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Nonnegative Rank Factorization of a Nonnegative Matrix A with $A^{\dagger}A \geq 0$

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In this article we obtain a nonnegative rank factorization of nonnegative matrices A satisfying one or both of the following conditions: (i) $AA^{\dagger} \geq 0$ (ii) $A^{\dagger}A \geq 0$, thus providing a new set of conditions that guarantee the existence of a nonnegative least-squares solution of a linear system. Indeed, the characterization of such matrices improves some of the previous known conditions for the existence of a nonnegative least-squares solution of a linear system.

Keywords: Idempotent matrices; Least-squares solution; Moore–Penrose inverse; Nonnegative rank factorization

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1 INTRODUCTION

A matrix $A = (a_{ij})$ is called nonnegative if $a_{ij} \geq 0$ for all i, j and this is expressed as $A \geq 0$. The ith row of a matrix A is denoted by $A_{(i)}$.

Let A be an $n \times m$ matrix. Consider the Penrose Equations, (1) $AXA = A$, (2) $XAX = X$, (3) $(AX)^T = AX$, (4) $(XA)^T = XA$ where X is an $m \times n$ matrix and T denotes the transpose.

For a rectangular matrix A and for a nonempty subset λ of $\{1, 2, 3, 4\}$, X is called a λ-*inverse* of A if X satisfies Eq. (i) for each $i \in \lambda$. In particular, the $\{1, 2, 3, 4\}$-*inverse* of A is the unique Moore–Penrose generalized inverse and is denoted $A^{\dagger}$. Nonnegative matrices having nonnegative Moore–Penrose inverses have been characterized previously by Berman and Plemmons [2,3]. The motivation of the study of λ-*monotone* matrices, i.e., matrices having a nonnegative λ-*inverse*, has its origin in the question of finding a nonnegative solution of the linear system $AX = B$ (see for example [6–8]), where A and B are $n \times n$ matrices. It is clear that for suitable λ, $A^{(\lambda)} \geq 0$ is simply a

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sufficient condition for the existence of a nonnegative best approximate solution. If B for example is $p(A) = \sum_{i=1}^{n} \alpha_i A^i$, $\alpha_i \geq 0$, then one may weaken the condition for $A^\dagger \geq 0$ to the condition that $A^\dagger A \geq 0$. Furthermore, Corollary 5 shows that if both $AA^\dagger$ and $A^{(1)} \geq 0$, then the linear system $Ax = b$ has a nonnegative least-squares solution; and the class of such matrices A is larger than the class of matrices A with $A^\dagger \geq 0$.

Section 2 establishes the main results. We conclude with an example of a nonnegative matrix A such that $AA^\dagger$ and $A^\dagger A$ are nonnegative, but $A^\dagger$ is not nonnegative (contains negative entries).

2 MAIN RESULTS

We state first the following well-known result due to Flor characterizing nonnegative idempotent matrices.

LEMMA 1 (Flor [5]) *If E is any nonnegative idempotent matrix then there exists a permutation matrix P such that*

$$PEP^T = \begin{bmatrix} J & JB & 0 & 0 \\ 0 & 0 & 0 & 0 \\ CJ & CJB & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where

$$J = \begin{bmatrix} x_1 y_1^T & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x_r y_r^T \end{bmatrix},$$

each x_i, y_i are positive vectors with $y_i^T x_i = 1$, and matrices $B, C \geq 0$ and the zeros in the matrices are zero blocks of appropriate size. In particular, if E is symmetric, then

$$E = \begin{bmatrix} J & 0 \\ 0 & 0 \end{bmatrix},$$

where

$$J = \begin{bmatrix} x_1 x_1^T & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x_r x_r^T \end{bmatrix},$$

each x_i is a positive unit vector.

We now present the decomposition theorem for nonnegative matrices A with $AA^\dagger \geq 0$.

