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# ON HERMITIAN POSITIVE DEFINITE SOLUTIONS OF MATRIX EQUATION $X - A^*X^{-2}A = I$ *

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**Abstract**

The Hermitian positive definite solutions of the matrix equation $X - A^*X^{-2}A = I$ are studied. A theorem for existence of solutions is given for every complex matrix $A$. A solution in case $A$ is normal is given. The basic fixed point iterations for the equation are discussed in detail. Some convergence conditions of the basic fixed point iterations to approximate the solutions to the equation are given.

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*Key words*: Matrix equation, Positive definite solution, Iterative methods.

## 1. Introduction

In this paper, we are concerned with the Hermitian positive definite solutions of the matrix equation

$$X - A^*X^{-2}A = I, \tag{1}$$

where $I$ is the $n \times n$ identity matrix and $A$ is an $n \times n$ complex matrix. The equation has been studied by several authors (see[6,8-11]) and some convergence conditions of the basic fixed point iterations to approximate the solutions to the equation are given. For the application areas in which the equation arises, see the references given in [6,8]. For the equation $X \pm A^*X^{-1}A = I$, there are many contributions in the literature on the theory, applications, and numerical solution(see,e.g.,[3-6,9-13]). Several authors[7,8,9,11,14] have studied the equation $X + A^*X^{-2}A = I$ and they have obtained theoretical properties of the equation.

Throughout this paper we use $\mathcal{C}^{n\times n}$ to denote the set of complex $n \times n$ matrices, and $\mathcal{H}^{n\times n}$ to denote the set of $n \times n$ Hermitian matrices. For $M \in \mathcal{C}^{n\times n}$ , $\|M\|$ stands for the spectral norm and $\lambda_i(M)$ represents the eigenvalues. For $X, Y \in \mathcal{H}^{n\times n}$, we write $X \geq Y (X > Y)$ if $X - Y$ is positive semi-definite (definite). For $M \in \mathcal{H}^{n\times n}$, let $\lambda_{max}(M)$ and $\lambda_{min}(M)$ be maximal and minimal eigenvalue of $M$, respectively.

In Section 2 we discuss existence of solutions and their properties and consider the solutions in case $A$ is normal or unitary. In Section 3 we give an estimation on the solutions. In Section 4, we discuss the convergence behavior of the basic fixed point iterations to approximate the solutions to Eq.(1). Some of results in [8,9,11] are improved. Several numerical examples are given in Section 5.

## 2. Existence of Solutions

In the sequel, a solution always means a Hermitian positive definite one.

**Lemma 1.** [9,10] *Eq.(1) has a solution for any* $A \in \mathcal{C}^{n\times n}$.

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**Theorem 1.** *For any invertible matrix $A \in \mathcal{C}^{n\times n}$, there exist unitary matrices $P$ and $Q$ and diagonal matrices $\Gamma > I$ and $\Sigma > 0$ with $\Gamma - \Sigma^2 = I$ such that*

$$A = P^* \Gamma Q \Sigma P.$$

*In this case $X = P^* \Gamma P$ is a solution of Eq.(1).*

*Proof.* For any $A \in \mathcal{C}^{n\times n}$, by Lemma 1 Eq.(1) has a solution. Suppose that $X$ is a solution. Then there exist a unitary matrix $P$ and a diagonal matrix $\Gamma$ such that $X = P^* \Gamma P$. Hence, the identity $X = I + A^* X^{-2} A$ gives

$$\Gamma - I = P A^* P^* \Gamma^{-2} P A P^*.$$

Noticing that $\Gamma > I$, then we have

$$\left((\Gamma - I)^{-\frac{1}{2}} P A^* P^* \Gamma^{-1}\right)\left(\Gamma^{-1} P A P^* (\Gamma - I)^{-\frac{1}{2}}\right) = I.$$

Let $Q = \Gamma^{-1} P A P^* (\Gamma - I)^{-\frac{1}{2}}$, that is $A = P^* \Gamma Q \Sigma P$ with $\Sigma = (\Gamma - I)^{\frac{1}{2}}$. Obviously, $Q$ is unitary and $\Gamma - \Sigma^2 = I$. It is easy to verify that $X = P^* \Gamma P$ is a solution of Eq.(1).

**Theorem 2.** *If $A$ is normal, in other words, there exists a unitary matrix $P$ such that $A = P^* \Lambda P$ where $\Lambda = diag(\lambda_1, \lambda_2, \cdots, \lambda_n)$, $\lambda_i$, $i = 1, 2, \cdots, n$ are the eigenvalues, then Eq.(1) has the following solution*

$$X = P^* diag(\mu_1, \mu_2, \cdots, \mu_n) P, \tag{2}$$

*where $\mu_i$ is the unique positive solution of the equation*

$$\mu_i - |\lambda_i|^2 \mu_i^{-2} = 1 \tag{3}$$

*for $i = 1, 2, \cdots, n$.*

*Proof.* Let $Y = PXP^*$. Consequently, Eq.(1) has a solution if and only if the following problem is solvable:

$$\exists Y > 0, \;\; Y - \Lambda^* Y^{-2} \Lambda = I. \tag{4}$$

Note that the equation (3) has only one positive solution $\mu_i$ and $\mu_i \in [1, +\infty)$. Let $Y = diag(\mu_1, \mu_2, \cdots, \mu_n)$. It is easy to verify $Y$ is a solution of (4).

