New method for square root of non-singular M-matrix

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Abstract:- Square root of a matrix play an important role in many applications of matrix theory. In this paper, we propose a new iterative method for square root of a non-singular M-matrix. We first transform the matrix equation $X^2 - A=0$ into special form of a non-symmetric algebraic Riccati equation (NARE), and then solve this special NARE by Newton method. Efficiency and effectiveness proved by theoretical analysis and numerical experiments.

Keywords: - Matrix square root, M-matrix, Non-symmetric algebraic Riccati equation, Newton method.

1. Introduction and Preliminaries

Let $A = (a_{ij}) \in \mathbb{C}^{n\times n}$ a matrix $X \in \mathbb{C}^{n\times n}$ is said to be a square root of A if,

$$X^2 = A. \qquad (1)$$

The study of square roots of a general (real or complex) matrix can he traced back to the early works of Sylvester, Cayley, Frobenius in the 19th century, followed by the works of Cecioni and Kreis in the early 20th century. There are many applications of square root of a matrix in a matrix theory, such as computation of the matrix logarithm, the boundary value problems and so on. For the background of the square root of matrix, we refer to [1].

The computation of square root real matrix A has been studies for many years by several authors [1-6] and references therein. The number of square roots varies from two to infinity, not every real matrix have real square root any matrix with no non-positive real eigenvalue has a unique square root for which every eigenvalue lies in the open right plane and sometimes called the principle square root, that is usually of interest. A class of matrices having no non-positive real eigenvalue is much studies class of non-singular M-matrices.

The Matrix square root methods can be divided into two classes, direct methods and iterative methods. In the class of direct methods, for example Schur method proposed by "Bjorck and Hammarling" [2] and the iterative methods depends on second class [7-11].

In this paper, we consider the computation of square root of the non-singular M-matrix

$$X^2 - A = 0 \qquad (2)$$

Where X, $A \epsilon \mathbb{R}^{nxn}$, and A is non-singular M-matrix. The solution of the matrix equation (2) is called M-matrix square root of A.

From reference [1, 2], we know that the equation (2) has a unique M-matrix square root when A is a non-singular M-matrix.

Our idea can be stated as follows.

By using transformation X = D – Y in [12], we can transform (1) into a special non-symmetric algebraic Riccati equation (NARE), because theory and methods of NARE is well developed and then apply Newton method to special NARE for computing minimal non-negative solution.

In the following, we first review some notations, definitions and basic results.

For any matrices $A = (a_{ii})$, $B = (b_{ii}) \in R^{n\times n}$, $\epsilon \mathbb{R}^{nxn}$, we write A $\geq$ B(A > B). if $a_{ii} \geq b_{ii} (a_{ii} > b_{ii})$ $for\ all\ i,\ j$. $\mathbb{C}_{>}$, $\mathbb{C}_{\geq}$, $\mathbb{C}_{<}$ and $\mathbb{C}_{\leq}$ are represent open left half plane, closed left half plane, open right half plane and closed left half plane respectively. The set of all given values of matrix A is represented by ρ(A) = $\max_i \{\lambda_i\}$, i = 1, 2, …, n.

Definition(1-1):-

The matrix A is called a Z-matrix if $a_{ii} < 0\ for\ all\ i, j$. Any Z-matrix A is called an M-matrix if there exists a non-negative matrix B such that A = sI - B and s $\geq$ ρ(B). In particular A is called a non-singular M-matrix if s > ρ(B) and singular M-matrix if s = ρ(B).

Definition(2-1):- [13]

Let A $\in C^{n\times n}$ with no eigenvalues on R^- (closed negative real axis), $A^{1/2}$ is the unique square root X of A whose spectrum lies in the open right half-plane, and it is primary matrix function of A. We refer to X as principal square root of A and we write X = $A^{1/2}$.

The following result on M-matrix can be found [14, 15]

Lemma(3-1):-.

Let A be a Z-matrix, then the following statements are equivalent:

(1) A is a non-singular M-matrix;

(2) $A^{-1} \geq 0$;

(3) There exists a vector $\upsilon > 0$ such that $A\upsilon > 0$;

(4) All eigenvalues of A have positive real part.