THEOREM 2 *Let A be a nonnegative $n \times n$ matrix of rank r. Then the following are equivalent:*

(i) *There exists an $A^{(1,3)}$ such that $AA^{(1,3)} \geq 0$.*
(ii) *There exists a permutation matrix P such that $PAP^T = FG$,*

where

$$F = \begin{bmatrix} x_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & x_r \\ 0 & \cdots & \cdots & 0 \end{bmatrix},$$

each x_i is a positive unit vector, and the zeros are zero vectors of appropriate size.

$$G = \begin{bmatrix} a_{1_1}^T & \cdots & a_{1_{r+1}}^T \\ \vdots & & \vdots \\ a_{r_1}^T & \cdots & a_{r_{r+1}}^T \end{bmatrix}$$

where each a_{i_j} is a nonnegative vector and $\operatorname{rank} G = r$.

(iii) $AA^\dagger \geq 0$.

Proof (i) $\Rightarrow$ (ii): So, assume there exists an $A^{(1,3)}$ such that $AA^{(1,3)} \geq 0$. Since $AA^{(1,3)}$ is a nonnegative symmetric idempotent, by Lemma 1, we have a permutation matrix P such that

$$PAA^{(1,3)}P^T = \begin{bmatrix} J & 0 \\ 0 & 0 \end{bmatrix}$$

where

$$J = \begin{bmatrix} x_1x_1^T & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x_rx_r^T \end{bmatrix},$$

each x_i is a positive unit vector.

Next, $AA^{(1,3)}A = A$ implies $(PAA^{(1,3)}P^T)(PAP^T) = PAP^T$. We partition PAP^T in conformity with the partitioning of $PAA^{(1,3)}P^T$. So let

$$PAP^T = \begin{bmatrix} A_{11} & \cdots & \cdots & A_{1,r+1} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ A_{r+1,1} & \cdots & \cdots & A_{r+1,r+1} \end{bmatrix}$$

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Then, $(PAA^{(1,3)}P^T)(PAP^T) = PAP^T$, and so,

$$\begin{bmatrix} x_1x_1^T & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & x_rx_r^T & 0 \\ 0 & \cdots & 0 & 0 \end{bmatrix} \begin{bmatrix} A_{11} & \cdots & \cdots & A_{1,r+1} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ A_{r+1,1} & \cdots & \cdots & A_{r+1,r+1} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & \cdots & A_{1,r+1} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ A_{r+1,1} & \cdots & \cdots & A_{r+1,r+1} \end{bmatrix}.$$

Thus, $(PAA^{(1,3)}P^T)(PAP^T) = PAP^T$ yields

$$\begin{bmatrix} x_1x_1^TA_{11} & \cdots & \cdots & x_1x_1^TA_{1,r+1} \\ \vdots & & & \vdots \\ x_rx_r^TA_{r1} & \cdots & \cdots & x_rx_r^TA_{r,r+1} \\ 0 & \cdots & \cdots & 0 \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & \cdots & A_{1,r+1} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ A_{r+1,1} & \cdots & \cdots & A_{r+1,r+1} \end{bmatrix}$$

This gives us $x_ix_i^TA_{ij} = A_{ij}$ for $i \le r$, $j \le r+1$ and $A_{r+1,j} = 0$ for all $j \le r+1$.

Next, we claim that in the block partitioning of PAP^T, for each i there exists j such that $A_{i,j}$ is not zero. We know that rank $PAA^{(1,3)}P^T = \operatorname{rank} A = r$. Write $A_i = [\,x_ix_i^TA_{i1} \quad \cdots \quad \cdots \quad x_ix_i^TA_{i,r+1}\,]$, the ith row in the block partitioning of $PAA^{(1,3)}P^T$. Clearly, rank $A_i \le 1$. If rank $A_i = 0$, then we have rank $A < r$, a contradiction. Thus, rank $A_i = 1$, and this implies that at least one of the $A_{i,j}$ is not zero.

