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A note on the fixed-point iteration for the matrix equations $X \pm A^*X^{-1}A = I$

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Abstract

The fixed-point iteration is a simple method for finding the maximal Hermitian positive definite solutions of the matrix equations $X \pm A^*X^{-1}A = I$ (the plus/minus equations). The convergence of this method may be very slow if the initial matrix is not chosen carefully. A strategy for choosing better initial matrices has been recently proposed by Ivanov et al. They proved that this strategy can improve the convergence in general and observed from numerical experiments that dramatic improvement happens for the plus equation with some matrices A. It turns out that the matrices A are normal for those examples. In this note we prove a result that explains the dramatic improvement in convergence for normal (and thus nearly normal) matrices for the plus equation. A similar result is also proved for the minus equation.

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1. Introduction

We consider the matrix equations

$$X + A^*X^{-1}A = Q \tag{1}$$

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and

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

where $Q \in \mathbb{C}^{n\times n}$ is Hermitian positive definite. We may assume $Q = I$ without loss of generality. A numerically efficient way for the reduction is as follows (assuming Q is not ill-conditioned). Let $Q = LL^*$ be the Cholesky factorization and set $\widetilde{X} = L^{-1}XL^{-*}$, $\widetilde{A} = L^{-1}AL^{-*}$. Then (1) and (2) become $\widetilde{X} \pm \widetilde{A}^*\widetilde{X}^{-1}\widetilde{A} = I$. So our discussions will be mostly about the equations

$$X + A^* X^{-1} A = I \tag{3}$$

and

$$X - A^* X^{-1} A = I. \tag{4}$$

Eq. (1) has been studied in a number of papers [1,4,5,8,10,13,14,16,18]. Several applications have been mentioned in [1]. More recently the equation has been used to solve a special quadratic eigenvalue problem efficiently [9]. Eq. (2) has been studied is several papers [2,6,10,13,16]; some applications have been mentioned in [6,11].

In this note we use the usual partial order for Hermitian matrices, that is, we write $X > Y (X \geqslant Y)$ if $X - Y$ is positive definite (semidefinite). We use $\|\cdot\|$ for the spectral norm, and $\rho(\cdot)$ for the spectral radius.

A necessary and sufficient condition for the existence of positive definite solutions of (1) has been given in [5]. It is also proved in [5] that if (1) has a positive definite solution, then it has a maximum positive definite solution X_L, which means that $X_L \geqslant X$ for any positive definite solution X. Moreover, $\rho(X_L^{-1}A) \leqslant 1$. The maximal solution is the required solution in applications. It is shown in [6] that (2) has a unique positive definite solution X_L, and $\rho(X_L^{-1}A) < 1$. This solution is the one of practical interest.

The following fixed-point iteration for (1) is studied in [5].

Algorithm 1

$$X_0 = Q,$$
$$X_k = Q - A^* X_{k-1}^{-1} A, \quad k = 1, 2, \ldots$$

It is shown in [5] that the sequence generated by this algorithm is monotonically decreasing and converges to X_L. The rate of convergence can be determined by computing the Fréchet derivative of the iterative function $f(X) = Q - A^*X^{-1}A$, and we have

$$\limsup_{k\to\infty} \sqrt[k]{\|X_k - X_L\|} \leqslant (\rho(X_L^{-1}A))^2 \tag{5}$$

(see [10] for details).

For the minus equation (2) the following fixed-point iteration is studied in [6].

Algorithm 2

$$X_0 = Q,$$
$$X_k = Q + A^* X_{k-1}^{-1} A, \quad k = 1, 2, \ldots$$

It is shown in [6] that the sequence produced by Algorithm 2 converges to X_L. Moreover, $\{X_{2k}\}$ is an increasing sequence and $\{X_{2k+1}\}$ is a decreasing sequence. The sequence $\{X_k\}$ still converges

to X_L if $X_0 = Q$ in Algorithm 2 is replaced with any $X_0 > 0$, see [6,17, Theorem 3.3], and we have

$$\limsup_{k\to\infty} \sqrt[k]{\|X_k - X_L\|} \leqslant (\rho(X_L^{-1}A))^2. \tag{6}$$

So the convergence of Algorithms 1 and 2 is fast if $\rho(X_L^{-1}A)$ is sufficiently small. On the other hand, the convergence is usually very slow when $X_L^{-1}A$ has eigenvalues on or near the unit circle, since equality usually holds in (5) and (6).

Meini [16] developed algorithms for (1) and (2) based on cyclic reduction; see [14] for a different derivation. The convergence of the algorithms is quadratic when $\rho(X_L^{-1}A) < 1$. For the plus equation, $\rho(X_L^{-1}A) = 1$ is possible. In that case, the convergence of Meini's method is shown in [9], and it is shown in [8] that the convergence is at least linear with rate $\frac{1}{2}$ if all eigenvalues of $X_L^{-1}A$ on the unit circle are semi-simple. It is shown recently in [3] that the convergence is at least linear with rate $\frac{1}{2}$ in all cases.

In general, Meini's method is very efficient for computing X_L for Eqs. (1) and (2). When the matrix Q is ill-conditioned in (2), Meini's method is not suitable since it uses Q^{-1} in the first step. In this case, we may use Algorithm 2 with $X_0 = I$ instead to compute X_L if $\rho(X_L^{-1}A)$ is not too close to 1. The method usually works well if X_L itself is not ill-conditioned. If $\rho(X_L^{-1}A)$ is very close to 1, then the convergence of the fixed-point iteration is usually very slow and the method proposed in [2] may be used.

Meini's method requires $\frac{19}{3}n^3$ flops each iteration, while the fixed-point iteration requires $\frac{7}{3}n^3$. So the fixed-point iteration may be more efficient if $\rho(X_L^{-1}A)$ is small and the required accuracy for X_L is not very high. It is of interest to devise an inexpensive strategy for choosing the initial guess X_0 such that the fixed-point iteration has faster convergence. Such an attempt is made in [13]. The main purpose of this note is to show that, while the strategy in [13] improves the convergence in general, significant improvement happens only when A is normal or nearly normal.

