# Iterative method for computing Moore-Penrose inverse based on Penrose equations

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#### **Abstract**

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

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#### 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. By  $P_{\mathcal{R}(A)}$  is denoted the orthogonal projection of  $\mathbb{R}^m$  onto  $\mathcal{R}(A)$ . Also for  $A\in\mathbb{C}_r^{n\times n}$  we denote its eigenvalues by

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

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

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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 [11]. Schultz in [11] found that the eigenvalues of  $I-AV_0$  must have magnitudes less than 1 to ensure the convergence. Since the residuals  $R_k = I - AV_k$  in each step (1.2) satisfy  $||R_{k+1}|| \le ||A|| ||R_k||^2$ , Newton method is the second order iterative method [3]. Similarly, in [8] the relation  $||AE_{m+1}|| \le ||AE_m||^2$  is verified for residuals of the form  $E_m = V_m - A^{-1}$ .

Ben-Israel in [1, 2, 3] used equation (1.2) and the starting value

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

where  $\alpha$  satisfies

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

Ben-Israel and Cohen [3] obtained additional results, still using equation (1.2), and derived an iterative approximation of the projector  $AA^{\dagger}$ . Newton's method is later investigated in [9].

Ben-Israel and Chanes in [4] proved that the sequence

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

converges to  $A^{\dagger}$  under the 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  $A^{\dagger}$  [1, 2].

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

$$Z_{k+1} = PZ_k + Q, \ Z_1 = Q,$$
 (1.7)

where

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

is powered by the successive matrix squaring (SMS) of an appropriate  $2 \times 2$  block matrix in [5]. By direct verification it is easy to verify

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

Ben-Israel in [3] proved  $V_k = Y_{2^k-1}$ , while Chen et al. in [5] shown  $Z_k = V_k$ . Tanabe in [13] 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 Y. Wei [14] and Y. Wei et al. [15] the authors considered two variants of 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 [7] defined successive improvements of a matrix X to solve the matrix equation AX = M, for nonsingular matrix A, using the recurrence relation

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

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 the 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 [3], process (1.5) is rewritten as

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

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), (1.8) is founded on the usage of Penrose equations (1) and (3).

Pierce in [10] 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 [10] for the sake of completeness.

If L is the desired limit matrix and  $X_k$  is the k-th 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  $E_k^{\ast}$  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 [10].

| Name          | Formula for $X_{k+1}$                | $error_1$  |
|---------------|--------------------------------------|--|
| $\alpha$      | $X_k(2I - AX_k)$                     | $E(2I - AA^{\dagger}) - A^{\dagger}AE$                             |
| $\beta$       | $X_kAX_k$                            | $EAA^{\dagger} + A^{\dagger}AE$                                    |
| $\gamma$      | $X_k(AX_k)^*$                        | $EAA^{\dagger} + A + E^*A^*$                                       |
| $\delta$      | $(X_kA)^*X_k$                        | $A^*E^*A^\dagger + A^\dagger AE$                                   |
| $\varepsilon$ | $(\gamma + \delta - \beta)$          | $A^{\dagger}E^*A^* + A^*E^*A^{\dagger}$                            |
| $\zeta$       | $X_k A X_k (2I - A X_k)$             | $EAA^{\dagger} + A^{\dagger}AE(2I - AA^{\dagger}) - A^{\dagger}AE$ |
| $\eta$        | $(\varepsilon \text{ then } \alpha)$ | 0  |
| $\theta$      | $X_k A X_k (2I - A X_k A X_k)$       | $EAA^{\dagger} - 2A^{\dagger}AEAA^{\dagger} + A^{\dagger}AE$       |

Table 1. Iterative methods from [10]

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 [10]. It is not difficult to verify that Algorithm  $\beta$  from Table 1 is based upon the usage of Equation (2). Algorithm  $\gamma$  uses equations (2) and (3), while Algorithm  $\delta$  uses equations (2) and (4). Algorithm  $\zeta$  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 are investigated as well as the first-order and the second-order terms in error estimates. A comparison with similar iterative algorithms is presented. Numerical results are given in the last section.

## 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 the equations (2), (4) and obtain

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

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

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

or equivalently

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

From the last equation we can formulate the following iterative method

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

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

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

for an appropriate real number  $\beta$ .

The following lemma will be useful in further considerations.

