chapter IV, the numerical accuracy seems to be governed by this ratio.

4. Homogeneous Case

When the Rank Modification Method is used to compute the solution to the constrained system of linear equations $Aw = f$, such that $b^T w = \tau$, then v must be set equal to b , so that the solution will satisfy the given constraint. Hence there is not complete flexibility in the selection of the vectors u and v . If the system of linear equation is homogeneous, then the solution is unique up to a scalar multiple. That is, if y is a right null vector of A , and w is any solution to the equation $Aw = 0$, then there exists a real number α such that $w = \alpha y$.

Let w be a solution to the homogeneous system of equations $Aw = 0$. Then as long as $b^T w \neq 0$, w can be scaled so that it satisfies the equation $b^T z = \tau$, where b is an n -dimensional vector, and τ is any real number.

Lemma 2.7. Let A be a matrix of order n , with rank $n - 1$. If w is a solution to the homogeneous system of linear equations $Aw = 0$ and b is an n -dimensional vector such that $b^T w \neq 0$, then for every nonzero number τ there exists a unique vector z such that $Az = 0$ and $b^T z = \tau$.

Proof. Let $z = \frac{\tau}{b^T w} w$. Then $Az = 0$ and $b^T z = \tau$. ■

Thus, the Rank Modification Method can be used to compute the solution to the constrained homogeneous system of equations $Aw = 0$ such that $b^T w = \tau$, without requiring that $v = b$.

Assume that zero is a simple eigenvalue of A . Suppose that one wishes to compute the solution to the homogeneous system of linear equations $Aw = 0$, such that $x^T w = \tau$ where $\tau \neq 0$ and x is a left null vector of A . Let $\hat{w}$ denote the computed solution to $Aw = 0$, that results when the Rank Modification Method is implemented on a finite precision machine. Let $\hat{z} = \alpha \hat{w}$, where $\alpha = x^T w / x^T \hat{w}$, assuming that $x^T \hat{w} \neq 0$. Then $x^T \hat{z} = \tau$, and $\hat{z}$ satisfies the following system of linear equations

$$(A + F)\hat{z} = 0,$$

where F is the matrix given in Theorem 2.9. The following corollary provides an explicit relationship between w and $\hat{z}$.

Corollary 2.2. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Let x be a left null vector of A , and F be a matrix of order n . If w and $\hat{z}$ are n -dimensional vectors such that

$$Aw = 0,$$

$$(A + F)\hat{z} = 0,$$

and

$$x^T w = x^T \hat{z},$$

then

$$w = (I + A^{\#}F)\hat{z}.$$

Proof. The result follows directly from Theorem 2.11. ■

Using the above corollary, an upper bound can be derived for the relative error term $\|w - \hat{z}\| / \|w\|$.

Corollary 2.3. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Let x be a left null vector of A and F be a matrix of order n . Let w and $\hat{z}$ be n -dimensional vectors such that

$$Aw = 0,$$

$$(A + F)\hat{z} = 0,$$

and

$$x^T w = x^T \hat{z}.$$

If $\|A^{\#}\| \|F\| < 1$, for some consistent matrix norm $\|\cdot\|$, then

$$\frac{\|w - \hat{z}\|}{\|w\|} \leq \frac{K(A)}{1 - \|A^\# \| \|F\|} \cdot \frac{\|F\|}{\|A\|}.$$

Proof. The result follows directly from Theorem 2.12 and Corollary 2.1. ■

If $x^T \hat{w} = 0$, then $\alpha = x^T w / x^T \hat{w}$ cannot be formed. The following lemma provides a condition for $x^T \hat{w} \neq 0$.

Lemma 2.8. Let A be a matrix of order n , with rank $n - 1$. Assume that zero is a simple eigenvalue of A . Let $\hat{w}$ be the solution of the homogeneous system of linear equations $(A + F)\hat{w} = 0$, where F is a matrix of order n . If $(I + A^\# F)^{-1}$ exists, then $x^T \hat{w} \neq 0$, where x is a left null vector of A .

Proof. Let y be a right null vector of A such that $x^T y = 1$.

Assume that

$$x^T \hat{w} = 0.$$

Multiplying the above equation on the left by y leads to the following equation

$$yx^T \hat{w} = 0.$$

From Lemma 2.5, it follows that $yx^T = I - A^\# A$, and thus

$$(I - A^\# A)\hat{w} = 0.$$

If $(A + F)\hat{w} = 0$, then $A\hat{w} = -F\hat{w}$. By using this result one obtains

$$(I + A^\# F)\hat{w} = 0.$$

This is a contradiction, because it was assumed that $(I + A^{\#}F)^{-1}$ exists. Therefore, it follows that $x^T \hat{w} \neq 0$. ■

The following theorem provides an explicit relationship between the left and right null vectors of A , under certain conditions.

Theorem 2.16. Let A be a matrix of order n , with rank $n - 1$.

Assume that A has a left null vector x such that $|x| > 0$. If

$y = (p_1/x_1, p_2/x_2, \dots, p_n/x_n)^T$, where $p_k = \det(A_k)$ for $k = 1, 2, \dots, n$ and A_k is the submatrix formed by deleting the k th row and the k th column of A , then

$$(1) \quad \text{adj}(A) = yx^T, \text{ and}$$

$$(2) \quad Ay = 0.$$

Proof. If rank of A is equal to $n - 1$, then $\dim N(A^T) = 1$.

Hence $N(A^T) = \langle x \rangle$. Since $\det(A) = 0$,

$$\text{adj}(A)A = 0.$$

It follows that each row of $\text{adj}(A)$ is in $N(A^T)$. Hence each row of $\text{adj}(A)$ is a scalar multiple of x . Therefore there exists a vector v such that

$$\text{adj}(A) = vx^T.$$

Thus, $(\text{adj}(A))_{k,k} = v_k x_k$, for $k = 1, 2, \dots, n$. However from the definition of $\text{adj}(A)$, it has to be the case that $v_k x_k = p_k$ for $k = 1, 2, \dots, n$. Solving for v_k yields

$$v_k = p_k/x_k \quad \text{for } k = 1, 2, \dots, n.$$

Therefore $y = v$ and $\text{adj}(A) = yx^T$.

Next, using this result together with the fact that

$$A \text{adj}(A) = 0,$$

one obtains

$$Ayx^T = 0.$$

Multiplying this equation on the right by $(1/x^T x)x$ yields

$$Ay = 0. \quad \blacksquare$$

The following example illustrates the previous theorem.

Example 2.5.

Let

$$A = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 2 \\ 3 & 3 & 0 \end{bmatrix} \quad \text{and } x = (6, 3, -2)^T.$$

Then $x^T A = 0$. Also, $p_1 = -6$, $p_2 = 3$, and $p_3 = 2$. So, applying Theorem 2.16 it follows that if $y = (1, -1, 1)^T$, then $Ay = 0$.

Theorem 2.16 would involve too much computation if it were used to compute y , but it can be used to obtain some interesting theoretical results. For instance, it can be used to derive upper and lower bounds for the condition number of the zero eigenvalue of A . If an eigenvalue of a matrix is ill-conditioned then its corresponding eigenvector will be ill-conditioned. Wilkinson [1965], p. 68 showed that $s(\lambda) = \|x\|_2 \|y\|_2 / |y^* x|$, where λ is a simple eigenvalue of A and

x and y are the eigenvectors that correspond to λ , can be considered a condition number for the eigenvalue λ . Using the same approach as Wilkinson, the term $r(\lambda) = \|x\|_{\infty} \|y_1\| / |y^T x|$ can be shown to be a condition number for the eigenvalue λ . Clearly $s(\lambda) \geq 1$ and $r(\lambda) \geq 1$.

The following theorem provides upper and lower bounds for $s(0)$ and $r(0)$.

Theorem 2.17. Let A be a matrix of order n , with rank $n - 1$.

Assume that zero is a simple eigenvalue of A . Assume that x is a left null vector of A such that $|x| > 0$. If $p_k = \det(A_k)$, where A_k is the submatrix formed by deleting the k th row and k th column of A , then

$$1) \frac{\|x\|_2}{\max_k |x_k|} \cdot \frac{\left(\sum_{k=1}^n p_k^2 \right)^{1/2}}{\left| \sum_{k=1}^n p_k \right|} \leq s(0) \leq \frac{\|x\|_2}{\min_k |x_k|} \cdot \frac{\left(\sum_{k=1}^n p_k^2 \right)^{1/2}}{\left| \sum_{k=1}^n p_k \right|} \quad (2.32)$$

and,

$$2) \frac{\sum_{k=1}^n |p_k|}{\left| \sum_{k=1}^n p_k \right|} \leq r(0) \leq \frac{\max_k |x_k|}{\min_k |x_k|} \cdot \frac{\sum_{k=1}^n |p_k|}{\left| \sum_{k=1}^n p_k \right|} \quad (2.33)$$

Proof. If $y = (p_1/x_1, p_2/x_2, \dots, p_n/x_n)^T$, then $Ay = 0$. Hence

$$y^T x = \sum_{k=1}^n p_k. \quad (2.34)$$

Using the fact that zero is a simple eigenvalue of A it follows that

$\sum_{k=1}^n p_k$ cannot equal zero. Therefore both inequalities are well defined.

1) Substituting equation (2.34) into the expression for $s(0)$ yields

$$s(0) = \frac{1}{\left| \begin{array}{c} n \\ \sum \\ k=1 \end{array} p_k \right|} \left[\sum_{k=1}^n \left(\frac{p_k}{x_k} \right)^2 \right]^{\frac{1}{2}} \|x\|_2.$$

Therefore the result (2.32) follows.

2) Substituting equation (2.34) into the expression for $r(0)$ yields

$$r(0) = \frac{1}{\left| \begin{array}{c} n \\ \sum \\ k=1 \end{array} p_k \right|} \left(\sum_{k=1}^n \left| \frac{p_k}{x_k} \right| \right) \|x\|_{\infty}.$$

Therefore the result (2.33) follows. ■

Assume that the term

$$\frac{\left(\sum_{k=1}^n |p_k|^{\ell} \right)^{1/\ell}}{\left| \begin{array}{c} n \\ \sum \\ k=1 \end{array} p_k \right|}, \text{ for } \ell = 1, 2 \quad (2.35)$$

is approximately equal to one. Then, if the vector x is known, the term $\max_k |x_k| / \min_k |x_k|$ or $\|x\|_2 / \min_k |x_k|$ might be used as an approximation to the condition number of the zero eigenvalue.

If the term (2.35) is very large, then the condition number $r(0)$ will also be too large. Therefore the zero eigenvalue will be ill-conditioned.

CHAPTER III

SINGULAR IRREDUCIBLE M-MATRICES

1. Introduction

This chapter concerns the problem of computing a right null vector of a singular irreducible M-matrix. The fundamental problem is to analyze and compute a vector y such that

$$Ay = 0 \tag{3.1}$$

where A is a singular irreducible M-matrix. M-matrices can be characterized in a large variety of ways (see Berman and Plemmons [1979], Ch. 6).

Also to be considered is the problem of computing the solution to the constrained homogeneous system of linear equations $Aw = 0$, such that $x^T w = \tau$ where x is a left null vector of A and τ is a nonzero real number.

A simple direct method is to be presented and compared to the Rank Modification Method. It will be shown that this direct method is actually a variation of the Rank Modification Method.

Theorem 3.1. (Berman and Plemmons [1979], p. 156) Let A be a singular irreducible M-matrix. Then

- (1) A has rank $n - 1$.
- (2) There exists a vector $y \gg 0$ such that $Ay = 0$.
- (3) Each principal submatrix of A other than A itself is a nonsingular M-matrix.
- (4) A is almost monotone. That is, $Ay \geq 0$ implies that $Ay = 0$.

If A is an M -matrix, then A^T is also an M -matrix. Hence there exists a vector $x \gg 0$ such that $x^T A = 0$. If A is nonsingular M -matrix, then $\det(A) > 0$ (e.g., Berman and Plemmons [1979], p. 134). Thus if A is a singular irreducible M -matrix, then zero is a simple eigenvalue of A . It is well known that, if A is a singular irreducible M -matrix, then $A^\#$ exists (see Plemmons [1976b]).

A perturbation analysis and a sensitivity analysis is performed on the homogeneous system of linear equations in Section 2. Next, a simple direct method for computing a solution to the equation $Ay = 0$ is developed in Section 3, and a complete backward error analysis is provided in Section 4. The scheme essentially corresponds to one step of inverse iteration as described in Wilkinson [1965], p. 619, for a certain eigenvector problem. In Section 5 an updating method for the proposed method is investigated. The relationship between the proposed method and the Rank Modification Method is given in Section 6. Finally, two special types of singular irreducible M -matrices will be investigated in Sections 7 and 8.

2. Perturbation Theory and Sensitivity Analysis

Assume that $A(t) = (a_{ij}(t))$ is a singular irreducible M -matrix for all t in some interval $[a, b]$, where $a_{ij}(t)$ is a differentiable function of t on the interval $[a, b]$. Let c be a fixed number in the interval $[a, b]$. Let x be a left null vector of $A(c)$. Then there exists a right null vector $y(t)$ associated with $A(t)$ for each t , such that $x^T y(t) = 1$, where

$$y(t) = (y_1(t), y_2(t), \dots, y_n(t))^T.$$

The purpose of this section is to present a simple expression for the derivative $y'(t)$ in terms of the entries $y_i(t)$, together with derivatives $\dot{a}_{ij}(t)$, and entries from $A^\#(c)$. Then using these expressions, the sensitivity of the right null vector of a singular irreducible matrix A relative to the change in the entries of A will be investigated.

The material in this section extends the recent work of Meyer [1980, 1982]. In these papers it was assumed that $A(t)$ was a column diagonally dominant M -matrix.

The following lemma provides an explicit relationship between $y(c)$ and $y(t)$.

Lemma 3.1. Assume that $A(t)$ is a singular irreducible M -matrix of order n for all $t \in [a, b]$. Let $c \in [a, b]$ and x denote a left null vector of $A(c)$. If $y(t)$ denotes the right null vector of $A(t)$, where $x^T y(t) = 1$ then for all $t \in [a, b]$,

$$y(c) = [I - A^\#(c)A(c)]y(t).$$

Proof. The rank of $A(c)$ is $n - 1$, hence $\dim N(A(c)) = 1$. Therefore $y(c)$ is unique up to a scalar multiple. From the definition of $A^\#(c)$ it follows that

$$[I - A^\#(c)A(c)]y(t) \in N(A(c)).$$

Applying Lemma 2.5, it follows that

$$I - A^\#(c)A(c) = y(c)x^T.$$

Multiplying the above equation on the left by $y(t)$ yields

$$[I - A^{\#}(c)A(c)]y(t) = y(c)x^T y(t).$$

Therefore $y(c) = [I - A^{\#}(c)A(c)]y(t)$. ■

If $y(c) = [I - A^{\#}(c)A(c)]y(t)$, then $y(c) - y(t) = [I - A^{\#}(c)A(c)]y(t) - [I - A^{\#}(c)A(t)]y(t)$, so that

$$y(c) - y(t) = -A^{\#}(c)[A(c) - A(t)]y(t).$$

Assume that $t \neq c$, then

$$\frac{y(c) - y(t)}{c - t} = -A^{\#}(c) \frac{A(c) - A(t)}{c - t} y(t).$$

If $A(t)$ is differentiable on the interval $[a, b]$, then $y(t)$ is a continuous function of t on $[a, b]$ (see Ortega [1972], p. 45). Thus taking the limit of the above equation as t approaches c yields

$$\lim_{t \rightarrow c} \frac{y(c) - y(t)}{c - t} = -A^{\#}(c)A'(c)y(c).$$

Therefore $y'(c)$ exists, and

$$y'(c) = -A^{\#}(c)A'(c)y(c). \quad (3.1)$$

The following theorem provides an expression for the derivative $y'(t)$, if it exists.

Theorem 3.2. Assume that $A(t)$ is a singular irreducible M-matrix of order n for all $t \in [a, b]$ and that $A(t)$ is a differentiable function of t on $[a, b]$. Let $c \in [a, b]$ and x denote a left null vector of $A(c)$.

Let $y(t)$ denote the right null vector of $A(t)$, where $x^T y(t) = 1$ for all $t \in [a, b]$. If $y'(t)$ exists, then

$$[I + A^\#(c)(A(t) - A(c))]y'(t) = -A^\#(c)A'(t)y(t).$$

Furthermore, if $[I + A^\#(c)(A(t) - A(c))]^{-1}$ exists, then

$$y'(t) = -[I + A^\#(c)(A(t) - A(c))]^{-1}A^\#(c)A'(t)y(t).$$

Proof. Applying Lemma 3.1 it follows that

$$y(c) = [I - A^\#(c)A(c)]y(t).$$

By assumption $A(t)y(t) = 0$, hence

$$y(c) = [I + A^\#(c)(A(t) - A(c))]y(t).$$

Differentiating this equation with respect to t yields

$$0 = A^\#(c)A'(t)y(t) + [I + A^\#(c)(A(t) - A(c))]y'(t),$$

so that

$$[I + A^\#(c)(A(t) - A(c))]y'(t) = -A^\#(c)A'(t)y(t).$$

Therefore, if $[I + A^\#(c)(A(t) - A(c))]^{-1}$ exists, then

$$y'(t) = -[I + A^\#(c)(A(t) - A(c))]^{-1}A^\#(c)A'(t)y(t). \quad \blacksquare$$

Corollary 3.1. Assume that $A(t)$ and $y(t)$ satisfy the hypothesis of Theorem 3.2. Then

$$y'(t) = [y(c)x^T + A^\#(c)A(t)]^{-1}A^\#(c)A'(t)y(t).$$

Proof. This result follows directly from Theorem 3.2, and the fact that $I - A^{\#}(c)A(c) = y(c)x^T$. ■

Corollary 3.2. Assume that $A(t)$ and $y(t)$ satisfy the hypothesis of Theorem 3.2. If $\|A^{\#}(c)\| \|A(t) - A(c)\| < 1$, for some consistent matrix norm $\|\cdot\|$, then

$$\frac{\|y'(t)\|}{\|y(t)\|} \leq \frac{K(A(c))}{1 - \|A^{\#}(c)\| \|A(t) - A(c)\|} \cdot \frac{\|A'(t)\|}{\|A(c)\|}$$

where $K(A(c)) = \|A(c)\| \|A^{\#}(c)\|$.

Proof. If $\|A^{\#}(c)\| \|A(t) - A(c)\| < 1$, then $[I + A^{\#}(c)(A(t) - A(c))]^{-1}$ exists. Thus, by applying Theorem 3.2, it follows that

$$y'(t) = -[I + A^{\#}(c)(A(t) - A(c))]^{-1} A^{\#}(c) A'(t) y(t),$$

hence

$$\frac{\|y'(t)\|}{\|y(t)\|} \leq \| [I + A^{\#}(c)(A(t) - A(c))]^{-1} \| \|A^{\#}(c)\| \|A'(t)\|.$$

Using the inequality $\|(I + B)^{-1}\| \leq 1/(1 - \|B\|)$, the result follows. ■

Therefore, if $K(A(c))$ is small and the term $\|A'(t)\| / \|A(c)\|$ is small, then $y(t)$ should have a relatively small derivatives. In particular, using Lemma 3.2 it follows that

$$\frac{\|y'(c)\|}{\|y(c)\|} \leq K(A(c)) \frac{\|A'(c)\|}{\|A(c)\|}.$$

Next, the sensitivity of the i th component of $y(c)$ is investigated. Multiplying equation (3.1) on the left by e_i^T leads to the following equation for the derivative $y_i'(c)$

$$y_i'(c) = A_i^\#(c)A'(c)y(c) \quad (3.2)$$

where $A_i^\#(c)$ denotes row i of $A^\#(c)$. Taking the absolute value of both sides of equation (3.2), and using some basic properties of norms it follows that

$$\frac{|y_i'(c)|}{\|y(c)\|_\infty} \leq \|A_i^\#(c)\|_1 \|A'(c)\|_1.$$

Therefore the sensitivity of the i th component of $y(c)$ to small perturbations $A(c)$ is directly governed by i th row of $A^\#(c)$.