**Theorem 3.** *If $A$ is a unitary matrix, then Eq.(1) has only one solution $X = \delta I$, where $\delta$ is the unique positive solution of the following equation*

$$\delta = 1 + \delta^{-2}.$$

*Proof.* It is easy to prove that $X = \delta I$ is a solution of Eq.(1). Suppose that $X$ is a solution of Eq.(1). We prove $X = \delta I$. We know that there exist a unitary matrix $U$ and a diagonal matrix $\Delta = diag(\delta_1, \delta_2, \cdots, \delta_n)$ such that $X = U^* \Delta U$. Hence, the identity $X = I + A^* X^{-2} A$ gives

$$V(\Delta - I) = \Delta^{-2} V,$$

where $V = (v_{ij}) = UAU^*$. Obviously, $V$ is unitary. Hence $detV \neq 0$, then there exists a permutation $\pi$ of the $n$ items $\{1, 2, \cdots, n\}$ such that $\prod_{i=1}^n v_{i,\pi(i)} \neq 0$. By computation, one derives for each $i$

$$v_{i,\pi(i)}(\delta_{\pi(i)} - 1) = \delta_i^{-2} v_{i,\pi(i)},$$

which implies

$$\delta_{\pi(i)} - 1 = \delta_i^{-2}, \;\; \text{for} \;\; i = 1, 2, \cdots, n.$$

Now we prove that $\delta_1 = \delta_2 = \cdots = \delta_n = \delta$. Let $\tau(x) = 1 + x^{-2}$. Obviously, $\delta_i > 1$, for $i = 1, 2, \cdots, n$. Then $\delta_{\pi(i)} = \tau(\delta_i) < \tau(1) = 2$. Therefore we have $\delta_{\pi(i)} > \tau(\tau(1)) = 5/4$. By induction, we get $\delta_i \in (\tau^{2k}(1), \tau^{2k-1}(1))$ for $i = 1, 2, \cdots, n$ and $k = 1, 2, \cdots$. It is easy to prove that $\lim_{k\to\infty} \tau^k(1) = \delta$. Hence, $\delta_i = \delta$, for $i = 1, 2, \cdots, n$. Then $\Delta = \delta I$ and $X = U^*\Delta U = \delta I$.

**Theorem 4.** *There do not exist two comparable solutions to Eq.(1), that is, it is impossible that for any two solutions $X^{(1)}$ and $X^{(2)}$ ($X^{(1)} \neq X^{(2)}$) of Eq.(1) $X^{(1)} \leq X^{(2)}$ or $X^{(2)} \leq X^{(1)}$.*

*Proof.* We distinguish two cases.

Case 1. Suppose that $A$ is invertible. Then we have

$$X = \sqrt{A(X-I)^{-1}A^*}.$$

Let $X^{(1)}$ and $X^{(2)}$ are two solutions of Eq.(1). If $X^{(1)} \leq X^{(2)}$, then $X^{(1)} \geq X^{(2)}$ by monotonicity of $\sqrt{A(X-I)^{-1}A^*}$, a contradiction to $X^{(1)} \neq X^{(2)}$. Similarly, $X^{(1)} \geq X^{(2)}$ is impossible.

Case 2. Suppose that $A$ is singular. If $A = 0$, then Eq.(1) has only one solution $X = I$. If $A \neq 0$, then exists an unitary matrix $T$ such that

$$A = T^* \begin{pmatrix} A_{11} & 0 \\ A_{21} & 0 \end{pmatrix} T$$

with $A_{11}$ invertible by Schur triangularization theorem. Let $Y = TXT^*$. Consequently, Eq.(1) has a solution if and only if the following problem is solvable:

$$\exists Y > 0,\ Y - \begin{pmatrix} A_{11}^* & A_{21}^* \\ 0 & 0 \end{pmatrix} Y^{-2} \begin{pmatrix} A_{11} & 0 \\ A_{21} & 0 \end{pmatrix} = I. \tag{5}$$

Let

$$Y = \begin{pmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{pmatrix},\ Y^{-2} = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}.$$

Then (5) is equivalent with

$$\begin{pmatrix} \begin{matrix} Y_{11} - A_{11}^*K_{11}A_{11} - A_{21}^*K_{21}A_{11} \\ -A_{11}^*K_{12}A_{21} - A_{21}^*K_{22}A_{21} \end{matrix} & Y_{12} \\ Y_{21} & Y_{22} \end{pmatrix} = I.$$

