A Stable Iteration to the Matrix Inversion

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Abstract. The matrix inversion plays a significant role in engineering and sciences. Any nonsingular square matrix has a unique inverse which can readily be evaluated via numerical techniques such as direct methods, decomposition scheme, iterative methods, etc. In this research article, first of all an algorithm which has fourth order rate of convergency with conditional stability will be proposed. Then, for solving stability issue, we introduce a coupled stable scheme that can evaluate the matrix inversion with very acceptable accuracy. Furthermore, the convergence and stability properties of the proposed schemes will be analyzed in details. Numerical experiments are adopted to illustrate the properties of the modified methods.

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Index to information contained in this paper

1 Introduction
2 A novel iterative method
3 The alternative coupled stable iterative methods
4 Numerical examples
5 Conclusions

1. Introduction

Given $A \in \mathbb{C}^{n \times n}$ is a nonsingular matrix. Let it is possible to make a branch cut in the complex plane from 0 to $\infty$ which does not intersect the set of eigenvalues of $A$ (or $\sigma(A)$), and $\Gamma$ be a contour in the cut plane winding once around each

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eigenvalue of $A$. Then the inverse of $A$ is defined as [3]

$$A^{-1} = \frac{1}{2\pi i} \oint_{\Gamma} z^{-1}(zI - A)^{-1} dz.$$  

(1)

Notice that the integral vanishes when $\Gamma$ is a counter-clockwise oriented circle centered at the origin of large enough radius. However, the matrix inversion can not be considered as a matrix function (See Chap. 1 in [4]). Moreover, the inversion of $A$ is given by the matrix which is satisfied in $AA^{-1} = I_n$ or $A^{-1}A = I_n$. The matrix inversion is a unique matrix.

The computation of matrix inversion has key role in practical applications like obtaining a rational approximation to the Fermi-Dirac functions which is appear in the density functional theory [11]. Another application of the matrix inversion includes in some particular circumstances, for instance, serval techniques to encrypt a message whenever the use of coding has become especially significant more recently [12].

It is well known that there are several approaches to the computation of matrix inversion which can be categorized as three considerable groups. First, direct methods that include Gaussian elimination with partial pivoting or Gauss-Jordan elimination. It should be mentioned that direct methods cannot correctly tackle sparse matrices possessing sparse inverses turn out in the numerical solution of integral equations. In order to solve this issue, some numerical procedures such as Conjugate Gradient for symmetric positive definite matrices and GMRES are effective for large sparse linear systems. However, when the coefficient matrix is ill-conditioned, solving a linear system of equations based on inversion is problematic. To antitode this, one can utilize an appropriate preconditioner to the system. Second part of the category is decomposition methods such as LU decomposition or QR factorization which require an affordable CPU time for computing the inverse when the dimension of the matrices is large. The last but not least, iterative approaches are drown mostly based on root finding methods. The other types of schemes, which can be considered as iterative methods. In such iterative methods, at each iteration an approximate inverse of a matrix can readily be yielded. Subsequently, the users have the ability to solve, for example, the linear systems iteratively or use the approximate inverses in Sensitivity analysis and the preconditioning of a linear system.

During past decade, several authors have been investigated the iterative methods for approximating the matrix inversion based on root finding methods. A fundamental iterative method introduced by Li [8] which can be used to compute an approximate inner inverse (see Def. 1.2) of a matrix for a given initial approximation:

$$X_{k+1} = X_k \left( \ell I - \frac{\ell(\ell - 1)}{2} AX_k + \cdots + (-1)^{\ell-1}(AX_k)^{\ell-1} \right), \quad \ell = 1, 2, \ldots$$  

(2)

Whenever $\ell = 2$, then it is straightforward (2) is the well-known Newton’s iteration
as
\[ X_{k+1} = X_k (2I - AX_k), \quad k = 0, 1, 2, \ldots \] (3)
and for the case \( \ell = 3 \), the particular case of (2) is the following important case:
\[ X_{k+1} = X_k (3I - 3AX_k + 3(AX_k)^2), \quad k = 0, 1, 2, \ldots \] (4)
Moreover, Krishnamurthy and Sen [6] provided the iterative method given by
\[ X_{k+1} = X_k (I + (I + Y_k (I + Y_k (I + Y_k))))), \quad k = 0, 1, 2, \ldots \] (5)
where, \( Y_k = I - AX_k \). Several years later, this iteration is modified for larger rate of convergency which applying Schröder’s general method and often called Schröder-Traub’s sequence as (one can refer to [10, 15])
\[ X_{k+1} = X_k (I + Y_k + Y_k^2 + \cdots + Y_k^{n-1}), \quad k = 0, 1, 2, \ldots \] (6)
or
\[ X_{k+1} = X_k (I + (I + Y_k (I + Y_k (\ldots + Y_k \ldots))), \quad k = 0, 1, 2, \ldots \] (7)
whereas it is requiring \( n \) Horner’s matrix multiplications.