Let A be a singular irreducible M -matrix of order n . Let x and y denote left and right null vectors of A such that $x^T y = 1$. Assume $B(t)$ is a matrix of order n such that $B(0) = 0$ and $A + B(t)$ is a differentiable singular irreducible M -matrix for all $t \in [a, b]$ where $ab \leq 0$. Let $y(t)$ denote the right null vector of $A + B(t)$ such that $x^T y(t) = 1$ for all $t \in [a, b]$. Applying Lemma 3.1, it follows that

$$y = [I - A^\# A]y(t) \quad t \in [a, b].$$

If $(A + B(t))y(t) = 0$, then $Ay(t) = -B(t)y(t)$. Hence

$$y = [I - A^\# B(t)]y(t).$$

Applying Theorem 3.2, an expression for the derivative of $y(t)$ can be found, where

$$y'(t) = -[I + A^{\#}B(t)]^{-1}A^{\#}B'(t)y(t).$$

In particular,

$$y'(0) = -A^{\#}B'(0)y(0).$$

Using the fact that $y = y(0)$ it follows that

$$y'(0) = -A^{\#}B'(0)y. \quad (3.3)$$

Taking the norm of both sides of the equation (3.3) it follows that

$$\frac{\|y'(0)\|}{\|y\|} \leq K(A) \cdot \frac{\|B'(0)\|}{\|A\|}.$$

Therefore the sensitivity of the problem of computing a vector y such that $Ay = 0$ and $x^T y = 1$, is governed by the term $K(A) = \|A\| \|A^{\#}\|$.

3. Partition Factorization Method

The method to be presented is a simple direct algorithm which was first suggested by Funderlic and Mankin [1981].

The direct solution of a system of linear equations generally involves some variation of Gaussian elimination. It is well known that an arbitrary matrix does not have an LU-decomposition, but for any matrix A there exists a permutation matrix P such that PA has an LU-decomposition. Therefore one must often use Gaussian elimination with row interchanges to ensure the completion of the algorithm. These permutations increase the time required to complete the algorithm, and if the matrix A has some special structure, the matrix PA may not. Therefore this type of pivoting should be avoided if possible.

If A is a nonsingular M -matrix, then A can be factored into $A = LU$, where L and U are lower and upper triangular M -matrices, respectively (see Fiedler and Pták [1962]). The following theorem is an extension of the above statement.

Theorem 3.3. (Funderlic and Plemmons [1981]) Let A be a M -matrix of order n , with the property that $x^T A \geq 0$ for some vector $x \gg 0$. Then for any permutation matrix P there exists a lower triangular M -matrix L with unit diagonal and an upper triangular M -matrix U such that

$$PAP^T = LU.$$

Therefore, if A is a large sparse singular M -matrix, with the property that $x^T A \geq 0$ for some vector $x \gg 0$, then a symmetric ordering scheme could be applied to A so that fill-in is reduced in the LU-decomposition process.

If A is a singular irreducible M -matrix, then there exists a vector $x \gg 0$ such that $x^T A = 0$. Thus, for any permutation matrix P , PAP^T has an LU-decomposition.

Usually some form of pivoting is required to ensure numerical stability when Gaussian elimination is applied to a matrix A . Set $A^{(1)} = A$ and let $A^{(k)}$ denote the result of the first $k - 1$ steps of Gaussian elimination applied to A , that is,

$$A^{(k)} = \left[\begin{array}{ccc} a_{11}^{(1)} & \text{---} & a_{1,k-1}^{(1)} & a_{1k}^{(1)} & \text{---} & a_{1n}^{(1)} \\ & \diagdown & | & | & & | \\ & & a_{k-1,k-1}^{(k-1)} & a_{k-1,k}^{(k-1)} & \text{---} & a_{k-1,n}^{(k-1)} \\ & & & & & \\ & & \bigcirc & & & \\ & & & a_{kk}^{(k)} & \text{---} & a_{kn}^{(k)} \\ & & & | & & | \\ & & & a_{nk}^{(k)} & \text{---} & a_{nn}^{(k)} \end{array} \right].$$

Gaussian elimination applied to some matrix A is a stable algorithm only when the elements of $A^{(k)}$ do not grow excessively during the course of the reduction. The growth factor g_A for Gaussian elimination on A is defined by

$$g_A = (\max_{i,j,k} |a_{ij}^{(k)}|) / (\max_{i,j} |a_{ij}|) \quad (3.4)$$

Hence, if Gaussian elimination applied to A is a stable algorithm, then the growth factor g_A will be small.

Suppose $x^T A \geq 0$ for some vector $x \gg 0$, and let

$$\beta_x = (\max_k x_k) / (\min_k x_k). \quad (3.5)$$

Then the following theorem establishes upper bounds on the entries l_{ij} and u_{ij} in terms of β_x .

Theorem 3.4. (Funderlic, et al [1982]) Let A be an M -matrix with the property that $x^T A \geq 0$ for some vector $x \gg 0$. If P is a permutation matrix, then PAP^T has an LU-decomposition, $PAP^T = LU$, where for all

$$1 \leq i, j \leq n,$$

$$1) \quad |l_{ij}| \leq \beta_x \quad \text{for } i, j = 1, 2, \dots, n,$$

$$2) \quad |u_{ij}| \leq \beta_x \max_k a_{kk} \quad \text{for } i, j = 1, 2, \dots, n.$$

Hence $g_A \leq \beta_x$, where β_x is given by (3.5).

Therefore, if x is given, or if some approximation to x has been computed, then β_x can be used to determine a sufficient condition for Gaussian elimination applied to A to be a stable algorithm.

The following simple algorithm can be used to compute a right null vector of a singular irreducible M-matrix.

Direct Factorization Method

Assume that A is a singular irreducible M-matrix. Then the following algorithm can be used to compute the vector y such that $Ay = 0$ and $y_n = 1$.

1. Apply Gaussian elimination to the matrix A , forming the factorization

$$A = LU.$$

2. Let

$$\bar{U} = \begin{bmatrix} u_{11} & u_{12} & \text{---} & u_{1,n-1} & u_{1n} \\ & u_{22} & \text{---} & u_{2,n-1} & u_{2n} \\ & & \diagdown & & \\ & \bigcirc & & u_{n-1,n-1} & u_{n-1,n} \\ & & & & 1 \end{bmatrix}. \quad (3.6)$$

3. Solve $\bar{U}y = e_n$ by back substitution.

The matrix $\bar{U}$ in step 2 of the algorithm can be written as

$$\bar{U} = U + e_n e_n^T.$$

Substituting this equation for $\bar{U}$ into the equation $\bar{U}y = e_n$ yields

$$(U + e_n e_n^T)y = e_n.$$

Thus, it follows that

$$Uy + (e_n^T y)e_n = e_n. \quad (3.7)$$

Clearly the back substitution of step 3 produces a vector y such that $y_n = 1$, hence $e_n^T y = 1$. Using this fact, equation (3.7) can be written as

$$Uy = 0.$$

Multiplying this equation on the left by L leads to the equation

$$LUy = 0,$$

or

$$Ay = 0.$$

Therefore the Direct Factorization Method produces a vector y such that $Ay = 0$, $y \gg 0$, and $y_n = 1$.

The above method does not use any form of pivoting, hence the elements of L and U could be quite large compared to the elements of A . Assume that this algorithm is executed on a machine, using floating point arithmetic with unit roundoff error μ . Then a simple backward

error analysis, using Reid [1971] and Stewart [1973], p. 150, shows that the computed solution $\hat{y}$ to $Ay = 0$ satisfies exactly a perturbed homogeneous system of linear equations $(A + E)\hat{y} = 0$.

Theorem 3.5. Let A be a singular irreducible M-matrix of order n . Suppose that the homogeneous system of linear equations $Ay = 0$ is solved for the positive vector y by applying Gaussian elimination to A without pivoting, using floating point arithmetic with unit roundoff error μ . Then there exists a matrix $E = (e_{ij})$ such that the computed solution $\hat{y}$ to $Ay = 0$ satisfies exactly the homogeneous system

$$(A + E)\hat{y} = 0 \quad (3.8)$$

such that for $1 \leq i, j \leq n$,

$$|e_{ij}| \leq \mu n(3.01 + 1.01(n+1) \max_{i,j} |\hat{\ell}_{ij}|) \max_{i,j,k} |\hat{a}_{ij}^{(k)}| \quad (3.9)$$

where $A = LU$ is the LU-decomposition of A , $\hat{\ell}_{ij}$ is the i, j entry in the floating version of L , and $\hat{a}_{ij}^{(k)}$ is the i, j entry in the floating version of $A^{(k)}$.

Proof. Consider the LU-decomposition of A by Gaussian elimination without pivoting. From Reid [1971], there exist a matrix $F = (f_{ij})$ such that the computed factors $\hat{L}$ and $\hat{U}$ satisfy

$$A + F = \hat{L}\hat{U}$$

where for all $1 \leq i, j \leq n$,

$$|f_{ij}| \leq \begin{cases} 2.01 \mu(i-1) \max_{i,j,k} |\hat{a}_{ij}^{(k)}| & \text{if } j \geq i, \\ 2.01 \mu j \max_{i,j,k} |\hat{a}_{ij}^{(k)}| & \text{if } j < i. \end{cases}$$

Thus by combining these inequalities in terms of i , it follows that

$$|f_{ij}| \leq 3.01 \mu n \max_{i,j,k} |\hat{a}_{ij}^{(k)}|. \quad (3.10)$$

The algorithm for the LU-decomposition of A by Gaussian eliminations yields

$$\hat{U} = \begin{bmatrix} \hat{u}_{11} & \hat{u}_{12} & \cdots & \hat{u}_{1,n-1} & \hat{u}_{1n} \\ & \hat{u}_{22} & \cdots & \hat{u}_{2,n-1} & \hat{u}_{2n} \\ & & \ddots & & \\ & & & \hat{u}_{n-1,n-1} & \hat{u}_{n-1,n} \\ & & & & 0 \end{bmatrix}.$$

Let

$$\hat{\hat{U}} = \begin{bmatrix} \hat{u}_{11} & \hat{u}_{12} & \cdots & \hat{u}_{1,n-1} & \hat{u}_{1n} \\ & \hat{u}_{22} & \cdots & \hat{u}_{2,n-1} & \hat{u}_{2n} \\ & & \ddots & & \\ & & & \hat{u}_{n-1,n-1} & \hat{u}_{n-1,n} \\ & & & & 1 \end{bmatrix}.$$

If the system of linear equations $\bar{U}y = e_n$ is solved using $\hat{\hat{U}}$, by back substitution in step 3, then by Stewart [1975], p. 150, there

exists a matrix $G = (g_{ij})$ such that the computed solution $\hat{y}$ to the linear system $\bar{U}y = e_n$ satisfies exactly the system

$$(\hat{U} + G)\hat{y} = e_n \quad (3.11)$$

where $1 \leq i, j \leq n$,

$$|g_{ij}| \leq 1.01 \mu(n+1) \max_{i,j} |\hat{u}_{ij}|.$$

Since $|\hat{u}_{ij}| \leq \max_{i,j,k} |\hat{a}_{ij}^{(k)}|$, it follows that

$$|g_{ij}| \leq 1.01 \mu(n+1) \max_{i,j,k} |\hat{a}_{ij}^{(k)}|. \quad (3.12)$$

Multiplying equation (3.11) on the left by L leads to

$$(\hat{L}\hat{U} + \hat{L}G)\hat{y} = \hat{L}e_n = e_n.$$

Since

$$\hat{L}\hat{U} = \hat{L}\hat{U} + e_n e_n^T$$

and $\hat{y}_n = 1$, it follows that

$$(\hat{L}\hat{U} + \hat{L}G)\hat{y} = 0.$$

Thus $\hat{y}$ satisfies the homogeneous system of linear equations

$$(A + F + \hat{L}G)\hat{y} = 0.$$

Let $E = F + \hat{L}G$, then

$$(A + E)\hat{y} = 0.$$

Then for each i and j , it follows that

$$|e_{ij}| \leq |f_{ij}| + \sum_{k=1}^i |\hat{\ell}_{ik}| |g_{kj}|,$$

thus

$$|e_{ij}| \leq |f_{ij}| + i \max_{i,j} |\hat{\ell}_{ij}| \max_{i,j} |g_{ij}|.$$

Applying (3.10) and (3.13), it follows that

$$|e_{ij}| \leq \mu n(3.01 + 1.01(n+1) \max_{i,j} |\hat{\ell}_{ij}|) \max_{i,j,k} |\hat{a}_{ij}^{(k)}|. \quad \blacksquare$$

Next, the general algorithm for computing a right null vector of a singular irreducible M-matrix will be developed. It was stated earlier that any irreducible singular M-matrix has the property that for each permutation matrix P , PAP^T has an LU-decomposition $PAP^T = LU$, where L is an M-matrix with unit diagonal, and where U is an M-matrix.

Let A_k denote the principal submatrix obtained by deleting the k th row and k th column of A . Accordingly, let P denote the permutation matrix such that PAP^T has the partitioned form

$$PAP^T = \begin{bmatrix} A_k & y_k \\ z_k^T & a_{kk} \end{bmatrix}. \quad (3.14)$$

Here A_k is an $(n-1) \times (n-1)$ nonsingular M-matrix, this follows from Theorem 3.1. The vectors z_k and y_k are $(n-1)$ -dimensional vectors with nonpositive entries.

Let $B = PAP^T$. Then the LU-decomposition of B can be written in the following partitioned form

$$B = \begin{bmatrix} L_k & 0 \\ \ell_k^T & 1 \end{bmatrix} \begin{bmatrix} U_k & u_k \\ 0 & 0 \end{bmatrix} \quad (3.15)$$

where L_k and U_k are $(n-1) \times (n-1)$ nonsingular M-matrices. The vectors ℓ_k and u_k are $(n-1)$ -dimensional vectors with nonpositive entries.

Multiplying together the factors in (3.15), it follows that

$$B = \begin{bmatrix} L_k U_k & L_k u_k \\ \ell_k^T U_k & \ell_k^T u_k \end{bmatrix}. \quad (3.16)$$

Using the partitioned form of B in (3.14) yields the following equations

$$A_k = L_k U_k, \quad (3.17)$$

$$u_k = L_k^{-1} y_k, \quad (3.18)$$

and

$$\ell_k^T = z_k^T U_k^{-1}. \quad (3.19)$$

If $Ay = 0$, then $PAP^T(Py) = 0$. Let $s = Py$, thus it follows that

$$Bs = 0.$$

Applying the equation $B = LU$, it follows that

$$LU s = 0. \quad (3.20)$$

Multiplying (3.20) on the left by L^{-1} yields

$$Us = 0. \quad (3.21)$$

The vector s can be written in the following partitioned form

$$s = \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}$$

where s_1 is an $(n - 1)$ -dimensional vector and s_2 is a scalar. Using this partitioned form of s and the partitioned form of U , equation (3.21) can be written as

$$\begin{bmatrix} U_k & u_k \\ 0 & 0 \end{bmatrix} \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

This is equivalent to the following system of linear equations

$$U_k s_1 + u_k s_2 = 0.$$

Solving for s_1 leads to

$$s_1 = -s_2 U_k^{-1} u_k. \quad (3.22)$$

Substituting equation (3.18) into (3.22) yields

$$s_1 = -s_2 U_k^{-1} L_k^{-1} y_k.$$

If $A_k = L_k U_k$, then $A_k^{-1} = U_k^{-1} L_k^{-1}$. Therefore

$$s_1 = -s_2 A_k^{-1} y_k$$

or

$$A_k s_1 = -s_2 y_k.$$

Setting $s_2 = 1$ yields

$$A_k s_1 = -y_k. \quad (3.23)$$

The following general scheme for computing y is based upon the system of linear equations (3.23).

Partition Factorization Method

Assume that A is a singular irreducible M -matrix. The following algorithm can be used to compute the right null vector y , of A , such that $y_k = 1$ for some k .

1. Choose k such that $1 \leq k \leq n$ and partition A into the form (3.14).
2. Solve $A_k s_1 = -y_k$, by applying Gaussian elimination to A_k without pivoting.
3. Set $y = P^T \begin{pmatrix} s_1 \\ 1 \end{pmatrix}$.

The Partition Factorization Method is mathematically the same as the Direct Factorization Method applied to PAP^T given by (3.14). This is true because the matrix $\bar{U}$ given by (3.6) in the Direct Factorization Method has the partitioned form

$$\bar{U} = \begin{bmatrix} U_k & L_k^{-1} y_k \\ 0 & 1 \end{bmatrix}.$$

Thus the backward error analysis given in Theorem 3.5 for the Direct Factorization Method also holds for the Partition Factorization Method.

There are some possible advantages to the flexibility of choosing an arbitrary submatrix A_k to factorize in the solution process for y . First, one might choose an A_k having a particular sparsity pattern. For example, if A has a dense row, then it could be excluded from the solution process. Secondly, the condition number $\|A_k\| \|A_k^{-1}\|$ may differ widely for $1 \leq k \leq n$, so one might expect better numerical results if a well-conditioned A_k were chosen. The following example illustrates the second observation.

Example 3.1

$$\text{Let } A = \begin{pmatrix} .5 & -.25 & -\epsilon \\ -.25 & .5 & -\epsilon \\ -.25 & -.25 & 2\epsilon \end{pmatrix}, \text{ where } 0 < \epsilon < \frac{1}{2}.$$

Clearly $e^T A = 0$, so it follows that A is a singular irreducible M-matrix.

$$(1) \text{ Let } A_1 = \begin{pmatrix} .5 & -\epsilon \\ -.25 & 2\epsilon \end{pmatrix}, \text{ then } A_1^{-1} = \frac{4}{3\epsilon} \begin{pmatrix} 2\epsilon & \epsilon \\ .25 & .5 \end{pmatrix}.$$

$$\text{So } \|A_1\|_1 = .75, \quad \|A_1^{-1}\|_1 = \frac{4}{3\epsilon} (.5 + \epsilon) \text{ and}$$

$$\|A_1\|_1 \|A_1^{-1}\|_1 = \frac{1}{\epsilon} (.5 + \epsilon).$$

$$(2) \text{ Let } A_3 = \begin{pmatrix} .5 & -.25 \\ -.25 & .5 \end{pmatrix}, \text{ then } A_3^{-1} = \frac{16}{3} \begin{pmatrix} .5 & .25 \\ .25 & .5 \end{pmatrix}.$$

$$\text{So } \|A_3\|_1 = .75, \quad \|A_3^{-1}\|_1 = 4 \text{ and } \|A_3\|_1 \|A_3^{-1}\|_1 = 3.$$

Thus, if ϵ is small enough, then $\|A_1\|_1 \|A_1^{-1}\|_1$ will be significantly larger than $\|A_3\|_1 \|A_3^{-1}\|_1$. In fact, as $\epsilon \rightarrow 0$, $\|A_1\|_1 \|A_1^{-1}\|_1$ becomes unbounded and $\|A_3\|_1 \|A_3^{-1}\|_1$ remains constant.

Suppose that one wishes to compute the solution to the constrained homogeneous system of linear equations $Aw = 0$, such that $b^T w = \tau$. Then the Partition Factorization Method can be used to compute w . When the Partition Factorization Method is applied to the problem the result is a vector y such that $Ay = 0$ and $y_k = 1$, for some k . The inner product $b^T w$ is to zero if and only if $b^T y$ is equal to zero. Hence, if $b^T y \neq 0$, then setting $w = (\tau/b^T y)y$ results in the solution to the homogeneous system of linear equations $Aw = 0$ such that $b^T w = \tau$. If $b^T y = 0$, then a solution exists to the constrained system if and only if $\tau = 0$.

4. Error Analysis for the Partition Factorization Method

Suppose that the Partition Factorization Method is executed on a machine, using floating point arithmetic with unit roundoff error μ . Let $\hat{w}^{(k)}$ denote the computed solution, where A_k was the submatrix used in step 2 of the algorithm. Then $\hat{w}^{(k)}$ is an approximation to the solution of the homogeneous linear system $Aw^{(k)} = 0$, where the k th entry in the vector $w^{(k)}$ is equal to one. Thus, by applying Theorem 3.5, it follows that $\hat{w}^{(k)}$ satisfies exactly the homogeneous system

$$(A + E)\hat{w}^{(k)} = 0, \quad (3.24)$$

where the matrix E is given in Theorem 3.5.

Let P denote the permutation matrix such that PAP^T has the following partitioned form (3.14), i.e.,

$$PAP^T = \begin{pmatrix} A_k & y_k \\ z_k^T & a_{kk} \end{pmatrix}.$$

Here A_k is the principal submatrix formed by deleting the k th row and k th column of A . The vectors y_k and z_k are $(n - 1)$ -dimensional vectors with nonpositive entries. The matrix PEP^T can be written in the following partitioned form

$$PEP^T = \begin{pmatrix} E_k & h_k \\ f_k^T & e_{kk} \end{pmatrix}. \quad (3.25)$$

Multiplying equation (3.24) on the left by P yields the following equation

$$(PA + PE)\hat{w}^{(k)} = 0. \quad (3.26)$$

Using the fact that $P^T P = I$, equation (3.26) can be written as

$$(PAP^T + PEP^T)\hat{s} = 0 \quad (3.27)$$

where $\hat{s} = P\hat{w}^{(k)}$.

