Honam Mathematical J. **35** (2013), No. 3, pp. 417–433
http://dx.doi.org/10.5831/HMJ.2013.35.3.417

NEWTON'S METHOD FOR SOLVING A QUADRATIC MATRIX EQUATION WITH SPECIAL COEFFICIENT MATRICES

Sang-Hyup Seo, Jong-Hyun Seo and Hyun-Min Kim[†,*]

Abstract. We consider the iterative solution of a quadratic matrix equation with special coefficient matrices which arises in the quasi-birth and death problem. In this paper, we show that the elementwise minimal positive solvent of the quadratic matrix equations can be obtained using Newton's method if there exists a positive solvent and the convergence rate of the Newton iteration is quadratic if the Fréchet derivative at the elementwise minimal positive solvent is nonsingular. Although the Fréchet derivative is singular, the convergence rate is at least linear. Numerical experiments of the convergence rate are given.

1. Introduction

We consider a quadratic matrix equation defined by

$$Q(X) = AX^2 + BX + C = 0, \tag{1.1}$$

where the coefficient matrices A, B and C are real $n \times n$ matrices. Then, the unknown matrix X must be an $n \times n$ matrix. In this paper, we study the quadratic matrix equation (1.1) for A and C are nonnegative matrices and $-B$ is a nonsingular M-matrix.

Definition 1.1. [3], [17, p. 42] Let a matrix $A \in \mathbb{R}^{n\times n}$. A is an *Z-matrix* if all its off-diagonal elements are nonpositive.

Received June 4, 2013. Accepted June 18, 2013.
2010 Mathematics Subject Classification. 65H10.
Key words and phrases. quadratic matrix equation, elementwise positive solvent, elementwise nonnegative solvent, M-matrix, Newton's method, convergence rate.
[†]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (2012R1A1A2008840).
[*]Corresponding author

It is clear that any Z-matrix A can be written as $sI - B$ with $B \geq 0$ and $s \in \mathbb{R}$. Then M-matrix can be defined as follows.

Definition 1.2. [3, p. 580] A matrix $A \in \mathbb{R}^{n\times n}$ is an *M-matrix* if $A = rI - B$ for some nonnegative matrix B with $r \geq \rho(B)$ where ρ is the spectral radius; it is a singular M-matrix if $r = \rho(B)$ and a nonsingular M-matrix if $r > \rho(B)$.

Definition 1.3. A positive solvent S_1 of the matrix equation $Q(X) = 0$ is an *elementwise minimal positive solvent* and a positive solvent S_2 of $Q(X) = 0$ is an *elementwise maximal positive solvent* if, for any positive solvent S of $Q(X)$,

$$S_1 \leq S \leq S_2. \tag{1.2}$$

Similarly, if nonnegative solvents S_1 and S_2 satisfy (1.2) for any nonnegative solvent S, S_1 is called an *elementwise minimal nonnegative solvent* and S_2 is called an *elementwise maximal nonnegative solvent.*

Nonlinear matrix equations like (1.1) often occur in some stochastic problems such as quasi-birth-and-death (QBD) processes. For example, let a matrix P be defined by

$$P = \begin{bmatrix} B_0 & B_1 & 0 & 0 & \\ A_{-1} & A_0 & A_1 & 0 & \ddots \\ 0 & A_{-1} & A_0 & A_1 & \ddots \\ 0 & 0 & A_{-1} & A_0 & \ddots \\ & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \tag{1.3}$$

where A_{-1}, A_0, A_1, B_0 and B_1 are $n \times n$ nonnegative matrices such that $A_1 + A_0 + A_1$ and $B_0 + B_1$ are stochastic. Then, P is a transition matrix of QBD processes. The purpose of QBD processes with a transition matrix P is to find the stationary probability vector π of P. If we have the minimal nonnegative solvent $R_{\min}$ of

$$X = X^2 A_{-1} + XA_0 + A_1 \tag{1.4}$$

and the minimal nonnegative solvent $G_{\min}$ of

$$X = A_{-1} + A_0 X + A_1 X^2, \tag{1.5}$$

then we can obtain the vector π. For details, see [1, 7, 13].

The equations (1.4) and (1.5) are applications of (1.1). (1.5) is equivalent to

$$A_1 X^2 + (A_0 - I_n)X + A_{-1} = 0$$

and (1.4) is equivalent to

$$A_{-1}^T Y^2 + (A_0^T - I_n)Y + A_1^T = 0.$$

In this case, A_{-1}, A_1 are nonnegative matrices and $I_n - A_0$ is a nonsingular M-matrix. So, the purpose of this paper is to find the minimal solvent of (1.1) with Newton's method and convergence rate of Newton iteration.

2. Positivity of matrices

Definition 2.1. [8, Definition 6.2.21, 6.2.22] Let $A \in \mathbb{R}^{n\times n}$. If there exists a permutation matrix $P \in \mathbb{R}^{n\times n}$ such that

$$P^T AP = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \text{ where } A_{11} \text{ and } A_{22} \text{ are square matrix,} \tag{2.1}$$

A is called *reducible*. If A is not reducible, it is called *irreducible*.

Nonnegative irreducible matrices have similar properties of positive matrices. For example, Perron's Theorem [8, Theorem 8.2.11] and Perron-Frobenius Theorem [8, Theorem 8.4.4] show similar results of positive matrices and nonnegative irreducible matrices.

Let A be a nonnegative irreducible matrix. Then, $A\mathbf{1}_n$ is a positive matrix where $\mathbf{1}_n$ is the n-column vector with all elements equal to 1. It yields that $A\mathbf{1}_{n\times n}$ and $\mathbf{1}_{n\times n}A$ are positive matrices where $\mathbf{1}_{n\times n}$ is the $n \times n$ matrix with all entries equal to 1. Furthermore, AB and BA are positive matrices for a positive matrix $B \in \mathbb{R}^{n\times n}$.

Lemma 2.2. [2, Corollary 52] *Let positive integers m, n, p, and q be given and let $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{p\times q}$. Then, $B \otimes A$ is always permutation equivalent to $A \otimes B$. When $m = n$ and $p = q$, $B \otimes A$ is always permutation similar to $A \otimes B$.*

From Definition 2.1 and Lemma 2.2, $A \otimes B$ and $B \otimes A$ are both irreducible or not for square matrices A and B.

