Journal of Computational and Applied Mathematics 235 (2011) 1604–1613

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Iterative method for computing the Moore–Penrose inverse based on Penrose equations

Marko D. Petković*, Predrag S. Stanimirović

University of Niš, Faculty of Science and Mathematics, Višegradska 33, 18000 Niš, Serbia

ARTICLE INFO

Article history:
Received 15 December 2009
Received in revised form 18 May 2010

MSC:
15A09

Keywords:
Moore–Penrose inverse
Iterative methods
Convergence
Penrose equations

ABSTRACT

An iterative algorithm for estimating the Moore–Penrose generalized inverse is developed. The main motive for the construction of the algorithm is simultaneous usage of Penrose equations (2) and (4). Convergence properties of the introduced method as well as their first-order and second-order error terms are considered. Numerical experiment is also presented.

1. Introduction

Let $\mathbb{C}^{m\times n}$ and $\mathbb{C}_r^{m\times n}$ denote the set of all complex $m\times n$ matrices and all complex $m\times n$ matrices of rank r, respectively. As usual, I denotes the unit matrix of an appropriate order. By A^*, $\mathcal{R}(A)$, rank(A) and $\mathcal{N}(A)$ we denote the conjugate transpose, the range, the rank and the null space of $A\in\mathbb{C}^{m\times n}$, respectively. The orthogonal projection of $\mathbb{R}^m$ onto $\mathcal{R}(A)$ is denoted by $P_{\mathcal{R}(A)}$. Also for $A\in\mathbb{C}_r^{n\times n}$ we denote its eigenvalues by

$$\lambda_1(A)\geq\cdots\geq\lambda_r(A)>\lambda_{r+1}(A)=\cdots=\lambda_n(A)=0. \tag{1.1}$$

The Moore–Penrose inverse of $A\in\mathbb{C}^{m\times n}$, denoted by $A^\dagger$, is the unique matrix satisfying the next Penrose equations

$$(1)\ AXA=A,\qquad (2)\ XAX=X,\qquad (3)\ (AX)^*=AX,\qquad (4)\ (XA)^*=XA.$$

The most frequently used iterative method for approximating the inverse A^{-1} is the famous Newton's method

$$V_{k+1}=V_k+V_k(I-AV_k)=V_k(2I-AV_k), \tag{1.2}$$

originated in [1]. Schultz in [1] found that the eigenvalues of $I-AV_0$ must have magnitudes less than 1 to ensure convergence. Since the residuals $R_k=I-AV_k$ in each step (1.2) satisfy $\|R_{k+1}\|\leq\|A\|\|R_k\|^2$, Newton's method is a second-order iterative method [2]. Similarly, in [3] the relation $\|AE_{m+1}\|\leq\|AE_m\|^2$ is verified for residuals of the form $E_m=V_m-A^{-1}$.

Ben-Israel in [4,5,2] used Eq. (1.2) and the starting value

$$X_0=\alpha A^*, \tag{1.3}$$

where α satisfies

$$0<\alpha<2/\lambda_1(AA^*). \tag{1.4}$$

* Corresponding author.
E-mail addresses: dexterofnis@gmail.com (M.D. Petković), pecko@pmf.ni.ac.rs (P.S. Stanimirović).

0377-0427/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2010.08.042

Ben-Israel and Cohen [2] obtained additional results, still using Eq. (1.2), and derived an iterative approximation of the projector $AA^{\dagger}$. Newton's method was later investigated in [6].

Ben-Israel and Chanes in [7] proved that the sequence

$$Y_k = \alpha \sum_{i=0}^{k} A^*(I - \alpha AA^*)^i, \quad k = 0, 1, \ldots \tag{1.5}$$

converges to $A^{\dagger}$ under assumption (1.4).

The iterative process (1.2) is generalized by the iterative scheme

$$U_{k+1} = U_k(2P_{\mathcal{R}(A)} - AU_k), \tag{1.6}$$

which converges to $A^{\dagger}$ [4,5].

The iterative method for computing the Moore–Penrose inverse of the form

$$Z_{k+1} = PZ_k + Q, \qquad Z_1 = Q, \tag{1.7}$$

where

$$P = I - \beta A^*A, \qquad Q = \beta A^*, \tag{1.8}$$

is powered by the successive matrix squaring (SMS) of an appropriate 2×2 block matrix in [8]. By direct verification it is easy to verify

$$Z_{k+1} = \sum_{i=0}^{k} P^i Q.$$

Ben-Israel in [2] proved that $V_k = Y_{2^k-1}$, while Chen et al. in [8] showed that $Z_k = V_k$. Tanabe in [9] applied the iterative scheme of the same form to the set of reflexive generalized inverses which obey only the Penrose equations (1) and (2). In the papers of Wei [10] and Wei et al. [11] the authors considered two variants of the SMS algorithm which approximate the Drazin inverse and the weighted Moore–Penrose inverse of A, respectively. An SMS algorithm to approximate an outer generalized inverse with prescribed range and null space of a given matrix $A \in \mathbb{C}_r^{m\times n}$ is derived in [12].

2. Motivation

Householder in [13] defined successive improvements of a matrix X to solve the matrix equation $AX = M$, for nonsingular matrix A, using the recurrence relation

$$X_{k+1} = X_k + C_k(M - AX_k). \tag{2.1}$$

A particular case of the general iterative scheme (2.1) is defined by the choice $M = I$ and $C_k = X_k$, which turns into Newton's iterative method (1.2). It is not difficult to verify that the iterations (1.2) are based on the usage of Penrose equation (2).