The vector $\hat{s}$ can be partitioned into the following form

$$\hat{s} = \begin{pmatrix} \hat{s}_1 \\ 1 \end{pmatrix}. \quad (3.28)$$

Here $\hat{s}_1$ is an $(n - 1)$ -dimensional vector. Substituting equations (3.14), (3.25), and (3.28) into equation (3.27) it follows that

$$\left[\begin{pmatrix} A_k & y_k \\ z_k^T & a_{kk} \end{pmatrix} + \begin{pmatrix} E_k & h_k \\ f_k^T & e_{kk} \end{pmatrix} \right] \begin{pmatrix} \hat{s}_1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

so that

$$\begin{pmatrix} A_k + E_k & y_k + h_k \\ z_k^T + f_k^T & a_{kk} + e_{kk} \end{pmatrix} \begin{pmatrix} \hat{s}_1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (3.29)$$

Clearly it follows that

$$(A_k + E_k) \hat{s}_1 = -(y_k + h_k). \quad (3.30)$$

Let $s = Pw^{(k)}$. The vector s can be written in the following partitioned form

$$s = \begin{pmatrix} s_1 \\ 1 \end{pmatrix} \quad (3.31)$$

where s_1 is an $(n - 1)$ -dimensional vector with positive entries. The homogeneous linear system of equations $Aw^{(k)} = 0$, can be written as

$$(PAP^T)s = 0. \quad (3.32)$$

Substituting equations (3.14) and (3.31) into (3.32) leads to

$$\begin{pmatrix} A_k & y_k \\ z_k^T & a_{kk} \end{pmatrix} \begin{pmatrix} s_1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (3.33)$$

Clearly it follows that

$$A_k s_1 = -y_k.$$

Using the above expressions an upper bound can be derived for the relative error formed by using $\hat{w}^{(k)}$ as an approximation to the exact solution $w^{(k)}$, i.e., the term

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} \quad \text{for } \ell = 1, 2. \quad (3.34)$$

Let x denote a left null vector of A , and $p_k = \det(A_k)$, for $k = 1, 2, \dots, n$. If $y = (p_1/x_1, \dots, p_n/x_n)^T$, then by applying Theorem 2.15 it follows that $Ay = 0$. Also, by the uniqueness of the vector y it follows that

$$w^{(k)} = \frac{x_k}{p_k} y. \quad (3.35)$$

If b is an n -dimensional vector, and Q is a permutation matrix of order n , then

$$\|Qb\|_\ell = \|b\|_\ell \quad \text{for } \ell = 1, 2.$$

Using this fact, it follows that

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} = \frac{\|Pw^{(k)} - P\hat{w}^{(k)}\|_\ell}{\|Pw^{(k)}\|_\ell} \quad \text{for } \ell = 1, 2,$$

hence

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} = \frac{\|s - \hat{s}\|_\ell}{\|s\|_\ell} \quad \text{for } \ell = 1, 2.$$

Applying equations (3.28) and (3.31), it follows that

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} = \frac{\|s_1 - \hat{s}_1\|_\ell}{\|s\|_\ell} \quad \text{for } \ell = 1, 2,$$

so that

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} = \frac{\|s_1\|_\ell}{\|s\|_\ell} \cdot \frac{\|s_1 - \hat{s}_1\|_\ell}{\|s_1\|_\ell} \quad \text{for } \ell = 1, 2. \quad (3.36)$$

Using equations (3.31) and (3.35) an explicit expression can be derived for $\|s_1\|_\ell / \|s\|_\ell$, that is,

$$\frac{\|s_1\|_\ell}{\|s\|_\ell} = \frac{\left[\sum_{j \neq k}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}}{\left[\sum_{j=1}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}} \quad \text{for } \ell = 1, 2. \quad (3.37)$$

Substituting equation (3.37) into equation (3.36) leads to

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} = \frac{\left[\sum_{j \neq k}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}}{\left[\sum_{j=1}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}} \cdot \frac{\|s_1 - \hat{s}_1\|_\ell}{\|s_1\|_\ell} \quad \text{for } \ell = 1, 2. \quad (3.38)$$

The term

$$\frac{\|s_1 - \hat{s}_1\|_\ell}{\|s_1\|_\ell} \quad \text{for } \ell = 1, 2,$$

is the relative error formed by using $\hat{s}_1$ as an approximation to s_1 .

Hence using standard perturbation analysis on the system of linear equations $A_k s_1 = -y_k$, and equation (3.30), and assuming that

$\|A_k^{-1}\|_\ell \|E_k\|_\ell < 1$ for $\ell = 1, 2$, it follows that

$$\frac{\|s_1 - \hat{s}_1\|_\ell}{\|s_1\|_\ell} \leq \frac{K_\ell(A_k)}{1 - \|A_k^{-1}\|_\ell \|E_k\|_\ell} \left[\frac{\|E_k\|_\ell}{\|A_k\|_\ell} + \frac{\|h_k\|_\ell}{\|y_k\|_\ell} \right] \quad \text{for } \ell = 1, 2,$$

where $K_\ell(A_k) = \|A_k\|_\ell \|A_k^{-1}\|_\ell$.

Applying the above inequality to equation (3.38) yields

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} \leq \frac{\left[\sum_{j \neq k}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}}{\left[\sum_{j=1}^n \left(\frac{p_j}{x_j} \right)^\ell \right]^{1/\ell}} \frac{K_\ell(A_k)}{1 - \|A_k^{-1}\|_\ell \|E_k\|_\ell} \left[\frac{\|E_k\|_\ell}{\|A_k\|_\ell} + \frac{\|h_k\|_\ell}{\|y_k\|_\ell} \right]$$

for $\ell = 1, 2.$ (3.39)

Clearly $\|s_1\|_\ell / \|s\|_\ell < 1$, thus

$$\frac{\|w^{(k)} - \hat{w}^{(k)}\|_\ell}{\|w^{(k)}\|_\ell} < \frac{K_\ell(A_k)}{1 - \|A_k^{-1}\|_\ell \|E_k\|_\ell} \left[\frac{\|E_k\|_\ell}{\|A_k\|_\ell} + \frac{\|h_k\|_\ell}{\|y_k\|_\ell} \right] \quad \text{for } \ell = 1, 2.$$

(3.40)

This inequality indicates that different submatrices A_k could yield results that vary significantly in terms of accuracy. Therefore $K_\ell(A_k)$ could be considered a condition number for the problem of computing the solution to the homogeneous system of linear equations $Aw = 0$, where $w_k = 1$, using the Partition Factorization Method.

The following theorem provides an upper bound for the smallest singular value of A_k .

Theorem 3.6. Let A be a matrix of order n . Let A_k denote the principal submatrix formed by deleting the k th row and k th column of A . If σ_{n-1} denotes the second smallest singular value of A and $\alpha_{n-1}^{(k)}$ denotes the smallest singular value of A_k , then

$$\alpha_{n-1}^{(k)} \leq \sigma_{n-1}.$$

Proof. Without loss of generality it will be assume that $k = n$.

Then A can be written in the following partitioned form

$$A = \begin{pmatrix} A_n & y_n \\ z_n^T & a_{nn} \end{pmatrix}. \quad (3.41)$$

Multiplying (3.41) on the left by A^T , and using the partitioned form of A , it follows that

$$A^T A = \begin{pmatrix} A_n^T A_n + z_n z_n^T & A_n^T y_n + a_{nn} z_n \\ y_n^T A_n + a_{nn} z_n^T & a_{nn}^2 + y_n^T y_n \end{pmatrix}.$$

Let $\sigma(A^T A) = \{\sigma_k^2\}_{k=1}^n$ where

$$0 \leq \sigma_n \leq \sigma_{n-1} \leq \dots \leq \sigma_1,$$

$\sigma(A_{nn}^T A_{nn}) = \{\alpha_k^2\}_{k=1}^{n-1}$ where

$$0 \leq \alpha_{n-1} \leq \alpha_{n-2} \leq \dots \leq \alpha_1, \text{ and}$$

$\sigma(A_n^T A_n + z_n z_n^T) = \{\gamma_k^2\}_{k=1}^{n-1}$ where

$$0 \leq \gamma_{n-1} \leq \gamma_{n-2} \leq \dots \leq \gamma_1.$$

The matrix $A_{nn}^T A_{nn} + z_n z_n^T$ is a principal leading submatrix of the symmetric matrix $A^T A$, therefore

$$0 \leq \sigma_n \leq \gamma_{n-1} \leq \sigma_{n-1} \leq \dots \leq \gamma_1 \leq \sigma_1. \quad (3.42)$$

Also, applying the results found on pages 97-98 in Wilkinson [1965], it follows that

$$\gamma_j^2 - \alpha_j^2 = m_j (z_n^T z_n) \quad \text{for } j = 1, 2, \dots, n-1$$

where $0 \leq m_k \leq 1$ and $\sum_{k=1}^{n-1} m_k = 1$. Hence

$$\alpha_j \leq \gamma_j \quad \text{for } j = 1, 2, \dots, n-1. \quad (3.43)$$

Applying (3.42) it follows that

$$0 \leq \alpha_j \leq \gamma_j \leq \sigma_j \quad \text{for } j = 1, 2, \dots, n-1,$$

or

$$0 \leq \alpha_j \leq \sigma_j \quad \text{for } j = 1, 2, \dots, n-1.$$

In particular, if $j = n-1$, then

$$0 \leq \alpha_{n-1} \leq \sigma_{n-1}.$$

Therefore the result follows. ■

If A is a singular irreducible M -matrix, then $\sigma_{n-1} > 0$, and $\alpha_{n-1}^{(k)} > 0$ for $k = 1, 2, \dots, n$. If σ_{n-1} is very small, then $\alpha_{n-1}^{(k)}$ will be close to zero for $k = 1, 2, \dots, n$. Therefore each submatrix A_k would be nearly singular. The following theorem provides a lower bound for $K_2(A_k)$ for $k = 1, 2, \dots, n$.

Theorem 3.7. Let A be a singular irreducible M -matrix, and A_k denote the principal submatrix formed by deleting the k th row and k th column of A . Then

$$\frac{\max_{j \neq k} \left[\sum_{\ell \neq k} a_{\ell j}^2 \right]^{1/2}}{\sigma_{n-1}} \leq K_2(A_k) \quad \text{for } k = 1, 2, \dots, n,$$

where σ_{n-1} denotes the second smallest singular value of A and

$$K_2(A_k) = \|A_k\|_2 \|A_k^{-1}\|_2.$$

Proof. If $\alpha_{n-1}^{(k)}$ denotes the smallest singular value of A_k , then $\|A_k^{-1}\|_2 = 1/\alpha_{n-1}^{(k)}$. Applying Theorem 3.6, it follows that

$$\frac{1}{\sigma_{n-1}} \leq \|A_k^{-1}\|_2. \quad (3.44)$$

If B is a square matrix, and b_j denotes the j th column of B , then $\max_j \|b_j\|_2 \leq \|B\|_2$. Hence

$$\max_{j \neq k} \left[\sum_{\ell \neq k} a_{\ell j}^2 \right]^{1/2} \leq \|A_k\|_2 \quad (3.45)$$

Therefore the result follows by combining inequalities (3.44) and (3.45). ■

Thus, if the second smallest singular value of A is very small,

and the term $\max_{j \neq k} \left[\sum_{\ell \neq k} a_{\ell j}^2 \right]^{1/2}$ is not small, then $K_2(A_k)$ will be large

for $k = 1, 2, \dots, n$.

Now returning to the inequality for the relative error, it can be easily seen that if σ_{n-1} is very small, then poor results could be

expected no matter which submatrix is used. This is exactly what has been observed in the numerical computations (see Chapter IV).

5. Updating the Partition Factorization Method

The material to be presented in this section is an extension of recent work by Funderlic and Mankin [1981].

Assume that the solution w to the homogeneous system of linear equations $Aw = 0$ has been computed using the Partition Factorization Method, with $k = n$, so that the n th component of w is equal to one.

Suppose that the n th column of A is modified so that the updated matrix A' remains a singular M-matrix. Let w' denote a solution to the homogeneous system of linear equations $A'w' = 0$. The following updating method computes the vector w' without applying the Partition Factorization Method again, as long as the LU-decomposition of A_n has been saved.

Let

$$A' = A + be_n^T$$

where b is an n -dimensional vector. Using the partitioned form of A ,

$$A = \begin{pmatrix} A_n & y_n \\ z_n^T & a_{nn} \end{pmatrix}, \quad (3.46)$$

the matrix A' can be partitioned as follows

$$A' = \left(\begin{array}{c|c} A_n & y_n + b_1 \\ \hline z_n^T & a_{nn} + b_2 \end{array} \right)$$

where b_1 is an $(n - 1)$ -dimensional vector. Let $w' = (u_1^T, u_2)$ where u_1 is an $(n - 1)$ -dimensional vector. If $A'w' = 0$, then

$$\begin{pmatrix} A_n & y_n & + b_1 \\ z_n^T & a_{nn} & + b_2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Then, clearly

$$A_n u_1 = -(y_n + b_1)$$

when u_2 has been set equal to zero, so that

$$u_1 = -A_n^{-1} y_n - A_n^{-1} b_1. \quad (3.47)$$

The vector w can be partitioned as follows

$$w = \begin{pmatrix} w_1 \\ 1 \end{pmatrix}$$

where w_1 is a $(n - 1)$ -dimensional vector. Then using (3.46), and the fact that $Aw = 0$, it follows that

$$A_n w_1 = -y_n,$$

or

$$w_1 = -A_n^{-1} y_n. \quad (3.48)$$

Substituting equation (3.48) into equation (3.47) yields

$$u_1 = w_1 - A_n^{-1} b_1.$$

Therefore one obtains

$$w' = w + c \quad (3.49)$$

where $c = \begin{pmatrix} -A_n^{-1}b_1 \\ 0 \end{pmatrix}$. So if the LU-decomposition of A_n had been saved, then $A_n^{-1}b_1$ can be easily computed. This result can be extended so that any column of A can be modified.

Theorem 3.8. Let A be a singular irreducible M-matrix, and let $w^{(k)}$ denote the solution to the homogeneous system of linear equations $Aw^{(k)} = 0$, such that the k th component of $w^{(k)}$ is equal to one. Suppose that b is an n -dimensional vector such that

$$A' = A + be_k^T$$

remains a singular M-matrix. Let P denote the permutation matrix such that

$$PAP^T = \begin{pmatrix} A_k & y_k \\ z_k^T & a_{kk} \end{pmatrix}$$

where A_k is the submatrix formed by deleting the k th row and k th column of A . Also, let

$$P^T b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

where b_1 is an $(n-1)$ -dimensional vector. If

$$w' = w + P^T \begin{pmatrix} -A_k^{-1}b_1 \\ 0 \end{pmatrix},$$

then $A'w' = 0$.

Proof. The proof is straightforward and is omitted. ■

The following example illustrates the previous theorem.

Example 3.2.

Let

$$A = \begin{bmatrix} 5 & -2 & -1 \\ -3 & 3 & -1 \\ -2 & -1 & 2 \end{bmatrix}.$$

If $b = (0, -1, 1)^T$, then $A' = A + be_3^T$ is a singular irreducible M-matrix. Suppose that the Partition Factorization Method has been used to compute the solution to the equation $Aw = 0$ such that $w_3 = 1$. Then $w = (5/9, 8/9, 1)^T$. The LU-decomposition of A_3 is

$$\begin{bmatrix} 1 & 0 \\ -3/5 & 1 \end{bmatrix} \begin{bmatrix} 5 & -2 \\ 0 & 9/5 \end{bmatrix}.$$

Using this LU-decomposition, $A_3^{-1}b_1$, where $b_1 = (0, -1)^T$, can be computed, thus

$$A_3^{-1}b_1 = \frac{1}{9} \begin{pmatrix} -2 \\ -5 \end{pmatrix}.$$

Applying Theorem 3.8, it follows that

$$w' = \begin{pmatrix} 5/9 \\ 8/9 \\ 1 \end{pmatrix} + \frac{1}{9} \begin{pmatrix} 2 \\ 5 \\ 0 \end{pmatrix},$$

and hence $w' = (7/9, 13/9, 1)$.

The following theorem provides necessary and sufficient conditions for the matrix $A' = A + be_k^T$ to be a singular M-matrix.

Theorem 3.9. Let A be a singular irreducible M-matrix of order n , and x denote a left null vector, then $A + be_k^T$ is a singular M-matrix if and only if $x^T b = 0$ and $A + be_k^T$ has nonpositive off diagonal entries.

Proof. Let y denote a right null vector of A . Then applying Corollary 2.1, it follows that $A + be_k^T$ is a singular matrix if and only if $x^T b = 0$ and $y^T e_k \neq 0$.

If $A + be_k^T$ is a singular M-matrix, then clearly $x^T b$ must equal zero and $A + be_k^T$ has nonpositive off diagonal entries.

If $x^T b = 0$, then $x^T(A + be_k^T) = 0$. Thus $A + be_k^T$ is a singular M-matrix (see Berman and Plemmons [1979], p. 155). ■

Theorem 3.8 can be used to determine the sensitivity of the right null vector to changes in the k th column of A .

Assume that A , $A + be_k^T$, P , w , and w' satisfy the hypothesis of Theorem 3.8, then

$$w' = w + P^T \begin{pmatrix} -A_k^{-1} b_1 \\ 0 \end{pmatrix}.$$

Solving the above equation for $w' - w$ yields

$$w' - w = P^T \begin{pmatrix} -A_k^{-1} b_1 \\ 0 \end{pmatrix}. \quad (3.50)$$

Taking the two norm of both sides of (3.50) leads to

$$\|w' - w\|_2 \leq \|A_k^{-1}\|_2 \|b_1\|_2 . \quad (3.51)$$

Multiplying (3.51) on both sides by $\|w\|_2^{-1}$ it follows that

$$\frac{\|w' - w\|_2}{\|w\|_2} \leq \frac{\|A_k^{-1}\|_2 \|b_1\|_2}{\|w\|_2} .$$

Then

$$\frac{\|w' - w\|_2}{\|w\|_2} \leq \frac{\|w_1\|_2}{\|w\|_2} \cdot \frac{\|A_k^{-1}\|_2 \|b_1\|_2}{\|w_1\|_2} . \quad (3.52)$$

Recalling that $w = P(w_1^T, 1)$, and $A_k w_1 = -y_k$ it follows that

$$\frac{\|w_1\|_2}{\|w\|_2} < 1, \quad (3.53)$$

and

$$\frac{1}{\|w_1\|_2} \leq \frac{\|A_k\|_2}{\|y_k\|_2} \quad (3.54)$$

Applying the inequalities (3.53) and (3.54) to the inequality (3.52), yields

$$\frac{\|w' - w\|_2}{\|w\|_2} < K_2(A_k) \frac{\|b_1\|_2}{\|y_k\|_2} .$$

Therefore the sensitivity of the vector w , where $w_k = 1$, to changes in the entries of the k th column of A is governed by the term $K_2(A_k)$.

6. Rank Modification Method

Suppose that the Rank Modification Method is to be used to compute a solution to the homogeneous system of linear equations $Aw = 0$. One of the major difficulties associated with this method is the selection of two vectors u and v such that $x^T u \neq 0$ and $y^T v \neq 0$ where x and y are left and right null vectors of A . If A is a singular irreducible M-matrix, then any vector u such that $u > 0$ or $u < 0$ will satisfy the equation $x^T u \neq 0$. Therefore when A is singular irreducible M-matrix the selection of the vectors u and v is not a problem.

Suppose one wishes to compute the solution to the constrained homogeneous system of linear equations $Aw = 0$ such that $b^T w = \tau$. Then, as long as $b^T y \neq 0$, any solution can be scaled to satisfy this constraint. Therefore there is considerable flexibility in the selection of the vectors u and v . Hence one might choose u and v so that $\|A\| \|(A + uv^T)^{-1}\|$ is as small as possible. The following theorem provides an explicit relationship between $(A + uv^T)^{-1}$ and $A^\#$.