2. Preliminaries

We start with a review of the main results in [13].

For the plus equation (3), it is assumed in [13] that $A \in \mathbb{C}^{n\times n}$ satisfies $\|A\| \leqslant \frac{1}{2}$. This condition on A is a sufficient condition for the existence of positive definite solutions of (3), and it is a necessary and sufficient condition when A is a normal matrix [4]. When Algorithm 1 is applied to (3), the initial matrix is $X_0 = I$. It is shown in [13] that the convergence of the fixed-point iteration can be improved by using other initial matrices. The algorithm proposed in [13] is the following.

Algorithm 3

$$X_0 = \gamma I, \tag{7}$$

$$X_k = I - A^* X_{k-1}^{-1} A, \quad k = 1, 2, \ldots, \tag{8}$$

where good choices of the parameter γ are suggested by the following result (see Theorems 2.4 and 2.5 in [13]).

Theorem 1. *Let A have singular values $\sigma_1, \sigma_2, \ldots, \sigma_n$ with $\frac{1}{2} \geqslant \sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n \geqslant 0$, and assume the numbers $\alpha, \beta \in \left[\frac{1}{2}, 1\right]$ are such that $\alpha(1-\alpha) = \sigma_n^2$ and $\beta(1-\beta) = \sigma_1^2$. Then*

(i) *For $\gamma \in [\alpha, 1]$, the sequence $\{X_k\}$ in Algorithm 3 is monotonically decreasing and converges to the maximum positive definite solution X_L of (3), and the fastest convergence is achieved for $\gamma = \alpha$.*
(ii) *For $\gamma \in \left[\frac{1}{2}, \beta\right]$, the sequence $\{X_k\}$ in Algorithm 3 is monotonically increasing and converges to X_L, and the fastest convergence is achieved for $\gamma = \beta$.*
(iii) *If $\gamma \in (\beta, \alpha)$ and $\sigma_1 < \frac{1}{2}$, then the sequence $\{X_k\}$ in Algorithm 3 converges to X_L.*

Based on Theorem 1 (i) and (ii), it is recommended in [13] that $\gamma = \alpha$ or $\gamma = \beta$ be used in Algorithm 3. A few remarks are now in order. First, the best performance of Algorithm 3 may be achieved for some $\gamma \in (\beta, \alpha)$ in special cases. This will be illustrated by one example in Section 5. In general, however, the use of $\gamma = \alpha$ or $\gamma = \beta$ may still be recommended. Now the question is which one would be better. The answer is that we should use $\gamma = \beta$ for Algorithm 3. There are several reasons for this recommendation. First, when A is singular we have $\alpha = 1$, so Algorithm 3 with $\gamma = \alpha$ is the same as Algorithm 1. When A is nonsingular we have $\alpha < 1$ and Theorem 1 (i) says the fastest convergence is achieved for $\gamma = \alpha$ when $\gamma \in [\alpha, 1]$ (in the sense that $X_k^{(\gamma)} > X_k^{(\alpha)} \geqslant X_L$ for all k and all $\gamma \in (\alpha, 1]$). However, the asymptotic rate of convergence may remain the same and the improvement in convergence may not be significant, even when the matrix A is normal. This will be illustrated by examples in Section 5. On the other hand, the use of $\gamma = \beta$ has a distinct advantage. We will show in Section 3 that linear convergence of Algorithm 3 is guaranteed for $\gamma = \beta$ even when $\rho(X_L^{-1}A) = 1$, if the matrix A is normal. For all examples in [13] where dramatic improvement of convergence happens with $\gamma = \beta$, the matrices A are normal. So our main result in Section 3 will reveal the underlying reason for the dramatic improvement. When A is nearly normal, this dramatic improvement of convergence will be more or less maintained, as shown by an example in Section 5. When A is a general non-normal matrix, however, the improvement offered by $\gamma = \beta$ is not expected to be very significant despite the conclusion in Theorem 1(ii).

For the minus equation (4) the following fixed-point iteration is studied in [13].

Algorithm 4

$$X_0 = \gamma I,$$
$$X_k = I + A^* X_{k-1}^{-1} A, \quad k = 1, 2, \ldots$$

It is shown in [13] that the convergence of Algorithm 4 will be faster if one uses special values for γ, as compared to the conventional choice $\gamma = 1$. Some good choices of the parameter γ are determined from singular values of A. Let A have singular values $\sigma_1 \geqslant \sigma_1 \geqslant \cdots \geqslant \sigma_n$. Then one may take $\gamma = \alpha$ or $\gamma = \beta$, where α is the real number with

$$\alpha(\alpha - 1) = \sigma_n^2, \quad \alpha \geqslant 1 \tag{9}$$

and β is the real number with

$$\beta(\beta - 1) = \sigma_1^2, \quad \beta \geqslant 1. \tag{10}$$

To allow comparison, we denote the sequence $\{X_k\}$ from Algorithm 4 by $\{X_k^{(\gamma)}\}$, and compare the three sequences $\{X_k^{(1)}\}$, $\{X_k^{(\alpha)}\}$, $\{X_k^{(\beta)}\}$.

Proposition 2 [13, Theorems 3.4 and 3.5]. *Let A be nonsingular. Then*

(i) *For each $k \geqslant 0$*

$$\|X_k^{(\alpha)} - A^*(X_k^{(\alpha)})^{-1}A - I\| < \|X_k^{(1)} - A^*(X_k^{(1)})^{-1}A - I\|. \tag{11}$$

(ii) *If*

$$\sigma_n^2(\sigma_n^2 + 1) \geqslant \sigma_1^2, \tag{12}$$

then for each $k \geqslant 0$

$$\|X_k^{(\beta)} - A^*(X_k^{(\beta)})^{-1}A - I\| < \|X_k^{(1)} - A^*(X_k^{(1)})^{-1}A - I\|. \tag{13}$$

When σ_n is small, the condition (12) is very restrictive. We will prove a result that is slightly weaker than (13), but without any assumption on A.