Hence we have

$$Y_{12} = 0,\ Y_{21} = 0,\ Y_{22} = I,\ \ Y = \begin{pmatrix} Y_{11} & 0 \\ 0 & I \end{pmatrix},\ \ Y^{-2} = \begin{pmatrix} Y_{11}^{-2} & 0 \\ 0 & I \end{pmatrix}.$$

Therefore, (5) is solvable if and only if

$$\exists Y_{11} > 0,\ Y_{11} - A_{11}^*Y_{11}^{-2}A_{11} = I + A_{21}^*A_{21}.$$

Thus we get

$$Y_{11} = \sqrt{A_{11}(Y_{11} - I - A_{21}^*A_{21})^{-1}A_{11}^*}. \tag{6}$$

Noting that $Q(Y_{11}) = \sqrt{A_{11}(Y_{11} - I - A_{21}^*A_{21})^{-1}A_{11}^*}$ is a decreasing operator in $[I + A_{21}^*A_{21}, \infty)$, we know that it is impossible that there exist two solutions of (6) $Y_{11}^{(1)}$ and $Y_{11}^{(2)}$ ($Y_{11}^{(1)} \neq Y_{11}^{(2)}$) such that $Y_{11}^{(1)} \geq Y_{11}^{(2)}$ or $Y_{11}^{(1)} \leq Y_{11}^{(2)}$.

## 3. Estimation of Solutions

**Lemma 2.** [10] *If $X$ is a solution to Eq.(1), then*

$$I \le X \le I + A^*A. \tag{7}$$

In the following theorem, we shall improve Lemma 2.

Define the sequence $\{\alpha_n\}$ by

$$\alpha_0 = 1 + \lambda_{max}(A^*A),\ \alpha_n = 1 + \frac{\lambda_{max}(A^*A)}{(1+\lambda_{min}(A^*A)/\alpha_{n-1}^2)^2}, \quad n = 1, 2, 3, \cdots \tag{8}$$

and the sequence $\{\beta_n\}$ by

$$\beta_0 = 1,\ \beta_n = 1 + \frac{\lambda_{min}(A^*A)}{(1+\lambda_{max}(A^*A)/\beta_{n-1}^2)^2}, \quad n = 1, 2, 3, \cdots. \tag{9}$$

Obviously, the two sequences $\{\alpha_n\}$ and $\{\beta_n\}$ can also be obtained by the following iterations

$$\beta_0 = 1, \quad \alpha_n = 1 + \frac{\lambda_{max}(A^*A)}{\beta_n^2}, \quad \beta_{n+1} = 1 + \frac{\lambda_{min}(A^*A)}{\alpha_n^2}, \quad n = 0, 1, 2, \cdots. \tag{10}$$

**Lemma 3.** *The sequences $\{\alpha_n\}$ and $\{\beta_n\}$ have the following properties:*

1. *The sequence $\{\alpha_n\}$ is convergent. Let $\alpha = \lim_{n\to\infty} \alpha_n$. Then $1 \le \alpha \le 1 + \lambda_{max}(A^*A)$ and $\alpha$ is the maximal positive solution of the following equation*

$$(\alpha - 1)\left(1 + \frac{\lambda_{min}(A^*A)}{\alpha^2}\right)^2 = \lambda_{max}(A^*A). \tag{11}$$

2. *The sequence $\{\beta_n\}$ is convergent. Let $\beta = \lim_{n\to\infty} \beta_n$. Then $1 \le \beta \le 1 + \lambda_{min}(A^*A)$ and $\beta$ is the minimal positive solution of the following equation*

$$(\beta - 1)\left(1 + \frac{\lambda_{max}(A^*A)}{\beta^2}\right)^2 = \lambda_{min}(A^*A). \tag{12}$$

3. $$\beta \le \alpha \tag{13}$$

*and we have*

$$(\alpha - 1)\beta^2 = \lambda_{max}(A^*A), \qquad (\beta - 1)\alpha^2 = \lambda_{min}(A^*A). \tag{14}$$

*Proof.* First prove that $\{\alpha_n\}$ is monotone decreasing and is bounded below by induction on $n$. It is easy to see that $1 \le \alpha_1 \le \alpha_0$. Now assume that $1 \le \alpha_n \le \alpha_{n-1}$. Noting that the function $f(x) = 1 + \frac{\lambda_{max}(A^*A)}{(1+\lambda_{min}(A^*A)/x^2)^2}$ is monotone increasing over $(0, +\infty)$, we have $1 \le f(\alpha_n) \le f(\alpha_{n-1})$, that is, $1 \le \alpha_{n+1} \le \alpha_n$. The result is proved. Hence the sequence $\{\alpha_n\}$ is convergent. By $1 \le \alpha_n \le \alpha_0 = 1 + \lambda_{max}(A^*A)$, let $n \to \infty$, we have $1 \le \alpha \le 1 + \lambda_{max}(A^*A)$. By (8), let $n \to \infty$, we know that $\alpha$ satisfies Eq.(11).