Theorem 3.10. Let A be a singular irreducible M-matrix of order n , and let x and y be left and right null vectors of A such that $x^T y = 1$. Let $G \in G$ where $G = (A + uv^T)^{-1}$. If b is an n -dimensional vector such that $b^T (A + uv^T) = x^T$, then

$$(A + uv^T)^{-1} = A^\# \left(I - \frac{1}{x^T u} ux^T \right) + yb^T. \quad (3.55)$$

Proof. It follows that

$$\begin{aligned}
& [A^\#(I - \frac{1}{x^T u} ux^T) + yb^T](A + uv^T) \\
&= A^\#A - \frac{1}{x^T u} A^\#ux^TA + A^\#uv^T - \frac{1}{x^T u} A^\#ux^Tuv^T \\
&\quad + yb^T(A + uv^T)
\end{aligned} \tag{3.56}$$

Using the fact that $x^TA = 0$, and $b^T(A + uv^T) = x^T$, equation (3.56) can be simplified. Here

$$\begin{aligned}
& [A^\#(I - \frac{1}{x^T u} ux^T) + yb^T](A + uv^T) \\
&= A^\#A + A^\#uv^T - A^\#uv^T + yx^T.
\end{aligned}$$

Thus

$$[A^\#(I - \frac{1}{x^T u} ux^T) + yb^T](A + uv^T) = A^\#A + yx^T, \tag{3.57}$$

and by applying Lemma 2.5, it follows that $A^\#A + yx^T = I$. Therefore the result follows. ■

Corollary 3.3. Let A be a singular irreducible M -matrix, and let x and y be left and right null vectors of A such that $x^Ty = 1$. If u is an n -dimensional vector such that $x^Tu \neq 0$, then

$$(A + ux^T)^{-1} = A^\#(I - \frac{1}{x^T u} ux^T) + \frac{1}{x^T u} yx^T. \tag{3.58}$$

Proof. The result follows directly from Theorem 3.9 with

$$b^T = \frac{1}{x^T u} x^T. \quad \blacksquare$$

Taking the norm of both sides of (3.55) leads to the following inequality

$$\|(A + uv^T)^{-1}\| \leq \|A^\# \| \|I - \frac{1}{x^T u} ux^T\| + \|yb^T\|. \quad (3.59)$$

Multiplying the inequality (3.59) on the left by $\|A\|$ yields

$$K(A, G) \leq K(A) \|I - \frac{1}{x^T u} ux^T\| + \|A\| \|yb^T\|$$

where $K(A, G) = \|A\| \|(A + uv^T)^{-1}\|$, $K(A) = \|A\| \|A^\#\|$, and $\|\cdot\|$ is any consistent matrix norm.

Next, it will be shown that the Partition Factorization Method can be considered a Rank Factorization Method. Assume that A has the following partitioned form

$$A = \begin{pmatrix} A_n & y_n \\ z_n^T & a_{nn} \end{pmatrix}.$$

Let $u = e_n$ and $v^T = e_n^T - (z_n^T a_{nn})$. Then $x^T u \neq 0$ and $y^T v \neq 0$. Thus the matrix $A + uv^T$ is nonsingular and

$$A + uv^T = \begin{pmatrix} A_n & y_n \\ 0 & 1 \end{pmatrix}.$$

The linear system $(A + uv^T)w = \tau u$ can be written as follows

$$\begin{pmatrix} A_n & y_n \\ 0 & 1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

where τ has been set equal to one and $w = (w_1^T, w_2)$, w_1 is an $(n-1)$ -

dimensional vector so that $w_1 = -A_n^{-1}y_n$ and $w_2 = 1$. These are the same equations that result when the Partition Factorization Method is applied to A , with $k = n$. Therefore the Partition Factorization Method, with $k = n$, is mathematically the same as the Rank Modification Method with $u = e_n$, $v^T = e_n^T - (z_n^T, a_{nn})$, and $\tau = 1$. This result can be extended to any k .

When Gaussian elimination is applied to $A + uv^T$, row pivoting must generally be used to ensure the completion of the algorithm. When the Partition Factorization Method is used, no pivoting is required to ensure the completion of Gaussian elimination applied to A_k .

Example 3.3. Let

$$A = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$

Clearly A is a singular irreducible M-matrix such that $e^T A = 0$ and $Ae = 0$. Let $u = -2e$ and $v = e$, then

$$A + uv^T = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} + \begin{pmatrix} -2 \\ -2 \\ -2 \end{pmatrix} (1 \ 1 \ 1),$$

or

$$A + uv^T = \begin{pmatrix} 0 & -3 & -3 \\ -3 & 0 & -3 \\ -3 & -3 & 0 \end{pmatrix}.$$

Thus pivoting must be used in the LU decomposition.

If A is a sparse matrix, then $A + uv^T$ might be a dense matrix. Therefore, based on these considerations, the Partition Factorization Method would seem to be the preferred algorithm.

7. Diagonally Dominant M-matrices

A matrix $A = (a_{ij})$ of order n , is (column) diagonally dominant if

$$|a_{jj}| \geq \sum_{i \neq j}^n |a_{ij}| \quad \text{for } j = 1, 2, \dots, n. \quad (3.60)$$

If A has nonpositive off-diagonal entries and nonnegative diagonal entries, then (3.60) can be written as

$$\sum_{i=1}^n a_{ij} \geq 0 \quad \text{for } j = 1, 2, \dots, n,$$

or using matrix notation it follows that

$$e^T A \geq 0. \quad (3.61)$$

Therefore, if A is a matrix of order n with nonpositive off-diagonal entries and nonnegative diagonal entries, then A is a column diagonally dominant matrix if and only if $e^T A \geq 0$. Thus, if A is a singular irreducible M-matrix, then A is column diagonally dominant matrix if and only if $e^T A = 0$.

The computation of the right null vector of a singular irreducible diagonally dominant M-matrix is of widespread interest (see, Funderlic and Mankin [1981], Funderlic and Plemmons [1981], and Funderlic, et al [1982]). More generally, this null vector is important in many areas of mathematical sciences, including Markov chains (e.g., Berman and Plemmons [1979], Ch. 8), compartmental models (e.g., Funderlic and Mankin [1981]), and input-output analysis in economics (e.g., Berman and Plemmons [1979], Ch. 9).

In Theorem 3.4 it was proved that if A is an M-matrix with the property that $x^T A \geq 0$ for some $x \gg 0$, then for any permutation matrix P , PAP^T has an LU-decomposition, $PAP^T = LU$. Also, an upper bound was stated for the moduli of the entries in the matrices L and U . The following theorem follows directly from Theorem 3.4.

Theorem 3.11. (Funderlic, et al [1982]) Let A be a diagonally dominant M-matrix. Then for each permutation matrix P , PAP^T has an LU-decomposition, $PAP^T = LU$, where for each i and j , $1 \leq i, j \leq n$

$$|l_{ij}| \leq 1,$$

$$|u_{ij}| \leq \max_k a_{kk}.$$

Hence $g_A = 1$, where g_A is given by

$$g_A = \max_{i,j,k} |a_{kj}^{(k)}| / \max_{i,j} |a_{ij}|.$$

When the LU-decomposition of A is computed on a machine, using floating point arithmetic with unit roundoff error μ , then the computed

factors $\hat{L}$ and $\hat{U}$ satisfy exactly the following equation

$$(A + E) = \hat{L}\hat{U}$$

where for all $1 \leq i, j \leq n$,

$$|e_{ij}| \leq 2.01 \mu \max_{i,j,k} |\hat{a}_{ij}^{(k)}|.$$

The computed growth factor $g_{\hat{A}}$ for Gaussian elimination applied to A is defined by

$$g_{\hat{A}} = (\max_{i,j,k} |\hat{a}_{ij}^{(k)}|) / (\max_{i,j} |a_{ij}|)$$

where $\hat{a}_{ij}$ is the i,j th entry in the floating point version of $A^{(k)}$.

If it is assumed that $g_A = g_{\hat{A}}$, then the above inequality can be written as

$$|e_{ij}| \leq 2.01 \mu g_A \max_{i,j} |a_{ij}|.$$

Suppose the Partition Factorization Method is executed on a machine, using floating point arithmetic with unit roundoff error μ . Then the following theorem shows that the Partition Factorization Method can be considered a stable algorithm.

Corollary 3.4. Let A be a singular irreducible diagonally dominant M -matrix of order n . Suppose the homogeneous system of linear equations $Aw = 0$ is solved for the positive vector w by applying Gaussian elimination to A without pivoting in floating point arithmetic with machine unit roundoff error μ . Then there exists a

matrix $E = (e_{ij})$ such that the computed solution $\hat{w}$ to $Aw = 0$ satisfies exactly the homogeneous system

$$(A + E)\hat{w} = 0$$

where for $1 \leq i, j \leq n$

$$|e_{ij}| \leq \mu n(3.02 + 1.01n) \max_k a_{kk}.$$

Proof. This result follows directly from Theorem 3.5 and the fact that

$$\max_{i,j} |a_{ij}| = \max_k a_{kk}$$

when A is a diagonally dominant matrix. ■

Therefore if $\max_k a_{kk}$ and the order of the matrix are not excessively large, then the Partition Factorization Method will be a stable algorithm when applied to a singular irreducible diagonally dominant M-matrix.

Recalling that a diagonally dominant singular irreducible M-matrix has the property that $e^T A = 0$, the following lemma provides an explicit expression for the right null vector of A .

Lemma 3.2. Let A be a singular irreducible diagonally dominant M-matrix. Let $y = (p_1, p_2, \dots, p_n)^T$ where $p_k = \det(A_k)$ for $k = 1, 2, \dots, n$ and A_k is the principal submatrix formed by deleting the k th row and k th column of A . Then $Ay = 0$.

Proof. This result is well known and it follows directly from Theorem 2.15, using $x = e$. ■

In Chapter II, it was stated that $r(\lambda) = \|x\|_{\infty} \|y\|_1 / |y^* x|$ where $x^T A = \lambda x^T$, $Ay = \lambda y$, and λ is a simple eigenvalue, can be considered a condition number for the eigenvalue λ . The following lemma proves that $r(0) = 1$, when A is a singular irreducible diagonally dominant M-matrix.

Lemma 3.3. Let A be a singular irreducible diagonally dominant M-matrix. Then

$$r(0) = 1.$$

Proof. Let $y = (p_1, p_2, \dots, p_n)^T$, where $p_k = \det(A_k)$ for $k = 1, 2, \dots, n$. Then, by Lemma 3.2 it follows that $Ay = 0$. Clearly, $e^T A = 0$. Thus

$$r(0) = \frac{\|e\|_{\infty} \|y\|_1}{|y^T e|}$$

or

$$r(0) = \frac{\sum_{j=1}^n |p_j|}{\sum_{j=1}^n p_j}.$$

Since A is a singular irreducible M-matrix, it follows that $p_k > 0$ for $k = 1, 2, \dots, n$, therefore $r(0) = 1$. ■

The fact that $r(0)$ is equal to one does not imply that the eigenvector associated with the zero eigenvalue is well conditioned.

In conclusion, if A is a singular irreducible diagonally dominant M-matrix, then the Partition Factorization Method is a preferred variation of the Rank Modification Method. Gaussian elimination applied to PAP^T is a stable algorithm, for any permutation matrix P . Consequently, Gaussian elimination applied to A_k is also a stable algorithm. Thus symmetric ordering schemes could be applied to either A or A_k , when A is large and sparse. When the Rank Modification Method is used, the matrix $A + uv^T$ will probably not be a diagonally dominant M-matrix, so some form of pivoting is required to ensure the stability and the completion of the Gaussian elimination algorithm. Also, if A is sparse, then the matrix $A + uv^T$ might be dense.

8. Tridiagonal M-matrices

Assume that A is a tridiagonal matrix. That is,

$$A = \begin{bmatrix} a_1 & b_1 & & & \\ c_1 & a_2 & b_2 & & \\ & c_2 & a_3 & & \\ & & & \ddots & \\ & & & & a_{n-1} & b_{n-1} \\ & & & & c_{n-1} & a_n \end{bmatrix}.$$

Research that involves concepts related to tridiagonal matrices is of widespread interest. Recently, papers have been published that investigate the stability of Gaussian elimination applied to a tridiagonal Toeplitz matrix (e.g., Gunzburger and Nicolaides [1982]), characterizations of tridiagonal D-stable matrices (e.g., Carlson, et

al [1982], Carlson [1982]), and the characterization of nonnegative nonsingular tridiagonal matrices that belong to the class of inverse M-matrices (e.g., Imann [1983]).

Clearly, if A is a tridiagonal irreducible matrix, then $b_k c_k \neq 0$ for $k = 1, 2, \dots, n - 1$. For notational purposes A will be denoted by

$$A = [c_j, a_j, b_j].$$

If $a_j = a$ for $j = 1, 2, \dots, n$ and $b_j = b$ for $j = 1, 2, \dots, n - 1$, then the following notation will be used to denote A

$$A = [c_j, a, b].$$

If $A = (a_{ij})$ is a Toeplitz matrix then there exists a sequence $\{\alpha_k\}_{k=-n+1}^{n-1}$ such that $a_{ij} = \alpha_{j-i}$ for $i, j = 1, 2, \dots, n$. Thus, if A is an irreducible tridiagonal Toeplitz matrix, then $A = [c, a, b]$ and $bc \neq 0$.

Assume that A is a tridiagonal irreducible M-matrix. Suppose that the Rank Modification Method is to be used to compute a solution to the homogeneous system of linear equations $Aw = 0$. In general, the matrix $A + uv^T$ will no longer be a tridiagonal matrix. The complete matrix A can be stored in a computer using only $3n - 2$ storage locations. If A were a full matrix, then n^2 storage locations would be required to store the matrix A . Therefore when A is a large matrix this special structure of A should be preserved. Thus the vectors u and v should be chosen so that $A + uv^T$ is also a tridiagonal matrix.

If A is an irreducible M -matrix, then there exists a vector $x \gg 0$ such that $x^T A \geq 0$. Let $\beta_x = (\max_k x_k) / (\min_k x_k)$. Then according to Theorem 3.4, β_x can be used as an upper bound for the elements l_{ij} and u_{ij} from the LU-decomposition of PAP^T , where P is an arbitrary permutation matrix. This upper bound can be very pessimistic. Another approach for investigating the stability of the Gaussian elimination algorithm applied to A is to directly examine the elements of L and U . The following proposition provides recurrence relationships for the elements of L and U when A is a tridiagonal irreducible M -matrix.

Proposition 3.1. Let $A = [c_j, a_j, b_j]$ be a tridiagonal irreducible M -matrix. Then the LU-decomposition of A exists, and the factors L and U are also tridiagonal matrices such that,

$$L = [m_j, 1, 0] \text{ and } U = [0, \alpha_j, b_j]$$

where

$$\alpha_1 = a_1 \quad m_1 = c_1/a_1,$$

$$\alpha_j = a_j - b_{j-1} m_{j-1} \quad \text{for } j = 2, 3, \dots, n,$$

and

$$m_j = c_j/\alpha_j \quad \text{for } j = 1, 2, \dots, n-1.$$

Proof. Since A is irreducible M -matrix, it follows that A has an LU-decomposition. The formulas for α_j and m_j can be found in Dahlquist, Björck, and Anderson [1974], p. 166. ■

The next two corollaries follow from the preceding proposition.

Corollary 3.5. Let $A = [c_j, a_j, b_j]$ be a tridiagonal M-matrix such that $c_j b_j \neq 0$ for $j = 1, 2, \dots, n-1$. If the LU-decomposition of A is $A = LU$, and the LU-decomposition of A^T is $A^T = \bar{L}\bar{U}$ where

$$\begin{aligned} L &= [m_j, 1, 0], \\ U &= [0, \alpha_j, b_j], \\ \bar{L} &= [\bar{m}_j, 1, 0], \end{aligned}$$

and

$$\bar{U} = [0, \bar{\alpha}_j, c_j],$$

then

$$\bar{\alpha}_j = \alpha_j \quad \text{for } j = 1, 2, \dots, n,$$

and

$$\bar{m}_j = \left(\frac{b_j}{c_j} \right) m_j \quad \text{for } j = 1, 2, \dots, n-1.$$

Proof. Applying Proposition 3.1 to the matrix A , it follows that

$$\alpha_j = a_j - b_{j-1} m_{j-1} \quad \text{for } j = 1, 2, \dots, n,$$

$$m_j = c_j / \alpha_j \quad \text{for } j = 1, 2, \dots, n-1.$$

Combining these equations leads to

$$\alpha_j = a_j - \frac{b_{j-1} c_{j-1}}{\alpha_{j-1}} \quad \text{for } j = 1, 2, \dots, n.$$

Also, applying Proposition 3.1 to the matrix A^T , it follows that

$$\begin{aligned}\bar{\alpha}_j &= a_j - c_{j-1}\bar{m}_{j-1} & \text{for } j = 1, 2, \dots, n, \\ \bar{m}_j &= b_j/\bar{\alpha}_j & \text{for } j = 1, 2, \dots, n-1.\end{aligned}$$

Combining these equations leads to

$$\bar{\alpha}_j = a_j - \frac{b_{j-1}c_{j-1}}{\bar{\alpha}_{j-1}} \quad \text{for } j = 1, 2, \dots, n.$$

Also, $\alpha_1 = \bar{\alpha}_1 = a_1$, so both α_j and $\bar{\alpha}_j$ satisfy the same recurrence relation with the same boundary condition. Therefore it follows that $\alpha_j = \bar{\alpha}_j$ for $j = 1, 2, \dots, n$. If $m_j = c_j/\alpha_j$, then

$$m_j = \frac{c_j}{b_j} \cdot \frac{b_j}{\bar{\alpha}_j} \quad \text{for } j = 1, 2, \dots, n-1,$$

so that $m_j = \left(\frac{c_j}{b_j}\right) \bar{m}_j$ for $j = 1, 2, \dots, n-1$. ■

Corollary 3.6. Let $A = [c_j, a_j, b_j]$ be a tridiagonal M-matrix such that $c_j b_j \neq 0$ for $j = 1, 2, \dots, n-1$. If $A = LU$ is the decomposition of A and $U = (u_{ij})$, then

$$\max_{i,j} |u_{ij}| \leq \max_j \{a_j, |b_j|\}.$$

Proof. Applying Proposition 3.1 it follows that $U = [0, \alpha_j, b_j]$ where $\alpha_j = a_j - b_{j-1}m_{j-1}$. From Theorem 3.3 it follows that $m_j \leq 0$ for $j = 1, 2, \dots, n-1$ and $\alpha_j \geq 0$ for $j = 1, 2, \dots, n$. Therefore $\alpha_j \leq a_j$ for $j = 1, 2, \dots, n$, and

$$\max_{i,j} |u_{ij}| \leq \max_j \{a_j, |b_j|\}. \quad \blacksquare$$

Therefore it follows that when Gaussian elimination is applied to a tridiagonal irreducible M-matrix the growth factor g_A is equal to one.

If A is an M-matrix with the property that $x^T A \geq 0$ for some vector x such that $x \gg 0$, then A has an LU-decomposition where the factors L and U are both M-matrices.

If a matrix A has an LU-decomposition $A = LU$ where L and U are M-matrices, then this does not imply that A is an M-matrix. The following example illustrates this statement.

Example 3.4.

Let

$$L = \begin{pmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ -3 & -3 & 1 \end{pmatrix} \text{ and } U = \begin{pmatrix} 1 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then

$$LU = \begin{pmatrix} 1 & -1 & -1 \\ -3 & 3 & 2 \\ -3 & 0 & 7 \end{pmatrix}.$$

Clearly, both L and U are M-matrices, but LU is not an M-matrix.

The following theorem proves that if A is an irreducible tridiagonal matrix that has an LU-decomposition where both L and U are M-matrices, then A is a M-matrix.

Theorem 3.12. Let $A = [c_j, a_j, b_j]$ be a tridiagonal matrix such that $c_j, b_j \neq 0$ for $j = 1, 2, \dots, n-1$. Assume that A has an LU-decomposition, $A = LU$. Then A is an M-matrix if and only if L and U are both M-matrices.

Proof. The proof follows from Proposition 3.1, and the fact that if D and E are M-matrices and DE has nonpositive off diagonal entries, then DE is an M-matrix (see Berman and Plemmons [1979], p. 159). ■

The next theorem provides necessary and sufficient conditions for a Toeplitz tridiagonal irreducible matrix to be an M-matrix. The following lemma will be used to prove this theorem.

Lemma 3.4. The recurrence relation

$$\sigma_{k+2} - a\sigma_{k+1} + (bc)\sigma_k = 0, \quad (3.62)$$

$$\sigma_1 = a, \sigma_0 = 1,$$

where $a > 0$ and $b, c < 0$, has positive solutions σ_k , for $k = 0, 1, \dots, n$ if and only if one of the following conditions hold

$$(1) \quad a^2 - 4bc > 0.$$

$$(2) \quad a^2 - 4bc = 0.$$

$$(3) \quad a^2 - 4bc < 0 \text{ and } \tan^{-1} \frac{\sqrt{4bc - a^2}}{a} < \frac{\pi}{n+1}.$$

Proof. The characteristic equation for the recurrence relation (3.62) is

$$\alpha^2 - a\alpha + bc = 0.$$

The roots of the above characteristic equation are

$$\lambda_1 = \frac{a + \sqrt{a^2 - 4bc}}{2}, \quad (3.63)$$

and

$$\lambda_2 = \frac{a - \sqrt{a^2 - 4bc}}{2}. \quad (3.64)$$

Case 1. Assume that $\lambda_1 \neq \lambda_2$. Then the solution to the recurrence relation (3.62) is

$$\sigma_k = A_1 \lambda_1^k + A_2 \lambda_2^k \quad (3.65)$$

where A_1 and A_2 are constants to be determined from the given boundary conditions.