Proposition 3. *For each $k \geqslant 0$*

$$\|X_{k+1}^{(\beta)} - A^*(X_{k+1}^{(\beta)})^{-1}A - I\| \leqslant \|X_k^{(1)} - A^*(X_k^{(1)})^{-1}A - I\|$$

and strict inequality holds when A is nonsingular.

Proof. The proof is a small modification of that of [13, Theorem 3.5]. Let

$$f(X) = I + A^*X^{-1}A.$$

Then $X_{k+1}^{(\beta)} = f(X_k^{(\beta)})$ with $X_0^{(\beta)} = \beta I$, and $X_{k+1}^{(1)} = f(X_k^{(1)})$ with $X_0^{(1)} = I$. Since $X_0^{(\beta)} \geqslant X_1^{(\beta)}$ by the choice of β, we have $X_1^{(\beta)} \leqslant X_2^{(\beta)}$. Since $X_1^{(\beta)} \geqslant X_0^{(1)}$, we have $X_2^{(\beta)} \leqslant X_1^{(1)}$. Thus

$$X_0^{(1)} \leqslant X_1^{(\beta)} \leqslant X_2^{(\beta)} \leqslant X_1^{(1)}.$$

Since f reverses the order, we have for each $k \geqslant 1$

$$X_{2k-2}^{(1)} \leqslant X_{2k-1}^{(\beta)} \leqslant X_{2k}^{(\beta)} \leqslant X_{2k-1}^{(1)}, \quad X_{2k}^{(1)} \leqslant X_{2k+1}^{(\beta)} \leqslant X_{2k}^{(\beta)} \leqslant X_{2k-1}^{(1)}.$$

It follows that $\|X_{k+1}^{(\beta)} - X_{k+2}^{(\beta)}\| \leqslant \|X_k^{(1)} - X_{k+1}^{(1)}\|$ for each $k \geqslant 0$. If A is nonsingular, we have $X_{2k}^{(\beta)} < X_{2k-1}^{(1)}$ for each $k \geqslant 1$, and thus $\|X_{k+1}^{(\beta)} - X_{k+2}^{(\beta)}\| < \|X_k^{(1)} - X_{k+1}^{(1)}\|$ for each $k \geqslant 0$. □

We see from Propositions 2 and 3 that the convergence of $\{X_k\}$ for $\gamma = \alpha, \beta$ should be no worse than that for $\gamma = 1$. As for the plus equation, we recommend the use of $\gamma = \beta$, since we can show that with this choice the convergence of Algorithm 4 is improved significantly when A is a (nearly) normal matrix.

3. Convergence analysis for the normal case

In this section we assume that A is a normal matrix and that $\|A\| \leqslant \frac{1}{2}$ for the plus equation. Even though we have explicit formulas for the maximal solutions of (3) and (4) for normal matrices, convergence analysis of Algorithms 3 and 4 with $\gamma = \beta$ for normal matrices (where β is given in Theorem 1 and (10), respectively) will help us to understand their rapid convergence for nearly normal matrices, where the formulas are no longer valid.

Since $A \in \mathbb{C}^{n\times n}$ is a normal matrix, it is unitarily diagonalizable (see [12], for example). Let $U = [u_1 u_2 \dots u_n]$ be a unitary matrix such that

$$U^* A U = \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n). \tag{14}$$

So the vectors $u_1, \dots, u_n$ are orthonormal eigenvectors of A corresponding to its eigenvalues $\lambda_1, \dots, \lambda_n$. We assume that the eigenvalues are arranged such that

$$|\lambda_1| = \cdots = |\lambda_{p-1}| > |\lambda_p| \geqslant \cdots \geqslant |\lambda_n|. \tag{15}$$

3.1. The plus equation

For the plus equation (3) with a normal matrix A, Engwerda conjectured in [4] and Zhan and Xie proved in [18] the formula for the maximal solution:

$$X_L = \frac{1}{2}\left[I + (I - 4A^*A)^{\frac{1}{2}}\right]. \tag{16}$$

From (16) and (14), we get

$$X_L = \frac{1}{2} U \left[I + (I - 4|\Lambda|^2)^{\frac{1}{2}}\right] U^*, \tag{17}$$

and then

$$X_L^{-1} A = U \operatorname{diag}(\eta_1, \dots, \eta_n) U^*, \tag{18}$$

where

$$\eta_i = \frac{2\lambda_i}{1 + \sqrt{1 - 4|\lambda_i|^2}}, \quad i = 1, \dots, n. \tag{19}$$

Thus, $u_1, \dots, u_n$ are orthonormal eigenvectors of $X_L^{-1}A$ corresponding to its eigenvalues $\eta_1, \dots, \eta_n$. In view of (15) and (19), we have

$$|\eta_1| = \cdots = |\eta_{p-1}| > |\eta_p| \geqslant \cdots \geqslant |\eta_n|. \tag{20}$$

To determine the rate of convergence for Algorithm 3, let

$$E_k = X_L - X_k, \quad k = 0, 1, \dots.$$

As in the proof of Theorem 2.3 in [10], for each $k \geqslant 1$ we have

$$E_k = (X_L^{-1}A)^* E_{k-1} (X_L^{-1}A) + (X_L^{-1}A)^* E_{k-1} X_{k-1}^{-1} E_{k-1} (X_L^{-1}A). \tag{21}$$