Later in [2], process (1.5) is rewritten as

$$Y_{k+1} = Y_k(I - \alpha AA^*) + \alpha A^* = Y_k + \alpha(I - Y_kA)A^*, \tag{2.2}$$

which indicates that it is based on the usage of the Penrose equations (1) and (4). Similarly, it is easy to verify that the method (1.7) and (1.8) is based on the usage of Penrose equations (1) and (3).

Pierce in [14] investigated some likely candidates for successive improvements toward $A^{\dagger}$ using some of the matrix equations (1)–(4). These methods are summarized in Table 1 and restated from [14] for the sake of completeness.

If L is the desired limit matrix and X_k is the kth estimate of L, then the convergence properties of the examined algorithm can be studied with the aid of the error matrix $E_k = X_k - L$. If an iterative algorithm is expressible as a simple matrix formula, E_{k+1} is a sum of several terms:

- zero-order term consisting of a matrix which does not depend upon E_k,
- one or more first-order matrix terms in which E_k or its conjugate transpose E_k^* appears only once,
- higher-order terms in which E_k or E_k^* appears at least twice.

All suitable algorithms have a zero-order term equal to 0. Hence the first-order terms determine the terminal convergence properties [14].

The calculation of the first-order terms' $error_1$ begins by substituting $X_k = A^{\dagger} + E$ and expanding the resulting formula. To produce these formulas, it is necessary to use the Hermitian property, some Penrose equations, or some simple algebraic transformations [14]. It is not difficult to verify that Algorithm β from Table 1 is based upon the usage of Eq. (2). Algorithm γ uses Eqs. (2) and (3), while Algorithm δ uses Eqs. (2) and (4). Algorithm ζ uses the matrix AU_k as the approximation of $P_{\mathcal{R}(A)}$ in (1.6).

In the present paper we present an iterative algorithm for computing the Moore–Penrose generalized inverse. The algorithm is based on the usage of Penrose equations (2) and (4). Conditions for the convergence of the method as well as the first-order and the second-order terms in error estimates are investigated. A comparison with similar iterative algorithms is presented. Numerical results are given in the last section.

Table 1
Iterative methods from [14].

Name	Formula for X_{k+1}	$error_1$
α	$X_k(2I - AX_k)$	$E(2I - AA^\dagger) - A^\dagger AE$
β	X_kAX_k	$EAA^\dagger + A^\dagger AE$
γ	$X_k(AX_k)^*$	$EAA^\dagger + A + E^*A^*$
δ	$(X_kA)^*X_k$	$A^*E^*A^\dagger + A^\dagger AE$
ε	$(\gamma + \delta - \beta)$	$A^\dagger E^*A^* + A^*E^*A^\dagger$
ζ	$X_kAX_k(2I - AX_k)$	$EAA^\dagger + A^\dagger AE(2I - AA^\dagger) - A^\dagger AE$
η	(ε then α)	0
θ	$X_kAX_k(2I - AX_kAX_k)$	$EAA^\dagger - 2A^\dagger AEAA^\dagger + A^\dagger AE$

3. The iterative method

Assume that $A \in \mathbb{C}^{m\times n}$ and $X = A^\dagger \in \mathbb{C}^{n\times m}$. We start from Eqs. (2), (4) and obtain

$$X^* = (XAX)^* = X^*(XA)^* = X^*XA.$$

Hence, for arbitrary $\beta \in \mathbb{R}$ it holds

$$X^* = X^* - \beta(X^*XA - X^*) = X^*(I - \beta XA) + \beta X^*,$$

or equivalently

$$X = (I - \beta XA)^*X + \beta X.$$

From the last equation we can formulate the following iterative method

$$X_{k+1} = (I - \beta X_kA)^*X_k + \beta X_k. \tag{3.1}$$

Assume that the starting value of the iterative method (3.1) is

$$X_0 = \beta A^*, \tag{3.2}$$

for an appropriate real number β.

The following lemma will be useful in further considerations.

Lemma 3.1. *For the sequence X_k generated by the iterative schemes (3.1) and (3.2) the following hold*

$$X_kA = (X_kA)^*, \qquad XAX_k = X_k, \qquad X_kAX = X_k, \quad k \geq 0. \tag{3.3}$$

Proof. We use mathematical induction. For $k = 0$ we have $X_0 = \beta A^*$ and all statements in (3.3) hold by direct verification. Under the assumption that the theorem is true for some integer k the following transformations are derived as consequences:

$$\begin{aligned}(X_{k+1}A)^* &= ((I - \beta X_kA)^*X_kA + \beta X_kA)^*\\ &= (X_kA)^*(I - \beta X_kA) + \beta(X_kA)^*\\ &= X_kA(I - \beta X_kA) + \beta X_kA\\ &= (I - \beta X_kA)^*X_kA + \beta X_kA\\ &= X_{k+1}A.\end{aligned}$$

In this way, we proved that the first statement of the lemma holds for $k + 1$. Similarly we prove the second statement as follows

$$\begin{aligned}XAX_{k+1} &= XA(I - \beta X_kA)^*X_k + \beta XAX_k\\ &= XAX_k - \beta XAX_kAX_k + \beta XAX_k\\ &= X_k - \beta X_kAX_k + \beta X_k\\ &= X_{k+1}.\end{aligned}$$

The third statement can be verified in a similar manner:

$$X_{k+1}AX = (I - \beta X_kA)^*X_kAX + \beta X_kAX = (I - \beta X_kA)^*X_k + \beta X_k = X_{k+1}.$$

This completes the proof of the lemma. □

From Lemma 3.1 follows that Eq. (3.1) can be written in the following form

$$X_{k+1} = (I - \beta X_kA)X_k + \beta X_k = (1 + \beta)X_k - \beta X_kAX_k. \tag{3.4}$$

Now we are ready to prove that the matrix sequence X_k defined by the starting value $X_0 = \beta A^*$ and the iterative rule (3.1), converges to the Moore–Penrose inverse $X = A^\dagger$.