Lemma(4-1):-

Let A, B be Z-matrices. *If* A is a nonsingular M-matrix and $A \leq B$, then B is also a nonsingular M-matrix. In particular, for any $a \geq 0$, $B = \alpha I + A$ is a nonsingular M-matrix.

Lemma(5-1):-

Let A be a M-matrix, $B \geq A$ be a Z-matrix. If A is non-singular or irreducible singular with $A \neq B$, then B is also a nonsingular M-matrix

Lemma(6-1):-

Let A be a non-singular M-matrix or an irreducible singular M-matrix. Partition of A as

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

Where A_{11} and A_{22} are square matrices, then A_{11} and A_{22} are non-singular M-matrices.

Lemma(7-1):-

Let A, B are two nonsingular M-matrices and $A \leq B$, then $A^{-1} \geq B^{-1}$

We now review some basic results on non-symmetric algebraic Riccati equation (NARE)

$$XCX - XD - AX + B = 0, \qquad (3)$$

where A, B, C and D are real matrices of sizes m x m, m x n, n x m and n x n respectively.

The NARE of this kind appears in transport theory, Wiener-Hopf factorization of Markov chains and etc. for which one can refer to [15-17] and the references there in. For the NARE (2), minimal non-negative solution is the practical interest. The following basic result is from [6].

Lemma(8- 1):-

From the coefficient matrices associated with the NARE (2), we can define an (m + n) x (m + n) matrix

$$M = \begin{pmatrix} D & -C \\ -B & A \end{pmatrix} \qquad (4)$$

If M is a non-singular M-matrix, then (2) has a unique minimal nonnegative solution S, and both D - CS and A - CS are non-singular M-matrices. Moreover, both D - CS and A - CS are irreducible when M is an irreducible (singular or nonsingular) M-matrix.

There have been many effective methods proposed for solving numerically the NARE (2) with M being an M-matrix, e.g., the fixed-point iteration, Newton iteration, Schur method, matrix sign function method, ALI method, Doubling algorithm and etc. [16, 17, 19-22].

The remaining of the paper is prepared as follows. In section 2, we review some existing numerical methods for computing matrix square root. In section 3, we first transform equation (2) into a special NARE and then solve this special NARE by applying Newton iteration method. In Section 4, we use some numerical experiments to show the effectiveness of the new method. Conclusion remarks are given in section 5.

2. Some previous methods

There have been some existing methods to solve matrix equation (2). In reference [13], Alefeld and Schneider first proposed to compute square root of M-matrix, since $A \in \mathbb{R}^{n\times n}$ is a non-singular M-matrix, so that

$$A = sI - B, B \geq 0, \ \ s > \rho(B).$$

This demonstration is not unique, but for the sake of computation, we can select

$$s = max_i\{a_{ii}\}.$$

Then we can write

$$A = s\,(I - P), \quad P = s^{-1} B \geq 0, \quad \rho(P) < 1. \qquad (5)$$

And the iteration process as follows:

$$Y_{k+1} = 0.5\,(P + Y_k^2),\ Y_0 = 0. \qquad (6)$$

The iteration method (6) can be explained in the following algorithm.

Algorithm(2-1):-[9, 13]

Step 1. Set $Y_0 = 0$, and ϵ. Set $k = 0$

Step 2. s = *max (diag* (A))

Step 3. $P = I - (1/s)\,A$

Step 4. $Y_{k+1} = 0.5(P + Y^2{}_k)$;

Step 5. $X = \sqrt{s}(I - Y)$

Step 6 . Let $Res(X) = \frac{\|x^2 - A\|_\infty}{\|A\|_\infty} < \in$, stop.

Otherwise set k=k+1 and go to step 4.

From reference (see [1]), convergence theorem, let $P \in \mathbb{R}^{n\times n}$ satisfy $P \geq 0$ (4) and $\rho(A) < 1$ and write $(I - P)^{1/2} = I - Y$.

Then in iteration (6)

$$Y_k \rightarrow Y$$

$$0 \leq Y_k \leq Y_{k+1} \leq Y,\ k \geq 0;$$

that is, the Y_k converge monotonically to Y from below.

In order to compute the square root of a matrix A, a natural approach is to apply Newton's method (see [9, 20]) to (2) and this algorithm can be stated as follows.

Algorithm(2-2):-[18, 20]

Step 1. Set $Y_0 = 0$, and ϵ. Set $k = 0$.