An important trouble in computing matrix inversion by utilizing iterative methods is that the most algorithms suffer stability issue. In the present work, we will introduce some iterative approaches for computing inverse of a square matrix \( A \) via concentrating on a particular scalar root finding method given in [1]. It is proven that by considering an appropriate initial matrix, the matrix iteration is convergent with the rate of convergency four. Furthermore, the stability of the proposed iteration is studied in details by proving some theorems. For solving instability of the algorithm, utilizing auxiliary variable, a new coupled iterative method is introduced which is stable. It was established that the numerical results will be very feasible for matrices with eigenvalues less that one. This strategy is applied for computing matrix square root and matrix \( p \)th roots in [5, 9]. For this purpose, normalization of the matrices has been used for getting better accuracy. Numerical implementations have been carried out to reveal the properties of the modified theory.

The organization of the paper is as follows: Section 2 reveal the basic concept of deriving iteration and its convergency. We will study the stable iteration by combining the normalization of the matrices in Sec. 3. In Section 4, we draw some numerical experiments to examine the proposed recursions. Concluding remarks will be given in Section 5. Throughout this paper, the following notation will be appeared. If \( W \in \mathbb{C}^{n \times n} \) with eigenvalues \( \lambda_1, \ldots, \lambda_n \), then the spectrum of \( W \) is defined by \( \sigma(W) = \{\lambda_1, \ldots, \lambda_n\} \) and spectral radius if \( W \) is defined by \( \rho(W) = \max_i |\lambda_i| \).
2. A novel iterative method

In this section, we provide some conditions to introduce new iterative method to approximate the matrix inversion. First of all, we apply the following iterative scheme introduced in [1]:

$$x_{\ell+1} = x_{\ell} - \mathcal{L}_f(x_{\ell}) \frac{\varphi(x_{\ell})}{\varphi'(x_{\ell})}, \quad \ell = 1, 2, \ldots \tag{8}$$

wherein

$$\mathcal{L}_f(x_{\ell}) = 1 + \frac{\varphi''(x_{\ell}) \varphi(x_{\ell})}{2 \varphi'(x_{\ell})} + \frac{\varphi'''(x_{\ell}) \varphi^2(x_{\ell})}{6 \varphi'(x_{\ell})}, \tag{9}$$

to the function $\varphi(x) = a - \frac{1}{x}$. Therefore, an iteration for finding the inversion of scalar $a$ will be attained as:

$$x_{k+1} = 4x_k - 6ax_k^2 + 4a^2x_k^3 - a^3x_k^3, \quad k = 1, 2, \ldots \tag{10}$$

This iterative scheme is fundamental recursion for proposing a new convergent iteration to the matrix inversion, which is the main contribution of this article. Now, considering the matrix version in Banach space, the recursive procedure would be yielded:

$$X_{k+1} = X_k \left(4I - 6AX_k + 4A^2X_k^2 - A^3X_k^3\right), \quad k = 1, 2, \ldots \tag{11}$$

It is clear that the above relation is a particular case of (2). We will illustrate that this recursion is not convergent in general and stability is also conditional, and therefore we solve these issues. Next lemma will be characterized that the sequences $X_k$ commutes with the matrix $A$.

**Lemma 2.1** Let $A \in \mathbb{C}^{n \times n}$ is a nonsingular matrix. If $AX_0 = X_0A$ is valid, then for the sequence $\{X_k\}_{k=0}^{\infty}$ in (14), one has that

$$AX_k = X_kA, \tag{12}$$

holds for all $k = 1, 2, \ldots$.

**Proof** By using a similar strategy mentioned in [5], Lemma can easily be proven. ■

Notice that the suggested recursive procedure in (11) has forth order convergence rate to compute matrix inversion. This point will be proven in the following theorem.