Theorem 3.1. *Iterative method (3.4) with the starting value defined in (3.2) converges to the Moore–Penrose inverse $X = A^{\dagger}$ under the assumptions*

$$\|(X_0 - X)A\| < 1, \quad 0 < \beta \leq 1. \tag{3.5}$$

For $\beta < 1$ the method has a linear convergence, while for $\beta = 1$ its convergence is quadratic. The first-order and the second-order terms, corresponding to the error estimation of (3.4) are equal to:

$$error_1 = (1 - \beta)E_k, \qquad error_2 = -\beta E_k A E_k, \tag{3.6}$$

respectively.

Proof. For the first part of the theorem, it suffices to verify that $\|X_n - X\| \to 0$ when $n \to +\infty$. Using the properties of the Moore–Penrose inverse X and results of Lemma 3.1 we obtain

$$\|X_{k+1} - X\| = \|X_{k+1}AX - XAX\| \leq \|X_{k+1}A - XA\|\|X\|.$$

Using (3.3) and (3.4) we have

$$\begin{aligned} X_{k+1}A - XA &= (1 + \beta)X_kA - \beta X_kAX_kA - XA \\ &= -(\beta X_kA - XA)(X_kA - XA). \end{aligned}$$

Later, taking into account

$$\beta X_kA - XA = \beta(X_kA - XA) - (1 - \beta)XA,$$

and using (3.3) we obtain

$$X_{k+1}A - XA = -\beta(X_kA - XA)^2 + (1 - \beta)(X_kA - XA).$$

The sequence of error matrices E_k defined by $E_k = X_k - X$ satisfy the following recurrence relation

$$E_{k+1}A = -\beta(E_kA)^2 + (1 - \beta)E_kA. \tag{3.7}$$

Let $t_k = \|E_kA\|$. Our goal is to show that $t_k \to 0$ when $k \to +\infty$. By mathematical induction we prove that $t_k < 1$. Condition of the theorem implies $t_0 = \|(X_0 - X)A\| < 1$. From Eq. (3.7) and the inductive hypothesis $t_k < 1$ we obtain

$$t_{k+1} \leq \beta t_k^2 + (1 - \beta)t_k < \beta t_k + (1 - \beta)t_k = t_k. \tag{3.8}$$

This completes the proof by induction since $t_{k+1} < t_k < 1$. Moreover, Eq. (3.8) implies $t_{k+1} < t_k$ for $k = 0, 1, \ldots$, i.e. t_k is a decreasing sequence. Since $t_k \geq 0$ is bounded, we conclude that t_k is convergent and $t_k \to t$ when $k \to +\infty$. Moreover $0 \leq t < 1$ holds. Again using (3.8) we obtain additionally

$$t \leq \beta t^2 + (1 - \beta)t.$$

The last inequality implies that either $t \geq 1$ or $t = 0$ and hence we conclude that $t = 0$. This completes the proof that $t_k \to 0$ when $k \to +\infty$.

Now, since Lemma 3.1 implies $\|X_k - X\| \leq t_k\|X\|$, we conclude that $X_k \to X$ when $k \to +\infty$. This proves the convergence of method (3.1) and the first part of the theorem.

Putting $X_k = X + E_k$ in (3.4) it is not difficult to verify that the error matrix E_{k+1} can be expressed in the form

$$E_{k+1} = (1 + \beta)E_k - \beta XAE_k - \beta E_kAX - \beta E_kAE_k,$$

which implies

$$\begin{aligned} error_1 &= (1 + \beta)E_k - \beta XAE_k - \beta E_kAX, \\ error_2 &= -\beta E_kAE_k. \end{aligned}$$

Using $E_k = X_k - X$ and Lemma 3.1 we obtain

$$\begin{aligned} error_1 &= (1 + \beta)(X_k - X) - \beta XA(X_k - X) - \beta(X_k - X)AX \\ &= (1 - \beta)(X_k - X) = (1 - \beta)E_k. \end{aligned}$$

This confirms the statements in (3.6). Obviously $error_1$ vanishes if and only if $\beta = 1$, while $error_2$ is always non-zero. Hence, the method has linear convergence for $\beta \neq 1$ and quadratic convergence for $\beta = 1$. This completes the proof of the theorem. □

From Theorem 3.1 we see that the convergence of the method (3.4) requires the condition $\|(\beta A^* - X)A\| < 1$. We need to write the previous condition in an equivalent form which does not contain the Moore–Penrose inverse X. The following well-known result (Lemma 3.2) will be used.

Lemma 3.2 ([15]). *Let $M \in \mathbb{C}^{n\times n}$ and $\varepsilon > 0$ be given. There is at least one matrix norm $\|\cdot\|$ such that*

$$\rho(M) \le \|M\| \le \rho(M) + \epsilon, \tag{3.9}$$

where $\rho(M) = \max\{|\lambda_1(M)|, \dots, |\lambda_n(M)|\}$ denotes the spectral radius of M.