Step 2. Let $Res(X) = \frac{\|x^2 - A\|_\infty}{\|A\|_\infty} < \in$, stop.

Step 3. Solve the following Sylvester equation for H_k

$$X_k H_k + H_k X_k = -F(X_k)$$

Step 4. Update $X_{k+1} = X_k + H_k$, For k = k + 1 and go to step 2.

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Applying the standard local convergence theorem to Algorithm(2- 2) [20], we conclude that the sequence $\{X_k\}$ generated by Algorithm(2- 2) converges quadratically to a square root X of A if the starting matrix X_0 is sufficiently close to X.

Later, some simplified Newton's methods were developed in [1, 20]. Unfortunately, these simplified Newton's methods have poor numerical stability.

3. New method

In this section, we will propose a new method to compute square root of M-matrix, which is motivated by reference [12]. We know that there have been many methods to solve NARE (3). If we let $C = I \; and \; D = A = 0$ in equation (3), so we will get equation (2), it means (2) is special form of NARE(3)

If we let in equation (3), we can get equation (2). So equation (2) is a special case of NARE (3). As theory and methods of NARE are well developed, so these methods can also be used to solve square root of M-matrix. Therefore, I will introduce a transformation in [12] and apply this transformation on equation on (2)

The transformation is as follows:

$$X = D - Y \qquad (7)$$

Where $D = diag(d_1, d_2, \ldots, d_n)$ is a positive diagonal matrix to be determined.

If we take equation (7) into equation (2), then we get

$$Y^2 - YD - DY + D^2 - A = 0 \qquad (8)$$

Which is a NARE of special form. As theory and methods of numerically solving the NARE are ver, we can solve the special NARE (8) directly.

The matrix (4) associated with the NARE is

$$M = \begin{pmatrix} D & -I \\ A - D^2 & D \end{pmatrix} \qquad (9)$$

Let A = (a_{ii}). If we choose the positive diagonal entries d_i (i = 1,2, ... ,n) such that

$$A - D^2 \leq 0, \text{ i.e.}$$

$$a_{ii} - d_i \leq 0, \; i = 1, 2, \ldots, n.$$

Then we easily verify that M of (9) is a Z-matrix. In fact, only if we choose d_i to satisfy

$$d_i \geq \sqrt{a_{ii}} > 0, \text{ for } i = 1, 2, \ldots, n. \qquad (10)$$

We can see that M is a non-singular M-matrix from the following theorem.

Theorem(1-3):-

If A be a non-singular M-Matrix and D be a diagonal matrix whose diagonal entries d_i satisfying (9). Then M defined in (8) is a non-singular M-matrix. Moreover,
if A is irreducible, then M is also irreducible.

From the above theorem and Lemma (8-1), we easily get the following corollary.

Corollary(2-3):-

Let A he a non-singular M-matrix. If D is a diagonal matrix whose diagonal entries d_i satisfying (9). Then

1. The NARE (7) has a minimal non-negative solution S_D, and $D - S_D$ is also non-singular M-matrices.
2. The equation (1) has a unique non-singular M-matrix square root $X = D - S_D$.

Remark(3-3):-

We use S_D to denote the unique minimal non-negative solution of the NARE (7) because the minimal solution is related with D. However, the M-matrix square root of the (2) is not related with choice of D.

Theorem(4-3):-.

Let A be nonsingular M-matrix. If D_i and D_2 are diagonal matrices whose diagonal entries satisfying (10), and $D_1 \geq D_2$. Then $S_{D1} \geq S_{D2}$.

Proof:-

Since the unique M-matrix square root X of the (2) is independent of D, we have
$X = D_1 - S_{D1} = D_2 - S_{D2}$. The lemma follows immediately from $D_1 \geq D_2$.

Now we apply the Newton iteration method to solve special NARE(8).For solving $\mathfrak{I}(Y) = 0$ can be described by Newton iteration for solving can be here.

Algorithm(5-3)

Step 1. Set $Y_0 = 0$.