Now we prove that $\alpha$ is the maximal positive solution of Eq.(11). For any positive solution $x$ of Eq.(11), we have $x \le 1 + \lambda_{max}(A^*A) = \alpha_0$. By $x = f(x)$ and the monotonicity of $f(x)$, $x = f(x) \le f(\alpha_0) = \alpha_1$. Proceeding in this way, we readily see that we can establish the inequality $x \le \alpha_n$ for $n = 0, 1, 2, \cdots$ by induction on $n$. Letting $n \to \infty$, we have $x \le \alpha$.

The results on $\{\beta_n\}$ are proved similarly.

For (13) it is sufficient to prove that $\beta_n \le \alpha_n, \quad n = 1, 2, 3, \cdots$ by induction. Now letting $n \to \infty$ on both sides of the equalities (10), we can get (14).

In the sequel, we always use $\alpha, \beta$ in the meaning of Lemma 3.

**Theorem 5.** *For the solution $X$ of Eq.(1), we have*

$$I + \frac{1}{\alpha^2} A^* A \le X \le I + \frac{1}{\beta^2} A^* A. \tag{15}$$

*Proof.* First show that

$$\beta I \le X \le \alpha I. \tag{16}$$

By Lemma 2, we have $I \le X \le (1 + \lambda_{max}(A^*A))I$, in other words, $\beta_0 I \le X \le \alpha_0 I$. By $X = I + A^* X^{-2} A$, we have $X = I + A^*(I + A^* X^{-2} A)^{-2} A$. Hence

$$\left(1 + \frac{\lambda_{min}(A^*A)}{\left(1 + \frac{\lambda_{max}(A^*A)}{\lambda^2_{min}(X)}\right)^2}\right) I \le X \le \left(1 + \frac{\lambda_{max}(A^*A)}{\left(1 + \frac{\lambda_{min}(A^*A)}{\lambda^2_{max}(X)}\right)^2}\right) I. \tag{17}$$

Since that $\beta_0 I \le X \le \alpha_0 I$ implies $\beta_0 \le \lambda_{min}(X)$ and $\lambda_{max}(X) \le \alpha_0$, we have $\beta_1 I \le X \le \alpha_1 I$ by (17). Applying this argument inductively, we see that $\beta_n I \le X \le \alpha_n I$ for all $n$. Now letting $n \to \infty$, we get $\beta I \le X \le \alpha I$.

Again, by $X = I + A^* X^{-2} A$, we have $I + \frac{1}{\lambda^2_{max}(X)} A^* A \le X \le I + \frac{1}{\lambda^2_{min}(X)} A^* A$. Noting (16), we get(15).

**Remark 1.** (16) is proved in [9]. Obviously, (15) improves (16).

## 4. Iterative Methods

**Lemma 4.** *Let*

$$F(X) = I + A^* X^{-2} A. \tag{18}$$

*Then*

$$F([\beta I, \alpha I]) \subseteq [\beta I, \alpha I]. \tag{19}$$

*Proof.* If $\beta I \le X \le \alpha I$, then

$$F(X) \le I + \frac{\lambda_{max}(A^*A)}{\lambda^2_{min}(X)} I \le \left(1 + \frac{\lambda_{max}(A^*A)}{\beta^2}\right) I = \alpha I$$

and

$$F(X) \ge I + \frac{\lambda_{min}(A^*A)}{\lambda^2_{max}(X)} I \ge \left(1 + \frac{\lambda_{min}(A^*A)}{\alpha^2}\right) I = \beta I,$$

that is $\beta I \le F(X) \le \alpha I$.

**Remark 2.** By Lemma 4 and Brouwer's fixed point theorem, we get that Eq.(1) has a solution in $[\beta I, \alpha I]$ for every $A \in \mathcal{C}^{n \times n}$.

**Theorem 6.** *If*

$$\beta > \sqrt[3]{2\lambda_{max}(A^*A)}, \tag{20}$$

*Then*

1. *Eq.(1) has a unique solution $X$ and the solution satisfies $\beta I \le X \le \alpha I$.*

2. *The solution can be obtained by the following matrix sequence:*

$$X_{n+1} = I + A^*X_n^{-2}A, \quad n = 0, 1, 2, \cdots \tag{21}$$

*for any* $X_0 \in [\beta I, \alpha I]$.

3. *The estimates*

$$\|X_n - X\| \leq \frac{q^n}{1-q}\|X_1 - X_0\|, \tag{22}$$

*and*

$$\|X_n - X\| \leq \frac{q}{1-q}\|X_n - X_{n-1}\|, \tag{23}$$

*hold where* $q = \frac{2\|A^*A\|}{\beta^3} < 1$.