According to Lemma 3.2, necessary and sufficient condition for the convergence of the iterative method is $\rho((\beta A^* - X)A) < 1$. The following lemma shows one property of the spectral radius function ρ.

Lemma 3.3 ([12, Lemma 2.1]). *If $P \in \mathbb{C}^{n\times n}$ and $S \in \mathbb{C}^{n\times n}$ are such that $P = P^2$ and $PS = SP$ then*

$$\rho(PS) \le \rho(S).$$

Now we are ready to prove the following convergence criterion which is similar as in [12].

Lemma 3.4. *Let the eigenvalues of matrix A^*A satisfy (1.1). Condition $\rho((\beta A^* - X)A) < 1$ is satisfied (i.e. method (3.4) with the initial value (3.2) is convergent) under the assumption*

$$\max_{1\le i\le r} |1 - \beta\lambda_i(A^*A)| < 1. \tag{3.10}$$

Proof. Let $P = XA$ and $S = \beta A^*A - I$. Since $P^2 = P$ and

$$\begin{aligned} PS &= \beta XAA^*A - XA = \beta(XA)^*A^*A - XA = \beta(AXA)^*A - XA \\ &= \beta A^*A - XA = \beta A^*AXA - XA = SP, \end{aligned}$$

from Lemma 3.3 we can conclude that

$$\rho((\beta A^* - X)A) \le \rho(\beta A^*A - I) = \max_{1\le i\le r} |1 - \beta\lambda_i(A^*A)| < 1.$$

This holds since $\mu_i = \beta\lambda_i(A^*A) - 1$ for $i = 1, \dots, n$ are the eigenvalues of the matrix $\beta A^*A - I$. □

Denote $s_k = \|E_k\|$ and $d_k = \|E_{k+1} - E_k\|$. In the next theorem we prove the convergence properties of the stated iterative method, i.e. behavior of the sequences t_k, s_k and d_k.

Theorem 3.2. *Iterative method (3.4) with the starting value defined in (3.2) satisfies*

$$\lim_{k\to+\infty} \frac{t_{k+1}}{t_k} = \lim_{k\to+\infty} \frac{s_{k+1}}{s_k} = \lim_{k\to+\infty} \frac{d_{k+1}}{d_k} = 1 - \beta. \tag{3.11}$$

Proof. From recurrent relation (3.7):

$$E_{k+1}A = -\beta(E_kA)^2 + (1 - \beta)E_kA,$$

we can conclude that

$$\begin{aligned} t_{k+1} = \|E_{k+1}A\| &\ge \|(1 - \beta)E_kA\| - \|\beta(E_kA)^2\| \\ &\ge (1 - \beta)\|E_kA\| - \beta\|E_kA\|^2 = t_k(1 - \beta - \beta t_k). \end{aligned}$$

On the other hand, it holds that

$$\begin{aligned} t_{k+1} = \|E_{k+1}A\| &\le \|(1 - \beta)E_kA\| + \|\beta(E_kA)^2\| \\ &\le (1 - \beta)\|E_kA\| + \beta\|E_kA\|^2 = t_k(1 - \beta + \beta t_k). \end{aligned}$$

The previous two inequalities directly imply

$$1 - \beta - \beta t_k \le \frac{t_{k+1}}{t_k} \le 1 - \beta + \beta t_k.$$

Since $t_k = \|E_kA\| \to 0$ (Theorem 3.1), by taking a limit of the previous equation we conclude that $t_{k+1}/t_k \to 1 - \beta$ when $k \to +\infty$.

According to Theorem 3.1 we can write

$$E_{k+1} = (1 - \beta)E_k - \beta E_kAE_k.$$

The previous equation implies

$$1 - \beta - \beta\frac{\|E_kAE_k\|}{\|E_k\|} \le \frac{\|E_{k+1}\|}{\|E_k\|} \le 1 - \beta + \beta\frac{\|E_kAE_k\|}{\|E_k\|}. \tag{3.12}$$

Now from $\|E_kAE_k\| \leq \|E_k\|^2\|A\|$ and $\|E_k\| \to 0$ when $k \to +\infty$ (Theorem 3.1) we conclude that

$$0 \leq \lim_{k\to+\infty} \frac{\|E_kAE_k\|}{\|E_k\|} \leq \lim_{k\to+\infty} \|E_k\|\|A\| = 0.$$

Applying a limit on both sides of Eq. (3.12) and using the previous equation yields $s_{k+1}/s_k \to 1-\beta$ when $k \to +\infty$.

In order to verify the statement for the sequence d_k, we start from $X_{k+1} - X_k = E_{k+1} - E_k$, which together with (3.6) implies

$$d_k = \|E_{k+1} - E_k\| = \|(1-\beta)E_k - \beta E_kAE_k - E_k\| = \beta\|E_k + E_kAE_k\|.$$

In a similar way, as in a verification of the previous statements of the theorem, it is possible to derive

$$\lim_{k\to+\infty} \frac{d_k}{s_k} = \lim_{k\to+\infty} \frac{d_k}{\|E_k\|} = \beta.$$

Now, we obtain

$$\lim_{k\to+\infty} \frac{d_{k+1}/s_{k+1}}{d_k/s_k} = 1,$$

which implies

$$\lim_{k\to+\infty} \frac{d_{k+1}}{d_k} = \lim_{k\to+\infty} \left(\frac{d_{k+1}/s_{k+1}}{d_k/s_k} \cdot \frac{s_{k+1}}{s_k}\right) = 1-\beta.$$

This completes the proof of the theorem. □

The following lemma shows one additional property of the sequence X_k. It will be useful for the consideration of numerical stability of method (3.4).

