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THE GENERALIZED INVERSE OF A NONNEGATIVE MATRIX

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ABSTRACT. Necessary and sufficient conditions are given in order that a nonnegative matrix have a nonnegative Moore-Penrose generalized inverse.

1. **Introduction.** Let A be an arbitrary $m \times n$ real matrix. Then the *Moore-Penrose generalized inverse* of A is the unique $n \times m$ real matrix A^+ satisfying the equations

$$A = AA^+A, \qquad A^+ = A^+AA^+,$$
$$(AA^+)^T = AA^+, \quad \text{and} \quad (A^+A)^T = A^+A.$$

The properties and applications of A^+ are described in a number of papers including Penrose [7], [8], Ben-Israel and Charnes [1], Cline [2], and Greville [6]. The main value of the generalized inverse, both conceptually and practically, is that it provides a solution to the following least squares problem: *Of all the vectors x which minimize $\|b - Ax\|$, which has the smallest* $\|x\|^2$? The solution is $x = A^+b$.

If A is nonnegative (written $A \geqq 0$), that is, if the components of A are all nonnegative real numbers, then A^+ is not necessarily nonnegative. In particular, if $A \geqq 0$ is square and nonsingular, then $A^+ = A^{-1} \geqq 0$ if and only if A is monomial, i.e., A can be expressed as a product of a diagonal matrix and a permutation matrix, so that $A^{-1} = DA^T$ for some diagonal matrix D with positive diagonal elements. The main purpose of this paper is to give necessary and sufficient conditions on $A \geqq 0$ in order that $A^+ \geqq 0$. Certain properties of such nonnegative matrices are then derived.

2. **Results.** In order to simplify the discussion to follow, it will be convenient to introduce a canonical form for a nonnegative symmetric

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idempotent matrix. Flor [5] has shown that if E is any nonnegative idempotent matrix of rank r, then there exists a permutation matrix P such that

$$PEP^T = \begin{pmatrix} J & JB & 0 & 0 \\ 0 & 0 & 0 & 0 \\ AJ & AJB & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

where A and B are arbitrary nonnegative matrices of appropriate sizes and

$$J = \begin{pmatrix} J_1 & & & 0 \\ & \cdot & & \\ & & \cdot & \\ & & & \cdot \\ 0 & & & J_r \end{pmatrix}$$

with each J_r a nonnegative idempotent matrix of rank 1. This gives the following lemma.

LEMMA 1. *Let $E \geqq 0$ be a symmetric idempotent matrix of rank r with q nonzero rows. Then there exists integers $\lambda_1, \cdots, \lambda_r$ and a permutation matrix P such that $q = \lambda_1 + \cdots + \lambda_r$ and such that PEP^T has the form*

$$(1) \qquad PEP^T = \left(\begin{array}{cccc|c} J_1 & & & 0 & \\ & \cdot & & & \\ & & \cdot & & 0 \\ & & & \cdot & \\ 0 & & & J_r & \\ \hline & & 0 & & 0 \end{array}\right)$$

where each J_i is a $\lambda_i \times \lambda_i$ positive idempotent matrix of rank 1.

The main result is given next. The theorem characterizes $A \geqq 0$ so that $A^+ \geqq 0$, and its proof indicates a method by which such an A^+ can be constructed readily.

THEOREM 1. *Let A be an $m \times n$ nonnegative matrix of rank r. Then the following statements are equivalent.*

(i) *A^+ is nonnegative.*

(ii) *There exists a permutation matrix P such that PA has the form*[2]

$$PA = \begin{pmatrix} B_1 \\ \cdot \\ \cdot \\ \cdot \\ B_r \\ 0 \end{pmatrix} \tag{2}$$

where each B_i has rank 1 and where the rows of B_i are orthogonal to the rows of B_j whenever $i \neq j$.

(iii) *$A^+ = DA^T$ for some diagonal matrix D with positive diagonal elements.*

PROOF. Suppose (i) holds so that A, $A^+ \geqq 0$. Since $E = AA^+$ is a symmetric idempotent, there exists a permutation matrix P so that $K = PEP^T$ has the form (1). Let $B = PA$. Then $B^+ = A^+P^T$, $BB^+ = K$, $KB = B$, and $B^+K = B^+$. Now B can be partitioned into the form (2), where r is the rank of A and where each B_i, $1 \leqq i \leqq r$, is a $\lambda_i \times n$ matrix with no zero rows, since A and B have the same number of nonzero rows. It remains to show each B_i has rank 1 and $B_iB_j^T = 0$, for $1 \leqq i \neq j \leqq r$. Let $C = B^+$. Then C can be partitioned into the form