Lemma 4. *Let A in (3) be a normal matrix, and $u_1, \dots, u_n$ be the orthonormal eigenvectors of A corresponding to its eigenvalues arranged as in (15). Then for Algorithm 3 with $\gamma = \beta$, where β is defined in Theorem 1, we have*

$$E_k u_i = 0, \quad i = 1, \dots, p-1, \ k = 0, 1, \dots$$

Proof. From (16) we get

$$E_0 = X_L - \beta I = \left(\frac{1}{2} - \beta\right) I + \frac{1}{2}(I - 4A^*A)^{\frac{1}{2}}.$$

Since $\beta \in \left[\frac{1}{2}, 1\right]$ and $\beta(1-\beta) = \sigma_1^2 = |\lambda_1|^2$, we have for $i = 1, \dots, p-1$

$$E_0 u_i = \left(\frac{1}{2} - \beta + \frac{1}{2}\sqrt{1 - 4|\lambda_1|^2}\right) u_i = \left(\frac{1}{2} - \beta + \frac{1}{2}\sqrt{(1-2\beta)^2}\right) u_i = 0.$$

Since $X_L^{-1} A u_i = \eta_i u_i$, it follows from (21) that $E_k u_i = 0$ for any $k \geqslant 0$. □

We can now prove our main result for the plus equation, which is similar in nature to Theorem 16 in [15].

Theorem 5. *Let A in (3) be a normal matrix and $\eta_1, \ldots, \eta_n$ be the eigenvalues of the matrix $X_L^{-1} A$, arranged as in (20). Then the rate of convergence of Algorithm 3 with $\gamma = \beta$ is*

$$r = \limsup_{k\to\infty} \sqrt[k]{\|E_k\|} = |\eta_p|^2.$$

Proof. As in [10], for any $\epsilon > 0$ there exist a k_0 such that for all $k \geqslant k_0$

$$E_k X_k^{-1} E_k \leqslant \epsilon E_k. \tag{22}$$

Combining (21) and (22) we have

$$0 \leqslant E_k \leqslant (1+\epsilon)^{k-k_0} ((X_L^{-1} A)^*)^{k-k_0} E_{k_0} (X_L^{-1} A)^{k-k_0}.$$

Therefore,

$$\begin{aligned} r &= \limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \\ &\leqslant \limsup_{k\to\infty} \sqrt[k]{\|(1+\epsilon)^{k-k_0} ((X_L^{-1} A)^*)^{k-k_0} E_{k_0} (X_L^{-1} A)^{k-k_0}\|} \\ &= (1+\epsilon) \limsup_{k\to\infty} \sqrt[k]{\max_{\|v\|_2=1} \|((X_L^{-1} A)^*)^{k-k_0} E_{k_0} (X_L^{-1} A)^{k-k_0} v\|_2} \\ &= (1+\epsilon) \limsup_{k\to\infty} \sqrt[k]{\|((X_L^{-1} A)^*)^{k-k_0} E_{k_0} (X_L^{-1} A)^{k-k_0} v^{(k)}\|_2}, \end{aligned}$$

where $\|v^{(k)}\|_2 = 1$. Write $v^{(k)}$ as a linear combination of the orthonormal vectors $u_1, \ldots, u_n$: $v^{(k)} = \sum_{i=1}^n a_i^{(k)} u_i$ with $\sum_{i=1}^n |a_i^{(k)}|^2 = 1$. Then

$$r \leqslant (1+\epsilon) \limsup_{k\to\infty} \sqrt[k]{\sum_{i=1}^n \|((X_L^{-1} A)^*)^{k-k_0} E_{k_0} (X_L^{-1} A)^{k-k_0} u_i\|_2}.$$

Using (21), (8), and the fact $X_L^{-1} A u_i = \eta_i u_i$, $i = 1, \ldots, n$, we can prove by induction that the u_i's are eigenvectors of E_k and X_k for all $k \geqslant 0$. Let $E_{k_0} u_i = b_i u_i$, $i = p, \ldots, n$. Then, applying Lemma 4, we obtain

$$\begin{aligned} r &\leqslant (1+\epsilon) \limsup_{k\to\infty} \sqrt[k]{\sum_{i=p}^n |b_i \|\eta_i|^{2(k-k_0)} \|u_i\|_2} \\ &\leqslant (1+\epsilon) \limsup_{k\to\infty} \sqrt[k]{|\eta_p|^{2(k-k_0)} \sum_{i=p}^n |b_i|} \\ &= (1+\epsilon)|\eta_p|^2. \end{aligned}$$

Since ϵ is arbitrary, we have $r \leqslant |\eta_p|^2$.

On the other hand, we have by (21)

$$E_k \geqslant (X_L^{-1}A)^* E_{k-1}(X_L^{-1}A) \geqslant ((X_L^{-1}A)^*)^k E_0 (X_L^{-1}A)^k.$$

Therefore,

$$\begin{aligned} r &= \limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \\ &\geqslant \limsup_{k\to\infty} \sqrt[k]{\|((X_L^{-1}A)^*)^k E_0 (X_L^{-1}A)^k\|} \\ &\geqslant \limsup_{k\to\infty} \sqrt[k]{\|((X_L^{-1}A)^*)^k E_0 (X_L^{-1}A)^k u_p\|_2} \\ &= \limsup_{k\to\infty} \sqrt[k]{|\eta_p|^{2k}|c_p|\|u_p\|_2} \\ &= |\eta_p|^2, \end{aligned}$$

where we have used $E_0 u_p = c_p u_p$ for $c_p = \frac{1}{2} - \beta + \frac{1}{2}\sqrt{1-4|\lambda_p|^2} > 0$. Thus $r = |\eta_p|^2$. □

For all three cases in Theorem 1, where A is not necessarily a normal matrix, we can show as in [10] that the iterates produced by Algorithm 3 satisfy (5). Theorem 5 says that when A is normal the rate of convergence of Algorithm 3 with $\gamma = \beta$ is not determined by the square of $\rho(X_L^{-1}A)$, but by the square of the next largest modulus for the eigenvalues of $X_L^{-1}A$. This is the underlying reason for the faster convergence. The improvement of convergence will be dramatic (from sublinear to linear) if $\rho(X_L^{-1}A) = 1$.