Lemma 3.5. *Sequence X_k defined by (3.4) and (3.2) satisfies $\mathcal{R}(X_k) = \mathcal{R}(A^*)$ and $\mathcal{N}(X_k) = \mathcal{N}(A^*)$ for each $k \geq 0$.*

Proof. Since $X_0 = \beta A^*$, the statement of the theorem obviously holds for $k = 0$. Let $y \in \mathcal{N}(X_k)$ be an arbitrary vector. From (3.4) we have

$$X_{k+1}y = (1+\beta)X_ky - \beta X_kAX_ky = 0.$$

Hence $y \in \mathcal{N}(X_{k+1})$, which implies $\mathcal{N}(X_k) \subseteq \mathcal{N}(X_{k+1})$. The statement $\mathcal{R}(X_k) \supseteq \mathcal{R}(X_{k+1})$ can be proved analogously. Hence, by mathematical induction we obtain $\mathcal{N}(X_k) \supseteq \mathcal{N}(X_0) = \mathcal{N}(A^*)$ and $\mathcal{R}(X_k) \subseteq \mathcal{R}(X_0) = \mathcal{R}(A^*)$. To prove the equality in these statements, let us consider $\mathcal{N} = \bigcup_{k\in\mathbb{N}_0} \mathcal{N}(X_k)$. Let $y \in \mathcal{N}$ be an arbitrary vector and let $y \in \mathcal{N}(X_{k_0})$ for some $k_0 \in \mathbb{N}_0$. Since $y \in \mathcal{N}(X_k)$ for all $k \geq k_0$ we have $X_ky = 0$ and using Theorem 3.1 we have

$$Xy = \lim_{k\to+\infty} X_ky = 0.$$

This implies $y \in \mathcal{N}(X) = \mathcal{N}(A^*)$ and $\mathcal{N} \subseteq \mathcal{N}(A^*)$. Furthermore it holds

$$\mathcal{N}(A^*) \subseteq \mathcal{N}(X_k) \subseteq \mathcal{N} \subseteq \mathcal{N}(A^*),$$

and hence we conclude that $\mathcal{N}(X_k) = \mathcal{N}(A^*)$.

Now the relation

$$\dim \mathcal{R}(X_k) = m - \dim \mathcal{N}(X_k) = m - \dim \mathcal{N}(A^*) = \dim \mathcal{R}(A^*)$$

and $\mathcal{R}(X_k) \subseteq \mathcal{R}(A^*)$ directly implies $\mathcal{R}(X_k) = \mathcal{R}(A^*)$. □

In the rest of this section we compare our method with known iterations available in the literature.

Remark 3.1. Note that for $\beta = 1$ method (3.4) reduces to the well-known Schultz method for computing the inverse and the Moore–Penrose inverse of a given matrix.

Remark 3.2. Let $A \in \mathbb{C}_r^{m\times n}$ and $R \in \mathbb{C}_s^{n\times m}$, $0 \leq s \leq r$ be given. The general iterative scheme used in paper [12] for iterative computation of $A^{(2)}_{T,S}$ inverse is given by (1.7), where $P = I - \beta RA$, $Q = \beta R$ and β is a relaxation parameter. In that way, we obtain the iterative scheme

$$X_{k+1} = (I - \beta RA)X_k + \beta R, \tag{3.13}$$

which comprises all iterative rules underlying the SMS technique. An essential difference between iterative schemes (3.4) and (3.13), embedded into the SMS algorithm, is that matrices P and Q (as well as the matrix R) are not constant during iterations in (3.4). A formal comparison points out that the matrix R from (3.13) is replaced by X_k. On the other hand, the value R in recurrence rule (3.13) is selected in advance and fixed throughout all iterations. For this purpose the acceleration procedure from the complete SMS algorithm is not applicable to our algorithm.

Remark 3.3. In order to compare our method (3.4) with the basic iterative method (1.7) of the SMS algorithm, let us mention that the first-order and the second-order terms in the error estimation of the iterative process (1.7) and (1.8) are equal to

$$error'_1 = (I - \beta A^*A)E_k, \qquad error'_2 = 0.$$

Let the eigenvalues $\lambda_j(A^*A)$ of A^*A be ordered as in (1.1). In view of Lemma 3.2 it immediately follows that

$$0 \le \|error'_1\| \le \left(\max_{1\le i\le m} |1 - \beta\lambda_i(A^*A)| + \varepsilon \right) \|E_k\|.$$

If (3.10) is satisfied, we can choose ϵ such that $\max_{1\le i\le m} |1 - \beta\lambda_i(A^*A)| + \varepsilon < 1$, which immediately gives

$$0 \le \|error'_1\| < \|E_k\|.$$

On the other hand, the norm of the first-order error estimate matrix in (3.6) satisfies the same lower and upper bounds:

$$0 \le \|error_1\| < \|E_k\|.$$

Therefore, the SMS original iterative scheme and our method are incomparable generally, and have identical lower and upper bounds for the norm of the first-order estimate matrix.

Remark 3.4. If we rewrite iterations (3.4) in the form

$$X_{k+1} = X_k(I - \beta AX_k) + \beta X_k,$$

we observed that our method is formally related to the iterative scheme (2.2) by the replacement of the matrix A^* in (2.2) by X_k.