So let us consider the equation $x_1x_1^TA_{11} = A_{11}$. Without loss of generality, assume rank $A_{11} = 1$. Now, rank $A_{11} = 1$ implies that $A_{11} = b_1a_1^T$ where $b_1 \ge 0$ and $a_1 \ge 0$, or $b_1 \le 0$ and $a_1 \le 0$. We may also assume that a_1 is a unit vector. Then by using $x_1x_1^TA_{11} = A_{11}$, we get, $x_1x_1^Tb_1a_1^T = b_1a_1^T \Rightarrow x_1x_1^Tb_1a_1^Ta_1 = b_1a_1^Ta_1 \Rightarrow \lambda_1x_1 = b_1$ where $\lambda_1 = x_1^Tb_1$. So, $A_{11} = \lambda_1x_1a_1^T$ and we define $a_{1_1}^T = \lambda_1a_1^T$. Note that if $b_1 \ge 0$ and $a_1 \ge 0$, then $\lambda_1 \ge 0$, while if $b_1 \le 0$ and $a_1 \le 0$, then $\lambda_1 \le 0$, so in either case, we have that $a_{1_1}^T$ is a nonnegative vector. Then we repeat the same for all equations $x_ix_i^TA_{ij} = A_{ij}$. Thus $A_{ij} = x_ia_{i_j}^T$ where $a_{i_j}^T$ is a nonnegative vector.

Therefore, we have the following:

$$PAP^T = \begin{bmatrix} x_1a_{1_1}^T & \cdots & \cdots & x_1a_{1_{r+1}}^T \\ \vdots & & & \vdots \\ x_ra_{r_1}^T & \cdots & \cdots & x_ra_{r_{r+1}}^T \\ 0 & \cdots & \cdots & 0 \end{bmatrix} = \begin{bmatrix} x_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & x_r \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} a_{1_1}^T & \cdots & a_{1_{r-1}}^T \\ \vdots & & \vdots \\ a_{r_1}^T & \cdots & a_{r_{r-1}}^T \end{bmatrix} = FG \text{ say.}$$

Note that FG is a full-rank factorization of PAP^T. It is clear that rank $F = r$. Furthermore, because rank PAP^T = rank $A = r$, we must have that rank $G \ge r$. However, G only has r rows, so the rank of G must be r. Therefore, we have a nonnegative full-rank factorization of PAP^T. Thus, we have shown (i) $\Rightarrow$ (ii).

Before we prove the next part of the theorem, we make the following remark. As argued above, no row of G is entirely a zero row. Therefore, in each row of G, there is at least one nonzero vector.

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(ii) $\Rightarrow$ (iii): So there exists a permutation matrix P such that $PAP^T = FG$ as above. We will show that $AA^\dagger \geq 0$. Let $B = PAP^T$. Because FG is a full-rank factorization of B, we have $B^\dagger = G^T(F^TBG^T)^{-1}F^T = G^T(F^TFGG^T)^{-1}F^T$. Now

$$F^TF = \begin{bmatrix} x_1^T & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & x_r^T & 0 \end{bmatrix} \begin{bmatrix} x_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & x_r \\ 0 & \cdots & \cdots & 0 \end{bmatrix} = \begin{bmatrix} x_1^Tx_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x_r^Tx_r \end{bmatrix}.$$

Therefore, because each x_i is a unit vector, $x_i^Tx_i = 1$. Hence $F^TF = I_r$, the $r \times r$ identity matrix. So we have $B^\dagger = G^T(GG^T)^{-1}F^T$. We first show that $PAP^TPA^\dagger P^T \geq 0$.

Now, $PAP^TPA^\dagger P^T = BB^\dagger = FGG^T(GG^T)^{-1}F^T = FF^T \geq 0$.

Therefore, $PAA^\dagger P^T \geq 0$. Finally, because P is a permutation matrix, $AA^\dagger \geq 0$, proving (ii) $\Rightarrow$ (iii).

(iii) $\Rightarrow$ (i): Obvious. ■

We now present an example showing that the class of nonnegative matrices A with $AA^\dagger \geq 0$ is not the same as the class of nonnegative matrices A with $A^\dagger A \geq 0$.