Theorem 2.3. *Let $B \in \mathbb{R}^{m\times m}$ be a positive matrix. Then, $A = [a_{ij}] \in \mathbb{R}^{n\times n}$ is irreducible if and only if $A\otimes B$ and $B\otimes A$ are irreducible.*

Proof. It is sufficient to show that $A \in \mathbb{R}^{n\times n}$ is reducible if and only if $A \otimes B$ is reducible. By Definition 2.1, we use only permutation matrices to know whether a matrix is reducible or not. So, without loss of generality, the positive matrix B can be replaced by the positive matrix $\mathbf{1}_{m\times m}$.

Suppose that $A \in \mathbb{R}^{n\times n}$ is reducible. Then, there exists a permutation matrix $P \in \mathbb{R}^{n\times n}$ such that

$$P^T AP = \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix}$$

where B_{11} and B_{22} are $p \times p$ and $q \times q$ square matrices, respectively. $A \otimes \mathbf{1}_{m\times m}$ is expressed by

$$A\otimes\mathbf{1}_{m\times m} = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{bmatrix} \text{ where } A_{ij} = \begin{bmatrix} a_{ij} & \cdots & a_{ij} \\ \vdots & \ddots & \vdots \\ a_{ij} & \cdots & a_{ij} \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

Consider $\mathcal{P} = P \otimes I_m$. Then,

$$\mathcal{P}^T \left(A \otimes \mathbf{1}_{m\times m}\right) \mathcal{P} = \begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ O & \mathcal{A}_{22} \end{bmatrix}$$

where O is a $mq \times mp$ zero matrix and $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$ are $mp \times mp$ and $mq \times mq$ square matrices, respectively. So, $A \otimes \mathbf{1}_{m\times m}$ is reducible.

Therefore, $A \otimes B$ is reducible and $B \otimes A$ is reducible by Lemma 2.2.

Conversely, suppose that $A \otimes \mathbf{1}_{m\times m}$ is reducible. Then, there exists a permutation matrix $\mathcal{P} \in \mathbb{R}^{mn\times mn}$ such that

$$\mathcal{P}^T (A \otimes \mathbf{1}_{m\times m})\mathcal{P} = \begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ O & \mathcal{A}_{22} \end{bmatrix}$$

where O is a $q' \times p'$ zero matrix and $\mathcal{A}_{11}$ and $\mathcal{A}_{12}$ are $p' \times p'$ and $q' \times q'$ square matrices, respectively.

Put $p = {}^{p'}/_{m}$ and $q = {}^{q'}/_{m}$. Then, $q+p = n$ because $m(p+q) = mp+mq = p' + q' = mn$. Since $O \in \mathbb{R}^{mq\times mp}$, there exist $\mathfrak{I} = \{i_1, i_2, \cdots, i_k\}$ and $\mathfrak{J} = \{j_1, j_2, \cdots, j_l\}$ such that

$$a_{ij} = 0 \text{ if } i \in \mathfrak{I} \text{ and } j \in \mathfrak{J}$$

where $q \le k \le mq$ and $p \le l \le mp$. If $\mathfrak{I} \cap \mathfrak{J} = \phi$, then A has a $q\times p$ zero submatrix which does not contain diagonal entries of A where $q+p = n$.

Suppose that $\mathfrak{I} \cap \mathfrak{J} \neq \phi$ and $i' \in \mathfrak{I} \cap \mathfrak{J}$. If $k = q$, then A has at most q zeros in a column and $A \otimes \mathbf{1}_{m\times m}$ has at most mq zeros in a column. Thus, O has m $a_{i',i'}$. It means that O contains a diagonal entry of $A\otimes\mathbf{1}_{m\times m}$. It's a contradiction. Therefore, $k \ge q+1$. Similarly, $l \ge p + 1$. So, A has a $q \times p$ zero submatrix which does not contain diagonal entries of A where $q + p = n$. Therefore, A is reducible. $\square$

Now, we see the properties of M-matrices.

Theorem 2.4. [3, Theorem 2.1], [14, Theorem 2.1] *For a Z-matrix A, the following are equivalent:*
1) A is a nonsingular M-matrix.
2) A^{-1} is nonnegative.
3) $Av > 0$ for some vector $v > 0$.
4) All eigenvalues of A have positive real parts.

Theorem 2.5. [3, Lemma 2.2], [5, Theorem 7.4] *Let $A \in \mathbb{R}^{m\times m}$ be a nonsingular M-matrix.*
1) $Av \geq 0$ implies $v \geq 0$.
2) If B is a Z-matrix and $B \geq A$, then B is also a M-matrix.

Using 1) in Theorem 2.5, we can yield the following theorem.

Theorem 2.6. *Let $A \in \mathbb{R}^{n\times n}$ be a nonsingular M-matrix and $v \in \mathbb{R}^n$. Then, $Av > 0$ implies $v > 0$.*

Proof. Let $A = [a_{ij}]$, $v = [v_1, v_2, \cdots, v_n]^T$ and $Av > 0$, then 2.5 1), $v \geq 0$. Now, suppose that $v \geq 0$ and there exists i such that $v_i = 0$. Then

$$(Av)_i = \sum_{j=1}^{n} a_{ij}v_j = \sum_{j=1}^{i-1} a_{ij}v_j + \sum_{j=i+1}^{n} a_{ij}v_j$$

Since for all $i \in \{1, 2, \cdots, n\}$, v_i is nonnegative and off-diagonal entries of A are nonpositive, $(Av)_i \leq 0$. It contradicts to the fact that $Av > 0$. Therefore, $v > 0$. □

Theorem 2.7. [8, Corollary 5.6.10] *Let $A \in \mathbb{R}^{n\times n}$ and $\epsilon > 0$ be given. There is a matrix norm $\|\cdot\|$ such that $\rho(A) \leq \|A\| \leq \rho(A) + \epsilon$.*

Theorem 2.8. [8, Corollary 5.6.16] *A matrix $A \in \mathbb{R}^{n\times n}$ is nonsingular if there is a matrix norm $\|\cdot\|$ such that $\|I_n - A\| < 1$. If this condition is satisfied,*

$$A^{-1} = \sum_{k=0}^{\infty}(I_n - A)^k$$

Theorem 2.9. [8, Theorem 6.2.23] *A matrix $A \in \mathbb{R}^{n\times n}$ is irreducible if and only if*

$$(I_n + |A|)^{n-1} > 0,$$

where $|A| = [|a_{ij}|]$.