3.2. The minus equation

For the minus equation (4) with a normal matrix A, we know from (14) that the unique positive definite solution X_L is given by

$$X_L = \frac{1}{2} U \left[I + (I + 4|\Lambda|^2)^{\frac{1}{2}} \right] U^*. \tag{23}$$

So

$$X_L^{-1}A = U \operatorname{diag}(\mu_1, \ldots, \mu_n) U^*, \tag{24}$$

where

$$\mu_i = \frac{2\lambda_i}{1 + \sqrt{1 + 4|\lambda_i|^2}}, \quad i = 1, \ldots, n. \tag{25}$$

Note that

$$|\mu_1| = \cdots = |\mu_{p-1}| > |\mu_p| \geqslant \cdots \geqslant |\mu_n|. \tag{26}$$

Let

$$\widetilde{E}_k = X_L - X_k, \quad k = 0, 1, \ldots \tag{27}$$

As in [10], for each $k \geqslant 1$ we have

$$\widetilde{E}_k = -(X_L^{-1}A)^* \widetilde{E}_{k-1}(X_L^{-1}A) - (X_L^{-1}A)^* \widetilde{E}_{k-1} X_{k-1}^{-1} \widetilde{E}_{k-1}(X_L^{-1}A). \tag{28}$$

Lemma 6. *Let A in (4) be a normal matrix, and $u_1, \ldots, u_n$ be the orthonormal eigenvectors of A corresponding to its eigenvalues $\lambda_1, \ldots, \lambda_n$ arranged as in (15). Then for Algorithm 4 with $\gamma = \beta$, where β is given in (10), we have*

$$\widetilde{E}_k u_i = 0, \quad i = 1, \ldots, p-1, \ k = 0, 1, \ldots$$

Proof. For $i = 1, \ldots, p-1$, a direct computation shows $\widetilde{E}_0 u_i = 0$. Since $X_L^{-1} A u_i = \mu_i u_i$, it follows from (28) that $\widetilde{E}_k u_i = 0$ for all $k \geqslant 0$. □

The following monotonicity properties will also be needed.

Lemma 7. *Let A in (4) be a normal matrix and $\{X_k\}$ be the sequence from Algorithm 4 with $\gamma = \beta$. Then $\{X_{2k}\}$ is a decreasing sequence, and $\{X_{2k+1}\}$ is an increasing sequence.*

Proof. We only need to show $X_0 \geqslant X_2$. Let A be factored as in (14). From $X_0 = \beta I$, we get after two iterations that

$$X_2 = U \operatorname{diag}\left(\frac{\beta + \sigma_1^2 + \beta\sigma_1^2}{\beta + \sigma_1^2}, \ldots, \frac{\beta + \sigma_n^2 + \beta\sigma_n^2}{\beta + \sigma_n^2} \right) U^*.$$

Since $\sigma_1^2 \geqslant \cdots \geqslant \sigma_n^2$ and $\sigma_1^2 = \beta(\beta - 1)$, we have

$$\begin{aligned} X_2 &\leqslant U \operatorname{diag}\left(\frac{\beta + \sigma_1^2 + \beta\sigma_1^2}{\beta + \sigma_1^2}, \ldots, \frac{\beta + \sigma_1^2 + \beta\sigma_n^2}{\beta + \sigma_n^2} \right) U^* \\ &= \beta U \operatorname{diag}\left(\frac{1 + \beta - 1 + \sigma_1^2}{\beta + \sigma_1^2}, \ldots, \frac{1 + \beta - 1 + \sigma_n^2}{\beta + \sigma_n^2} \right) U^* = \beta I = X_0. \end{aligned}$$

This completes the proof. □

We note that $X_0 \geqslant X_2$ is not always true when $X_0 = \beta I$ and A is not a normal matrix.
We now prove our main result for the minus equation.

Theorem 8. *Let A in (4) be a normal matrix, and $\mu_1, \ldots, \mu_n$ be the eigenvalues of $X_L^{-1} A$, arranged as in (26). Then the rate of convergence of Algorithm 4 with $\gamma = \beta$ is*

$$r = \limsup_{k \to \infty} \sqrt[k]{\|\widetilde{E}_k\|} = |\mu_p|^2.$$

Proof. By Lemma 7 we have

$$\widetilde{E}_{2k+1} = X_L - X_{2k+1} \geqslant 0, \quad \widetilde{E}_{2k} = X_L - X_{2k} \leqslant 0.$$

As in [10], for any $\epsilon \in (0, 1)$ there exists a k_0, such that for all $k \geqslant k_0$

$$\widetilde{E}_k X_k^{-1} \widetilde{E}_k \leqslant \epsilon (-1)^{k+1} \widetilde{E}_k. \tag{29}$$

Combining (28) and (29) we have for $k > k_0$

$$\begin{aligned} 0 &\leqslant (-1)^{k+1} \widetilde{E}_k \\ &= (X_L^{-1} A)^* (-1)^k \widetilde{E}_{k-1} (X_L^{-1} A) + (-1)^k (X_L^{-1} A)^* \widetilde{E}_{k-1} X_{k-1}^{-1} \widetilde{E}_{k-1} (X_L^{-1} A) \end{aligned}$$

$$\leqslant (1+\epsilon)(X_L^{-1}A)^*(-1)^k\widetilde{E}_{k-1}(X_L^{-1}A)$$
$$\leqslant (1+\epsilon)^{k-k_0}((X_L^{-1}A)^*)^{k-k_0}(-1)^{k_0+1}\widetilde{E}_{k_0}(X_L^{-1}A)^{k-k_0}.$$