*Proof.* Let

$$F(X) = I + A^*X^{-2}A,$$

$$\Omega = \{X : \ \beta I \leq X \leq \alpha I\}$$

Obviously, $\Omega$ is a nonempty convex closed set and $F(X)$ is continuous in $\Omega$. By Lemma 4, we know that $F(\Omega) \subseteq \Omega$.

We prove that $F$ is a contraction operator on $\Omega$. For $X_1, \ X_2 \in \Omega$, we have

$$\begin{aligned}
& \|F(X_1) - F(X_2)\| \\
= \ & \|A^*(X_1^{-2} - X_2^{-2})A\| \\
= \ & \|A^*[X_1^{-1}(X_1 - X_2)X_2^{-2} + X_1^{-2}(X_1 - X_2)X_2^{-1}]A\| \\
\leq \ & (\|X_1^{-1}(X_1 - X_2)X_2^{-2} + X_1^{-2}(X_1 - X_2)X_2^{-1}\|)\|A^*A\| \\
\leq \ & (\|X_1^{-1}\|\|X_2^{-2}\| + \|X_1^{-2}\|\|X_2^{-1}\|)\|A\|^2\|X_1 - X_2\| \\
\leq \ & \frac{2\|A^*A\|}{\beta^3}\|X_1 - X_2\| \\
= \ & q\|X_1 - X_2\|.
\end{aligned}$$

Noting that $q = \frac{2\|A^*A\|}{\beta^3} < 1$, we know that $F$ is a contraction operator. By Banach's fixed point principle[1], we get the theorem.

**Theorem 7.** *(20) holds if and only if*

$$\frac{1}{2}\lambda_{max}(A^*A) + \frac{3}{4}\sqrt[3]{4\lambda_{max}^2(A^*A)} - 1 < \lambda_{min}(A^*A) \leq \lambda_{max}(A^*A) < 4. \tag{24}$$

*Proof.* We proceed in two steps.

(i) Prove that (24) is rational, in other words, there exists $A \in \mathbf{C}^{n\times n}$ satisfying (24). It is sufficed to prove

$$\frac{1}{2}\lambda_{max}(A^*A) + \frac{3}{4}\sqrt[3]{4\lambda_{max}^2(A^*A)} - 1 < \lambda_{max}(A^*A).$$

that is

$$\lambda_{max}^{\frac{1}{3}}(A^*A) + 2\lambda_{max}^{-\frac{2}{3}}(A^*A) > \frac{3}{\sqrt[3]{2}}.$$

Noting that $\lambda_{max}(A^*A) < 4$, we have that $\frac{1}{2}\lambda_{max}^{\frac{1}{3}}(A^*A) \neq 2\lambda_{max}^{-\frac{2}{3}}(A^*A)$. By geometric-mean inequality, we have

$$\begin{aligned}
\lambda_{max}^{\frac{1}{3}}(A^*A) + 2\lambda_{max}^{-\frac{2}{3}}(A^*A) &= \frac{1}{2}\lambda_{max}^{\frac{1}{3}}(A^*A) + \frac{1}{2}\lambda_{max}^{\frac{1}{3}}(A^*A) + 2\lambda_{max}^{-\frac{2}{3}}(A^*A) \\
&> 3\sqrt[3]{\frac{1}{2}\lambda_{max}^{\frac{1}{3}}(A^*A)\cdot\frac{1}{2}\lambda_{max}^{\frac{1}{3}}(A^*A)\cdot 2\lambda_{max}^{-\frac{2}{3}}(A^*A)} \\
&= \frac{3}{\sqrt[3]{2}}.
\end{aligned}$$

(ii) Now we prove that (24) $\Leftrightarrow$ (20). Note that $\beta$ is the minimal positive solution of the following equation

$$(x-1)\left(1+\frac{\lambda_{max}(A^*A)}{x^2}\right)^2 = \lambda_{min}(A^*A). \tag{25}$$

Let

$$f(x) = (x-1)\left(1+\frac{\lambda_{max}(A^*A)}{x^2}\right)^2 - \lambda_{min}(A^*A). \tag{26}$$

Then

$$f'(x) = \left(1+\frac{\lambda_{max}(A^*A)}{x^2}\right)\frac{\lambda_{max}(A^*A)}{x^2}\left(\frac{x^2}{\lambda_{max}(A^*A)}+\frac{4}{x}-3\right). \tag{27}$$