From the three previous theorems, we obtain the next result.

Theorem 2.10. *Let $A = rI_n - B \in \mathbb{R}^{n\times n}$ be a nonsingular irreducible M-matrix. Then, A^{-1} is positive.*

Proof. Since A is a nonsingular irreducible M-matrix, B is a nonnegative irreducible matrix and $r > \rho(B)$. Put $C = \frac{1}{r}B$. Then, C is also nonnegative irreducible matrix and $\rho(C) < 1$. Putting $\epsilon = \frac{1-\rho(C)}{2}$, there is a matrix norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$ such that $\rho(C) \leq \|C\| \leq \rho(C)+\epsilon < 1$ by Theorem 2.7. Since there is a matrix norm $\|\cdot\|$ such that $\|C\| < 1$,

$$(I_n - C)^{-1} = \sum_{k=0}^{\infty} C^k$$

by Theorem 2.8.

$$\begin{aligned} A^{-1} &= (rI_n - B)^{-1} \\ &= \frac{1}{r}(I_n - C)^{-1} \\ &= \frac{1}{r}\sum_{k=0}^{\infty} C^k \end{aligned}$$

where $C^0 = I_n$. By Theorem 2.9,

$$(I_n + C)^{n-1} = \sum_{i=0}^{n-1} \binom{n-1}{i} C^i > 0.$$

So, $\sum_{k=0}^{n-1} C^k > 0$, also. Therefore,

$$A^{-1} = \frac{1}{r}\sum_{k=0}^{\infty} C^k \geq \frac{1}{r}\sum_{k=0}^{n-1} C^k > 0. \qquad \square$$

3. Convergence of Newton's Method

The Fréchet derivative of the quadratic matrix equation (1.1) at X in the direction H is given by

$$Q'_X(H) = AHX + (AX + B)H. \tag{3.1}$$

The second Fréchet derivative of the quadratic matrix equation (1.1) at X is given by

$$Q^{(2)}_X(K, H) = A(KH + HK). \tag{3.2}$$

For the equation (1.1), each step of Newton iteration can be simplified

$$(3.3)\qquad \begin{cases} AH_iX_i + (AX_i + B)H_i = -Q(X_i), \\ X_{i+1} = X_i + H_i, \end{cases} \qquad i = 1, 2, \cdots .$$

Also supposing that Q'_{X_i} is nonsingular, the Newton iteration (3.3) can be rewritten as

$$X_{i+1} = X_i - (Q'_{X_i})^{-1}(Q(X_i))$$

which is equivalent to

$$(3.4)\qquad AX_{i+1}X_i + (AX_i + B)X_{i+1} = AX_i^2 - C$$

The general approach for solving (3.4) is to solve the $n^2 \times n^2$ linear system derived by vec function and Kronecker product [11, 15] such as

$$\mathcal{D}_{X_i}\text{vec}(H) = \text{vec}(-Q(X_i))$$

where

$$(3.5)\qquad \mathcal{D}_X = \left[\left(X^T \otimes A + I \otimes AX\right) + I \otimes B)\right].$$

Clearly from Definition 1.2, if $-B$ is an M-matrix, then so is $-I \otimes B$. For convinence we write

$$(3.6)\qquad -\mathcal{D}_X = -I \otimes B - \left(X^T \otimes A + I \otimes AX\right) = rI_{n^2} - \mathbf{N}(X)$$

where $\mathbf{N}(X) = I \otimes T_0 + X^T \otimes A + I \otimes AX$.

In this paper, we use the Frobenius norm $||\cdot||_F$ for matrices. For convenience, the notation $||\cdot||$ is used instead of $||\cdot||_F$ and we define $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

Theorem 3.1. *Let A in the quadratic matrix equation* (1.1) *be a nonnegative irreducible matrix, and C in* (1.1) *be a nonnegative matrix, and let $-B$ in* (1.1) *be a nonsingular M-matrix. If there is a positive matrix Y such that $Q(Y) \leq 0$, then for the Newton iteration* (3.3) *with $X_0 = 0$, the sequence $\{X_i\}$ is well defined, $X_0 \leq X_1 \leq X_2 \leq \cdots$, and converges to the elementwise nonnegative solvent S. Furthermore*

$$-\mathcal{D}_{X_i} = -\left[\left(X_i^T \otimes A + I_n \otimes AX_i\right) + I_n \otimes B)\right]$$

is a nonsingular M-matrix at each iterate X_i and $-\mathcal{D}_S$ is an M-matrix.

Proof. The proof is by mathematical induction. Let Y be any positive matrix such that

$$(3.7)\qquad Q(Y) = AY^2 + BY + C \leq 0.$$

By Theorem 2.4, $(-B)^{-1} \geq 0$. $X_1 = -B^{-1}C \geq 0$. So, the statements

$$(3.8)\qquad X_k \leq X_{k+1},\ X_k < Y,$$

and

$$-\mathcal{D}_{X_k} \text{ is a nonsingular } M\text{-matrix} \tag{3.9}$$

are true for $k = 0$.

We now suppose that (3.8) and (3.9) are true for $k = i \in \mathbb{N}_0$.

From (3.4) and (3.7), we obtain that

$$\begin{aligned} &A(Y - X_{i+1})X_i + (AX_i + B)(Y - X_{i+1}) \\ &\quad \le AYX_i + AX_iY - AX_i^2 - AY^2 \\ &\quad = -A(Y - X_i)^2 < 0. \end{aligned} \tag{3.10}$$

By Theorem 2.6, we obtain that $\text{vec}(Y - X_{i+1}) > 0$, i.e., $X_{i+1} < Y$.