4. Influence of roundoff errors

Roundoff errors always occur when the floating point arithmetics is used. In this section we consider the influence of the roundoff errors on our iterative method (3.4). The consequence is that the computed value $\tilde{X}_s$, in sth iteration, differs from the original value X_s by error matrix Δ_s. Our goal is to consider the propagation of the error Δ_s through further iterations. In other words, we consider the same iterative process

$$\tilde{X}_{k+1} = (1 + \beta)\tilde{X}_k - \beta\tilde{X}_kA\tilde{X}_k, \quad k \ge s, \tag{4.1}$$

where $\tilde{X}_s = X_s + \Delta_s$. If the matrix A is not of full rank, iterative process (4.1) can diverge. Theorem 4.1 shows that it happens when $\operatorname{rank}(\tilde{X}_s) > \operatorname{rank}(X_s) = \operatorname{rank}(A)$.

We assume that the matrix norm $\|\cdot\|$ is induced by the corresponding vector norm. Since all matrix norms are equivalent, the theorem also holds in a general case, for an arbitrary matrix norm.

Theorem 4.1. *Consider the iterative method (3.4) and assume that the roundoff error in sth iteration initiates* $\operatorname{rank}(\tilde{X}_s) > \operatorname{rank}(X_s) = \operatorname{rank}(A)$. *Then, the resulting method (4.1) diverges and* $\|\tilde{X}_k\| \ge c \cdot (1 + \beta)^{k-s}$, *where* $c > 0$ *is the constant which depends only on* $\tilde{X}_s$.

Proof. Since $\mathcal{N}(\tilde{X}_s) \subseteq \mathcal{N}(\tilde{X}_sA\tilde{X}_s)$ and $\operatorname{rank}(\tilde{X}_sA\tilde{X}_s) \le \operatorname{rank}(A) < \operatorname{rank}\tilde{X}_s$, we conclude that the inclusion is strict and there exists a non-zero vector $y \in \mathcal{N}(\tilde{X}_sA\tilde{X}_s) \setminus \mathcal{N}(\tilde{X}_s)$. Then $\tilde{X}_sA\tilde{X}_sy = 0$ and $\tilde{X}_sy \ne 0$.

We prove by mathematical induction that $\tilde{X}_ky = (1 + \beta)^{k-s}\tilde{X}_sy$ and $\tilde{X}_kA\tilde{X}_ky = 0$ for every $k \ge s$. The initial condition $k = s$ is already proven. We assume that the statement holds for some $k \ge 0$. From (3.4) and induction hypothesis we have

$$\tilde{X}_{k+1}y = (1 + \beta)\tilde{X}_ky - \beta\tilde{X}_kA\tilde{X}_ky = (1 + \beta)\tilde{X}_ky = (1 + \beta)^{k-s+1}\tilde{X}_sy.$$

Moreover, from the previous equation and inductive hypothesis we have

$$\begin{aligned}\tilde{X}_{k+1}A\tilde{X}_{k+1}y &= (1 + \beta)\tilde{X}_{k+1}A\tilde{X}_ky \\ &= (1 + \beta)((1 + \beta)\tilde{X}_k - \beta\tilde{X}_kA\tilde{X}_k)A\tilde{X}_ky \\ &= (1 + \beta)^2\tilde{X}_kA\tilde{X}_ky - (1 + \beta)\beta\tilde{X}_kA\tilde{X}_kA\tilde{X}_ky = 0.\end{aligned}$$

This finishes the mathematical induction.

Now we directly have

$$\|\tilde{X}_k\| \ge \frac{\|\tilde{X}_ky\|}{\|y\|} = (1 + \beta)^{k-s}\frac{\|\tilde{X}_sy\|}{\|y\|} = c \cdot (1 + \beta)^{k-s},$$

where $c = \|\tilde{X}_sy\|/\|y\| > 0$ since $y \notin \mathcal{N}(\tilde{X}_s)$. Also $\|\tilde{X}_k - X\| \ge \|\tilde{X}_k\| - \|X\| \to +\infty$ when $k \to +\infty$. This completes the proof. □

Theorem 4.1 will be used in the following section for explanation of the numerical instability of our iterative method.

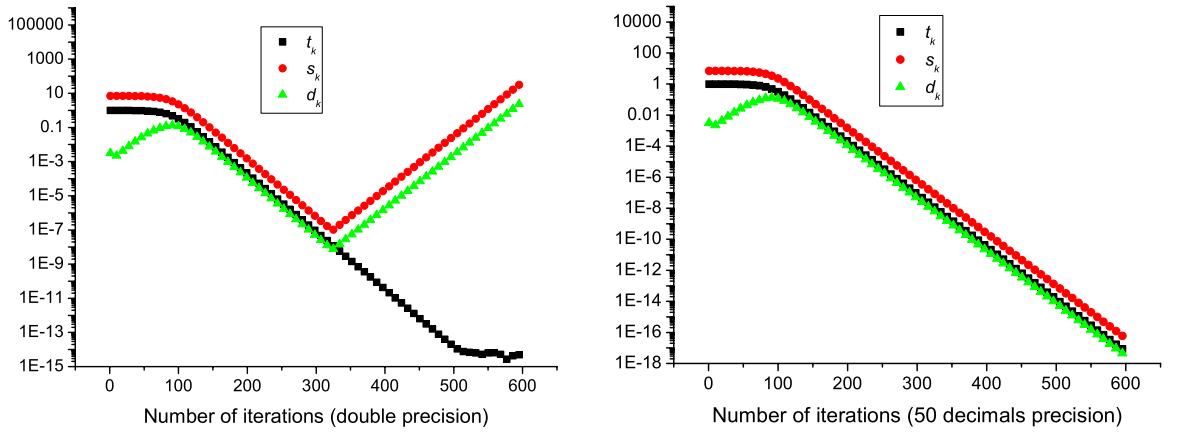

Fig. 1. Residual norms $t_k = \|E_kA\| = \|(X_k - X)A\|$, $s_k = \|X_k - X\|$ and $d_k = \|X_{k+1} - X_k\|$ through iterations in lin–log scale.