Therefore,

$$\begin{aligned} r &= \limsup_{k\to\infty}\sqrt[k]{\|\widetilde{E}_k\|} \\ &\leqslant \limsup_{k\to\infty}\sqrt[k]{\|(1+\epsilon)^{k-k_0}((X_L^{-1}A)^*)^{k-k_0}\widetilde{E}_{k_0}(X_L^{-1}A)^{k-k_0}\|} \\ &= (1+\epsilon)\limsup_{k\to\infty}\sqrt[k]{\|((X_L^{-1}A)^*)^{k-k_0}\widetilde{E}_{k_0}(X_L^{-1}A)^{k-k_0}v^{(k)}\|_2}, \end{aligned}$$

where $\|v^{(k)}\|_2 = 1$. Write $v^{(k)} = \sum_{i=1}^n a_i^{(k)}u_i$ with $\sum_{i=1}^n |a_i^{(k)}|^2 = 1$. Then

$$r \leqslant (1+\epsilon)\limsup_{k\to\infty}\sqrt[k]{\sum_{i=1}^n \|((X_L^{-1}A)^*)^{k-k_0}\widetilde{E}_{k_0}(X_L^{-1}A)^{k-k_0}u_i\|_2}.$$

As for the plus equation, we can prove by induction that the u_i's are eigenvectors of $\widetilde{E}_k$ and X_k for all $k \geqslant 0$. Applying Lemma 6 and setting $\widetilde{E}_{k_0}u_i = d_iu_i$, $i = p, \ldots, n$, we obtain

$$r \leqslant (1+\epsilon)\limsup_{k\to\infty}\sqrt[k]{\sum_{i=p}^n |d_i\|\mu_i|^{2(k-k_0)}\|u_i\|_2} \leqslant (1+\epsilon)|\mu_p|^2.$$

Since ϵ is arbitrary, we have $r \leqslant |\mu_p|^2$.

On the other hand, by (28) and (29) we have for $k > k_0$

$$\begin{aligned} (-1)^{k+1}\widetilde{E}_k &\geqslant (1-\epsilon)(X_L^{-1}A)^*(-1)^k\widetilde{E}_{k-1}(X_L^{-1}A) \\ &\geqslant (1-\epsilon)^{k-k_0}((X_L^{-1}A)^*)^{k-k_0}(-1)^{k_0+1}\widetilde{E}_{k_0}(X_L^{-1}A)^{k-k_0} \\ &\geqslant 0. \end{aligned}$$

Therefore,

$$\begin{aligned} r &= \limsup_{k\to\infty}\sqrt[k]{\|\widetilde{E}_k\|} \\ &\geqslant \limsup_{k\to\infty}\sqrt[k]{(1-\epsilon)^{k-k_0}\|((X_L^{-1}A)^*)^{k-k_0}\widetilde{E}_0(X_L^{-1}A)^{k-k_0}\|} \\ &\geqslant (1-\epsilon)\limsup_{k\to\infty}\sqrt[k]{\|((X_L^{-1}A)^*)^{k-k_0}\widetilde{E}_0(X_L^{-1}A)^{k-k_0}u_p\|_2} \\ &\geqslant (1-\epsilon)\limsup_{k\to\infty}\sqrt[k]{|\mu_p|^{2(k-k_0)}|c_p|\|u_p\|_2} \\ &= (1-\epsilon)|\mu_p|^2, \end{aligned}$$

where we have used $\widetilde{E}_0u_p = c_pu_p$ for $c_p = \frac{1}{2} - \beta + \frac{1}{2}\sqrt{1+4|\lambda_p|^2} < 0$. Since ϵ is arbitrary, we obtain $r \geqslant |\mu_p|^2$. Thus $r = |\mu_p|^2$. □

We have shown in Theorem 8 that when A is normal the rate of convergence of Algorithm 4 with $\gamma = \beta$ is not determined by the square of $\rho(X_L^{-1}A)$, but is determined by the square of the next largest modulus for the eigenvalues of $X_L^{-1}A$. This is the underlying reason for the faster convergence. However, we cannot expect the improvement of convergence to be as dramatic as for the plus equation, because for the minus equation we always have $\rho(X_L^{-1}A) < 1$.

4. Convergence improvement of the fixed-point iteration for the matrix equation $X + BX^{-1}A = C$

We now consider the more general equation

$$X + BX^{-1}A = C, \tag{30}$$

where A, B, C are $n \times n$ matrices. Suppose that the equation has a solution X_L and that for a proper X_0 the sequence generated by

$$X_k = C - BX_{k-1}^{-1}A, \quad k = 1, 2, \ldots$$

converges to X_L. Let $E_k = X_L - X_k$. Then we have

$$E_k = (BX_{k-1}^{-1})E_{k-1}(X_L^{-1}A) = (BX_{k-1}^{-1})\cdots(BX_0^{-1})E_0(X_L^{-1}A)^k. \tag{31}$$

From this we know that

$$\limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \leqslant \rho(BX_L^{-1})\rho(X_L^{-1}A).$$

So the convergence of the fixed-point iteration is linear if $\rho(BX_L^{-1})\rho(X_L^{-1}A) < 1$. If $\rho(BX_L^{-1}) \cdot \rho(X_L^{-1}A)$ is equal or very close to 1, the convergence may be very slow. However, it is possible to speed up the convergence by choosing X_0 properly. Let $X_L^{-1}A$ have eigenvalues $\eta_1, \ldots, \eta_n$, and corresponding linearly independent (generalized) eigenvectors $u_1, \ldots, u_n$ (as they appear in the Jordan canonical form). Suppose that

$$|\eta_1| = \cdots = |\eta_{p-1}| > |\eta_p| \geqslant \cdots \geqslant |\eta_n|$$

and that X_0 satisfies $X_0u_i = X_Lu_i$, $i = 1, \ldots, p-1$. Then $E_0u_i = 0$ for $i = 1, \ldots, p-1$. It follows from (31) that

$$\limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \leqslant \rho(BX_L^{-1}) \limsup_{k\to\infty} \sqrt[k]{\|E_0(X_L^{-1}A)^k v_k\|},$$

where $\|v_k\| = 1$. Writing $v_k = \sum_{i=1}^n a_i^{(k)}u_i$, we get

$$\limsup_{k\to\infty} \sqrt[k]{\|E_0(X_L^{-1}A)^k v_k\|} = \limsup_{k\to\infty} \sqrt[k]{\|E_0(X_L^{-1}A)^k \sum_{i=p}^n a_i^{(k)}u_i\|} \leqslant |\eta_p|.$$

So

$$\limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \leqslant \rho(BX_L^{-1})|\eta_p| \tag{32}$$

and the convergence is improved.