**Theorem 2.2** Assume $A \in \mathbb{C}^{n \times n}$, is nonsingular square matrix. If the initial guess $X_0$ satisfies $\|E_0\| = \|I - AX_0\| < 1$, therefore the iterative procedure (11) converges to $A^{-1}$ with the order of four.
**Proof** Let $E_k = I - AX_k$. Then, we can obtain that

\[ E_{k+1} = I - AX_{k+1} \]

\[ = I - A(4X_k - 6AX_k^2 + 4A^2X_k^3 - A^3X_k^4) \]

\[ = I - 4(AX_k) + 6(AX_k)^2 - 4(AX_k)^3 + (AX_k)^4 \]

\[ = (I - AX_k)^4 \]

\[ = (E_k)^4. \]

Subsequently, since $\|E_0\| < 1$, for any subordinate matrix norm, we attain

\[ \|E_{k+1}\| \leq \|E_k\|^4 \leq \ldots \leq \|E_0\|^{4k} \to 0 \]

whenever $k \to \infty$. In other words, $I - AX_k \to 0$ or $X_k \to A^{-1}$ as $k \to \infty$. Now, we get

\[ A^{-1} + e_{k+1} = X_{k+1} \]

\[ = 4X_k - 6AX_k^2 + 4A^2X_k^3 - A^3X_k^4 \]

\[ = (A^{-1} + e_k)(4I - 6A(A^{-1} + e_k) + 4A^2(A^{-1} + e_k)^2 - A^3(A^{-1} + e_k)^3) \]

\[ = (A^{-1} + e_k)(I - Ae_k + A^2e_k^2 + A^3e_k^3) \]

\[ = A^{-1} + e_k + Ae_k^2 - A^2e_k^3 + e_k - Ae_k^2 + A^2e_k^3 - A^3e_k^4 \]

\[ = A^{-1} - e_k(Ae_k)^3. \]

By removing $A^{-1}$ from both sides of the equality, we have

\[ e_{k+1} = -e_k(Ae_k)^3. \]

After taking any subordinate norm once again, it would be yielded that

\[ \|e_{k+1}\| \leq \|A\|^3\|e_k\|^4 \]

Consequently, it is indicated that the sequence $\{X_k\}$ has at least fourth order rate of convergence.

Theorem 2.1 illustrated that the order of convergence of the matrix sequence $\{X_k\}_{k=1}^\infty$ given by (11) is equal to 4, provided that $A$ is a nonsingular matrix. In Fig. 1, we depict the behavior of the scalar iteration for computing inverse of $a = 1$ and $a = 2$. Fractal behavior and divergency of scalar version of iteration can be
observed in plotted figures. In continue, we will see that the iteration is conditional stable.

![Figure 1. The behavior of iteration (14) for $a = 1$ and $a = 2$.](image)

It is remarkable that the initial guess is important in convergency of the iteration. In our computation we use the following initial matrices as indicated in several references like [12–14, 16]:

$$X_0 = \frac{A^*}{\|A\|1\|A\|\infty}, \quad (13)$$

and

$$X_0 = \frac{A^*}{tr(AA^*)}, \quad (14)$$

where $W^*$ is conjugate transpose of the matrix $W$.

**Remark 2.3** If $\rho(A) > 1$, then $B = A/\|A\|$ can be substituted. In this case, it is clear that $\rho(B) \leq 1$.

Subsequently, we can obtain the matrix sequence $\{R_k\}_{k=1}^{\infty}$ as following.

**Algorithm (I).** Let $A \in \mathbb{C}^{n \times n}$ and $B = A/\|A\|$. The iterative method for computing inverse of $A$ with $\rho(A) > 1$ can be stated as:

$$R_0 = I,$$

$$R_{k+1} = R_k \left(4I - 6(AR_k) + 4(AR_k)^2 - (AR_k)^3\right),$$

$$X_k = \|A\|R_k.$$  

In Algorithm (I), it is clear that $\lim_{k \to \infty} R_k = B^{-1}$, and $\lim_{k \to \infty} X_k = A^{-1}$. We then have

$$\|X_{k+1} - A^{-1}\| = \|A\|\|R_{k+1} - B^{-1}\| = \mathcal{O}(\|X_k - A^{-1}\|^4), \quad (15)$$

where $\mathcal{O}$ denotes big $O$. Notice that the matrix $B$ could also be proposed by $B = A/\rho(A)$ if $\rho(A)$ is available. Since $\rho(A) \leq \|A\|$, it is more appropriate that the
upper bound $\|A\|$ will be considered. Now, we are interested to know that whether the iterations in Algorithm (I) are stable or not. First we give the following theorem.

**Theorem 2.4** The sequence $\{X_k\}_{k=1}^\infty$ introduced in Algorithm (I) is conditionally stable.

*Proof* The proof would be done based on strategy which applied in [5, 7]. It is hence omitted. ■

According to Theorem 2.1, it was seen that the proposed scheme has turn out to be stable whenever $A$ is ill-conditioned or the size of the input matrix $A$ is large. For solving this issue, two stable and convergent iterations will be proposed by employing matrix auxiliary variables in the next section.