If $k = 0$, then equation (3.65), along with the boundary condition $\sigma_0 = 1$, yields

$$1 = A_1 + A_2,$$

so that $A_2 = 1 - A_1$. If $k = 1$, then equation (3.65), along with the boundary condition $\sigma_1 = a$, yields

$$a = A_1 \lambda_1 + A_2 \lambda_2,$$

or

$$a = A_1 \lambda_1 + (1 - A_1) \lambda_2.$$

Solving for A_1 yields

$$A_1 = \frac{a - \lambda_2}{\lambda_1 - \lambda_2}.$$

Applying equation (3.63) it follows that

$$A_1 = \frac{\lambda_1}{\lambda_1 - \lambda_2}.$$

If $A_2 = 1 - A_1$, then $A_2 = -\lambda_2/(\lambda_1 - \lambda_2)$. Substituting these equations for A_1 and A_2 in terms of λ_1 and λ_2 into (3.65) leads to

$$\sigma_k = \frac{1}{\lambda_1 - \lambda_2} \left(\lambda_1^{k+1} - \lambda_2^{k+1} \right). \quad (3.66)$$

Clearly λ_1 and λ_2 are real numbers if and only if $a^2 - 4bc > 0$.

If λ_1 and λ_2 are real numbers then $\sigma_k > 0$ for all k . Thus if $a^2 - 4bc > 0$ then $\sigma_k > 0$ for $k = 0, 1, \dots, n$.

Clearly λ_1 and λ_2 are complex numbers if and only if $a^2 - 4bc < 0$.

Assume that λ_1 and λ_2 are complex numbers, then equations (3.63) and (3.64) can be written as

$$\lambda_1 = \delta + wi, \quad (3.67)$$

$$\lambda_2 = \delta - wi, \quad (3.68)$$

where $\delta = a/2$ and $w = \frac{1}{2} \sqrt{4bc - a^2}$. Then the solution to the recurrence relation (3.62) is

$$\sigma_k = B_1 \rho^k \cos(k\theta) + B_2 \rho^k \sin(k\theta)$$

where

$$B_1 = A_1 + A_2,$$

$$B_2 = i(A_1 - A_2),$$

$$\theta = \tan^{-1}(w/\delta),$$

and

$$\rho = \sqrt{w^2 + \delta^2}.$$

Using the equations $\lambda_1 - \lambda_2 = 2wi$ and $\lambda_1 + \lambda_2 = 2\delta$, it clearly follows that $B_1 = 1$ and $B_2 = \delta/w$. Since $w/\delta > 0$, it follows that $\theta \in (0, \pi/2)$.

The equation for σ_k can be written as

$$\sigma_k = \rho^k \frac{\sin((k+1)\theta)}{\sin(\theta)} \quad (3.69)$$

where $\rho = \sqrt{bc}$. Thus $\sigma_k > 0$ for $k = 0, 1, \dots, n$ if and only if $\sin((k+1)\theta)/\sin(\theta) > 0$ for $k = 0, 1, \dots, n$.

Assume that $\theta \in (0, \pi/2)$. Then $\sin(\theta) > 0$. Also, $\sin((k+1)\theta) > 0$ for $k = 0, 1, \dots, n$ if and only if $0 < \theta(k+1) < \pi$ for $k = 0, 1, \dots, n$. Therefore $\sin(k+1)\theta > 0$ for $k = 0, 1, \dots, n$ if and only if

$$0 < \theta < \frac{\pi}{n+1}.$$

Therefore, $\sigma_k > 0$ for $k = 0, 1, 2, \dots, n$ if

$$0 < \theta < \frac{\pi}{n+1}.$$

Since $\theta = \tan^{-1}(w/\delta)$ it follows that

$$0 < \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) < \frac{\pi}{n+1}.$$

Therefore if $a^2 - 4bc < 0$, then

$$0 < \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) < \frac{\pi}{n+1},$$

if and only if $\sigma_k > 0$ for $k = 0, 1, 2, \dots, n$.

Case 2. Assume that λ_1 is equal to λ_2 . This will occur if and only if $a^2 - 4bc = 0$. Then the roots of the characteristic equation for the recurrence relation (3.62) are

$$\lambda_1 = \lambda_2 = \frac{a}{2}.$$

Thus the solution to the recurrence relation (3.62) is

$$\sigma_k = (A_2 k + A_1) \lambda_1^k \quad (3.70)$$

where A_1 and A_2 are constants to be determined from the given boundary conditions.

If $k = 0$, then equation (3.70), along with the boundary condition $\sigma_0 = 1$, yields

$$A_1 = 1.$$

If $k = 1$, then equation (3.70), along with the boundary condition $\sigma_1 = a$, yields

$$a = (A_2 + 1) \frac{a}{2},$$

so that

$$A_2 = 1.$$

Thus it follows that

$$\sigma_k = (k+1)\lambda_1^k. \quad (3.71)$$

Clearly, $\sigma_k > 0$ for all k .

Therefore $\sigma_k > 0$ for $k = 0, 1, \dots, n$ if and only if one of the following conditions holds

- (1) $a^2 - 4bc > 0$,
- (2) $a^2 - 4bc = 0$,
- (3) $a^2 - 4bc < 0$ and $\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) < \frac{\pi}{n+1}$. ■

Theorem 3.13. Let $A = [c, a, b]$ be a Toeplitz tridiagonal matrix.

If $a > 0$ and $b, c < 0$, then A is a nonsingular M-matrix if and only if one of the following conditions holds

- (1) $a^2 - 4bc > 0$,
- (2) $a^2 - 4bc = 0$,
- (3) $a^2 - 4bc < 0$ and $\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) < \frac{\pi}{n+1}$.

Proof. Let σ_k denote the k th principal leading minor of A . Then A is a nonsingular M-matrix if and only if $\sigma_k > 0$ for $k = 1, 2, \dots, n$. Let $\sigma_0 = 1$. Then it can be proven that the σ_k 's satisfies the following recurrence relation

$$\sigma_{k+1} - a\sigma_k + bc\sigma_{k-1} = 0.$$

Therefore applying Lemma 3.4, the result follows. ■

If $A = [c, a, b]$ is a singular irreducible M-matrix, then $\sigma_k > 0$ for $k = 1, 2, \dots, n-1$ and $\sigma_n = 0$. The following corollary provides

necessary and sufficient conditions for $A = [c, a, b]$ to be a singular irreducible M-matrix.

Corollary 3.7. Let $A = [c, a, b]$ be a Toeplitz tridiagonal matrix of order n . If $a > 0$ and $b, c < 0$, then A is a singular M-matrix if and only if $a^2 - 4bc < 0$ and

$$\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) = \frac{\pi}{n+1}.$$

Proof. Let σ_k denote the k th principal leading minor of A and $\sigma_0 = 1$. Then the σ_k 's satisfy the following recurrence relation

$$\sigma_{k+1} - a\sigma_k + bc\sigma_{k-1} = 0.$$

In the proof of Lemma 3.4 it was shown that, if $a^2 - 4bc \geq 0$, then $\sigma_k > 0$ for all k . Thus it must hold that $a^2 - 4bc < 0$. Hence the solution to the recurrence relation is

$$\sigma_k = \rho^k \frac{\sin((k+1)\theta)}{\sin(\theta)}$$

where $\theta = \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right)$ and $\rho = \sqrt{bc}$. Let A_n denote the submatrix of A formed by deleting the n th row and n th column of A . Applying Theorem 3.13, it follows that A_n is a nonsingular M-matrix if and only if $0 < \theta < \pi/n$.

The minor σ_n is equal to zero if and only if

$$\sin((n+1)\theta) = 0.$$

Therefore

$$\theta = \frac{\pi}{(n+1)} i$$

where i is any integer. Since $0 < \theta < \pi/n$, it follows that

$\theta = \pi/(n+1)$. Hence $\sigma_n = 0$ if and only if $\theta = \pi/(n+1)$.

Therefore A is a singular irreducible M -matrix if and only if

$$a^2 - 4bc < 0 \text{ and } \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) = \frac{\pi}{n+1}. \quad \blacksquare$$

The above corollary gives a very simple method for determining whether or not a Toeplitz tridiagonal matrix is a singular irreducible M -matrix. The following example illustrates the previous corollary.

Example 3.5.

Let $A = [c, a, b]$ be a Toeplitz tridiagonal matrix of order 5, where $a = -2$, $b = -4$, and $c = 1/3$. Then it follows that

$$\frac{\sqrt{4bc - a^2}}{a} = \frac{\sqrt{3}}{3},$$

and $\tan(\pi/6) = \sqrt{3}/3$. Therefore A is singular irreducible M -matrix.

The following theorem provides a recurrence relation for the entries in a vector x such that $x^T A \geq 0$ and $x \gg 0$, when A is a Toeplitz tridiagonal irreducible M -matrix.

Theorem 3.14. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M -matrix such that $bc \neq 0$. If $x = (x_k)$ where the x_k 's satisfy the following recurrence relation

$$\begin{aligned} cx_{k+1} + ax_k + bx_{k-1} &= 0, \\ x_1 &= 1, x_0 = 0, \end{aligned} \tag{3.72}$$

then $x \gg 0$ and $x^T A \geq 0$. Furthermore, if A is a singular matrix, then $x^T A = 0$.

Proof. The characteristic equation for the recurrence relation (3.72) is

$$c\lambda^2 + a\lambda + b = 0.$$

The roots of the above characteristic equation are

$$\mu_1 = \frac{a}{2|c|} + \frac{1}{2|c|} \sqrt{a^2 - 4bc}, \quad (3.73)$$

and

$$\mu_2 = \frac{a}{2|c|} - \frac{1}{2|c|} \sqrt{a^2 - 4bc}. \quad (3.74)$$

Case 1. Assume that $\mu_1 \neq \mu_2$. Then the solution to the recurrence relation (3.72) is

$$x_k = A_1 \mu_1^k + A_2 \mu_2^k \quad (3.75)$$

where A_1 and A_2 are constants to be determined from the given boundary conditions.

If $k = 0$, then equation (3.75), along with the boundary condition $x_0 = 0$, yields

$$0 = A_1 + A_2,$$

so that $A_2 = -A_1$. If $k = 1$, then equation (3.75), along with the boundary condition $x_1 = 1$, yields

$$1 = A_1 \mu_1 + A_2 \mu_2,$$

or using the fact that $A_2 = -A_1$ it follows that

$$1 = A_1 \mu_1 - A_1 \mu_2.$$

Solving for A_1 yields

$$A_1 = \frac{1}{\mu_1 - \mu_2},$$

thus

$$A_2 = \frac{-1}{\mu_1 - \mu_2}.$$

Substituting these equations for A_1 and A_2 into equation (3.75) yields

$$x_k = \frac{\mu_1^k - \mu_2^k}{\mu_1 - \mu_2}. \quad (3.76)$$

If $a^2 - 4bc > 0$, then μ_1 and μ_2 are real numbers, and clearly $x_k > 0$ for all k . If $a^2 - 4bc < 0$ then μ_1 and μ_2 are complex numbers and equation (3.75) can be written as

$$x_k = \rho^k [B_1 \cos(k\theta) + B_2 \sin(k\theta)] \quad (3.77)$$

where

$$B_1 = A_1 + A_2,$$

$$B_2 = i(A_1 - A_2),$$

$$\mu_1 = \alpha + i\beta, \quad \mu_2 = \alpha - i\beta$$

$$\rho = \sqrt{\alpha^2 + \beta^2},$$

$$\theta = \tan^{-1}(\beta/\alpha),$$

$$\alpha = \frac{a}{2|c|}, \text{ and } \beta = \frac{1}{2|c|} \sqrt{4bc - a^2}.$$

Using the above equations it follows that, $B_1 = 0$, $B_2 = (\rho \sin(\theta))^{-1}$,
 $\theta = \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right)$, and $\rho = \sqrt{b/c}$. Therefore equation (3.77)
 can be rewritten as

$$x_k = (b/c)^{(k-1)/2} \frac{\sin(k\theta)}{\sin(\theta)}.$$

If $\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) \leq \frac{\pi}{n+1}$, then $0 < \theta \leq \frac{\pi}{n+1}$. Thus
 $\sin(k\theta) > 0$ for $k = 1, \dots, n$ and $\sin((n+1)\theta) \geq 0$. Therefore
 $x_k > 0$ for $k = 1, 2, \dots, n$ and $x_{n+1} \geq 0$.

Case 2. Assume that $\mu_1 = \mu_2$. This is equivalent to $a^2 - 4bc = 0$.
 Thus $\mu_1 = a/2|c|$, and the solution to the recurrence relation (3.72)
 is

$$x_k = (A_1 k + A_0) \left(\frac{a}{2|c|} \right)^k \quad (3.78)$$

where A_1 and A_2 are constants to be determined from the given boundary
 conditions. If $k = 0$, then equation (3.78), along with the boundary
 condition $x_0 = 0$, yields

$$A_0 = 0.$$

If $k = 1$, then equation (3.78), along with the boundary condition
 $x_1 = 1$, yields

$$A_1 = \frac{2|c|}{a}.$$

Substituting these equations for A_0 and A_1 into equation (3.78) yields

$$x_k = k \left(\frac{a}{2|c|} \right)^{k-1}.$$

Clearly, it follows that $x_k > 0$ for all k .

Therefore $x_k > 0$ for $k = 1, 2, \dots, n$ and $x_{n+1} \geq 0$, if A is an irreducible M-matrix.

Let $z^T = x^T A$. Then it follows that

$$z_k = \begin{cases} cx_2 + ax_1 & \text{if } k = 1, \\ cx_{k+1} + ax_k + bx_{k-1} & \text{if } 2 \leq k \leq n-1, \\ ax_n + bx_{n-1} & \text{if } k = n. \end{cases}$$

Applying the recurrence relation (3.72), it follows that

$z_k = 0$ for $k = 1, 2, \dots, n-1$, and

$$cx_{n+1} + z_n = 0.$$

Solving for z_n yields

$$z_n = |c| x_{n+1}.$$

Therefore the results follows.

If A is a singular irreducible M-matrix, then by applying Theorem 3.1, it follows that $x^T A = 0$. ■

Assume that A is a singular irreducible M-matrix. Then Theorem 3.14 can be used to compute a right null vector of A . Let

$y = (y_1, y_2, \dots, y_n)^T$ where the y_k 's satisfy the following recurrence relation,

$$by_{k+1} + ay_k + cy_{k-1} = 0,$$

$$y_1 = 1, \quad y_0 = 0.$$

Then $Ay = 0$. This recurrence relation provides a simple method for computing a right null vector of a Toeplitz tridiagonal singular irreducible M-matrix.

The following definition for a strongly stable LU-decomposition can be found in Wendroff [1966], p. 146.

Definition 3.1. Let A be a matrix of order n . Suppose an LU-decomposition exists for A . Let $(\max_{i,j} |a_{ij}|)^{-1} A = LU$. If there exists constants α and β , independent of the elements and order of A such that for all $1 \leq i, j \leq n$,

$$|l_{ij}| \leq \alpha,$$

and

$$|u_{ij}| \leq \beta,$$

then the LU-decomposition of A is said to be strongly stable.

Next a strict upper bound on the moduli of the elements of L will be derived, where $A = LU$ is the LU-decomposition of a Toeplitz tridiagonal irreducible M-matrix. The following lemma provides a useful expression for the multipliers encountered during the Gaussian elimination process.

Lemma 3.5. (Gunzburger and Nicolaides [1982]). Let A be a Toeplitz tridiagonal M -matrix of order n . If $A = LU$ is the LU-decomposition of A and $L = [m_j, 1, 0]$, then

$$m_j = c \frac{\sigma_{j-1}}{\sigma_j} \quad \text{for } j = 1, 2, \dots, n-1$$

where σ_k denotes the k th principal leading minor of A and $\sigma_0 = 1$.

Let $M_A = \max_j |m_j|$, where m_j is the j th multiplier of A . The following two lemmas will be used in the proof of the next theorem.

Lemma 3.6. If $a > 1$ and

$$f_a(x) = \frac{a^x - 1}{a^{x+1} - 1}, \quad (3.79)$$

then

- (a) $f_a(x)$ is a strictly increasing function for all $x \geq 1$,
- (b) $0 < f_a(x) < 1$ for all $x \geq 1$.

Proof. (a) Differentiating equation (3.79) with respect to x leads to the following equation for the derivative of $f_a(x)$

$$f'_a(x) = \frac{a^x(a-1) \ln(a)}{(a^{x+1} - 1)^2}.$$

Thus $f'_a(x)$ is positive for all $x \geq 1$, and $f_a(x)$ is a strictly increasing function for all $x \geq 1$.

(b) If $a > 1$, then $a^{x+1} > a^x > 1$ for $x \geq 1$. Thus

$$1 > \frac{a^x - 1}{a^{x+1} - 1} > 0.$$

So that $0 < f_a(x) < 1$ for all $x \geq 1$. ■

Lemma 3.7. Assume that $0 < \theta \leq \frac{\pi}{(n+1)}$, where n is a positive integer such that $n \geq 2$, and

$$g_\theta(x) = \frac{\sin(x\theta)}{\sin((x+1)\theta)} \quad (3.80)$$

then

(a) $g_\theta(x)$ is a strictly increasing function for all

$$x \in [1, n-1],$$

(b) $\frac{1}{2} < g_\theta(x) < 2$, for all $x \in [1, n-1]$ and $\theta \in (0, \pi/(n+1)]$.

Proof. (a) Differentiating equation (3.80) with respect to x leads to the following equation for the derivative of $g_\theta(x)$.

$$g'_\theta(x) = \frac{\theta \sin(\theta)}{[\sin((x+1)\theta)]^2}$$

Thus $g'_\theta(x)$ is positive for $x \in [1, n-1]$, and $g_\theta(x)$ is a strictly increasing function for $x \in [1, n-1]$.

(b) The proof of part (b) will be omitted. ■

The following theorem provides closed form expressions for the multipliers of A , and for M_A , where $M_A = \max_j |m_j|$.

Theorem 3.15. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M -matrix of order n , such that $bc \neq 0$. Assume $A = LU$ is the LU-decomposition of

A, and $L = [m_j, 1, 0]$.

(1) If $a^2 - 4bc > 0$, then

$$m_j = \frac{c}{\lambda_2} \left(\frac{\gamma^j - 1}{\gamma^{j+1} - 1} \right) \quad \text{for } j = 1, 2, \dots, n-1,$$

$$M_A = \frac{|c|}{\lambda_2} \left(\frac{\gamma^{n-1} - 1}{\gamma^n - 1} \right)$$

where $\gamma = \lambda_1/\lambda_2$,

$$\lambda_1 = \frac{a + \sqrt{a^2 - 4bc}}{2},$$

and

$$\lambda_2 = \frac{a - \sqrt{a^2 - 4bc}}{2}.$$

(2) If $a^2 - 4bc = 0$, then

$$m_j = \frac{2c}{a} \left(\frac{j}{j+1} \right) \quad \text{for } j = 1, 2, \dots, n-1,$$

$$M_A = \frac{2|c|}{a} \left(\frac{n-1}{n} \right).$$

(3) If $a^2 - 4bc < 0$ and $\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) \leq \frac{\pi}{n+1}$ then

$$m_j = (c/b)^{\frac{1}{2}} \frac{\sin(j\theta)}{\sin((j+1)\theta)} \quad \text{for } j = 1, 2, \dots, n-1,$$

$$M_A = (c/b)^{\frac{1}{2}} \frac{\sin((n-1)\theta)}{\sin(n\theta)}$$

$$\text{where } \theta = \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right).$$

Proof. (1) Assume that $a^2 - 4bc > 0$. Applying Lemma 3.5, and equation (3.66) it follows that

$$m_j = c \left(\frac{\lambda_1^j - \lambda_2^j}{\lambda_1^{j+1} - \lambda_2^{j+1}} \right) \quad \text{for } j = 1, 2, \dots, n-1, \quad (3.81)$$

where λ_1 and λ_2 are given by equations (3.63) and (3.64). Let $\gamma = \lambda_1/\lambda_2$. Applying this equation for γ to equation (3.81) leads to

$$m_j = \frac{c}{\lambda_2} f_\gamma(j) \quad \text{for } j = 1, 2, \dots, n-1$$

where

$$f_\gamma(x) = \frac{\gamma^x - 1}{\gamma^{x+1} - 1}.$$

In Lemma 3.6 it was shown that $f_\gamma(x)$ is a strictly increasing function, hence it follows that $M_A = \frac{|c|}{\lambda_2} f_\gamma(n-1)$.