First prove (24) $\Rightarrow$ (20). By geometric-mean inequality and $\lambda_{max}(A^*A) < 4$, we have

$$\frac{x^2}{\lambda_{max}(A^*A)}+\frac{4}{x} = \frac{x^2}{\lambda_{max}(A^*A)}+\frac{2}{x}+\frac{2}{x} \geq 3\sqrt[3]{\frac{4}{\lambda_{max}(A^*A)}} > 3$$

as $x > 0$. Then $f'(x) \geq 0$ as $x > 0$. Thus, $f(x)$ is monotone increasing over $(0, +\infty)$, and therefore $f(x) = 0$ has a unique positive solution. Noting that

$$\begin{aligned}
&f(\sqrt[3]{2\lambda_{max}(A^*A)}) \\
= \;& (\sqrt[3]{2\lambda_{max}(A^*A)} - 1)\left(1+\sqrt[3]{\frac{\lambda_{max}(A^*A)}{4}}\right)^2 - \lambda_{min}(A^*A) \\
= \;& \frac{1}{2}\lambda_{max}(A^*A) + \frac{3}{4}\sqrt[3]{4\lambda_{max}^2(A^*A)} - 1 - \lambda_{min}(A^*A) < 0
\end{aligned}$$

and $f(\infty) > 0$, we get (20).

Second, we prove that (20) $\Rightarrow$ (24). Assume, on the contrary, that

$$\lambda_{max}(A^*A) < 4, \;\; \frac{1}{2}\lambda_{max}(A^*A) + \frac{3}{4}\sqrt[3]{4\lambda_{max}^2(A^*A)} - 1 \geq \lambda_{min}(A^*A)$$

or

$$\lambda_{max}(A^*A) \geq 4$$

For the first case, since that $f(x) = 0$ has a unique positive solution, $f(x)$ is monotone increasing over $(0, +\infty)$ and $f(\sqrt[3]{2\lambda_{max}(A^*A)}) \geq 0$, then $\beta \leq \sqrt[3]{2\lambda_{max}(A^*A)}$, a contradiction to (20).

For the second case, by

$$f(1) = -\lambda_{min}(A^*A) \leq 0$$

and

$$f(2) = \left(1 + \frac{\lambda_{max}(A^*A)}{4}\right)^2 - \lambda_{min}(A^*A) \geq \lambda_{max}(A^*A) - \lambda_{min}(A^*A) \geq 0,$$

we have $1 \leq \beta \leq 2 \leq \sqrt[3]{2\lambda_{max}(A^*A)}$, a contradiction to (20).

**Remark 3.** By Theorem 6 and 7, we can easily get the following result in [9]: if $\lambda_{max}(A^*A) < \frac{1}{2}$, then the statements 1, 2 and 3 in Theorem 6 hold.

**Remark 4.** The condition (24) has been found by M.Reurings[11], but the proof in [11] is very complicated.

**Theorem 8.** *If*

$$4 < \lambda_{min}(A^*A) \leq \lambda_{max}(A^*A) < (\gamma - 1)\left(1 + \frac{\lambda_{min}(A^*A)}{\gamma^2}\right)^2, \tag{28}$$

*where $\gamma$ is a unique positive solution in $(1, +\infty)$ of the equation*

$$2\gamma(\gamma - 1)^2 = \lambda_{max}(A^*A), \tag{29}$$

*then*

1. *Eq.(1) has a unique solution satisfying*

$$\eta I \leq X \leq \xi I, \tag{30}$$

   *where $\eta \in (\gamma, \sqrt{\lambda_{min}(A^*A)})$ satisfies*

$$(\eta - 1)(1 + \frac{\lambda_{min}(A^*A)}{\eta^2})^2 = \lambda_{max}(A^*A) \tag{31}$$

   *and*

$$\xi = 1 + \frac{\lambda_{min}(A^*A)}{\eta^2}. \tag{32}$$

2. *The solution can be obtained by the following matrix sequence:*

$$X_{n+1} = \sqrt{A(X_n - I)^{-1}A^*}, \quad n = 0, 1, 2, \cdots \tag{33}$$

   *for any $X_0 \in [\eta I, \xi I]$.*

3. *The estimates*

$$\|X_n - X\| \leq \frac{p^n}{1-p}\|X_1 - X_0\| \tag{34}$$

   *and*

$$\|X_n - X\| \leq \frac{p}{1-p}\|X_n - X_{n-1}\| \tag{35}$$

   *hold, where $p = \frac{\|A^*A\|}{2\eta(\eta-1)^2} < 1$.*

*Proof.* We proceed in seven steps.

(i) Prove that Eq.(29) in $(1, +\infty)$ has only a solution and the solution $\gamma \in (2, \sqrt{\lambda_{max}(A^*A)})$. Let $h(x) = 2x(x-1)^2 - \lambda_{max}(A^*A)$. By $h'(x) = 2(x-1)(3x-1) > 0$ as $x \in (1, +\infty)$ and $h(2) = 4 - \lambda_{max}(A^*A) < 0$, $h(\sqrt{\lambda_{max}(A^*A)}) = \sqrt{\lambda_{max}(A^*A)}(2\sqrt{\lambda_{max}(A^*A)} - 1)(\sqrt{\lambda_{max}(A^*A)} - 2) > 0$, we get the statement.