### 3. The alternative coupled stable iterative methods

In this section, new stable variant of iterative method for computing the matrix inversion will be introduced. For this purpose, we first consider an auxiliary variable in the form $M_k = AX_k$. It can be easily shown that $\lim_{k \to \infty} X_k = I$ and $\lim_{k \to \infty} M_k = A$. Furthermore, each matrices $X_k$, $M_k$, and $A$ commutes with the others. Now, the new variant of the matrix iterations are obtained as following:

\[
X_{k+1} = X_k \left(4I - 6AX_k + 4(AX_k)^2 - (AX_k)^3\right)
= X_k \left(4I - AX_k(6I - AX_k(4I - AX_k))\right)
= X_k \left(4I - M_k(6I - M_k(4I - M_k))\right),
\]

and

\[
M_{k+1} = AX_{k+1}
= AX_k \left(4I - M_k(6I - M_k(4I - M_k))\right)
= M_k \left(4I - M_k(6I - M_k(4I - M_k))\right).
\]

Consequently, the following algorithm will be given.

**Algorithm (II).** Let $A \in \mathbb{C}^{n \times n}$. The coupled iterative method for computing the matrix inversion is defined by the recursive relation

\[
X_0 = I, \quad M_0 = A
X_{k+1} = X_k \left(4I - M_k(6I - M_k(4I - M_k))\right),
M_{k+1} = M_k \left(4I - M_k(6I - M_k(4I - M_k))\right).
\]
In Algorithm (II), it is straightforward that whenever \( \lim_{k \to \infty} X_k = A^{-1} \), then \( \lim_{k \to \infty} M_k = I_n \).

In this part, we present stability analysis of the coupled iteration for computing matrix inversion. According to [2], an iteration \( X_{k+1} = g(X_k) \) is stable in a neighborhood of a solution \( X = g(X) \), if the error matrices \( E_k = X_k - X \) satisfy

\[
E_{k+1} = L(E_k) + O(\|E_k\|^2),
\]

where \( L \) is a linear operator with bounded powers. In other words, there exist a constant \( \varepsilon > 0 \) such that for all \( k > 0 \) and an arbitrary unit norm, we have \( L^k(E) < \varepsilon \). This means small perturbation introduced in a certain step will not be amplified in the subsequent iterations. Thus, we give the following theorem.

**Theorem 3.1** The sequences \( \{X_k\}_{k=1}^\infty \) and \( \{M_k\}_{k=1}^\infty \) in Algorithm (II) are stable.

**Proof** Consider the iterations in Algorithm (II) and introduce the error matrices \( E_k = X_k - A^{-1} \) and \( F_k = M_k - I \). For the sake of simplicity, we perform a first order error analysis and we remove all the terms that are quadratic in the errors. Assume equality up to second order terms is denoted with the symbol \( \cong \). Thus, from \( M_k = I + F_k \), one has

\[
E_{k+1} = X_{k+1} - A^{-1} \\
= X_k(4I - (I + F_k)(6I - (I + F_k)(4I - (I + F_k)))) - A^{-1} \\
= X_k(4I - (3I + F_k)(3I + 2F_k)) - A^{-1} \\
\cong X_k(4I - (3I + F_k)) - A^{-1} \\
= X_k(I - F_k) - A^{-1} \\
= X_k + X_kF_k - A^{-1} \\
= E_k - X_kF_k.
\]
Furthermore, we yield
\[ F_{k+1} = M_{k+1} - I \]
\[ = M_k (4I - M_k (6I - M_k (4I - M_k))) - I \]
\[ \approx (I + F_k) (I - F_k) - I \]
\[ = I - F_k^2 - I \]
\[ = -F_k^2. \]

In conclusion, it can be written
\[
\begin{pmatrix}
E_{k+1} \\
F_{k+1}
\end{pmatrix}
= \begin{pmatrix}
I - X_k \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
E_k \\
F_k
\end{pmatrix}
= L \begin{pmatrix}
E_k \\
F_k
\end{pmatrix}. \tag{17}
\]

The coefficient matrix \( L \) is idempotent (\( L^2 = L \)) and hence has bounded powers. Thus the proposed iterations are stable. \( \blacksquare \)

Once again if \( \rho(A) > 1 \), therefore the substitution \( B = A/\| A \| \) can be applied. Hence, we propose the following.