From that $X_{i+1} < Y$ and $X_i \le X_{i+1}$, we get the inequation

$$\begin{aligned} &A(Y - X_{i+1})X_{i+1} + (AX_{i+1} + B)(Y - X_{i+1}) \\ &\quad \le -AY^2 + AYX_{i+1} + AX_{i+1}Y - AX_{i+1}^2 \\ &\qquad -AX_{i+1}^2 + AX_{i+1}X_i + AX_iX_{i+1} - AX_i^2 \\ &\quad = -A(Y - X_{i+1})^2 - A(X_{i+1} - X_i)^2 < 0. \end{aligned} \tag{3.11}$$

Applying the Vec operator to (3.11), we get

$$\begin{aligned} &\text{vec}\left(-[A(Y - X_{i+1})X_{i+1} + (AX_{i+1} + B)(Y - X_{i+1})]\right) \\ &\quad = -[X_{i+1}^T \otimes A + I_n \otimes (AX_{i+1} + B)]\text{vec}(Y - X_{i+1}) \\ &\quad = -\mathcal{D}_{X_{i+1}}\text{vec}(Y - X_{i+1}) > 0. \end{aligned}$$

Since $-\mathcal{D}_{X_{i+1}}$ is a Z-matrix, (3.9) is true for $k = i + 1$ by Theorem 2.4.

By (3.4), we have

$$\begin{aligned} &A(X_{i+2} - X_{i+1})X_{i+1} + (AX_{i+1} + B)(X_{i+2} - X_{i+1}) \\ &\quad = AX_{i+2}X_{i+1} - AX_{i+1}^2 + AX_{i+1}X_{i+2} + BX_{i+2} - AX_{i+1}^2 - BX_{i+1} \\ &\qquad = -A(X_{i+1} - X_i)^2 \le 0 \end{aligned} \tag{3.12}$$

It shows that $-\mathcal{D}_{X_{i+1}}\text{vec}(X_{i+2} - X_{i+1}) \ge 0$. By Theorem 2.5, we obtain $X_{i+2} \ge X_{i+1}$.

Since the Newton sequence $\{X_i\}$ is monotone increasing and bounded above, it has a limit, $\lim_{i\to\infty} X_i = S$ [12]. Therefore, $\{X_i\}$ converges to a nonnegative solvent S. □

Lemma 3.2. *Let A, B and C in the quadratic matrix equation* (1.1) *have same conditions in Theorem 3.1. If there is a nonnegative matrix Y such that $Q(Y) \le 0$, the sequence $\{X_i\}$ is well defined for the Newton iteration* (3.3) *and satisfies $X_0 \le X_1 \le X_2 \le \cdots$ with $X_0 = 0$, and $-\mathcal{D}_{X_i}$ is a nonsingular M-matrix for $i \in \mathbb{N}_0$, then the sequence converges to the elementwise minimal nonnegative solvent S.*

Proof. At first, we will prove that

$$X_k \leq Y \tag{3.13}$$

is true for $k \in \mathbb{N}_0$ by mathematical induction. Let Y be any nonnegative matrix such that

$$Q(Y) = AY^2 + BY + C \leq 0. \tag{3.14}$$

Obviously, the statement (3.13) is true for $k = 0$.

We now suppose that (3.13) is true for $k = i \in \mathbb{N}_0$. Like (3.10), we get that

$$\begin{aligned} A(Y - X_{i+1})X_i + (AX_i + B)(Y - X_{i+1}) \\ \leq -A(Y - X_i)^2 \leq 0. \end{aligned}$$

By Theorem 2.5, $\mathrm{vec}(Y - X_{i+1}) \geq 0$, i.e., $X_{i+1} \leq Y$.

Since the Newton sequence $\{X_i\}$ is monotone increasing and bounded above, it has a limit, $\lim_{i\to\infty} X_i = S$. From the fact that $X_1 \geq 0$ and $X_k \leq Y$ for all $k \in \mathbb{N}_0$, we get $0 \leq S \leq Y$. Since we can take for Y any nonnegative solvent, it follows that S is the elementwise minimal nonnegative solvent. □

By Theorem 3.1 and Lemma 3.2, we get the next result.

Corollary 3.3. *For the quadratic matrix equation* (1.1) *that has same conditions in Theorem 3.1, the Newton sequence* $\{X_i\}$ *with* $X_0 = 0$ *converges to the elementwise minimal nonnegative solvent* S.

Now, we will give an assumption to (1.1).

Assumption 3.4. *For the quadratic matrix* (1.1)
I) The coefficient matrices A *and* C *are nonnegative and irreducible.*
II) $-B = rI - T_0$ *is a nonsingular irreducible* M*-matrix where* $T_0 \geq 0$.

Applying Assumption 3.4 to Theorem 3.1, we obtain the next results.

Corollary 3.5. *Suppose the quadratic matrix equation satisfies Assumption 3.4. If there is a positive matrix* Y *such that* $Q(Y) \leq 0$, *then for the Newton iteration* (3.3) *with* $X_0 = 0$, *the sequence* $\{X_i\}$ *is well defined,* $X_0 < X_1 < X_2 < \cdots$, *and converges to the elementwise minimal positive solvent* S. *Furthermore*

$$-\mathcal{D}_{X_i} = -\left[\left(X_i^T \otimes A + I_n \otimes AX_i\right) + I_n \otimes B)\right]$$

is a nonsingular irreducible M*-matrix at each iterate* X_i *except* X_0, *and* $-\mathcal{D}_S$ *is an irreducible* M*-matrix.*

Proof. Since C is a nonnegative matrix and $-B$ is a nonsingular M-matrix, $-\mathcal{D}_{X_i}$ is a nonsingular M-matrix for all $i \in \mathbb{N}_0$ and $-\mathcal{D}_S$ is an M-matrix by Theorem 3.1.

We need to show that $X_i < X_{i+1}$ for all $i \in \mathbb{N}_0$ and $-\mathcal{D}_{X_i}$ and $-\mathcal{D}_S$ are irreducible for all $i \in \mathbb{N}$. We use the mathematical induction.

Since $X_1 = -B^{-1}C > 0 = X_0$, the statement

$$X_{k+1} > X_k \tag{3.15}$$

is true for $k = 0$.

Now, suppose that (3.15) is true for $k = i$. From (3.12) and $A(X_{i+1} - X_i)^2 > 0$, we obtain

$$-\mathcal{D}_{X_{i+1}} \text{vec}(X_{i+2} - X_{i+1}) > 0.$$

Since $-\mathcal{D}_{X_{i+1}}$ is a nonsingular M-matrix, (3.15) is true for $k = i + 1$ by Theorem 2.6.