(ii) Prove that (31) has one solution $\eta \in (\gamma, \sqrt{\lambda_{max}(A^*A)})$. Let $g(x) = (x-1)(1+\frac{\lambda_{min}(A^*A)}{x^2})^2 - \lambda_{max}(A^*A)$. By

$$\begin{aligned} & g(\gamma) > 0, \\ g(\sqrt{\lambda_{max}(A^*A)}) &= (\sqrt{\lambda_{max}(A^*A)}-1)(1+\tfrac{\lambda_{min}(A^*A)}{\lambda_{max}(A^*A)})^2 - \lambda_{max}(A^*A) \\ &\le 4(\sqrt{\lambda_{max}(A^*A)}-1) - \lambda_{max}(A^*A) \\ &= -(2-\sqrt{\lambda_{max}(A^*A)})^2 < 0 \end{aligned}$$

and the continuity of $g(x)$, we get the statement.

(iii) Prove that the solution $\eta \in (\gamma, \sqrt{\lambda_{max}(A^*A)})$ for Eq.(31) is unique and $\eta \le \sqrt{\lambda_{min}(A^*A)}$. By computation, we have

$$\begin{aligned} g'(x) &= \left(1+\tfrac{\lambda_{min}(A^*A)}{x^2}\right)\tfrac{1}{x^3}\left(x^3 - 3\lambda_{min}(A^*A)x + 4\lambda_{min}(A^*A)\right) \\ &= \left(1+\tfrac{\lambda_{min}(A^*A)}{x^2}\right)\tfrac{1}{x^3}\left(x(x^2-\lambda_{min}(A^*A)) + 2\lambda_{min}(A^*A)(2-x)\right). \end{aligned}$$

Obviously, $g'(x) < 0$ as $x \in (2, \sqrt{\lambda_{min}(A^*A)}]$. Then $g(x)$ is monotone decreasing over $(2, \sqrt{\lambda_{min}(A^*A)})$. For any $x \in [\sqrt{\lambda_{min}(A^*A)}, \sqrt{\lambda_{max}(A^*A)}]$, we have

$$\begin{aligned} g(x) &\le (\sqrt{\lambda_{max}(A^*A)}-1)(1+\frac{\lambda_{min}(A^*A)}{(\sqrt{\lambda_{min}(A^*A)})^2})^2 - \lambda_{max}(A^*A) \\ &= -(2-\sqrt{\lambda_{max}(A^*A)})^2 < 0. \end{aligned}$$

Then

$$\gamma < \sqrt{\lambda_{min}(A^*A)}$$

and $\eta \in (\gamma, \sqrt{\lambda_{min}(A^*A)})$ is unique.

(iv) Prove $p < 1$. By $2 < \gamma < \eta < \sqrt{\lambda_{min}(A^*A)}$, we have $2\eta(\eta-1)^2 > 2\gamma(\gamma-1)^2 = \lambda_{max}(A^*A)$.

(v) Prove $\eta \le \xi$. Note that $2 < \eta < \sqrt{\lambda_{min}(A^*A)}$ and $\xi = 1 + \frac{\lambda_{min}(A^*A)}{\eta^2} > 2$. By (31) and (32), we get $\xi^2(\eta-1) = \lambda_{max}(A^*A) \ge \lambda_{min}(A^*A) = \eta^2(\xi-1)$. Therefore, $\xi^2(\eta-1) \ge \eta^2(\xi-1)$, that is $(\xi-\eta)\xi\eta(1-\frac{1}{\xi}-\frac{1}{\eta}) \ge 0$. Noting that $\eta > 0$, $\xi > 0$ and $1-\frac{1}{\xi}-\frac{1}{\eta} > 0$, we get $\eta \le \xi$.

Let

$$G(X) = \sqrt{A(X-I)^{-1}A^*}, \quad X \in \Gamma = [\eta I, \xi I]. \tag{36}$$

(vi) Prove that $G(\Gamma) \subseteq \Gamma$. For all $X \in \Gamma$, we have $\frac{1}{\xi-1}I \le (X-I)^{-1} \le \frac{1}{\eta-1}I$. Then

$$\eta I = \sqrt{\frac{\lambda_{min}(A^*A)}{\xi-1}} \le \sqrt{A(X-I)^{-1}A^*} \le \sqrt{\frac{\lambda_{max}(A^*A)}{\eta-1}}I = \xi I,$$

that is, $G(X) \in \Gamma$.