**Lemma 3.1.** For the sequence  $X_k$  generated by the iterative scheme (3.1), (3.2) the following holds

$$X_k A = (X_k A)^*, \quad X A X_k = X_k, \quad X_k A X = X_k, \quad k \ge 0.$$
 (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:

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

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

$$XAX_{k+1} = XA(I - \beta X_k A)^* X_k + \beta XAX_k$$
$$= XAX_k - \beta XAX_k AX_k + \beta XAX_k$$
$$= X_k - \beta X_k AX_k + \beta X_k$$
$$= X_{k+1}.$$

Third statement can be verified in a similar manner:

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

This completes the proof of the lemma.  $\Box$ 

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

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

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

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

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:

$$error_1 = (1 - \beta)E_k, \quad error_2 = -\beta E_k A E_k,$$
 (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

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

Using (3.3) and (3.4) we have

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

Later, taking into account

$$\beta X_k A - XA = \beta (X_k A - XA) - (1 - \beta)XA,$$

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

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

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

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

The last inequality implies that either  $t \ge 1$  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  $||X_k - X|| \le t_k ||X||$ , we conclude  $X_k \to X$  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

$$error_1 = (1 + \beta)E_k - \beta XAE_k - \beta E_kAX,$$
  
 $error_2 = -\beta E_kAE_k.$ 

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

$$error_1 = (1 + \beta)(X_k - X) - \beta X A(X_k - X) - \beta (X_k - X) A X$$
  
=  $(1 - \beta)(X_k - X) = (1 - \beta)E_k$ .

This confirms 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 for  $\beta = 1$ . This completes the proof of the theorem.  $\square$ 

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.** [6] 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 convergence of the iterative method is  $\rho((\beta A^* - X)A) < 1$ . The following lemma shows the one property of the spectral radius function  $\rho$ .

**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 eigenvalues of matrix  $A^*A$  satisfy (1.1). Condition  $\rho((\beta A^* - X)A) < 1$  is satisfied (i.e. the 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

$$PS = \beta X A A^* A - X A = \beta (X A)^* A^* A - X A = \beta (A X A)^* A - X A$$
$$= \beta A^* A - X A = \beta A^* A X A - X A = S P,$$

from Lemma 3.3 we can conclude that

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

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

Denote by  $s_k = ||E_k||$  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

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

*Proof.* From the recurrent relation (3.7):

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

we can conclude that

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

On the other hand, it holds that

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

Previous two inequalities directly implies

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

Since  $t_k = ||E_k A|| \to 0$  (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

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

Previous equation implies

$$1 - \beta - \beta \frac{\|E_k A E_k\|}{\|E_k\|} \le \frac{\|E_{k+1}\|}{\|E_k\|} \le 1 - \beta + \beta \frac{\|E_k A E_k\|}{\|E_k\|}.$$
 (3.12)

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

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

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

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

In the similar way, as in a verifications 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.  $\Box$ 

The following lemma shows one additional property of the sequence  $X_k$ . It will be useful for the consideration on the numerical stability of the 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  $X_0 = \beta A^*$ , statement of the theorem obviously holds for k = 0. Let  $y \in \mathcal{N}(X_k)$  be 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  $\mathcal{N}(X_k) \subseteq \mathcal{N}(X_{k+1})$ . 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 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 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  $X_k y = 0$  and using Theorem 3.1 we have

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

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

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

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

Now 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  $\mathcal{R}(X_k) = \mathcal{R}(A^*)$ .  $\square$ 

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 Shultz 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  $R \in \mathbb{C}_s^{n \times m}$ ,  $0 \le s \le r$  be given. The general iterative scheme used in the paper [12] for iterative computation of  $A_{T,S}^{(2)}$  inverse is given by (1.7), where  $P = I - \beta RA$ ,  $Q = \beta R$  and  $\beta$  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 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, value R in the 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), (1.8) are equal to

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

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

$$0 \le \|error_1'\| \le \left(\max_{1 \le i \le m} |1 - \beta \lambda_i(A^*A)| + \varepsilon\right) \|E_k\|.$$

If (3.10) is satisfied, we can choose  $\epsilon$  such that  $\max_{1 \leq i \leq m} |1 - \beta \lambda_i(A^*A)| + \epsilon < 1$ , 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:

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

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

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

we observed that our method is formally related with 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). Consequence is that the computed value  $\tilde{X}_s$ , in sth iteration, differs from the original value  $X_s$  by error matrix  $\Delta_s$ . Our goal is to consider the propagation of the error  $\Delta_s$  through further iterations. In other words, we consider the same iterative process