5. Numerical experiment

We implemented the iterative method (3.4) in package MATHEMATICA 7.0 [16] and tested it on several test matrices.

Example 5.1. Let us consider the following matrix

$$A = \begin{bmatrix} 0.8846 & 0.807516 & 0.381614 & 0.671798 \\ 0.854492 & 0.91836 & 0.611953 & 0.664359 \\ 0.673669 & 0.459477 & 0.383368 & 0.575746 \\ 0.865487 & 0.803065 & 0.523343 & 0.687009 \\ 1.14976 & 0.964402 & 0.594889 & 0.918999 \end{bmatrix}.$$

Note that $\operatorname{rank}(A) = 3$. The choice $\beta = 0.075$ satisfies the convergence criterion (3.10), since the eigenvalues of A^*A are

$$(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = (11.0908, 0.04375, 0.020103, 0)$$

and $\max_{1\le i\le 3} |1 - \beta\lambda_i| = 0.998492 < 1$. The Moore–Penrose inverse $X = A^\dagger$ is equal to

$$X = \begin{bmatrix} 1.2218 & -1.73664 & 0.477176 & -0.373851 & 0.849832 \\ 2.32302 & 1.54411 & -3.62337 & 0.0625838 & -0.745567 \\ -4.7017 & 2.95821 & 2.4219 & 1.11348 & -0.928495 \\ -0.573185 & -1.36973 & 1.99102 & -0.113338 & 0.782951 \end{bmatrix}.$$

We investigated the matrix norms

$$t_k = \|E_kA\| = \|(X_k - X)A\|, \qquad s_k = \|X_k - X\| = \|E_k\|, \qquad d_k = \|X_{k+1} - X_k\|$$

throughout the iterations. Total number of iterations was $N_{\text{iter}} = 600$. Values of t_k, s_k and d_k are plotted in Fig. 1(left).

It can be observed that convergence starts after a few initial steps. When the convergence starts, all plotted norms first exponentially decrease. Also the ratios t_{k+1}/t_k, s_{k+1}/s_k and d_{k+1}/d_k are close to $1-\beta$ in that case. This numerical experiment is in accordance with the convergence properties derived in Theorem 3.2.

However, continuing with the iterations persistently, we observed that these ratios exponentially increase with the quotients equal to $1 + \beta$. The reason for such a behavior is roundoff errors, which is in accordance with Theorem 4.1. To show that, we enlarged working precision to 50 decimals and run the same test. Results are shown in Fig. 1(right). Since the residual norms are now equal to $t_{600} = 5.77129 \cdot 10^{-18}$, $s_{600} = 4.070436 \cdot 10^{-17}$ and $d_{600} = 3.052827 \cdot 10^{-18}$ after $N_{\text{iter}} = 600$ iterations, we conclude that the convergence is still stable.

Moreover, numerical results on the other test matrices suggest that the following conjecture is valid.

Conjecture 5.1. *Assume that the roundoff error in sth iteration initiates increasing of rank of X_s. Then holds*

$$\lim_{k\to+\infty} \frac{t_{k+1}}{t_k} = \lim_{k\to+\infty} \frac{s_{k+1}}{s_k} = \lim_{k\to+\infty} \frac{d_{k+1}}{d_k} = 1 + \beta.$$

We choose the matrix X_k minimizing d_k as the output matrix, since s_k and d_k have the minimum at the same point $k = 324$. On the other hand, t_k has the minimum at the point $k = 579$. At this point, the absolute difference norm has value $s_k = 6.82$, meaning that X_k is far from X.

Finally, note that we should specify the total number of iterations N_{iter}. It should be larger than the index of X_k minimizing d_k. Another approach is to perform iterations until the ratio d_{k+1}/d_k is close enough to $1+\beta$. However, we still need to limit the maximal number of iterations due to the fact that it cannot be estimated analytically as in [12]. Note that for small k, values d_k are increasing (Fig. 1) but the slope is smaller than $1+\beta$.

Hence, there are two possible choices for the stopping criterion:

$C1$. Fix the total number of iterations N_{iter} and choose the X_k such that the difference norm $d_k = \|X_{k+1} - X_k\|$ is minimal.

$C2$. Perform the iterations until $|d_{k+1}/d_k - \beta - 1| > \epsilon$ (or the maximum number of iterations is not achieved) and return the same X_k as in the previous case.

Implementations based on the stopping criteria $C1$ and $C2$ are denoted by `It24C1` and `It24C2`, respectively. Complete MATHEMATICA code is included in the Appendix.

It is worthy to note that the underlying iterative method in [12] suffers from the same problem. In [12] the problem is solved by calculating the prescribed number of iterative steps N_{iter} as the function of a given precision $\|X - X_k\|/\|X\| \leq \delta$ (see the recommended number of iterative steps in the relation (2.28) from [12]). Similar calculations are not available for the iterative process used in the present paper since the fixed matrix R from [12] takes variable values, as is mentioned in Remark 3.2.