Example 3 Consider the matrix

$$A = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

This matrix is of the form described in Theorem 2.

For this matrix,

$$A^\dagger = \begin{bmatrix} \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{1}{3} \\ -\frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} & \frac{2}{3} \\ \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} & \frac{1}{3} \end{bmatrix}.$$

Then we can see that

$$AA^\dagger = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

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while

$$A^{\dagger}A = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{bmatrix}.$$

The characterization of nonnegative matrices A with $A^{\dagger}A \geq 0$ is presented below without proof as the proof is just the dual of the proof of Theorem 2.

THEOREM 4 *Let A be a nonnegative $n \times n$ matrix of rank r. Then the following are equivalent*:

(i) *There exists an $A^{(1,4)}$ such that $A^{(1,4)}A \geq 0$.*
(ii) *There exists a permutation matrix P such that $PAP^T = FG$,*

where

$$F = \begin{bmatrix} a_{1_1} & \cdots & a_{1_r} \\ \vdots & & \vdots \\ a_{r+1_1} & \cdots & a_{r+1_r} \end{bmatrix},$$

each a_{i_j} is a nonnegative vector with rank $F = r$, and

$$G = \begin{bmatrix} x_1^T & 0 & \cdots & 0 & 0 \\ 0 & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & x_r^T & 0 \end{bmatrix},$$

each x_i is a positive unit vector, and the zeros are zero vectors of appropriate size.

(iii) $A^{\dagger}A \geq 0$.

We remark that by considering the transpose of the matrix A in Example 3, we have a nonnegative matrix A with $A^{\dagger}A \geq 0$, but $AA^{\dagger}$ and $A^{\dagger}$ are not nonnegative, thus showing that the the class of nonnegative matrices A with $A^{\dagger}A \geq 0$ is not the same as the class of nonnegative matrices A with $AA^{\dagger} \geq 0$.

In addition, if we know that there exists a nonnegative $A^{(1)}$, then we get the following Corollary.

COROLLARY 5 *Let A be a nonnegative matrix. Under any one of the conditions in Theorem 2, such that G as described in that theorem contains a monomial submatrix of rank r, then the system $Ax = b$, where b is a nonnegative vector, has a nonnegative least-squares solution.*

Proof It is known that a least-squares solution of the linear system $Ax = b$ is given by the consistent linear system $Ax = AA^{(1,3)}b$ (cf. [1], Corollary 1, p. 104). Furthermore, a solution of $Ax = AA^{(1,3)}b$ is given by $x = A^{(1)}AA^{(1,3)}b$ ([1], Theorem 2, p. 40). Now, by Theorem 2, we have that $AA^{(1,3)} \geq 0$, and by the additional hypothesis on G there exists an $A^{(1)} \geq 0$ ([6], Theorem 4.4). Thus, $A^{(1)}AA^{(1,3)}b$ is a nonnegative least-squares solution of the linear system $Ax = b$. ■

To show that the class of matrices described in Corollary 5 is larger than the class of nonnegative matrices A with $A^\dagger \geq 0$, we present the following example.

Example 6 Consider the matrix

$$A = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

which is of the form described in Corollary 5.
For this matrix,

$$A^\dagger = \begin{bmatrix} \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \\ 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & -\frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} \\ -\frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} \end{bmatrix}, \qquad AA^\dagger = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

and

$$A^{(1)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \end{bmatrix},$$

a nonnegative $\{1\}$-inverse of A.

This example illustrates the fact that there exists a nonnegative matrix A such that $AA^\dagger \geq 0$, $A^{(1)} \geq 0$ but $A^\dagger$ is not necessarily nonnegative.

We now characterize nonnegative matrices A with $AA^\dagger \geq 0$ and $A^\dagger A \geq 0$ in the following theorem.

Note that the proof seems very complicated considering that we have already characterized nonnegative matrices A with either $AA^\dagger \geq 0$ or $A^\dagger A \geq 0$. This is due to the factorization not being unique as well as the fact that we would have different permutation matrices in each decomposition.