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

where  $\tilde{X}_s = X_s + \Delta_s$ . If the matrix A is not of full rank, iterative process (4.1) can diverges. 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, theorem also holds in general case, for 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, 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  $\mathcal{N}(\tilde{X}_s) \subseteq \mathcal{N}(\tilde{X}_s A \tilde{X}_s)$  and  $\operatorname{rank}(\tilde{X}_s A \tilde{X}_s) \leq \operatorname{rank}(A) < \operatorname{rank}\tilde{X}_s$ , we conclude that the inclusion is strict and there exists non-zero vector  $y \in \mathcal{N}(\tilde{X}_s A \tilde{X}_s) \setminus \mathcal{N}(\tilde{X}_s)$ . Then  $\tilde{X}_s A \tilde{X}_s y = 0$  and  $\tilde{X}_s y \neq 0$ .

We prove by mathematical induction that  $\tilde{X}_k y = (1+\beta)^{k-s} \tilde{X}_s y$  and  $\tilde{X}_k A \tilde{X}_k y = 0$  for every  $k \geq s$ . Initial condition k = s is already proven. We assume that the statement holds for some  $k \geq 0$ . 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

$$\tilde{X}_{k+1}A\tilde{X}_{k+1}y = (1+\beta)\tilde{X}_{k+1}A\tilde{X}_{k}y$$

$$= (1+\beta)((1+\beta)\tilde{X}_{k} - \beta\tilde{X}_{k}A\tilde{X}_{k})A\tilde{X}_{k}y$$

$$= (1+\beta)^{2}\tilde{X}_{k}A\tilde{X}_{k}y - (1+\beta)\beta\tilde{X}_{k}A\tilde{X}_{k}A\tilde{X}_{k}y = 0.$$

This finishes the mathematical induction.

Now we directly have

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

where  $c = \|\tilde{X}_s y\|/\|y\| > 0$  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.  $\square$ 

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

## 5 Numerical experience

We implemented 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 rank(A) = 3. Choice  $\beta = 0.075$  satisfies the convergence criterion (3.10), since the eigenvalues of  $A^*A$  are

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

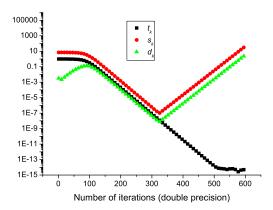
and  $\max_{1 \le i \le 3} |1 - \beta \lambda_i| = 0.998492 < 1$ . The Moore-Penrose inverse  $X = A^{\dagger}$  is equal to

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

We investigated the matrix norms

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

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



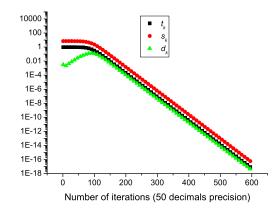


Figure 1: Residual norms  $t_k = ||E_k A|| = ||(X_k - X)A||$ ,  $s_k = ||X_k - X||$  and  $d_k = ||X_{k+1} - X_k||$  through iterations in lin-log scale.

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 experience 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 behavior are 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 on 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  $N_{iter} = 600$  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  $d_k$  has minimum in the same point k=324. On the other hand,  $t_k$  has minimum in 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 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 of 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 given precision  $||X - X_k||/||X|| \le \delta$  (see the recommended number of iterative steps in the relation (2.28) from [12]). Similar calculation are not available for the iterative process used in the present paper since the fixed matrix R from [12] takes variable values, as it is mentioned in Remark 3.2.

## 6 Conclusion

In the literature it is 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 estimates of the Moore-Penrose generalized inverse, using Penrose equations (2) and (4). Convergence properties of the introduced method are considered as well as the formula for their first-order and the second-order error estimates. 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.

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## A Implementation details

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

Function It24C1 takes the matrix A (A) and values  $\beta$  (beta) and  $N_{iter}$  (Niter) as input arguments. It returns the matrix  $X_k$  such that value  $d_k$  (norm) 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];
];</pre>
```

Function It24C2 has the matrix A (A) and values  $\beta$  (beta) and  $\epsilon$  (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 which 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;
   DoΓ
    Xk1 = (1 + beta) Xk - beta*Xk.A.Xk;
    normd = Norm[Xk1 - Xk];
    If [normd < minnormd,</pre>
    minnormd = normd; Xkmin = Xk;
    ];
    If[Abs[normd/normd1 - 1 - beta] < eps,</pre>
     Break[];
    ];
    normd1 = normd;
    Xk = Xk1;
    , {i, 1, Niter}
   ];
   Return[Xkmin];
];
```

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