Since X_k is positive for all $k \in \mathbb{N}$ and S is positive, $X_k^T \otimes A$ and $S^T \otimes A$ are irreducible by Theorem 2.3. Therefore, $-\mathcal{D}_{X_k}$ and $-\mathcal{D}_S$ are irreducible because the off-diagonal entries of $I_n \otimes (AX_k + B)$ and $I_n \otimes (AS + B)$ are nonnegative.

Finally, from the fact that $X_1 > 0$ and $X_k < Y$ for all $k \in \mathbb{N}_0$, we get $0 < S \leq Y$. Since we can take for Y any positive solvent, it follows that S is the elementwise minimal positive solvent. □

Theorem 3.6. *If the matrix $-\mathcal{D}_S$ in Theorem 3.1 is a nonsingular M-matrix, then for $X_0 = 0$, the Newton sequence $\{X_i\}$ converges to S quadratically.*

Proof. By the hypothesis, the Fréchet derivative Q'_S is an invertible map. Since the sequence $\{X_i\}$ is converges to S, there exists $K \in \mathbb{N}$ such that $k \geq K$ implies that $\|X_k - S\| < \epsilon$ for any sufficiently small $\epsilon > 0$. Therefore, by [10, Theorem 4.1.9], the sequence $\{X_i\}_{i=K}^{\infty}$ converges to S quadratically. □

4. Convergence Rate for a Singular M-matrix $-\mathcal{D}_S$

In the case of $-\mathcal{D}_S$ is a singular M-matrix, we will see the Newton sequence also converges to the solvent but linearly. If Q'_S is non-invertible, then Q'_S has a null space $\mathcal{N} = \text{Ker}(Q'_S)$ and closed range $\mathcal{M} = \text{Im}(Q'_S)$. Suppose that the direct sum $\mathcal{N} \oplus \mathcal{M} = \mathbb{R}^{n \times n}$. Then we can define $\mathcal{P}_{\mathcal{N}}$

to be the projection onto $\mathcal{N}$ parallel to $\mathcal{M}$ and $\mathcal{P}_{\mathcal{M}} = I - \mathcal{P}_{\mathcal{N}}$. For a nonzero matrix $N_0 \in \mathcal{N}$, define the map $\mathcal{B}_{N_0} : \mathcal{N} \to \mathcal{N}$ given by

$$\mathcal{B}_{N_0}(N) = \mathcal{P}_{\mathcal{N}} Q_S^{(2)}(N_0, N). \tag{4.1}$$

Our main result is an application of the following theorem which establish local convergence in contrast with Theorem 3.1.

Theorem 4.1. [9, Thm.1.1] *Let $\mathcal{B}_{N_0}$ in* (4.1) *be invertible for some nonzero $N_0 \in \mathcal{N}$ and let $\mathcal{N} = span\{N_0\} \oplus \mathcal{N}_1$ for some subspace $\mathcal{N}_1$. Write $\tilde{X} = X - S$ and let*

$$W(\rho, \theta, \eta) = \left\{ X \;\middle|\; \begin{array}{l} 0 < \|\tilde{X}\| < \rho, \|\mathcal{P}_{\mathcal{M}}(\tilde{X})\| \le \theta \|\mathcal{P}_{\mathcal{N}}(\tilde{X})\|, \\ \|(\mathcal{P}_{\mathcal{N}} - \mathcal{P}_0)(\tilde{X})\| \le \eta \|\mathcal{P}_{\mathcal{N}}(\tilde{X})\| \end{array} \right\}, \tag{4.2}$$

where $\mathcal{P}_0$ is the projection onto span$\{N_0\}$ parallel to $\mathcal{N}_1 \oplus \mathcal{M}$. If $X_0 \in W(\rho_0, \theta_0, \eta_0)$ for ρ_0, θ_0, η_0 sufficiently small, then the Newton sequence $\{X_i\}$ is well defined and $\|{Q'_{X_i}}^{-1}\| \le c\|\tilde{X}_i\|^{-1}$ for all $i \ge 1$ and some constant $c > 0$. Moreover,

$$\lim_{i\to\infty} \frac{\|\tilde{X}_{i+1}\|}{\|\tilde{X}_i\|} = \frac{1}{2}, \qquad \lim_{i\to\infty} \frac{\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\|}{\|\mathcal{P}_{\mathcal{N}}(\tilde{X}_i)\|^2} = 0.$$

To prove convergence rate of Newton's method of the case that $-\mathcal{D}_S$ is singular, we will show that (1.1) satisfies the conditions of Theorem 4.1. Before proving the following lemma, we use unvec operator from $\mathbb{R}^{n^2}$ onto $\mathbb{R}^{n\times n}$ which is the inverse of the vec operator.

Lemma 4.2. *Suppose the quadratic matrix equation* (1.1) *satisfies Assumption 3.4. If the matrix $-\mathcal{D}_S$ in Theorem 3.1 is a singular M-matrix, then* 0 *is a simple eigenvalue of $-\mathcal{D}_S$, $\mathcal{N} \oplus \mathcal{M} = \mathbb{R}^{n\times n}$, $\mathcal{N}$ is one-dimensional and the map $\mathcal{B}_{N_0}$ is invertible for some nonzero $N_0 \in \mathcal{N}$.*

Proof. From (3.6), $-\mathcal{D}_S = rI_{n^2} - \mathbf{N}(S)$ where $\mathbf{N}(S) = I_n \otimes T_0 + S^T \otimes A + I_n \otimes AS$. Since S is positive and A is irreducible, $S^T \otimes A$ is irreducible by Theorem 2.3. Hence, $\mathbf{N}(S)$ is also irreducible. Then, by Perron-Frobenius Theorem, [8, Theorem 8.4.4] $\rho(\mathbf{N}(S)) = r$ is a simple eigenvalue of $\mathbf{N}(S)$ with a positive eigenvector. Thus, we can find n^2 linearly independent vectors $x_1, x_2, \cdots x_{n^2}$ such that $x_1 > 0$ and

$$X^{-1}\mathcal{D}_S X = \begin{bmatrix} 0 & 0 \\ 0 & \mathcal{D}_{22} \end{bmatrix}, \text{ where } X = \left[\begin{array}{c|c|c|c} x_1 & x_2 & \cdots & x_{n^2} \end{array}\right] \tag{4.3}$$

and $\mathcal{D}_{22}$ is an $(n^2-1)\times(n^2-1)$ nonsingular matrix. By the same way, we also have a positive vector y such that $y^T\mathcal{D}_S = 0$ (i.e., $y \in \operatorname{Ker}\left({\mathcal{D}_S}^T\right)$).