(vii) Prove that $G : \Gamma \to \Gamma$ is a $p$-contraction. For $Y_1, Y_2 \in \Gamma$, let $P_1 = A(Y_1-I)^{-1}A^*$ and $P_2 = A(Y_2-I)^{-1}A^*$. Then $P_1 \ge \eta^2 I$ and $P_2 \ge \eta^2 I$. By a classical result(see Theorem X.3.8 in[2],p.304), we have

$$\begin{aligned} \|G(Y_1)-G(Y_2)\| &= \|\sqrt{P_1}-\sqrt{P_2}\| \\ &\le \tfrac{1}{2\eta}\|P_1-P_2\| \\ &\le \tfrac{1}{2\eta}\|A\|^2\|(Y_1-I)^{-1}-(Y_2-I)^{-1}\| \\ &= \tfrac{1}{2\eta}\|A\|^2\|(Y_1-I)^{-1}(Y_2-Y_1)(Y_2-I)^{-1}\| \\ &\le \tfrac{1}{2\eta}\|A\|^2\|(Y_1-I)^{-1}\|\|Y_2-Y_1\|\|(Y_2-I)^{-1}\| \\ &\le \tfrac{\|A\|^2\|}{2\eta(\eta-1)^2}\|Y_1-Y_2\| \\ &\le p\|Y_1-Y_2\|. \end{aligned}$$

By Banach's fixed point theorem [1] we obtain the convergence and the error estimates.

## 5. Numerical Examples

We now use simple numerical examples to illustrate our results. All computations were performed using MATLAB, version 6.0.

**Example 1.** Consider Eq.(1) with

$$A = \begin{pmatrix} 0 & 6\sqrt{2} \\ 8 & 0 \end{pmatrix}.$$

It is easy to know $\lambda_{max}(A * A) = 72, \lambda_{min}(A * A) = 64$. Let us consider diagonal positive definite solutions. Let $X = diag(x_1, x_2)$. Then we have

$$\begin{cases} x_1 = 1 + 64/x_2^2, \\ x_2 = 1 + 72/x_1^2. \end{cases}$$

The system has three positive solutions. One of them is $x_1 = \beta, x_2 = \alpha$. Hence we know that with $\alpha, \beta$ the inequalities (15) and (16) in Theorem 5 are sharp. By computation, we can get at least the following three solutions:

$$X = \begin{pmatrix} 1.012619 & 0 \\ 0 & 71.216726 \end{pmatrix}, \quad \begin{pmatrix} 4.827975 & 0 \\ 0 & 4.088890 \end{pmatrix},$$

and

$$\begin{pmatrix} 62.720012 & 0 \\ 0 & 1.018303 \end{pmatrix}.$$

**Example 2.** Consider Eq.(1) with

$$A = \begin{pmatrix} 0.12525491782700 & -0.76991965836417 & 0.46747345506882 \\ 0.88788502515975 & 0.17638000655582 & 0.20977698164743 \\ -0.35556154646883 & 0.40861155116318 & 0.81618623751850 \end{pmatrix}$$

By computation, we get

$$\begin{aligned} &\lambda_{max}(A^*A) = 1, && \lambda_{min}(A^*A) = 0.75, \\ &\alpha = 1.59722868268156, && \beta = 1.29398627960329, \\ &q = 0.92308348565281. \end{aligned}$$

The matrix $A$ satisfies the conditions of Theorem 6 and 7. Then Eq.(1) has a unique solution satisfying

$$\beta I \le X \le \alpha I$$

Choose $X_0 = 1.4I$. With the iterative method (21), after 178 iterations we obtain the following result

$$X_{178} = \begin{pmatrix} 1.52381998957013 & -0.05077203374296 & -0.00391727224933 \\ -0.05077203374296 & 1.34137319253121 & 0.01866946845041 \\ -0.00391727224933 & 0.01866946845041 & 1.44272036829284 \end{pmatrix}$$

whose error $\|X_{178} - X\|$ is less than $10^{-14}$.

**Example 3.** *Consider Eq.(1) with*

$$A = \begin{pmatrix} 2.03480656930046 & -7.76558407441603 & -2.56864825089238 \\ 5.29358053743931 & 3.34249802779581 & -5.41476349037101 \\ 5.85290165142532 & -0.08493435128064 & 5.49360438671923 \end{pmatrix}.$$

*By computation, we get* $\lambda_{max}(A^*A) = 72$ *and* $\lambda_{min}(A^*A)$=64, $\gamma$=4, *and* $\eta$=4.08889007016108, $\xi$=4.82797510390027. *The matrix A satisfies the conditions of Theorem 8. Then Eq.(1) has a unique solution X satisfying*

$$\eta I \leq X \leq \xi I$$

*Choosing* $X_0 = 4.2I$, *202 iterations with the iterative method (33) yield*

$$X_{202} = \begin{pmatrix} 4.50211434339476 & -0.09933738565402 & -0.10626059612285 \\ -0.09933738565402 & 4.44069140329871 & 0.01187341828058 \\ -0.10626059612285 & 0.01187341828058 & 4.38964314270634 \end{pmatrix}$$

with the error $\|X_{202} - X\|$ less than $10^{-14}$.

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