In general it is difficult to find X_0 (other than X_L itself) such that $X_0u_i = X_Lu_i$ ($i = 1, \ldots, p-1$). However, an important equation from the study of recurrent quasi-birth-death processes [15] has the form (30), with A, B, $I - C$ elementwise nonnegative, and $A + B + I - C$ stochastic.

Moreover, for the desired solution X_L the matrix $X_L^{-1}A$ is such that $1 = \eta_1 > |\eta_2| \geqslant \cdots \geqslant |\eta_n|$ and $u_1 = e$, the vector of ones. So $X_L e = Ae$. Thus $X_0 u_1 = X_L u_1$ is satisfied by any X_0 with $X_0 e = Ae$. (To apply the fixed-point iteration we need to ensure that X_0 is invertible.) For the plus/minus equations with a normal matrix A, we have shown in Section 3 that $X_0 u_i = X_L u_i$ $(i = 1, \ldots, p-1)$ for $X_0 = \beta I$, without computing X_L and u_i. In this case, (32) becomes $\limsup_{k\to\infty} \sqrt[k]{\|E_k\|} \leqslant |\eta_1 \eta_p|$. Note that we have proved in Section 3, by a refined analysis, that $\limsup_{k\to\infty} \sqrt[k]{\|E_k\|} = |\eta_p|^2$. If A is a general non-normal matrix, however, the choice $X_0 = \gamma I$ is unlikely to improve the convergence of the fixed-point iteration significantly, since $X_0 u_i = X_L u_i$ would mean that u_i $(i = 1, \ldots, p-1)$ are linearly independent eigenvectors of X_L corresponding to the same eigenvalue γ.

5. Numerical experiments

In this section we compare the algorithms $Alg_+(\gamma)$ and Alg_+M, where $Alg_+(\gamma)$ is Algorithm 3 (with $X_0 = \gamma I$) and Alg_+M is Meini's algorithm [16] for the plus equation (3). We also compare the algorithms $Alg_-(\gamma)$ and Alg_-M, where $Alg_-(\gamma)$ is Algorithm 4 (with $X_0 = \gamma I$) and Alg_-M is Meini's algorithm [16] for the minus equation (4). The purpose here is to show the usefulness as well as the limitation of $Alg_\pm(\beta)$.

Our numerical experiments are performed in MATLAB 7.3 on a Sun workstation. In all examples, each algorithm is stopped as soon as an approximation $\widetilde{X}$ to X_L satisfies

$$\|\widetilde{X} \pm A^*\widetilde{X}^{-1}A - I\|_\infty \leqslant 10^{-10}$$

for the plus/minus equations. We note that $Alg_\pm(\gamma)$ requires about $\frac{7}{3}n^3$ flops each iteration and all singular values of A can be found in $\frac{8}{3}n^3$ flops [7] (we just need the largest and the smallest singular value to determine β and α, respectively). $Alg_\pm M$ requires $\frac{19}{3}n^3$ flops each iteration.

The first four examples are for the plus equation.

Example 1. We consider a normal matrix $A \in \mathbb{R}^{n\times n}$, given in [16] as follows:

(1) Choose $\xi \in [0, \frac{1}{2})$.
(2) For $i = 1, \ldots, n$:
  (a) for $j = i, \ldots, n$, set $a_{i,j} = i^2 + j$;
  (b) compute $s_1 = \sum_{j=1}^{i-1} a_{i,j}$, $s_2 = \sum_{j=i}^{n} a_{i,j}$;
  (c) for $j = i, \ldots, n$, set

$$a_{i,j} = a_{i,j}\frac{0.5 - \xi - s_1}{s_2}, \quad a_{j,i} = a_{i,j}.$$

For this example, we have $\|A\| = \frac{1}{2} - \xi$. If $\xi = 0$ then $\|A\| = \frac{1}{2}$, $\rho(X_L^{-1}A) = 1$, and the convergence of $Alg_+(1)$ is expected to be sublinear. We take $n = 100$ and report in Table 1 the number of iterations required for each algorithm and for different values of ξ. In the table, "$*$" means that the stopping criterion is not satisfied in 50,000 iterations. For this example, $Alg_+(\beta)$ has the best performance. The iterates provided by $Alg_+(\alpha)$ are slightly better than the corresponding iterates from $Alg_+(1)$ (in agreement with Theorem 1(i)), but the number of iterations required remains the same.

Table 1
Number of iterations for Example 1

ξ	$Alg_+(\beta)$	$Alg_+(1)$	$Alg_+(\alpha)$	Alg_+M
0.4	3	5	5	3
0.1	5	16	16	5
0.01	5	50	50	6
0.001	6	143	143	8
0.0001	6	396	396	9
0	6	$*$	$*$	17

Example 2. We consider a nearly normal matrix $A = QRQ^{\mathrm{T}}$, where Q is a random orthogonal matrix and

$$R = \begin{pmatrix} 0.499 & 0.00003 & 0.00001 \\ 0 & 0.2 & 0.00002 \\ 0 & 0 & 0.1 \end{pmatrix}.$$

We have $\|A\| = 0.4990$, $\alpha = 0.9899$, $\beta = 0.5316$. $Alg_+(1)$ and $Alg_+(\alpha)$ need 144 iterations each, while $Alg_+(\beta)$ requires only 18 iterations. Alg_+M needs 8 iterations. $Alg_+(\beta)$ still has the best performance, since the computational work for 8 iterations of Alg_+M is roughly that for 22 iterations of $Alg_+(\beta)$.