Now, $Q'_S(N) = ANS + (AS + B)N = 0$ if and only if $\mathcal{D}_S\text{vec}(N) = 0$. From (4.3), $\mathcal{D}_S\text{vec}(N) = 0$ if and only if $\text{vec}(N) = X(a, 0, \cdots, 0)^T = ax_1$ for some $a \in \mathbb{R}$, in which case we write $N = a\text{unvec}(x_1)$. Thus $\mathcal{N} = \{a\text{unvec}(x_1)|a \in \mathbb{R}\}$. Simiarly, $\mathcal{M} = \{b_2\text{unvec}(x_2) + \cdots + b_{n^2}\text{unvec}(x_{n^2})| b_2, \cdots, b_{n^2} \in \mathbb{R}\}$. Therefore, $\mathcal{N}$ is one-dimensional and $\mathbb{R}^{n\times n} = \mathcal{N} \oplus \mathcal{M}$. From (3.2) and (4.1), to prove the map $\mathcal{B}$ is invertible, we only need to show

$$\mathcal{P}_{\mathcal{N}}\left(A(\text{unvec}(x_1))^2\right) \neq 0.$$

Since $x_1 > 0$, we have $\text{vec}(A(\text{unvec}(x_1))^2) > 0$ and it represented by

$$\text{vec}\left(A(\text{unvec}(x_1))^2\right) = k_1x_1 + k_2x_2 + \cdots + k_{n^2}x_{n^2}$$

for some real numbers $k_1, k_2, \cdots, k_{n^2}$. By Fundamental theorem of linear algebra in [16] and Lemma 6.3.10 in [8], we have

$$y^T\text{vec}\left(A(\text{unvec}(x_1))^2\right) = k_1y^Tx_1.$$

Furthermore, Since $\text{vec}(A(\text{unvec}(x_1))^2)$, y, and x_1 are positive vectors, $y^T\text{vec}(A(\text{unvec}(x_1))^2) > 0$ and $y^Tx_1 > 0$. Therefore, $k_1 > 0$ and

$$\mathcal{P}_{\mathcal{N}}\left(A(\text{unvec}(x_1))^2\right) = k_1\text{unvec}(x_1) > 0. \qquad \square$$

Lemma 4.3. *Let S be a solvent for the quadratic matrix equation $Q(X) = 0$ in (1.1), let $\{X_i\}$ be a Newton sequence in (3.4) where $i = 0, 1, 2, \cdots$ and let $\tilde{X}_i = X_i - S$. Then*

$$\|Q(X_i)\| \leq a\|\tilde{X}_i\|^2 + b\|\tilde{X}_i\|\|\tilde{X}_{i-1}\| + c\|\tilde{X}_{i-1}\|^2$$

for some positive real number a, b, c.

Proof. From Taylor's Theorem with the second derivative (3.2), we have

$$Q(X_i) = Q(S) + Q'_S(\tilde{X}_i) + \frac{1}{2}Q_S^{(2)}(\tilde{X}_i, \tilde{X}_i) = Q'_S(\tilde{X}_i) + A\tilde{X}_i^2. \tag{4.4}$$

From (3.3) we have

$$AX_iX_{i-1} + (AX_{i-1} + B)X_i = AX_{i-1}^2 - C,$$

and clearly

$$BS = -AS^2 - C.$$

By subtraction, we obtain

$$\begin{aligned} AX_iX_{i-1} + AX_{i-1}X_i + B(X_i - S) &= AX_{i-1}^2 + AS^2 \\ AX_iX_{i-1} - ASX_{i-1} + AX_{i-1}X_i - AX_{i-1}S + B\tilde{X}_i &= A(X_{i-1} - S)^2 \\ A\tilde{X}_iX_{i-1} + AX_{i-1}X_i + B\tilde{X}_i &= A\tilde{X}_{i-1}^2 \end{aligned}$$

Writing $S = X_{i-1} - \tilde{X}_{i-1}$ in (4.4)

$$\begin{aligned} Q(X_i) &= A\tilde{X}_i(X_{i-1} - \tilde{X}_{i-1}) + \left(A(X_{i-1} - \tilde{X}_{i-1}) + B\right)\tilde{X}_i + A\tilde{X}_i^2 \\ &= A\tilde{X}_{i-1}^2 - A\tilde{X}_i\tilde{X}_{i-1} - A\tilde{X}_{i-1}\tilde{X}_i + A\tilde{X}_i^2. \end{aligned}$$

Since $\|\cdot\|$ is a multiplicative matrix norm on $\mathbb{R}^{n\times n}$, we have required result. □

Lemma 4.4. *For any fixed $\theta > 0$, let*

$$\mathcal{Q} = \{i | \|\mathcal{P}_{\mathcal{M}}(X_i - S)\| > \theta \|\mathcal{P}_{\mathcal{N}}(X_i - S)\|\}$$

where $\{X_i\}$ is a Newton sequence in Corollary 3.5. Then there exist an integer i_0 and a constant $c > 0$ such that $\|X_i - S\| \le c\|X_{i-1} - S\|^2$ for all i in $\mathcal{Q}$ for $i \ge i_0$.