6. Conclusion

In the literature it is a frequently used idea to exploit some Penrose equations to derive iterative methods for approximating the Moore–Penrose or other generalized inverses. We survey these methods and derive an algorithm for improving the estimates of the Moore–Penrose generalized inverse, using Penrose equations (2) and (4). Convergence properties of the introduced method as well as the formula for their first-order and the second-order error estimates are considered. Numerical examples are presented. A comparative study with respect to the basic iterative processes underlying in the SMS method and with the Shultz method is presented.

Acknowledgements

The authors wish to thank the anonymous referee for valuable comments which improved the quality of the paper. The authors gratefully acknowledge support from the research project 144011 of the Serbian Ministry of Science.

Appendix. Implementation details

We give the complete MATHEMATICA code of the functions `It24C1` and `It24C2`.

Function `It24C1` takes the matrix A (`A`) and values β (`beta`) and N_{iter} (`Niter`) as input arguments. It returns the matrix X_k such that value d_k (`normd`) is minimal.

```
It24C1[A_, beta_, Niter_]:=
  Module[{minnormd, Xk, Xk1, Xkmin, normd, i, ind},

   Xk = beta*Transpose[A];
   minnormd = +Infinity;
   Do[
    Xk1 = (1 + beta) Xk - beta*Xk.A.Xk;
    normd = Norm[Xk1 - Xk];
    If [normd < minnormd,
     minnormd = normd; Xkmin = Xk;
     ];
    Xk = Xk1;
     , {i, 1, Niter}
   ];
   Return[Xkmin];
];
```

Function `It24C2` has the matrix A (`A`) and values β (`beta`) and ϵ (`eps`) as input arguments. It performs iterations until $|d_{k+1}/d_k - 1 - \beta| < \epsilon$ or maximal number of iterations is reached. Maximal number of iterations is given by the option value `MaxIterations` whose default is set to 2000.

```
Options[It24C2] = {MaxIterations -> 2000};

It24C2[A_, beta_, eps_, OptionsPattern[]]:=
  Module[{normd1, minnormd, Xk, Xk1, Xkmin, normd, i, ind,
    Niter = OptionValue[MaxIterations]},

   Xk = beta*Transpose[A];
   minnormd = +Infinity;
   Do[
    Xk1 = (1 + beta) Xk - beta*Xk.A.Xk;
    normd = Norm[Xk1 - Xk];
    If [normd < minnormd,
     minnormd = normd; Xkmin = Xk;
    ];

    If[Abs[normd/normd1 - 1 - beta] < eps,
     Break[];
    ];
    normd1 = normd;
    Xk = Xk1;
     , {i, 1, Niter}
   ];
   Return[Xkmin];
];
```

References

[1] G. Schulz, Iterative Berechmmg der reziproken matrix, Z. Angew. Math. Mech. 13 (1933) 57–59.
[2] A. Ben-Israel, D. Cohen, On iterative computation of generalized inverses and associated projections, SIAM J. Numer. Anal. 3 (1966) 410–419.
[3] H.S. Najafi, M.S. Solary, Computational algorithms for computing the inverse of a square matrix, quasi-inverse of a non-square matrix and block matrices, Appl. Math. Comput. 183 (2006) 539–550.
[4] A. Ben-Israel, An iterative method for computing the generalized inverse of an arbitrary matrix, Math. Comp. 19 (1965) 452–455.
[5] A. Ben-Israel, A note on an iterative method for generalized inversion of matrices, Math. Comp. 20 (1966) 439–440.
[6] V. Pan, R. Sehreiber, An improved Newton iteration for the generalized inverse of a matrix, with applications, SIAM J. Sci. Stat. Comput. 12 (1991) 1109–1130.
[7] A. Ben-Israel, A. Chanes, Contributions to the theory of generalized inverses, SIAM J. 11 (1963) 667–669.
[8] L. Chen, E.V. Krishnamurthy, I. Macleod, Generalized matrix inversion and rank compuation by successive matrix powering, Parallel Comput. 20 (1994) 297–311.
[9] K. Tanabe, Neumann-type expansion of generalized inverses of a matrix and the hyperpower iterative method, Linear Algebra Appl. 10 (1975) 163–175.
[10] Y. Wei, Successive matrix squaring algorithm for computing Drazin inverse, Appl. Math. Comput. 108 (2000) 67–75.
[11] Y. Wei, H. Wu, J. Wei, Successive matrix squaring algorithm for parallel computing the weighted generalized inverse $A^{\dagger}_{MN}$, Appl. Math. Comput. 116 (2000) 289–296.
[12] P.S. Stanimirović, D.S. Cvetković-Ilić, Successive matrix squaring algorithm for computing outer inverses, Appl. Math. Comput. 203 (2008) 19–29.
[13] A.S. Householder, The Theory of Matrices in Numerical Analysis, Blaisdell, New York, 1964 (Chapter 7).
[14] W.H. Pierce, A self-correcting matrix iteration for the Moore–Penrose generalized inverse, Linear Algebra Appl. 244 (1996) 357–363.
[15] R.A. Horn, C.R. Johnson, Matrix Analysis, Cambridge University Press, Cambridge, New York, New Rochelle, Melbourne, Sydney, 1986.
[16] S. Wolfram, The Mathematica Book, 5th ed., Wolfram Media, Cambridge University Press, Champaign, IL, USA, 2003, 61820.