(2) Assume that $a^2 - 4bc = 0$. Applying Lemma 3.5 and equation (3.71) it follows that

$$m_j = \frac{2c}{a} \left(\frac{j}{j+1} \right) \quad \text{for } j = 1, 2, \dots, n-1.$$

Clearly, it follows that $M_A = \frac{2|c|}{a} \left(\frac{n-1}{n} \right)$.

(3) Assume that $a^2 - 4bc < 0$. Applying Lemma 3.5 and equation (3.69) it follows that

$$m_j = \sqrt{c/b} \frac{\sin(j\theta)}{\sin((j+1)\theta)}$$

or

$$m_j = \sqrt{c/b} g_\theta(j)$$

where $g_\theta(x) = \sin(x\theta)/\sin((x+1)\theta)$.

In Lemma 3.7 it was shown that $g_\theta(x)$ is a strictly increasing function for $x \in [1, n-1]$, hence it follows that

$$M_A = \sqrt{c/b} \frac{\sin((n-1)\theta)}{\sin(n\theta)} \quad \blacksquare$$

The above theorem provides an upper bound for the multipliers encountered during the Gaussian elimination process.

In a recent paper by Gunzburger and Nicolaidis [1982] it was shown that it is possible to find a Toeplitz tridiagonal matrix $A = [c, a, b]$ where $b = -1$, $c = -1$, and $0 < a < 2$, such that the multipliers of A may become arbitrarily large. It will be shown, however, that if $A = [c, a, b]$ is a Toeplitz tridiagonal M-matrix, then the moduli of the multipliers are bounded above by either 2 or $2(c/b)$.

Lemma 3.8. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M-matrix of order n , such that $bc \neq 0$. If $|b| \leq |c|$, then $M_{A^T} \leq M_A$.

Proof. If $|b| \leq |c|$, then $b/c \leq 1$. Applying Corollary 3.5 it follows that, letting $\bar{m}_j$ denote the j th multiplier for A^T ,

$$\bar{m}_j = (b/c)m_j \quad \text{for } j = 1, 2, \dots, n-1. \quad (3.82)$$

Taking the absolute value of both sides of equation (3.82) leads to the equation

$$|\bar{m}_j| = \frac{b}{c} |m_j|,$$

so that

$$|\bar{m}_j| \leq |m_j|.$$

Therefore the result follows. ■

Theorem 3.4 states that, if A is a M -matrix with the property that $x^T A \geq 0$ for some vector $x \gg 0$, then A has an LU-decomposition $A = LU$ where

$$|\ell_{ij}| \leq \beta_x$$

where $\beta_x = (\max_k x_k) / (\min_k x_k)$.

If A is Toeplitz tridiagonal irreducible M -matrix, then Theorem 3.14 provides a formula for the entries of a positive vector x such that $x^T A \geq 0$. It has been stated that using β_x as an upper bound for the entries in the matrix A can be quite pessimistic at times. The following example illustrates this statement.

Example 3.6

Let $A = [-3/20, 2, -5]$ be a matrix of order 10. Then $a^2 - 4bc = 1$. Thus A is a nonsingular irreducible M -matrix. Applying Theorem 3.15 it follows that

$$M_A = \frac{(3/20)}{(1/2)} \cdot \frac{3^9 - 1}{3^{10} - 1} \doteq .1.$$

Therefore $\max_{i,j} |\ell_{ij}| = 1$.

Applying Theorem 3.14 it follows that

$$\beta_x \doteq 1.5 \times 10^9.$$

Clearly β_x is significantly larger than M_A , where $M_A = \max_j |m_j|$.

To show that A has a strongly stable LU-decomposition a constant α needs to be found such that $M_A \leq \alpha$, where α is independent of n and the elements of A . The following lemmas will be used in the next theorem.

Lemma 3.9. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M -matrix of order n , such that $bc \neq 0$. If $|c| \leq a$ and $|c| \leq |b|$, then $M_A < 2$.

Proof. If A is column diagonally dominant, then it is well known that $\max_{i,j} |\ell_{ij}| \leq 1$. Therefore assume that A is not column diagonally dominant. Thus it must be true that $a < |b| + |c|$.

Assume that $a^2 - 4bc > 0$. Then

$$M_A = \frac{|c|}{\lambda_2} f_Y(n-1)$$

where $\lambda_2 = \frac{a - \sqrt{a^2 - 4bc}}{2}$, and $f_Y(x)$ is defined in Lemma 3.6.

Applying Lemma 3.6 it follows that

$$M_A < \frac{|c|}{\lambda_2}.$$

If $a < |b| + |c|$, then it follows that $\frac{|c|}{\lambda_2} < 1$.

Therefore $M_A < 1$.

Assume that $a^2 - 4bc = 0$. Then

$$M_A = \frac{2|c|}{a} \left(\frac{n-1}{n} \right).$$

Since $|c| \leq a$, it follows that $M_A < 2$.

Assume that $a^2 - 4bc < 0$, and $\tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right) \leq \frac{\pi}{n+1}$.

Then

$$M_A = \sqrt{c/b} g_\theta(n-1)$$

where $\theta = \tan^{-1} \left(\frac{\sqrt{4bc - a^2}}{a} \right)$ and $g_\theta(x)$ is defined in Lemma 3.7.

Applying Lemma 3.7 it follows that $g_\theta(n-1) < 2$, so that

$$M_A < 2 \sqrt{c/b},$$

or

$$M_A < 2. \quad \blacksquare$$

Lemma 3.10. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M-matrix of order n , such that $bc \neq 0$. Then the following two inequalities cannot both be true

$$a < |b|, \quad a < |c|.$$

Proof. The second principal minor σ_2 of A is

$$\sigma_2 = a^2 - bc.$$

Thus it must hold that

$$a^2 - bc \geq 0.$$

If $a < |b|$ and $a < |c|$, then $a^2 - bc < 0$. This is a contradiction. ■

Theorem 3.16. Let $A = [c, a, b]$ be a Toeplitz tridiagonal M-matrix of order n , such that $bc \neq 0$. Then either $M_A < 2$ or $M_{A^T} < 2$.

Proof. At least one of the following inequalities must hold.

$$|b| \leq a \quad \text{or} \quad |c| \leq a.$$

Assume that $|c| \leq a$. If $|b| < |c|$, then $|b| < a$. Hence by applying Lemma 3.9 to A^T , it follows that $M_{A^T} < 2$. If $|c| \leq |b|$, then by applying Lemma 3.9 to A , it follows that $M_A < 2$.

Assume that $|b| \leq a$. If $|b| < |c|$, then by applying Lemma 3.9 to A^T , it follows that $M_{A^T} < 2$. If $|c| \leq |b|$, then by applying Lemma 3.9 to A , it follows that $M_A < 2$.

Therefore either $M_A < 2$ or $M_{A^T} < 2$. ■

If $A = LU$ is the LU-decomposition of A , then by applying Corollary 3.6 it follows that

$$\max_{i,j} |u_{ij}| \leq \max\{a, |b|\}.$$

Thus there was no growth in the elements of the matrix U . Also, if $A^T = \bar{L}\bar{U}$ is the LU-decomposition of A^T , then by applying Corollary 3.6 it follows that

$$\max_{i,j} |\bar{u}_{ij}| \leq \max\{a, |c|\}.$$

Therefore, either A or A^T will have a strongly stable LU-decomposition. It is not true in general that, if A has a strongly stable LU-decomposition, then A^T will have a strongly stable LU-decomposition. The following example illustrates this statement.

Example 3.7

Let

$$A = \begin{pmatrix} 2\varepsilon & -1 \\ -\varepsilon^2 & 2\varepsilon \end{pmatrix}$$

where $0 < \varepsilon < 1/2$. Then A has the following LU-decomposition

$$A = \begin{pmatrix} 1 & 0 \\ -\varepsilon/2 & 1 \end{pmatrix} \begin{pmatrix} 2\varepsilon & -1 \\ 0 & 3\varepsilon/2 \end{pmatrix}.$$

Clearly A has a strongly stable LU-decomposition. Next,

$$A^T = \begin{pmatrix} 2\varepsilon & -\varepsilon^2 \\ -1 & 2\varepsilon \end{pmatrix}.$$

Then A^T has the following LU-decomposition

$$A^T = \begin{pmatrix} 1 & 0 \\ -1/(2\varepsilon) & 1 \end{pmatrix} \begin{pmatrix} 2\varepsilon & -\varepsilon^2 \\ 0 & 3\varepsilon/2 \end{pmatrix}.$$

In this case A^T does not have a strongly stable LU-decomposition.

Assume that $M_{A^T} < 2$. Then by applying Corollary 3.6 it follows that

$$M_A < (c/b)2.$$

So the growth of the multipliers of A is bounded by $2(c/b)$. Therefore A

may not have a strongly stable LU-decomposition, but the moduli of the multipliers are bounded above by $2(c/b)$, and there is no growth in the entries of the matrix U .

Finally, assume that A is an irreducible tridiagonal matrix and that $x^T A = \lambda x^T$, where x is an n -dimensional vector. If $Ay = \lambda y$, then the following theorem provides a relationship between x and y .

Theorem 3.17. Let $A = [c_j, a_j, b_j]$ be a tridiagonal matrix of order n , such that $b_j c_j \neq 0$ for $j = 1, 2, \dots, n-1$. Assume that λ is an eigenvalue of A and x is the left eigenvector corresponding to λ . If $y_1 = x_1$ and

$$y_k = x_k \prod_{j=1}^{k-1} \left(\frac{c_j}{b_j} \right) \quad \text{for } k = 2, \dots, n, \quad (3.83)$$

then

$$Ay = \lambda y. \quad (3.84)$$

Proof. If $x^T A = \lambda x^T$, then the following equations must hold

$$a_1 x_1 + c_1 x_2 = \lambda x_1 \quad (3.85)$$

$$b_{k-1} x_{k-1} + a_k x_k + c_k x_{k+1} = \lambda x_k \quad \text{for } k = 2, 3, \dots, n-1, \quad (3.86)$$

$$b_{n-1} x_{n-1} + a_n x_n = \lambda x_n. \quad (3.87)$$

The equation (3.84) will be proven correct by directly showing that the k th component of Ay is equal to λy_k for $k = 1, 2, \dots, n$. The proof will be broken into three cases, $k = 1$, $k = 2, \dots, n-1$, and $k = n$.

Assume that $k = 1$. Then

$$(Ay)_1 = a_1 y_1 + b_1 y_2,$$

or

$$(Ay)_1 = a_1 x_1 + c_1 x_2.$$

Using equation (3.85) it follows that

$$(Ay)_1 = \lambda x_1,$$

so that $(Ay)_1 = \lambda y_1$.

Assume that $k = 2, 3, \dots, n - 1$. Then

$$(Ay)_k = c_{k-1} y_{k-1} + a_k y_k + b_k y_{k+1}.$$

and applying equation (3.83) yields

$$\begin{aligned} (Ay)_k &= c_{k-1} x_{k-1} \prod_{j=1}^{k-2} \left(\frac{c_j}{b_j} \right) + a_k x_k \prod_{j=1}^{k-1} \left(\frac{c_j}{b_j} \right) \\ &\quad + b_k x_{k+1} \prod_{j=1}^k \left(\frac{c_j}{b_j} \right), \end{aligned}$$

so that

$$(Ay)_k = \prod_{j=1}^{k-1} \left(\frac{c_j}{b_j} \right) \left[b_{k-1} x_{k-1} + a_k x_k + c_k x_{k+1} \right].$$

Using equation (3.86) it follows that

$$(Ay)_k = \prod_{j=1}^{k-1} \left(\frac{c_j}{b_j} \right) \lambda x_k,$$

so that $(Ay)_k = \lambda y_k$.

Assume that $k = n$. Then

$$(Ay)_n = c_{n-1}y_{n-1} + a_n y_n$$

and applying equation (3.83) yields

$$(Ay)_n = c_{n-1}x_{n-1} \prod_{j=1}^{n-2} \left(\frac{c_j}{b_j} \right) + a_n x_n \prod_{j=1}^{n-1} \left(\frac{c_j}{b_j} \right),$$

so that

$$(Ay)_n = \prod_{j=1}^{n-1} \left(\frac{c_j}{b_j} \right) \left[b_{n-1}x_{n-1} + a_n x_n \right].$$

Using equation (3.87) it follows that

$$(Ay)_n = \prod_{j=1}^{n-1} \left(\frac{c_j}{b_j} \right) \lambda x_n,$$

so that $(Ay)_n = \lambda y_n$. ■

Corollary 3.8. Let $A = [c_j, a_j, b_j]$ be a tridiagonal diagonally dominant singular M-matrix of order n , such that $b_j c_j \neq 0$ for $j = 1, 2, \dots, n-1$. If $y_1 = 1$ and

$$y_k = \prod_{j=1}^{k-1} \left(\frac{c_j}{b_j} \right) \quad \text{for } k = 2, 3, \dots, n,$$

then $Ay = 0$.

Proof. If A is a diagonally dominant singular M -matrix, then $e^T A = 0$. Therefore the stated result follows directly from Theorem 3.17, where $x = e$. ■

Thus, if A is tridiagonal column diagonally dominant singular irreducible M -matrix, then one can use Corollary 3.8 to easily compute the right null vector of A .

CHAPTER IV

COMPUTING STATIONARY DISTRIBUTIONS OF MARKOV CHAINS

1. Introduction

This chapter is concerned with applying the methods of Chapters II and III to computing the stationary distribution vector p of an ergodic finite Markov chain C with rate transition matrix Q . Here Q is an $n \times n$ irreducible, row stochastic matrix and p is an n -dimensional vector with positive probabilities satisfying

$$Q^T p = p. \quad (4.1)$$

Since Q is an irreducible nonnegative matrix ($Q \geq 0$), by the Perron-Frobenius Theory (see, e.g., Varga [1962], p. 30 or Berman and Plemmons [1979], p. 27), $p = (p_i)$ is the unique positive vector satisfying

$$\|p\|_1 = 1.$$

The computation of the stationary distributions of a Markov chain is of widespread interest (Kemeny and Snell [1960], Golub and Seneta [1973], Paige, Styan, and Wachter [1975], Meyer [1975], W. J. Stewart [1978], G. W. Stewart [1980], Hunter [1982], Kemeny [1981]). More generally, the stationary distribution vector p satisfying (4.1) is important in many areas of the mathematical sciences, including queueing networks (e.g., Kaufman [1982]), input-output economic models (e.g., Berman and Plemmons [1979], Chapter 9, and Duchin and Szyld [1979]) and in compartmental analysis tracer models (e.g., Sheppard

and Householder [1951] and Funderlic and Mankin [1981]). Such computations are also related to the discrete Neuman problem in partial differential equations (e.g., Plemmons [1976a]). Techniques for computing p where Q is large and sparse have traditionally been iterative and often involve some variation of the power method for computing eigenvectors (e.g., W. J. Stewart [1978]), although more recently methods based upon matrix splitting such as the Gauss-Seidel method have been investigated (see Kaufman [1982] for an interesting study of such methods). Combined direct-iterative methods have recently been considered by Koury, McAllister and Stewart [1982], and by Funderlic and Plemmons [1982]. Our interest here is in the Rank Modification Method and the Partition Factorization Method (PF Method).

2. Direct Methods

Paige, Styan and Wachter [1975] have considered a variety of direct methods for computing the stationary distributions vector p for a ergodic Markov chain with row transition matrix Q . They recommended two methods which are based upon the transformation of $I - Q^T$ into a nonsingular matrix by a rank one modification, followed by the solution of an associated nonsingular system of linear equations. Specifically they showed that if u is any n -dimensional vector such that $e^T u \neq 0$, then

$$I - Q^T + ue^T \tag{4.2}$$

is nonsingular and p is the solution to the nonsingular system of linear equations

$$(I - Q^T + ue^T)p = u. \quad (4.3)$$

Recently this rank one modification concept has been extended to a more general method by Hunter [1982]. In this paper it was proven that if u and v are n -dimensional vectors such that $u^T e \neq 0$ and $v^T p \neq 0$, then

$$I - Q^T + uv^T \quad (4.4)$$

is nonsingular and p is then the solution to the nonsingular system of linear equations

$$(I - Q^T + uv^T)p = u.$$

Also, recently this rank one modification concept has been extended to more general problems by Kemeny [1981].

Based upon the numerical comparison of a collection of direct methods for computing p available at that time, Paige, Styan and Wachter [1975] recommended the use of the nonsingular system (4.3) with two possible choices of u . The resulting nonsingular systems of linear equations were

$$[I - Q^T + (Q^T e_k) e^T]p = Q^T e_k, \quad (4.5)$$

$$[I - Q^T + e_k e^T]p = e_k. \quad (4.6)$$

The methods will be named as follows:

Paige, Styan and Wachter Method 1 (PSW Method 1)

Let Q be the rate transition matrix of an n state ergodic Markov chain C . The following method can be used to compute the stationary

distribution vector p of the chain C .

- 1) Apply Gaussian elimination to the matrix $I - Q^T + (Q^T e_j) e^T$ to produce the following factorization

$$P[I - Q^T + (Q^T e_k) e^T] = LU$$

where P is the permutation matrix that results from row pivoting and $1 \leq k \leq n$.

- 2) Solve $Lz = P(Q^T e_k)$ using forward substitution.
- 3) Solve $Up = z$ using back substitution.

Paige, Styan and Wachter Method 2 (PSW Method 2)

Let Q be the rate transition matrix of an n -state ergodic Markov chain C . The following method can be used to compute the stationary distribution vector p of the chain C .

- 1) Apply Gaussian elimination to the matrix $I - Q^T + e_k e^T$ to produce the following factorization

$$P[I - Q^T + e_k e^T] = LU$$

where P is the permutation matrix that results from row pivoting and $1 \leq k \leq n$.

- 2) Solve $Lz = P e_k$ using forward substitution.
- 3) Solve $Up = z$ using back substitution.

If $A = I - Q^T$, then A is a diagonally dominant irreducible singular M -matrix. This follows because the off diagonal entries of A are nonpositive and $e^T A = 0$. Clearly, the stationary distribution vector p is the right null of A such that $\|p\|_1 = 1$.

There are other direct methods which have been used in the past to compute the stationary distribution vector p of Q . Suppose A has been partitioned into the following form

$$A = \begin{pmatrix} A_n & y_n \\ z_n^T & a_{nn} \end{pmatrix} \quad (4.7)$$

where A_n is the submatrix formed by deleting the n th row and n th column of A . Let $\tilde{A}$ be defined as

$$\tilde{A} = \begin{pmatrix} A_n & y_n \\ e^T & 1 \end{pmatrix}$$

where e is the $(n - 1)$ -dimensional vector of all one's. It can be easily shown that $\tilde{A}$ is a nonsingular matrix and if p is the solution to the nonsingular system of linear equations $\tilde{A}p = e_n$, then p is the solution to the homogeneous system of linear equations $Ap = 0$ such that $e^T p = 0$. This method will be named as follows:

Replace Last Row Method (RLR Method)

Let Q be the rate transition matrix of an n state ergodic Markov chain, C . The following method can be used to compute the stationary distribution vector p of the chain C .

- 1) Let $A = I - Q^T$. Suppose that A has been partitioned into the form (4.7). Consider the matrix $\tilde{A}$ defined above.
- 2) Apply Gaussian elimination with row pivoting to the matrix $\tilde{A}$ to produce the following factorization

$$\tilde{PA} = LU$$

where P is the permutation matrix that results from row pivoting.

- 3) Solve $Lz = Pe_n$ using forward substitution.
- 4) Solve $Up = z$ using back substitution.

Another method that can be found in the literature is Muller's Method (see Muller [1980]). Let $\bar{A} = (\bar{a}_{ij})$ be a matrix of order n , such that

$$\bar{a}_{ij} = \begin{cases} a_{ij} & \text{if } i \neq n \text{ and } j \neq n, \\ a_{ij} + 1 & \text{if } i = n \text{ and } j = n \end{cases}$$

where $A = I - Q^T$. Then $\bar{A}$ is an irreducibly diagonally dominant matrix. Also, $\bar{A}$ is a nonsingular matrix (see Varga [1962], p. 23). If w is the solution to the system of linear equations $\bar{A}w = e_n$, then w is a right null vector of A . This suggests the following scheme for computing the stationary distribution vector p :

Muller's Method (MU Method)

Let Q be the rate transition matrix of an n state ergodic Markov chain C . The following method can be used to compute the stationary distribution vector p of the chain C .