Step 2. For $k = 1, 2,\ldots$, until convergence, computing Y_{k+1} from the following equation

$$Y_{k+1} = Y_k - (\mathfrak{I}'(Y_k))^{-1}\mathfrak{I}(Y_k). \qquad (10)$$

Step 3. $\mathfrak{I}'(Y_k)\Delta_k = -\mathfrak{I}(Y_k)$, $Y_{k+1} = Y_k + \Delta_k$, $Y_0 = 0$, $k = 0, 1, 2,\ldots,$

or equivalently

$$(D - Y_k)Y_{k+1} + Y_{k+1}(D - Y_k) = D^2 - A - Y^2_k,\ Y_0 = 0,\quad k=0,1,2,\ldots,$$

In each iteration it needs to solve a Sylvester matrix equation. In [21, 22] it is proved that the sequence $\{Y_k\}$ generated by the Newton iteration is monotonically increasing and quadratically converges to S_D, the minimal nonnegative solution of the NARE.

4 Numerical experiments

In this section, numerical experiments are done to verify our theoretical analysis. We get unique non-singular M-matrix square root of (2) by solving (8), which is depends on the transformation $X = D - Y$ in [12] and compare our new algorithm(5-3) with some other algorithms i-e Algorithm(1-2) and "Algorithm(2-2). We present computational results of each experiment in terms of iteration numbers CPU time and residue. The residue is defined by

$$Res = \frac{\|x^2 - A\|\infty}{\|X^2\|\infty + \|A\|\infty}.$$

In this whole process executions all iterations are run in MATLAB2007 on personal computer, and are terminated when the current iterate satisfies

$$\frac{\|x^2 - A\|_\infty}{\|A\|_\infty} < le - 6.$$

Experiment (1-4):-

Consider equation (1) with coefficient matrix

$$A = \begin{pmatrix} 1 & -1 & \\ -1 & 2 & \ddots \\ \ddots & \ddots & -1 \\ & -1 & n \end{pmatrix}_{256\times256}$$

Table 4.1. Computational results of experiment 1, with $X_0 = 0.5I$.

Algorithms	Number of Iteration.	CPU time	Res
Algorithm (1-2)	262	17.7824	4.9861e-07
Algorithm (2-2)	08	1.8591	2.3099e-07
Algorithm (5-3)	04	0.5522	2.622e-09

Experiment(2-4):-

Consider equation (1) with coefficient matrix is given

$$A = \begin{pmatrix} 3 & -1 & \\ & 3 & \ddots \\ & \ddots & -1 \\ -1 & & 3 \end{pmatrix}_{256\times256}$$

Table 4.2. Computational results of experiment 2, with Xo = 0.81

Algorithms	Number of iterations	CPU time	Res
Algorithm (1-2)	07	0.329302	3.7193e-07
Algorithm (2-2)	06	0.25560	1.5938e-07
Algorithm (5-3)	03	0.07096	1.0846e-08

Experiment(3-4):-

Consider equation (1) with coefficient matrix given below

$A = rand(n.\ n);$ $A = diag(Ae) - A + I,$ where $e = (1, 1,\dots, 1)^T$ and $n=256.$

Table 4.3. Computational results of experiment 3, with $X_0 = 0.3I$.

Algorithms	Number of iterations	CPU time	Res
Algorithm (1-2)	104	1.830531	4.9622e-07
Algorithm (2-2)	7	3.5845	1.4468e-07
Algorithm (5-3)	6	1.05992	8.5039e-08

Experiment(4-4):-

Consider equation (1) with coefficient matrix A given below

$$A = \begin{pmatrix} 3 & -1 & & \\ & 3 & \ddots & \\ & & \ddots & -1 \\ -1 & & & 5 \end{pmatrix}_{256\times256}$$

Table 4.4. Computational results of experiment 4, with $X_0 = 0.41$.

Algorithms	Number of iterations	CPU time	Res
Algorithm(1-2)	13	0.724079	1.8719e-07
Algorithm (2-2)	06	1.385610	2.883e-10
Algorithm (5-3)	03	0.628560	7.2308e-09

From Table 1-4. We can see that our new algorithm(5-3) by utilizing general transformation is faster and more effective than existing ones i-e algorithm(1-2) and algorithm(2-2) in terms of number of iterations, CPU time and the residue.

5. Concluding Remarks

We have proposed a new iterative method for the square root of a non-singular M-matrix. First transform this problem to special NARE using transformation $X = D - Y$, and then solved this special NARE by Newton method due to it is quadratically converges to its solution Theoretical analysis and numerical experiments showed that our method is effective and efficient.

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