THEOREM 7 *Let A be a nonnegative $n \times n$ matrix of rank r. Then the following are equivalent:*

(i) *There exists an $A^{(1,3)}$ and an $A^{(1,4)}$ such that $AA^{(1,3)} \geq 0$ and $A^{(1,4)}A \geq 0$.*
(ii) *There exists permutation matrices P and P_1 such that $PAP^T = FG$, where F and G are as in Theorem 2 and we have that*

$$GP_1^T = \begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix} \begin{bmatrix} a'^T_{1_1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a'^T_{1_r} & 0 \end{bmatrix}$$

where each $a'^T_{i_1}$, and z_i are nonnegative vectors and $\begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix}$ is invertible.

(iii) $AA^\dagger \geq 0$ *and* $A^\dagger A \geq 0$.

Proof (i) $\Rightarrow$ (ii): So $AA^{(1,3)} \geq 0$ and $A^{(1,4)}A \geq 0$ for some $A^{(1,3)}$ and $A^{(1,4)}$. By Theorem 2 there exists a permutation matrix P such that $PAP^T = FG$, where

$$F = \begin{bmatrix} x_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & x_r \\ 0 & \cdots & \cdots & 0 \end{bmatrix},$$

each x_i is a positive unit vector, and the zeros are zero vectors of appropriate size.

$$G = \begin{bmatrix} a^T_{1_1} & \cdots & a^T_{1_{r+1}} \\ \vdots & & \vdots \\ a^T_{r_1} & \cdots & a^T_{r_{r+1}} \end{bmatrix}$$

where each a_{i_j} is a nonnegative vector and *rank* $G = r$. Again, let $B = PAP^T$ and so $B^\dagger = G^T(GG^T)^{-1}F^T$, since $F^TF = I$. Therefore, $B^\dagger B = G^T(GG^T)^{-1}F^TFG = G^T(GG^T)^{-1}G$. Now because we have the additional assumption that $A^{(1,4)}A \geq 0$, $B^\dagger B = PA^\dagger P^T PAP^T = PA^\dagger AP^T \geq 0$ also. Furthermore, because $B^\dagger B$ is a symmetric idempotent we have a permutation matrix P_1 such that

$$P_1 B^\dagger B P_1^T = \begin{bmatrix} J_1 & 0 \\ 0 & 0 \end{bmatrix}$$

where

$$J_1 = \begin{bmatrix} x'_1 x'^T_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x'_r x'^T_r \end{bmatrix}$$

each x'_i positive unit vectors. Note the number of (positive) blocks on the diagonal is r because $\operatorname{rank} J_1 = \operatorname{rank} A^\dagger A$.

Now, we also have that

$$P_1 B^\dagger B P_1^T = P_1 G^T (GG^T)^{-1} G P_1^T = P_1 G^T (G P_1^T P_1 G^T)^{-1} G P_1^T.$$

So, let $G_1 = GP_1^T$. Then $P_1 B^\dagger B P_1^T = G_1^T (G_1 G_1^T)^{-1} G_1$.

Consider $P_1 B^\dagger B P_1^T$. Each diagonal block $x'_i x'^T_i$ is rank 1. Let x'_i be an $l_i \times 1$ vector. The rows of $P_1 B^\dagger B P_1^T$ in each of the r sets that contain rows 1 through l_1, rows $l_1 + 1$ through $l_1 + l_2, \ldots,$ rows $l_1 + \cdots + l_{r-1} + 1$ through $l_1 + \cdots + l_r$, are multiples of each other, and the rows $l_1 + \cdots + l_r + 1$ through $l_1 + \cdots + l_{r+1}$ are rows of zeros. Therefore, the same must be true of $G_1^T (G_1 G_1^T)^{-1} G_1$.