- 1) Let $A = I - Q^T$ and $\bar{A} = (\bar{a}_{ij})$ denote the matrix of order n , such that

$$\bar{a}_{ij} = \begin{cases} a_{ij} & \text{if } i \neq n \text{ and } j \neq n, \\ a_{ij} + 1 & \text{if } i = n \text{ and } j = n, \end{cases}$$

where $A = (a_{ij})$.

- 2) Apply Gaussian elimination to the matrix $\bar{A}$ to produce the following factorization

$$\bar{A} = LU.$$

- 3) Solve $Lz = e_n$ using forward substitution.
 4) Solve $Uw = z$ using back substitution.
 5) Set $p = \frac{1}{\|w\|_1} w$.

The LU-decomposition of A is

$$A = \begin{pmatrix} L_n & 0 \\ z_n^T U_n^{-1} & 1 \end{pmatrix} \begin{pmatrix} U_n & L_n^{-1} y_n \\ 0 & 0 \end{pmatrix}$$

where $A_n = L_n U_n$ is the LU-decomposition of A_n . It can be easily shown that the LU-decomposition of $\bar{A}$ is

$$\bar{A} = \begin{pmatrix} L_n & 0 \\ z_n^T U_n^{-1} & 1 \end{pmatrix} \begin{pmatrix} U_n & L_n^{-1} y_n \\ 0 & 1 \end{pmatrix}. \quad (4.8)$$

Therefore Muller's Method is mathematically the same as the Direct Factorization Method or the Partition Factorization Method, with $k = n$. It should be noted that when the Partition Factorization Method is used to compute the stationary distribution vector that the computed vector w needs to be scaled so that the resulting vector is a probability vector.

If $A = I - Q^T$, where Q is a stochastic matrix, then $\max_{i,j} |a_{ij}| \leq 1$. Let $\hat{p}$ be the approximation to the stationary distribution vector p , solved by Gaussian elimination applied to $I - Q^T$ without pivoting in floating point arithmetic with machine unit roundoff error μ . Then, applying Corollary 3.4, there exists a matrix E such that $\hat{p}$ satisfies the homogeneous system

$$(I - Q^T + E)\hat{p} = 0,$$

where for $1 \leq i, j \leq n$,

$$|e_{ij}| \leq \mu n (3.02 + 1.01 n).$$

3. Rank Modification Method

Assume that A is a singular irreducible diagonally dominant M-matrix. Then $e^T A = 0$. The statement that, p is the unique solution to the homogeneous system of linear equations $Ap = 0$ such that $e^T p = 1$, is equivalent to the statement that p is the unique solution to the homogeneous system of linear equations $Ap = 0$ such that $\|p\|_1 = 1$. Using this fact it can be easily shown that all of the direct methods discussed in Section 2 can be viewed as a Rank Modification Method:

- 1) PSW Method 1. Let $u = Q^T e_j$ and $v = e$.

- 2) PSW Method 2. Let $u = e_j$ and $v = e$.
- 3) RLR Method. Let $u = e_n$ and $v^T = e^T - (z_n^T, a_{nn})$.
- 4) MU Method. Let $u = e_n$ and $v = e_n$.

It has already been shown that the Partition Factorization Method can be viewed as a Rank Modification Method.

When any of the above methods is used to compute the stationary distribution of a Markov chain, the computed solution $\hat{p}$ should be scaled so that $\|\hat{p}\|_1 = 1$ or equivalently $e^T \hat{p} = 1$. Let $\hat{p}$ be the scaled approximation to the stationary distribution vector p , computed by using the Rank Modification Method in floating point arithmetic with machine roundoff error μ . If $\|A^\# \| \|F\| < 1$, for some consistent matrix norm $\|\cdot\|$, then by applying Corollary 2.2 it follows that

$$\frac{\|p - \hat{p}\|}{\|p\|} \leq \frac{K(A)}{1 - \|F\| \|A^\#\|} \cdot \frac{\|F\|}{\|A\|}$$

where the matrix F is due to the roundoff errors produced by the method and $K(A) = \|A\| \|A^\#\|$.

It was observed that for the numerical results computed using the Partition Factorization Method and the Paige, Styan and Wachter Methods 1 and 2, that the accuracy of the result was independent of which method was used.

4. Numerical Comparisons

Numerical comparisons were performed for the Partition Factorization (PF) Method and the Paige, Styan, and Wachter (PSW)

Methods 1 and 2. Note that in computing the stationary distribution vector p for a stochastic matrix of order n , in each of the three algorithms being tested there are n possibly different systems of linear equations that can be used to obtain p .

The computer program for each algorithm was executed on an IBM 3081 computer at the Triangle Universities Computation Center. The software was written in FORTRAN and compiled using the IBM Extended Optimizing Compiler in single and double precision floating point arithmetic.

The relative error was computed by comparing the single precision result with the double precision approximate solution, found by using the IMSL subroutine EIGRF. The relative error reported was computed as $\|p - \hat{p}\|_1 / \|p\|_1$ where p is the double precision approximation and will be referred to as the "exact solution" and $\hat{p}$ the single precision approximation computed by one of the three algorithms. The vectors p and $\hat{p}$ are both normalized so that $\|p\|_1 = 1$ and $\|\hat{p}\|_1 = 1$. Hence the relative error is bounded above by two. The residual error computed was $\|\hat{p} - Q^T \hat{p}\|_1$ and would theoretically be zero if $\hat{p} = p$. The condition numbers, of the submatrices A_k , are computed relative to the one norm.

One of the problems associated with the PSW Methods is that the sparse structure of the matrix A may be modified and the resulting updated matrix may no longer be sparse. In order to measure this effect, the numbers of nonzero entries in the matrix A and in the rank one modified matrix in the PSW Methods 1 and 2 are reported when A is sparse.

Various test problems were used to compare the three algorithms being considered. One type of matrix used is a nearly completely decomposable (NCD) matrix. The stochastic matrix

$$Q = Q^* + \epsilon C$$

where $\epsilon > 0$, Q^* is a block diagonal stochastic matrix and C has row sums zero, is called a nearly completely decomposable matrix. If Q^* has m diagonal blocks then Q^* has one as an eigenvalue of multiplicity at least m . Therefore the matrix Q has at least $m - 1$ eigenvalues close to one. The parameter ϵ is called the degree of coupling and is a measure of the decomposability of the matrix Q . Such matrices often arise in the analysis of queueing networks (e.g., Koury, McAllister, and Stewart [1982]).

The following list of test problems were used to compare the PF Method and the PSW Methods 1 and 2.

Test Problem One

This matrix is of order ten and the condition numbers for the submatrices A_k of order nine range from $2.046 \text{ E} + 01$ to $2.090 \text{ E} + 17$. The transition matrix and the numerical results can be found in Appendix A.

Test Problem Two

This matrix is of order eight and is commonly called Courtois' Matrix (see Courtois [1977]). This matrix has been used to test several algorithms (e.g., Koury, McAllister, and Stewart [1982], Stewart [1980] and Vantilbourg [1981]). It is nearly completely decomposable and the degree of coupling is 0.001. The condition

numbers for the submatrices A_k of order seven range from $1.021 \text{ E} + 04$ to $2.041 \text{ E} + 04$. The transition matrix and the numerical results can be found in Appendix B.

Test Problem Three

This matrix is of order six and the condition numbers for the submatrices A_k of order five range from $1.644 \text{ E} + 01$ to $1.425 \text{ E} + 07$. The transition matrix and the numerical results can be found in Appendix C.

Test Problem Four

This is a class of matrices of order ten which are nearly completely decomposable. This particular class of matrices was used in the paper by Paige, Styan, and Wachter [1975] for test purposes. The transition matrix and the numerical results can be found in Appendix D.

Test Problem Five

This matrix is of order 84 is banded and sparse. It arose from the queueing network analysis of a job line production model, studied in the Industrial Engineering Department at North Carolina State University. The condition numbers for submatrices A_k of order 83 range from $2.668 \text{ E} + 02$ to $6.034 \text{ E} + 02$. The transition matrix and the numerical results can be found in Appendix E.

Test Problem Six

This is a class of matrices of order three. The transition matrix and the numerical results can be found in Appendix F.

Test Problem Seven

This matrix is of order 20 and sparse. The condition numbers for the submatrices A_k of order 19 range from $2.821 \text{ E} + 01$ to $1.802 \text{ E} + 02$.

The transition matrix and the numerical results can be found in Appendix G.

Special Notation

If B is a square matrix, then $N(B)$ denotes the percent of nonzero entries in B . If B is also nonsingular then the term $K_1(B)$ denotes the condition number of the matrix and is defined by $K_1(B) = \|B\|_1 \|B^{-1}\|_1$.

The term maximum relative error means the maximum of all the relative error terms for the n possible different linear systems for a particular problem and algorithm. Similar definitions are applied to the terms minimum relative error and maximum and minimum residual errors.

5. Concluding Remarks

The chapter is concluded with some observations concerning the performances of the nonsingular rank one modification methods recommended by Paige, Styan and Wachter [1975] (PSW Methods 1 and 2) and the Partition Factorization (PF) Method. We comment first about the particular test problems considered in the preceding section and then give some general observations.

1. In Test Problem One all three algorithms produced five or more decimal digits of accuracy in IBM single precision in each situation. (Here the PF Method was tested using each of the ten principal submatrices A_k of A having order nine. The PSW Method 1 was tested using each of the ten rows of Q and the PSW Method 2 was tested using each unit vector e_j , $1 \leq j \leq 10$). Some fill-in to $I - Q^T$ occurred as a result of PSW rank one modifications. Notice that

the one condition numbers of the A_k range up to near $2.0 \text{ E} + 17$. However, the PF Method still obtains uniformly good results using each A_k . The second smallest singular value of $I - Q^T$ is near .14 and thus the overall problem of computing P is apparently well-conditioned.

2. Test Problem Two is Courtois' matrix which is nearly completely decomposable. Here the three methods obtain moderately accurate results in IBM single precision (between three and six decimal digits) in each situation.

3. Between only one and two decimal digits of accuracy are obtained by the three methods applied to Test Problem Three. However, the residual error is small in each case. Observe that the second smallest singular value of $I - Q^T$ is around 10^{-6} .

4. Test Problem Four represents a class of test situations involving a nearly completely decomposable matrix in which the degree of coupling decreases from 10^{-1} to 10^{-7} , resulting in a comparable decrease in the second smallest singular value of $I - Q^T$. Here the PF Method produces the smallest maximum relative error in each case.

5. For the job line production model in Test Problem Five, all three methods obtained relatively accurate results. However, the PSW Methods 1 and 2 destroy the sparse banded structure of $I - Q^T$. In a recent paper by Funderlic and Plemmons [1982], this transition matrix was used to test a combined direct-iterative algorithm. Similar numerical accuracy was obtained.

6. Test Problem Six represents a class of test matrices where the maximum one condition numbers of A_k , for $k = 1, 2, 3$, increase

from $5.0 \text{ E} + 05$ to $5.0 \text{ E} + 08$. However, the three algorithms obtained relatively accurate results.

7. In Test Problem Seven all three algorithms obtained relatively accurate results. However, the PSW Methods 1 and 2 destroy the random sparse structure of $I - Q^T$.

8. In general for all the problems tested, the residual error was between 10^{-6} and 10^{-9} , even though in many cases the relative error was large. Thus, the residual error may not always be a good measure of the accuracy of the approximation to p .

9. Recall that pivoting generally is necessary in the LU-decompositions of the nonsingular rank one updates of $I - Q^T$ in PSW Methods 1 and 2. However, the PF Method requires no pivoting for numerical stability. Thus it facilitates the possible application of symmetric pivoting to preserve sparsity (see Funderlic and Plemmons [1982]) without the use of any threshold pivoting parameter.

10. Finally, observe that the three methods all obtained comparable accuracy on each test problem. In particular, the PF Method obtained uniformly good or uniformly poor results on a given test problem (depending upon the magnitude of the second smallest singular value), even though there was often a considerable variation of the condition numbers of the principal submatrices used in the PF Method. This leads us to infer that the accuracy obtained by the PF Method is relatively independent of the choice of principal submatrices, up to the constraints of the machine precision. Thus the choice of the principal submatrix A_k for the PF Method could be based upon other considerations, such as sparsity. For example, if Q has

one dense column, say the k th, then the extreme fill-in in computing the LU-decomposition might be avoided by using A_k in the PF Method.

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APPENDIXES

APPENDIX A

TEST PROBLEM ONE

The following matrix is the rate transition matrix for Test Problem One:

$$Q = \begin{bmatrix} .2 & 0 & 0 & .6 & 0 & 0 & 0 & 0 & 0 & .2 \\ 0 & .1 & 0 & 0 & .6 & 0 & .3 & 0 & 0 & 0 \\ 0 & .1 & 0 & 0 & 0 & 0 & 0 & .8 & 0 & .1 \\ 0 & 0 & .6 & 0 & .3 & 0 & 0 & 0 & 0 & .1 \\ 0 & .5 & 0 & 0 & .5 & 0 & 0 & 0 & 0 & 0 \\ 0 & .5 & 0 & 0 & .2 & 0 & 0 & 0 & .3 & 0 \\ 0 & 0 & 0 & 0 & .7 & 0 & .2 & 0 & 0 & .1 \\ .1 & 0 & .9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & .1 & 0 & 0 & 0 & .8 & 0 & 0 & 0 & .1 \\ 0 & .4 & 0 & 0 & 0 & .4 & 0 & 0 & 0 & .2 \end{bmatrix}$$

The following is the "exact solution" for Test Problem One:

$$p = (3.18129230 \text{ E-16}, 3.13420278 \text{ E-01}, 2.93617551 \text{ E-15}, \\ 3.07485879 \text{ E-16}, 5.43805217 \text{ E-01}, 7.88809424 \text{ E-03}, \\ 1.17532604 \text{ E-01}, 2.56247898 \text{ E-15}, 2.36642827 \text{ E-03}, \\ 1.49873790 \text{ E-02})^T.$$

The second smallest singular value of the matrix A is 1.424 E-01.

The percent of nonzero entries in the matrix A is 33%.

TABLE A.1
RELATIVE ERROR FOR TEST PROBLEM ONE

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	2.525 E-06	2.479 E-06	3.676 E-06
Minimum	1.454 E-07	1.757 E-07	6.856 E-08

TABLE A.2
RESIDUAL ERROR FOR TEST PROBLEM ONE

Residual Error	PF Method	PSW Method 1	PSW Method 2
Maximum	4.452 E-06	7.882 E-07	7.881 E-07
Minimum	4.555 E-07	1.827 E-07	1.830 E-07

TABLE A.3
PERCENT OF NONZERO ENTRIES IN
THE MATRICES FORMED BY THE
PSW METHODS FOR TEST
PROBLEM ONE

	$N(A + (Q^T e_j) e^T)$	$N(A + e_j e^T)$
Maximum	51%	40%
Minimum	40%	37%

APPENDIX B

TEST PROBLEM TWO

The following matrix is the rate transition matrix for Test Problem Two:

$$Q = \begin{bmatrix} .85 & 0 & .149 & .0009 & 0 & .00005 & 0 & .00005 \\ .1 & .65 & .249 & 0 & .00009 & .00005 & 0 & .00005 \\ .1 & .8 & .0996 & .0003 & 0 & 0 & .0001 & 0 \\ 0 & .0004 & 0 & .7 & .2995 & 0 & .0001 & 0 \\ .0005 & 0 & .0004 & .399 & .6 & .0001 & 0 & 0 \\ 0 & .00005 & 0 & 0 & .00005 & .6 & .2499 & .15 \\ .00003 & 0 & .00003 & .00004 & 0 & .1 & .8 & .0999 \\ 0 & .00005 & 0 & 0 & .00005 & .1999 & .25 & .55 \end{bmatrix}$$

The following is the "exact solution" for Test Problem Two:

$$p = (8.92826528 \text{ E-02}, 9.27576375 \text{ E-02}, 4.04883120 \text{ E-02}, \\ 1.58533191 \text{ E-01}, 1.18938207 \text{ E-01}, 1.20385481 \text{ E-01}, \\ 2.77795252 \text{ E-01}, 1.01819266 \text{ E-01})^T.$$

The second smallest singular value of the matrix A is 1.906 E-04.

The percent of nonzero entries in the matrix Q is 64%.

TABLE B.1
RELATIVE ERROR FOR TEST PROBLEM TWO

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	1.710 E-04	1.180 E-03	1.097 E-03
Minimum	3.957 E-05	3.905 E-04	1.111 E-04

TABLE B.2
RESIDUAL ERROR FOR TEST PROBLEM TWO

Residual Error	PF Method	PSW Method 1	PSW Method 2
Maximum	1.149 E-06	1.009 E-06	9.946 E-07
Minimum	1.891 E-07	7.152 E-07	7.860 E-07

TABLE B.3
 PERCENT OF NONZERO ENTRIES IN
 THE MATRICES FORMED BY THE
 PSW METHODS FOR TEST
 PROBLEM TWO

	$N(A + (Q^T e_j) e^T)$	$N(A + e_j e^T)$
Maximum	83%	69%
Minimum	77%	67%

APPENDIX C

TEST PROBLEM THREE

The following matrix is the rate transition matrix for Test

Problem Three:

$$Q = \begin{bmatrix} 0.999999 & 1.0 \text{ E-}07 & 2.0 \text{ E-}07 & 3.0 \text{ E-}07 & 4.0 \text{ E-}07 \\ 0.4 & 0.3 & 0 & 0 & 0.3 \\ 5.0 \text{ E-}07 & 0 & 0.999999 & 0 & 5.0 \text{ E-}07 \\ 5.0 \text{ E-}07 & 0 & 0 & 0.999999 & 5.0 \text{ E-}07 \\ 2.0 \text{ E-}07 & 3.0 \text{ E-}07 & 1.0 \text{ E-}07 & 4.0 \text{ E-}07 & 0.999999 \end{bmatrix}$$

The following is the "exact solution" for Test Problem Three:

$$p = (3.15217329 \text{ E-}01, 1.95652135 \text{ E-}07, 9.81883865 \text{ E-}02, \\ 2.35144881 \text{ E-}01, 3.51449206 \text{ E-}01)^T.$$

The second smallest singular value of the matrix A is 1.007 E-06.

TABLE C.1
RELATIVE ERROR FOR TEST PROBLEM THREE

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	2.265 E-02	3.888 E-02	2.265 E-02
Minimum	1.313 E-02	6.115 E-03	1.313 E-02

TABLE C.2
RESIDUAL ERROR FOR TEST PROBLEM THREE

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	3.040 E-08	4.172 E-07	3.636 E-07
Minimum	5.900 E-09	3.576 E-07	3.576 E-07

APPENDIX D

TEST PROBLEM FOUR

Let

$$\bar{Q}(\epsilon) = \begin{bmatrix} .1 & .3 & .1 & .2 & .3 & 0 & 0 & 0 & 0 & 0 \\ .2 & .1 & .1 & .2 & .4 & 0 & 0 & 0 & 0 & 0 \\ .1 & .2 & .2 & .4 & .1 & 0 & 0 & 0 & 0 & 0 \\ .4 & .2 & .1 & .2 & .1 & 0 & 0 & 0 & 0 & 0 \\ .6 & .3 & 0 & 0 & .1 & 0 & 0 & 0 & 0 & 0 \\ \epsilon & 0 & 0 & 0 & 0 & .1 & .2 & .2 & .4 & .1 \\ 0 & 0 & 0 & 0 & 0 & .2 & .2 & .1 & .3 & .2 \\ 0 & 0 & 0 & 0 & 0 & .1 & .5 & 0 & .2 & .2 \\ 0 & 0 & 0 & 0 & 0 & .5 & .2 & .1 & 0 & .2 \\ 0 & 0 & 0 & 0 & 0 & .1 & .2 & .2 & .3 & .2 \end{bmatrix}$$

where $0 < \epsilon$.

If s_j denotes the inverse of the sum of the entries in row j of the matrix $\bar{Q}(\epsilon)$ and $D = \text{diag} (s_1, s_2, \dots, s_n)$ then $Q(\epsilon) = D\bar{Q}(\epsilon)$ is a nearly completely decomposable matrix of order 10. Let $A(\epsilon) = I - Q(\epsilon)^T$. The degree of coupling of $Q(\epsilon)$ is $\epsilon/(1 + \epsilon)$, and the percent of nonzero entries in the matrix $A(\epsilon)$ is 50%.