Example 3 [13, Example 1]. For the non-normal matrix

$$A = \begin{pmatrix} 0.471 & 0.002 & 0.040 \\ 0.002 & 0.472 & -0.002 \\ -0.040 & -0.001 & 0.471 \end{pmatrix},$$

we have $\|A\| = 0.4749$, $\alpha = 0.6710$, $\beta = 0.6566$. $Alg_+(1)$ requires 32 iterations; $Alg_+(\alpha)$ requires 28 iterations; $Alg_+(\beta)$ requires 27 iterations. We have also tried $Alg_+(\gamma)$ with many different $\gamma \in (\beta, \alpha)$, the number of iteations required is either 27 or 28. Alg_+M needs six iterations. So Alg_+M has the best performance.

Example 4. For the non-normal matrix

$$A = \begin{pmatrix} 0.1304 & 0.1639 & -0.0437 \\ 0.0182 & 0.4045 & 0.0313 \\ 0.1661 & 0.1425 & 0.0285 \end{pmatrix},$$

we have $\|A\| = 0.4757$, $\alpha = 0.9970$, $\beta = 0.6539$. For this example 23 iterations are needed for $Alg_+(1)$, $Alg_+(\alpha)$ and $Alg_+(\beta)$. We also note that $Alg_+(\gamma)$ with $\gamma = 0.72755$ only needs nine iterations (but this good value of γ is obtained by trial and error). Alg_+M needs five iterations and thus has the best performance for this example.

We now give a few examples for the minus equation.

Example 5. For the normal matrix

$$A = \begin{pmatrix} -1.8519 & 0.0131 & 0.0370 & 1.4361 \\ 0.0131 & 0.1001 & -0.0797 & 0.1191 \\ 0.0370 & -0.0797 & 0.2006 & -0.0343 \\ 1.4361 & 0.1191 & -0.0343 & -1.2283 \end{pmatrix},$$

we have $\alpha = 1.0093$, $\beta = 3.5530$, $\rho(X_L^{-1}A) = 0.8477$. $Alg\_(1)$ and $Alg\_(\alpha)$ require 77 iterations each; $Alg\_(\beta)$ needs 9 iterations; Alg_M takes 7 iterations. The iterates provided by $Alg\_(\alpha)$ are slightly better than the corresponding iterates from $Alg\_(1)$ (in agreement with Proposition 2), but the number of iterations required remains the same. $Alg\_(\beta)$ has the best performance for this example.

Example 6. We consider a nearly normal matrix $A = QRQ^{\mathrm{T}}$, where Q is a random orthogonal matrix and

$$R = \begin{pmatrix} 0.1 & 0.0002 & 0.00003 & 0.00002 \\ 0 & 0.2 & 0.00001 & 0.00003 \\ 0 & 0 & 3.99 & 0.00001 \\ 0 & 0 & 0 & 0.499 \end{pmatrix}.$$

We have $\alpha = 1.0099, \beta = 4.5212, \rho(X_L^{-1}A) = 0.8825$. $Alg\_(1)$ and $Alg\_(\alpha)$ need 102 iterations each, while $Alg\_(\beta)$ requires only 14 iterations. Alg_M needs 7 iterations. So $Alg\_(\beta)$ still has the best performance.

Example 7. For the non-normal matrix

$$A = \begin{pmatrix} 2.9130 & 11.1804 & 4.0826 & 1.5700 \\ -0.0300 & -3.1354 & -14.1875 & 7.2807 \\ -1.6573 & 0.6205 & 5.9407 & -1.6480 \\ 7.6587 & -4.8459 & 1.3134 & -0.7988 \end{pmatrix},$$

we have $\alpha = 2.0360$, $\beta = 18.9393$, $\rho(X_L^{-1}A) = 0.9317$. For this example $Alg\_(1)$ requires 191 iterations; $Alg\_(\alpha)$ requires 189 iterations; $Alg\_(\beta)$ requires 184 iterations. But Alg_M needs only 8 iterations and thus has the best performance.

6. Conclusions

To compute the maximal solution X_L of the matrix equation (3) with $\|A\| \leqslant \frac{1}{2}$, we can speed up the convergence of the fixed-point iteration by using a good initial matrix. The recommended initial matrix is $X_0 = \beta I$, where β is determined by the largest singular value of A. Significant (and sometimes dramatic) improvement is achieved by this special initial matrix if A is normal or nearly normal. If A is a general non-normal matrix, the improvement is usually not significant. But if $\rho(X_L^{-1}A)$ is small the convergence of the fixed-point iteration is fast for $X_0 = \gamma I$ and any $\gamma \in \left[\frac{1}{2}, 1\right]$ since (5) is always true. It is still advisable to use $\gamma = \beta$ in this case, since it is very likely that the number of iterations can be reduced by at least one, offsetting the computational work required for determining β. If A is a general non-normal matrix and $X_L^{-1}A$ has eigenvalues on or near the unit circle, then Meini's algorithm [16] is the best choice we have available.

To compute the unique positive definite solution X_L of the matrix equation (4), we can also use $X_0 = \beta I$ to speed up the convergence of the fixed-point iteration, where β is again determined by the largest singular value of A. Significant improvement is achieved by this special initial matrix if A is normal or nearly normal. If A is a general non-normal matrix, the improvement is usually not significant. But if $\rho(X_L^{-1}A)$ is small the convergence of the fixed-point iteration is fast for any $X_0 > 0$. If A is a general non-normal matrix and $X_L^{-1}A$ has eigenvalues near the unit circle, then Meini's algorithm [16] is the best choice.

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