Note that, in general, we have for any matrices C, D $(CD)_{(i)} = C_{(i)} D$ where $X_{(i)}$ denotes the ith row of matrix X. Therefore, we have the following:

$(G_1^T (G_1 G_1^T)^{-1} G_1)_{(i)} = (G_1^T)_{(i)} ((G_1 G_1^T)^{-1} G_1)$ for all i. And, we know that the second row is a multiple of the first, so we have that $(G_1^T (G_1 G_1^T)^{-1} G_1)_{(2)} = \lambda_2 (G_1^T (G_1 G_1^T)^{-1} G_1)_{(1)}$ for some positive number λ_2.

Therefore, we have that $(G_1^T)_{(2)} ((G_1 G_1^T)^{-1} G_1) = (G_1^T (G_1 G_1^T)^{-1} G_1)_{(2)} = \lambda_2 (G_1^T (G_1 G_1^T)^{-1} \times G_1)_{(1)} = \lambda_2 (G_1^T)_{(1)} ((G_1 G_1^T)^{-1} G_1)$.

Thus, we get $(G_1^T)_{(2)} ((G_1 G_1^T)^{-1} G_1) = \lambda_2 (G_1^T)_{(1)} ((G_1 G_1^T)^{-1} G_1)$, and so we multiply both sides of this equation by G_1^T on the right to get that $(G_1^T)_{(2)} = \lambda_2 (G_1^T)_{(1)}$. Continuing this process we obtain that the rows in each of the r sets consisting of rows 1 through l_1, rows $l_1 + 1$ through $l_1 + l_2, \ldots,$ rows $l_1 + \cdots + l_{r-1} + 1$ through $l_1 + \cdots + l_r$, of G_1^T are multiples of each other.

Also, we know that the last l_{r+1} rows of $P_1 B^\dagger B P_1^T$ are rows of zeros, and exactly as above, we get that the last l_{r+1} rows of G_1^T are rows of zeros.

This gives us that

$$G_1^T = \begin{bmatrix} a'_{1_1} & \cdots & a'_{r_1} \\ \vdots & & \vdots \\ a'_{1_r} & \cdots & a'_{r_r} \\ 0 & \cdots & 0 \end{bmatrix}.$$

Therefore, the rows of the submatrix $[a'_{1_i} \quad a'_{2_i} \quad \cdots \quad a'_{r_i}]$ are multiples of each other, $1 \le i \le r$. Hence, we have $\operatorname{rank}\, [a'_{1_i} \quad a'_{2_i} \quad \cdots \quad a'_{r_i}] = 1$. Therefore, we have that the columns of $[\,a'_{1_i} \quad a'_{2_i} \quad \cdots \quad a'_{r_i}\,]$ are all multiples of a nonzero column. For convenience, let us assume $a'_{1_i} \neq 0$. Then

$$[\,a'_{1_i} \quad a'_{2_i} \quad \cdots \quad a'_{r_i}\,] = [\,a'_{1_i} \quad \beta_{2i}a'_{1_i} \quad \cdots \quad \beta_{ri}a'_{1_i}\,] = a'_{1_i}[\,1 \quad \beta_{2i} \quad \cdots \quad \beta_{ri}\,]$$

where the β_{ji} are nonnegative real numbers. Note that some of them could be zero. So, let $z_i^T = [\,1 \quad \beta_{2i} \quad \cdots \quad \beta_{ri}\,]$ and then we have that each z_i is an $r \times 1$ vector and

$$P_1 G^T = G_1^T = \begin{bmatrix} a'_{1_1} z_1^T \\ \vdots \\ a'_{1_r} z_r^T \\ 0 \end{bmatrix}$$

where the zero is a zero block of appropriate size.

So we can rewrite this as

$$GP_1^T = [\,z_1 \quad \cdots \quad z_r\,] \begin{bmatrix} a'^T_{1_1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a'^T_{1_r} & 0 \end{bmatrix}.$$

Now we need only to show that $[\,z_1 \quad \cdots \quad z_r\,]$ is invertible. We know that $B^\dagger = G^T(GG^T)^{-1}F^T = B^\dagger = G^T(GP_1^T P_1 G^T)^{-1}F^T$.