TABLE D.1
 SECOND SMALLEST SINGULAR
 VALUE OF $A(\epsilon)$ FOR TEST
 PROBLEM FOUR

ϵ	Second Smallest Singular Value of $A(\epsilon)$
1.0 E-01	4.211 E-01
1.0 E-03	4.898 E-04
1.0 E-05	4.898 E-06
1.0 E-07	4.899 E-08

TABLE D.2
 MAXIMUM RELATIVE ERROR
 FOR TEST PROBLEM FOUR

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-01	4.417 E-06	6.738 E-06	7.304 E-06
1.0 E-03	2.320 E-04	5.506 E-04	2.876 E-04
1.0 E-05	1.586 E-02	2.501 E-02	3.901 E-02
1.0 E-07	8.294 E-01	*	*

TABLE D.3
MINIMUM RELATIVE ERROR
FOR TEST PROBLEM FOUR

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-01	1.661 E-06	1.177 E-06	2.052 E-06
1.0 E-03	6.453 E-05	6.164 E-05	7.774 E-05
1.0 E-05	8.296 E-03	7.814 E-03	7.034 E-03
1.0 E-07	6.424 E-01	8.167 E-01	8.167 E-01

TABLE D.4
MAXIMUM RESIDUAL ERROR
FOR TEST PROBLEM FOUR

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-01	8.102 E-06	1.143 E-06	1.512 E-06
1.0 E-03	7.825 E-06	1.501 E-06	1.262 E-06
1.0 E-05	7.946 E-06	1.281 E-06	1.352 E-06
1.0 E-07	6.395 E-06	*	*

TABLE D.5
MINIMUM RESIDUAL ERROR
FOR TEST PROBLEM FOUR

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-01	4.395 E-07	6.556 E-07	6.034 E-07
1.0 E-03	4.145 E-07	5.997 E-07	6.631 E-07
1.0 E-05	5.772 E-07	5.557 E-07	6.630 E-07
1.0 E-07	2.236 E-07	5.774 E-07	5.848 E-07

TABLE D.6
CONDITION NUMBERS OF THE
PRINCIPAL SUBMATRICES OF
 $A(\epsilon)$ OF ORDER NINE FOR
TEST PROBLEM FOUR

ϵ	Min $K_1(A(\epsilon)_j)$ j	Max $K_1(A(\epsilon)_j)$ j
1.0 E-01	7.494 E+01	1.755 E+02
1.0 E-03	6.284 E+03	9.216 E+03
1.0 E-05	6.261 E+05	9.135 E+05
1.0 E-07	6.261 E+07	9.134 E+07

TABLE D.7

PERCENT OF NONZERO ENTRIES IN
 THE MATRICES FORMED BY THE
 PSW METHODS FOR TEST
 PROBLEM FOUR

	$N(A(\epsilon) + (Q(\epsilon)^T e_j) e^T)$	$N(A(\epsilon) + e_j e^T)$
Maximum	75%	56%
Minimum	60%	54%

APPENDIX E

TEST PROBLEM FIVE

The entries in the rate transition matrix for Test Problem Five and the "exact solution" will not be given. The second smallest singular value of the matrix A is $3.305 \text{ E-}02$. The percent of nonzero entries in the matrix A is 5%. Figure E.1 shows the zero/nonzero structure of the matrix A . Figure E.2 shows the zero/nonzero structure of the matrix $A + (A^T e_{43}) e^T$.

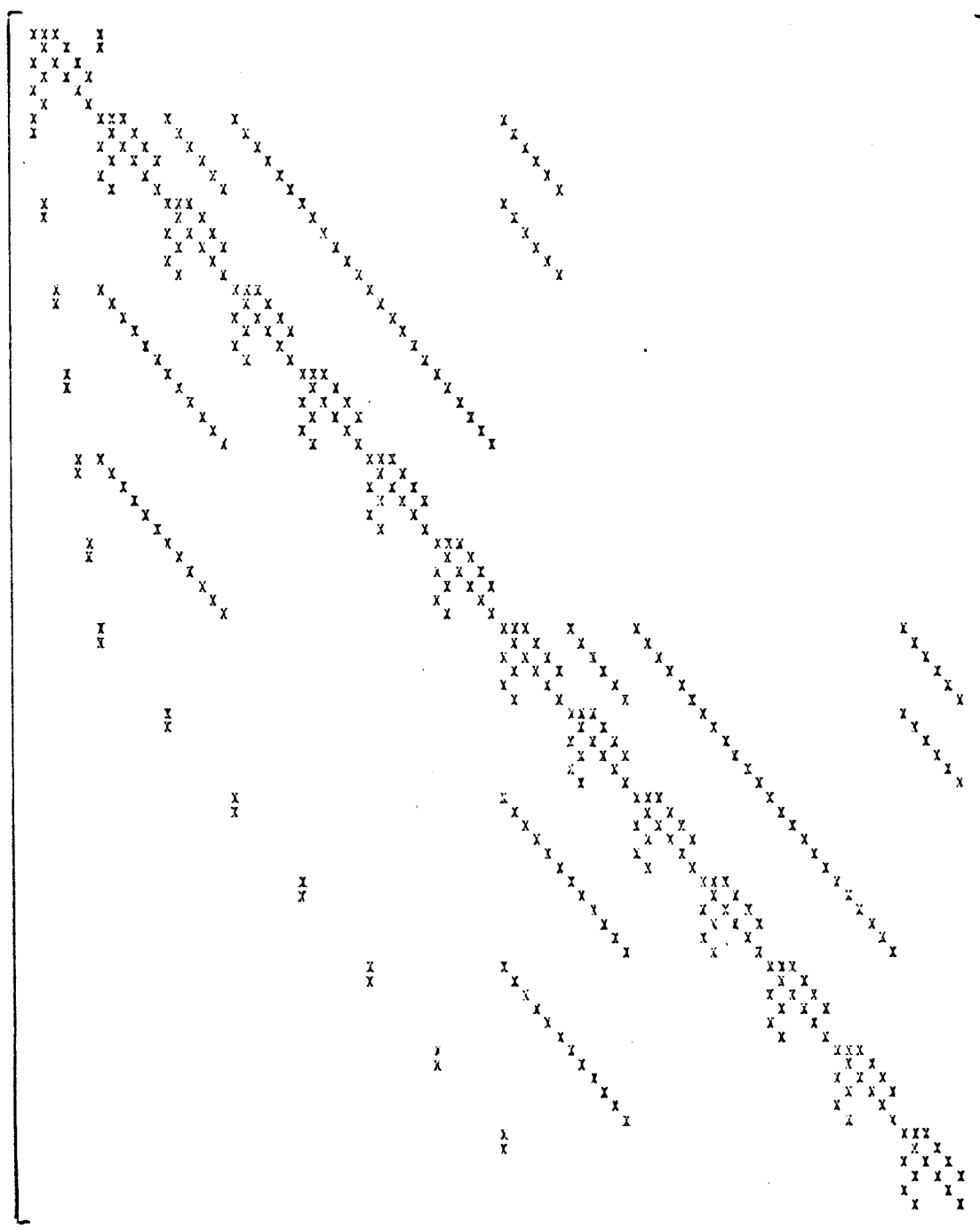


FIGURE E.1

ZERO/NONZERO STRUCTURE OF THE MATRIX
A FOR TEST PROBLEM FIVE

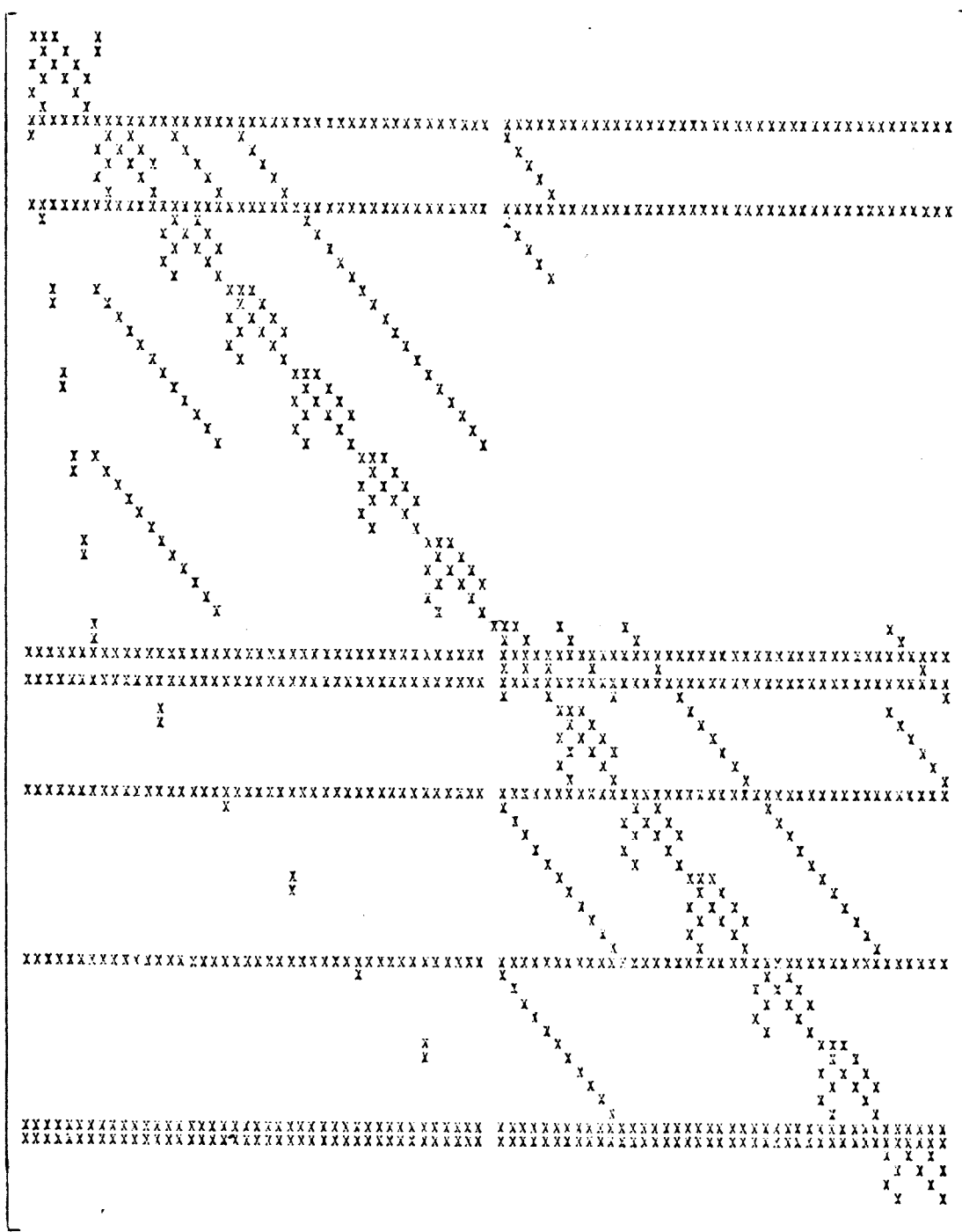


FIGURE E.2

ZERO/NONZERO STRUCTURE OF THE MATRIX

$$A + (Q^T e_4) e^T \text{ FOR TEST PROBLEM FIVE}$$

TABLE E.1
RELATIVE ERROR FOR TEST PROBLEM FIVE

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	2.479 E-05	3.706 E-05	3.580 E-05
Minimum	3.735 E-06	6.990 E-06	2.756 E-05

TABLE E.2
RESIDUAL ERROR FOR TEST PROBLEM FIVE

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	3.580 E-05	4.461 E-06	9.070 E-06
Minimum	1.925 E-06	2.888 E-06	5.493 E-06

TABLE E.3
 PERCENT OF NONZERO ENTRIES IN
 THE MATRICES FORMED BY THE
 PSW METHODS FOR TEST
 PROBLEM FIVE

	$N(A + (Q^T e_j) e^T)$	$N(A + e_j e^T)$
Maximum	14%	6%
Minimum	6%	6%

APPENDIX F

TEST PROBLEM SIX

The following matrix is the rate transition matrix for Test Problem Six:

$$Q(\epsilon) = \begin{bmatrix} .50 & .25 & .25 \\ .25 & .50 & .25 \\ \epsilon & \epsilon & 1 - 2\epsilon \end{bmatrix}$$

where $0 \leq \epsilon \leq .5$.

The following is the exact solution for Test Problem Six:

$$p(\epsilon) = \frac{1}{1 + 8\epsilon} (4\epsilon, 4\epsilon, 1)^T.$$

Let $A(\epsilon) = I - Q(\epsilon)^T$. The second smallest singular value of the matrix $A(\epsilon)$ is approximately equal to 4.330 E-01.

TABLE F.1
MAXIMUM RELATIVE ERROR
FOR TEST PROBLEM SIX

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-06	3.705 E-07	8.417 E-07	1.430 E-06
1.0 E-07	8.000 E-07	6.265 E-07	8.847 E-07
1.0 E-08	1.333 E-07	2.772 E-07	1.400 E-07
1.0 E-09	1.333 E-08	1.600 E-08	1.400 E-08

TABLE F.2
MINIMUM RELATIVE ERROR
FOR TEST PROBLEM SIX

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-06	1.787 E-07	2.125 E-07	4.767 E-07
1.0 E-07	1.695 E-07	1.297 E-07	5.655 E-07
1.0 E-08	8.000 E-08	1.595 E-07	1.333 E-07
1.0 E-09	8.000 E-09	1.400 E-08	1.333 E-08

TABLE F.3
 MAXIMUM RESIDUAL ERROR
 FOR TEST PROBLEM SIX

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-06	7.967 E-08	1.689 E-07	1.430 E-06
1.0 E-07	6.355 E-08	6.265 E-07	8.847 E-07
1.0 E-08	5.999 E-08	1.042 E-07	2.000 E-08
1.0 E-09	5.000 E-09	2.000 E-09	2.000 E-09

TABLE F.4
 MINIMUM RESIDUAL ERROR
 FOR TEST PROBLEM SIX

ϵ	PF Method	PSW Method 1	PSW Method 2
1.0 E-06	2.655 E-08	2.657 E-08	4.767 E-07
1.0 E-07	2.118 E-08	1.297 E-07	5.655 E-07
1.0 E-08	2.000 E-08	5.960 E-08	1.500 E-08
1.0 E-09	2.000 E-09	1.500 E-09	2.000 E-09

TABLE F.5
 CONDITION NUMBERS OF THE
 PRINCIPAL SUBMATRICES OF
 $A(\epsilon)$ OF ORDER TWO FOR
 TEST PROBLEM SIX

ϵ	Min $K_1(A(\epsilon)j)$ j	Max $K_1(A(\epsilon)j)$ j
1.0 E-06	3.000 E 00	5.000 E+05
1.0 E-07	3.000 E 00	5.000 E+06
1.0 E-08	3.000 E 00	5.000 E+07
1.0 E-09	3.000 E 00	5.000 E+08

APPENDIX G

TEST PROBLEM SEVEN

The entries in the rate transition matrix for Test Problem Seven and the "exact solution" will not be given. The second smallest singular value of the matrix A is $4.009 \text{ E-}01$. The percent of nonzero entries in the matrix A is 23%. Figure G-1 shows the zero/nonzero structure of the matrix A . Figure G-2 shows the zero/nonzero structure of the matrix $A + (Q^T e_6) e_6^T$.

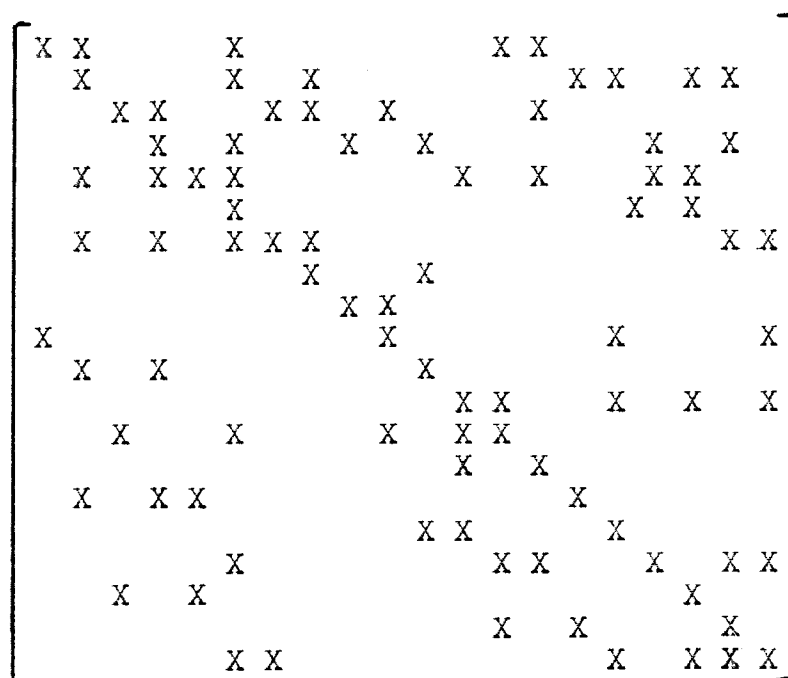


FIGURE G.1

ZERO/NONZERO STRUCTURE OF THE MATRIX
A FOR TEST PROBLEM SEVEN

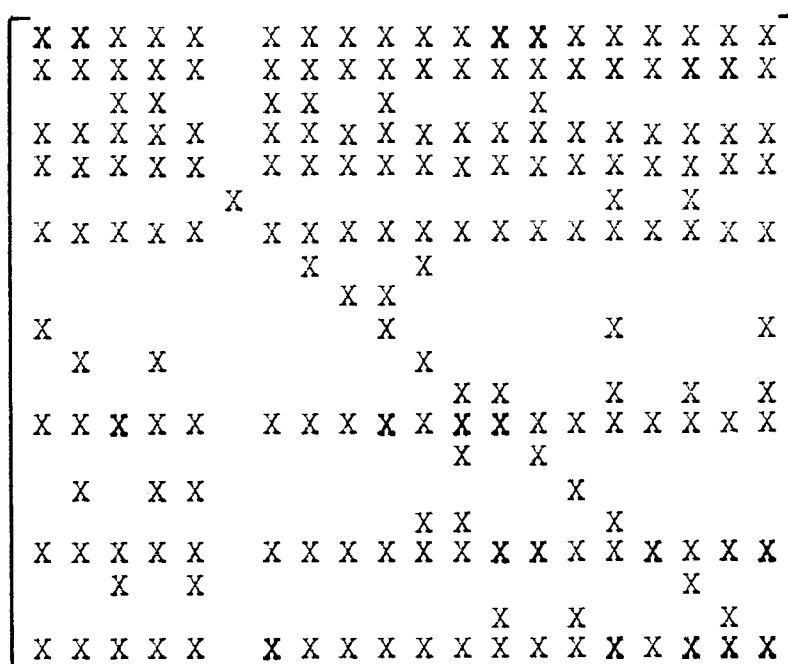


FIGURE G.2

ZERO/NONZERO STRUCTURE OF THE MATRIX

 $A + (Q^T e_6) e^T$ FOR TEST PROBLEM SEVEN

TABLE G.1
RELATIVE ERROR FOR TEST PROBLEM SEVEN

Relative Error	PF Method	PSW Method 1	PSW Method 2
Maximum	2.644 E-06	2.422 E-06	2.437 E-06
Minimum	9.547 E-07	6.336 E-07	8.533 E-07

TABLE G.2
RESIDUAL ERROR FOR TEST PROBLEM SEVEN

Residual Error	PF Method	PSW Method 1	PSW Method 2
Maximum	1.790 E-05	1.557 E-06	1.404 E-06
Minimum	1.005 E-06	6.034 E-07	4.954 E-07

TABLE G.3
 PERCENT OF NONZERO ENTRIES IN
 THE MATRICES FORMED BY THE
 PSW METHODS FOR TEST
 PROBLEM SEVEN

	$N(A + (Q^T e_j) e^T)$	$N(A + e_j e^T)$
Maximum	45%	27%
Minimum	27%	26%

VITA

William Joseph Harrod was born in Chicago, Illinois, on December 25, 1953. In June, 1976 he received a Bachelor of Arts degree with a major in Mathematics from Emory University in Atlanta, Georgia. From August, 1976 until August, 1978 he attended the Graduate School at Clemson University in Mathematics. In September, 1978 he entered the Graduate School at The University of Tennessee, Knoxville, in Mathematics. He received the Master of Science degree, with a major in Mathematics, in August, 1981 and the Doctor of Philosophy degree with a major in Mathematics in December, 1982.