$$C = (C_1, \cdots, C_r, 0)$$

where, for $1 \leqq i \leqq r$, C_i is an $n \times \lambda_i$ matrix with no zero columns. Moreover, since CB is symmetric, a column of B is nonzero if and only if the corresponding row of C is nonzero. Now $KB = B$ implies that $J_iB_i = B_i$, so that B_i has rank 1, for $1 \leqq i \leqq r$. It remains to show that the rows of B_i are orthogonal to the rows of B_j for $i \neq j$. Since $BC = K$ has the form (1),

$$\begin{aligned} B_iC_j &= J_i, \quad \text{if} \quad i = j, \quad \text{and} \\ &= 0, \quad \text{if} \quad i \neq j, \end{aligned}$$

for $1 \leqq i, j \leqq r$. Suppose the lth column of B_i is nonzero. Then $B_iC_k = 0$ for $k \neq i$ implies that the lth row of C_k is zero. However, since the lth row of C is nonzero, the lth row of C_i is nonzero. In this case, the lth column of B_k is zero for all $k \neq i$, since $B_kC_i = 0$. Thus

$$B_iB_j^T = 0 \quad \text{for all} \quad 1 \leqq i \neq j \leqq r,$$

and (ii) is established.

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[2] Note that the zero block may not be present.

Now assuming (ii) holds, let $B = PA$ have the form (2). Then for $1 \leqq i \leqq r$, there exist column vectors x_i, y_i such that $B_i = x_i y_i^T$. Furthermore, B_i^+ is the nonnegative matrix

$$B_i^+ = (\|x_i\|^2 \, \|y_i\|^2)^{-1} B_i^T$$

and moreover $B^+ = (B_1^+, \cdots, B_r^+, 0)$, since $B_i B_j^T = 0$ for $i \neq j$. In particular then, $B^+ = DB^T$ where D is a diagonal matrix with positive diagonal elements and thus $A^+ = DA^T$, yielding (iii).

Clearly (iii) implies (i) so the proof is complete.

The next theorem considers doubly stochastic matrices, that is, square matrices $B \geqq 0$ whose row sums and column sums are 1. The matrix $A \geqq 0$ is said to be diagonally equivalent to a doubly stochastic matrix if there exist diagonal matrices D_1 and D_2 such that $D_1 A D_2$ is doubly stochastic. Classes of nonnegative matrices with this property have been the subject of several recent papers (for example, see Djoković **[4]**). Part of the following theorem identifies another such class.

THEOREM 2. *Let $A \geqq 0$ be square with no zero rows or columns. If $A^+ \geqq 0$ then A is diagonally equivalent to a doubly stochastic matrix. Moreover, if A is doubly stochastic then A^+ is doubly stochastic if and only if the equation $A = AXA$ has a doubly stochastic solution, in which case $A^+ = A^T$.*

PROOF. The first statement follows since there exist permutation matrices P and Q such that

$$PAQ = \begin{pmatrix} B_1 & & 0 \\ & \ddots & \\ 0 & & B_r \end{pmatrix}$$

where each B_i is a positive square matrix.

For the second statement note that a doubly stochastic idempotent matrix E is necessarily symmetric; for in particular, there exists a permutation matrix P such that PEP^T has the form (1), where each row and column is nonzero and where each J_i is a positive, idempotent doubly stochastic matrix of rank 1. Then each entry of J_i is $1/\lambda_i$ so that PEP^T and, accordingly, E are symmetric matrices. This means that A^+ is the only possible doubly stochastic solution to the equations $A = AYA$ and $Y = YAY$, since AY and YA are symmetric and A^+ is unique. Thus A^+ is doubly stochastic if and only if $A = AXA$ has a doubly stochastic solution, in which case $A^+ = XAX$, and so $A^+ = A^T$ by Theorem 1.

The final result determines the singular values of A (i.e., the positive square roots of the nonzero eigenvalues of $A^T A$) whenever $A^+ \geqq 0$.

THEOREM 3. *Let $A \geqq 0$ be an $m \times n$ real matrix with $A^+ \geqq 0$ and let PA have the form* (2). *Let $\{x_i, y_i\}_{i=1}^r$ be column vectors so that $B_i = x_i y_i^T$ for $1 \leqq i \leqq r$. Then the singular values of A are the numbers $\|x_i\| \cdot \|y_i\|$.*

PROOF. The eigenvalues of AA^T are the eigenvalues of BB^T. But these are the eigenvalues of the matrices $B_i B_i^T$ for $1 \leqq i \leqq r$, that is, the numbers $\|x_i\|^2 \cdot \|y_i\|^2$.

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