Now,

$$GP_1^T P_1 G^T = [\,z_1 \quad \cdots \quad z_r\,] \begin{bmatrix} a'^T_{1_1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a'^T_{1_r} & 0 \end{bmatrix} \begin{bmatrix} a'_{1_1} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & a'_{1_r} \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} z_1^T \\ \vdots \\ z_r^T \end{bmatrix}$$

$$= [\,z_1 \quad \cdots \quad z_r\,] \begin{bmatrix} \left\| a'_{1_1} \right\|^2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \left\| a'_{1_r} \right\|^2 \end{bmatrix} \begin{bmatrix} z_1^T \\ \vdots \\ z_r^T \end{bmatrix}.$$

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We know that this product is invertible. Each matrix in the product is an $r \times r$ matrix. So the product is an $r \times r$ matrix that is invertible, and hence the product has rank r. But then each matrix in the product has rank $\geq r$, and so each matrix is of rank r. But then, each matrix is invertible. Specifically, $\begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix}$ is invertible. So we have proved (i) $\Rightarrow$ (ii).

(ii) $\Rightarrow$ (iii): By invoking Theorem 2 we have $AA^\dagger \geq 0$. Thus we need only to show that $A^\dagger A \geq 0$. To prove this, we will show that $P_1 P A^\dagger A P^T P_1^T \geq 0$.

First, notice that $PA^\dagger AP^T = G^T(GG^T)^{-1}G$.

Next we compute

$$P_1 P A^\dagger A P^T P_1^T = P_1 G^T (G P_1^T P_1 G^T)^{-1} G P_1^T$$

$$= P_1 G^T \left[\begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix} \begin{bmatrix} \|a'_{1_1}\|^2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \|a'_{1_r}\|^2 \end{bmatrix} \begin{bmatrix} z_1^T \\ \vdots \\ z_r^T \end{bmatrix} \right]^{-1} G P_1^T$$

$$= \begin{bmatrix} a'_{1_1} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & a'_{1_r} \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} z_1^T \\ \vdots \\ z_r^T \end{bmatrix} \begin{bmatrix} z_1^T \\ \vdots \\ z_r^T \end{bmatrix}^{-1} \begin{bmatrix} \frac{1}{\|a'_{1_1}\|^2} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \frac{1}{\|a'_{1_r}\|^2} \end{bmatrix}$$

$$\begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix}^{-1} \begin{bmatrix} z_1 & \cdots & z_r \end{bmatrix} \begin{bmatrix} a'^T_{1_1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a'^T_{1_r} & 0 \end{bmatrix}$$

$$= \begin{bmatrix} a'_{1_1} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \vdots & & \ddots & a'_{1_r} \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\|a'_{1_1}\|^2} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \frac{1}{\|a'_{1_r}\|^2} \end{bmatrix} \times \begin{bmatrix} a'^T_{1_1} & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a'^T_{1_r} & 0 \end{bmatrix}.$$

In this product, all of the matrices are nonnegative, and so the product is nonnegative. Thus, we have shown that $P_1PA^{\dagger}AP^TP_1^T \geq 0$ and hence, $A^{\dagger}A \geq 0$. Proving (ii) $\Rightarrow$ (iii).

(iii) $\Rightarrow$ (i): Obvious. ■

We conclude this section with an example that shows that the class of matrices characterized in Theorem 7 is in fact strictly larger than the class of nonnegative matrices A having $A^{\dagger} \geq 0$.

Example 8 Consider the matrix

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

For this matrix,

$$A^{\dagger} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

which has negative entries. However, it is easily verified that

$$AA^{\dagger} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and

$$A^{\dagger}A = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

both of which are nonnegative.

This example is of interest for another reason. We find that $AA^{\dagger}$ and $A^{\dagger}A$ are nonnegative, with decompositions as a direct sum of three and two blocks of Type *I* respectively. Whereas $AA^{\dagger}$ is a direct sum of three blocks, [1], [1] and [0], $A^{\dagger}A$ is a direct sum of two blocks,

$$\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

and [1].

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