**Algorithm (III).** Let \( A \in \mathbb{C}^{n \times n} \) and \( B = A/\| A \| \). The stable coupled iterative method for computing the inversion of \( A \) is expressed as follows:

\[ R_0 = I, \quad M_0 = A \]
\[ R_{k+1} = R_k (4I - M_k (6I - M_k (4I - M_k))) \]
\[ M_{k+1} = M_k (4I - M_k (6I - M_k (4I - M_k))) \]
\[ X_k = \| A \| \cdot R_k. \]

In Algorithm (III), it is apparent that \( \lim_{k \to \infty} R_k = B^{-1}, \lim_{k \to \infty} X_k = A^{-1} \). Thus, the matrix inversion can be computed efficiently.

4. **Numerical examples**

In this section, we support the theory which has been developed so far with several numerical implementations. All experiments have been carried out by using MATLAB (R2018b). In addition, the accuracy is measured by means of the size of:
\[
E_k(\hat{X}) = \frac{\| A \hat{X}_k - I \|_F}{\| A \|_F} < 10^{-16}, \tag{18}
\]
whenever \( \hat{X} \) is the computed inverse of \( A \) and \( \| \cdot \|_F \) is Frobenius norm.
Test 1. The first example is made considering \( n \times n \) lower bidiagonal matrices defined as

\[
A = \begin{pmatrix}
\frac{1}{x_1} & 1 & \cdots & \frac{1}{x_n} \\
\frac{1}{x_1} & \frac{1}{x_2} & \cdots & \frac{1}{x_n} \\
\vdots & \vdots & \ddots & \vdots \\
-\frac{1}{x_{n-1}} & x_n & \cdots & x_n
\end{pmatrix}_{n \times n},
\]

whereas, \( x = (x_1, \cdots, x_n)^t \in \mathbb{R}^n \) and \( x_n > 0 \) for \( i = 1, \cdots, n \). The inverse of the matrix which has pretty form will be obtain analytically by induction as follows:

\[
A^{-1} = \begin{pmatrix}
x_1 & x_2 & \cdots & x_n \\
x_2 & x_3 & \cdots & x_n \\
\vdots & \vdots & \ddots & \vdots \\
x_n & x_n & \cdots & x_n
\end{pmatrix}_{n \times n}.
\]

Now, considering the vectors \( x = (1, 2, \cdots, 5)^t \), \( x = (1, 2, \cdots, 10)^t \), and \( x = (1, 2, \cdots, 40)^t \) the inverse of \( A \) is computed via using the proposed iterations and it is compared by other approaches. The residual errors and number of iterations are measured and reported in Table 1. It should be noted that in spite of we have used double precision arithmetic precision, we present error by short form. According to the results, we can see that the Algorithm (III) has very accurate advantage with less number of iterations in comparison other methods.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
Method & \multicolumn{2}{c|}{n = 5} & \multicolumn{2}{c|}{n = 10} & \multicolumn{2}{c|}{n = 40} \\
\hline
Iter. & Err. & Iter. & Err. & Iter. & Err. \\
\hline
Iteration 1.4 & 7 & 4.4251e-16 & 11 & 8.2214e-16 & 14 & 8.8543e-16 \\
Iteration 1.5 & 5 & 1.2730e-16 & 7 & 4.5801e-16 & 9 & 7.5635e-16 \\
Algorithm I. & 5 & 1.1232e-16 & 7 & 3.2543e-16 & 9 & 4.2596e-16 \\
Algorithm II. & 4 & 1.2416e-16 & 6 & 2.4563e-16 & 8 & 3.2486e-16 \\
Algorithm III. & 4 & 1.2314e-16 & 6 & 2.4186e-16 & 8 & 3.1873e-16 \\
\hline
\end{tabular}
\caption{Comparison errors and iterations in Test 1.}
\end{table}

Test 2. In this example, a particular tridiagonal matrix is assumed in order to compute the inversion. Let us consider
where $a > 0$ and $b > 0$. The general form of the inversion of this matrix is given by $A^{-1} = \frac{1}{a} B$, whenever $B$ is defined for $i, j = 1, 2, \cdots, n$ as

$$B = (b_{ij}) = \min_{0 \leq i, j \leq n} \{ ai - b, aj - b \}.$$ 

In order to tackle the computation of inversion, we assumed the values of $a = 2$ and $b = 1$ for several values of $n$ by using Algorithm III. Here, we measure the residual error and the number of iteration. The results are demonstrated in Table 2. According to this table, it can easily be seen that by increasing the dimension, the number of iteration should be enhanced to achieve favorable accuracy.

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5. Conclusions

In this paper, a particular root finding approach applied to derive an iterative scheme for computing matrix inversion. The stability issue of the iteration has been solved by using auxiliary variables. Moreover, for some matrices with large spectral radios, the normalization of matrices is considered for circling the eigenvalues. Numerical implementations reveal that the stable coupled method can compute inversion with good accuracy without using the matrix $A$ directly.
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