Proof. Let $\tilde{X}_i = X_i - S$. Using Taylor's Theorem with the second derivative (3.2) and the fact that $Q'_S\left(\mathcal{P}_{\mathcal{N}}(\tilde{X}_i)\right) = 0$,

$$Q(X_i) = Q(S) + Q'_S(\tilde{X}_i) + \frac{1}{2}Q_S^{(2)}(\tilde{X}_i, \tilde{X}_i) = Q'_S\left(\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\right) + A\tilde{X}_i^2. \tag{4.5}$$

Since $Q'_S|_{\mathcal{M}} : \mathcal{M} \to \mathcal{M}$ is invertible, $\left\|Q'_S\left(\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\right)\right\| \ge c_1\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\|$ for some constant $c_1 > 0$. For $i \in \mathcal{Q}$, we have

$$\|\tilde{X}_i\| \le \left\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\right\| + \left\|\mathcal{P}_{\mathcal{N}}(\tilde{X}_i)\right\| \le (\theta^{-1} + 1)\left\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\right\|. \tag{4.6}$$

Thus by (4.5),

$$\|Q(X_i)\| \ge c_1\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\| - c_2\|\tilde{X}_i\|^2 \ge \left(c_1(\theta^{-1} + 1)^{-1} - c_2\|\tilde{X}_i\|\right)\|\tilde{X}_i\|.$$

On the other hand, from Lemma 4.3, we have

$$\|Q(X_i)\| \le c_3\|\tilde{X}_i\|^2 + c_4\|\tilde{X}_{i-1}\|\|\tilde{X}_i\| + c_5\|\tilde{X}_i\|^2.$$

From (4.6) and the fact that $X_i \ne S$ for any i, we have

$$c_1(\theta^{-1} + 1)^{-1} - c_2\|\tilde{X}_i\| \le c_3\|\tilde{X}_i\| + c_4\|\tilde{X}_{i-1}\| + c_5\frac{\|\tilde{X}_{i-1}\|^2}{\|\tilde{X}_i\|}.$$

Since $\tilde{X}_i$ converges to 0 by Theorem 3.1, we can find an i_0 such that $\|\tilde{X}_i\| \le c\|\tilde{X}_{i-1}\|^2$ for all $i \ge i_0$. □

Corollary 4.5. *Assume that, for given $\theta > 0$, $\|\mathcal{P}_{\mathcal{M}}(X_i - S)\| > \theta\|\mathcal{P}_{\mathcal{N}}(X_i - S)\|$ for all i large enough. Then $X_i \to S$ quadratically.*

In the case of Q'_S is singular practically the Newton sequence converges linearly, according to the corollary we conclude that *the error will generally be dominated by its $\mathcal{N}$ component*[4]. From Lemma 4.2 and 4.4 we have following main theorem.

Theorem 4.6. *If $\mathcal{D}_S$ is a singular M-matrix and the convergence of the Newton sequence $\{X_i\}$ in Corollary 3.5 is not quadratic, then $\|{Q'_{X_i}}^{-1}\| \le c\|X_i - S\|^{-1}$ for all $i \ge 1$ and some constant $c > 0$. Moreover,*

$$\lim_{i\to\infty} \frac{\|\tilde{X}_{i+1}\|}{\|\tilde{X}_i\|} = \frac{1}{2}, \qquad \lim_{i\to\infty} \frac{\|\mathcal{P}_{\mathcal{M}}(\tilde{X}_i)\|}{\|\mathcal{P}_{\mathcal{N}}(\tilde{X}_i)\|^2} = 0.$$

5. Numerical Experiments

In this paper, the tolerance of the Newton algorithm is $n \times 10^{-16}$ and we will stop the iteration if $\|Q(X_{i+1})\|/(\|A\|\|X_{i+1}\|^2 + \|B\|\|X_{i+1}\| + \|C\|)$ is less than tolerance.

Example 5.1. Consider the matrix equation (1.1) for a QBD process. We construct $n \times n$ matrices

$$A = W,\ B = W - I_n,\ \text{and}\ \ C = W + \sqrt{\delta} I_n \tag{5.1}$$

where

$$W = \frac{1 - \sqrt{\delta}}{3(n-1)}(\mathbf{1}_{n\times n} - I_n)$$

for $0 < \delta < 1$. Then, $(3W + \delta I_n)\mathbf{1}_n = \mathbf{1}_n$. Note that as δ approaches zero, the problem becomes more unstable [6][12]. The matrices A, B and C satisfy the Assumption 3.4. So, the problem has the elementwise minimal positive solvent S if it exists. The result is obtained with matrices A, B and C in (5.1) of size $n = 8$ and $n = 16$ with from $\delta = 10^{-1}$ to $\delta = 10^{-16}$.

The results of Figures 5.1, 5.2 and Table 5.1 show that the Newton sequence of the problem converges to a solvent linearly as δ approaches to zero whatever n is. In fact, in the case of $\delta = 10^{-1}$, the minimal eigenvalues of $-\mathcal{D}_S$ are about 0.31623 in both cases $n = 8$ and $n = 16$. But, in the case of $\delta = 10^{-16}$, the minimal eigenvalues of $-\mathcal{D}_S$ are about 4.0916×10^{-8} and 8.0053×10^{-8} when $n = 8$ and $n = 16$, respectively. Then, we can see that the convergence rate of Newton sequence approaches linear if δ approaches to zero because $-\mathcal{D}_S$ becomes nearly singular.

δ	$n = 8$	$n = 16$	δ	$n = 8$	$n = 16$
10^{-1}	3.1623e−001	3.1623e−001	10^{-9}	3.1623e−005	3.1623e−005
10^{-2}	1.0000e−001	1.0000e−001	10^{-10}	1.0000e−005	1.0000e−005
10^{-3}	3.1623e−002	3.1623e−002	10^{-11}	3.1626e−006	3.1626e−006
10^{-4}	1.0000e−002	1.0000e−002	10^{-12}	9.9996e−007	1.0037e−006
10^{-5}	3.1623e−003	3.1623e−003	10^{-13}	3.1628e−007	3.2818e−007
10^{-6}	1.0000e−003	1.0000e−003	10^{-14}	1.0125e−007	1.1738e−007
10^{-7}	3.1623e−004	3.1623e−004	10^{-15}	4.8129e−008	8.3301e−008
10^{-8}	1.0000e−004	1.0000e−004	10^{-16}	4.0916e−008	8.0053e−008

TABLE 5.1. The smallest eigenvalues of $-\mathcal{D}_S$

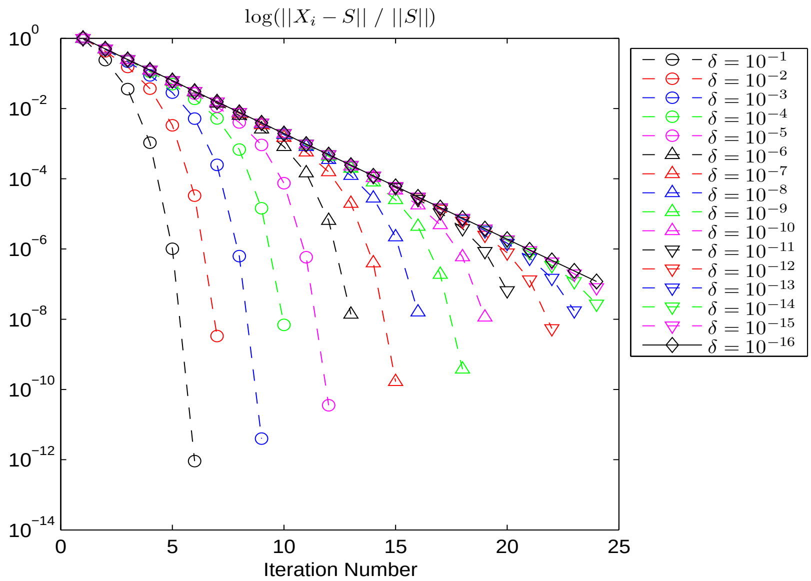

FIGURE 5.1. The convergence rate in Example 5.1 where $n = 8$

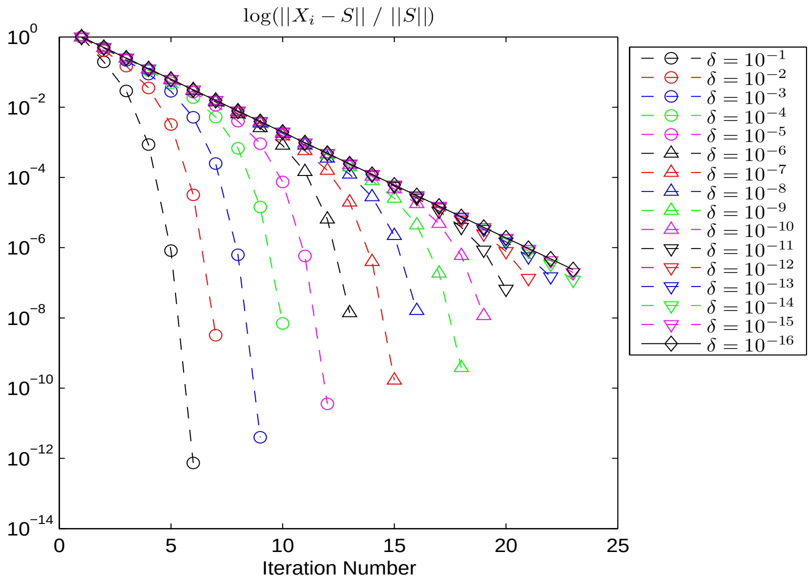

FIGURE 5.2. The convergence rate in Example 5.1 where $n = 16$

References

[1] Dario A. Bini, Guy Latouche, and Beatrice Meini, *Numerical methods for structured Markov chains*, Oxford University Press Oxford, 2005.

[2] B.J. Broxson, *The Kronecker product*, Master's thesis, University of North Florida, 2006.

[3] Chun-Hua Guo and Nicholas J. Higham, *Iterative solution of a nonsymmetric algebraic RICCATI equation*, SIAM Journal on Matrix Analysis and Applications, **29** (2007), 396-412.

[4] Chun-Hua Guo and Peter Lancaster, *Analysis and modification of newton's method for algebraic RICCATI equations*, Mathematics of Computation, **67** **(223)** (1998), 1089-1105.

[5] S. Hautphenne, G. Latouche, and Marie-Ange Remiche, *Newton's iteration for the extinction probability of a Markovian binary tree*, Linear Algebra and its Applications, **428** (2008), 2791-2804.

[6] C. He, B. Meini, N. H. Rhee, and K. Sohraby, *A quadratically convergent Bernoulli-like algorithm for solving matrix polynomial equations in markov chains*, Electronic transactions on numerical analysis, **17** (2004), 151-167.

[7] Qi-Ming He and Marcel F. Neuts, *On the convergence and limits of certain matrix sequences arising in quasi-birth-and-death Markov chains*, Journal of Applied Probability, **38(2)** (2001), 519-541.

[8] Roger A. Horn and Charles R. Johnson, *Matrix Analysis*, Cambridge University Press, 1985.
[9] C. T. Kelley, *A shamanskii-like acceleration scheme for nonlinear equations at singular roots*, Mathematics of Computation, **47(176)** (1986), 609-623.
[10] Hyun-Min Kim, *Numerical methods for solving a quadratic matrix equation*, PhD thesis, Department of Mathematics, University of Manchester, 2000.
[11] W. Kratz and E. Stickel, *Numerical solution of matrix polynomial equations by Newton's method*, IMA Journal of Numerical Analysis, **7** (1987), 355-369.
[12] G. Latouche, *Newton's iteration for nonlinear equations in Markov chains*, IMA Journal of Numerical Analysis, **14** (1994), 583-598.
[13] G. Latouche and V. Ramaswami, *Introduction to Matrix Analytic Methods in Stochastic Modeling*, ASA-SIAM, 1999.
[14] George Poole and Thomas Boullion, *A survey on M-matrices*, SIAM review, **16(4)** (1974), 419-427.
[15] Jong Hyeon Seo and Hyun-Min Kim, *Solving matrix polynomials by Newton's method with exact line searches*, Journal of KSIAM, **12(2)** (2008), 55-68.
[16] G. Strang, *Linear Algebra and Its Applications*, Thomson, Brooks/Cole, 4th edition, 2006.
[17] David M. Young, *Iterative Solution of Large Linear Systems*, Academic Press, 1971.

Sang-Hyup Seo
Department of Mathematics, Pusan National University,
Busan 609-735, Republic of Korea.

Jong-Hyun Seo
Department of Mathematics, Pusan National University,
Busan 609-735, Republic of Korea.

Hyun-Min Kim
Department of Mathematics, Pusan National University,
Busan 609-735, Republic of Korea.
E-mail: hyunmin@pusan.ac.kr