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Sufficient conditions to be exceptional

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Abstract: A copositive matrix A is said to be exceptional if it is not the sum of a positive semidefinite matrix and a nonnegative matrix. We show that with certain assumptions on A^{-1}, especially on the diagonal entries, we can guarantee that a copositive matrix A is exceptional. We also show that the only 5-by-5 exceptional matrix with a hollow nonnegative inverse is the Horn matrix (up to positive diagonal congruence and permutation similarity).

Keywords: copositive matrix; positive semidefinite; nonnegative matrix; exceptional copositive matrix; irreducible matrix

MSC: 15A18, 15A48, 15A57, 15A63

1 Introduction

All of the matrices considered will be symmetric matrices with real entries. We will say a matrix is a *nonnegative matrix* if all of its entries are nonnegative, and likewise for a vector. A symmetric matrix $A \in \mathbf{R}^{n\times n}$ is *positive semidefinite* (*positive definite*) if $x^TAx \geq 0$ for all $x \in \mathbf{R}^n$ ($x^TAx > 0$ for all $x \in \mathbf{R}^n$, $x \neq 0$). A symmetric matrix $A \in \mathbf{R}^{n\times n}$ is called *copositive* (*strictly copositive*) if $x^TAx \geq 0$ for all $x \in \mathbf{R}^n$, $x \geq 0$ ($x^TAx > 0$ for all $x \in \mathbf{R}^n$, $x \geq 0$, $x \neq 0$). We will let $e_i \in \mathbf{R}^n$ denote the vector with ith component one and all other components zero. A *permutation matrix* is an n-by-n matrix whose columns are $e_1, \ldots, e_n$ in some order. For $n \geq 2$, an n-by-n matrix is said to *irreducible* [9] if under similarity by a permutation matrix, it cannot be written in the form

$$\begin{pmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{pmatrix},$$

with A_{11} and A_{22} square matrices of order less than n. We call an n-by-n matrix *hollow* if all of its diagonal entries are zero.

2 When the inverse is nonnegative and hollow

The results in this paper grew out of a question that arose from studying symmetric, nonnegative, hollow, invertible matrices in [4]. Theorem 1, despite its short proof and the fact that we will extend it in Section 3, is the core theorem of this paper.

Theorem 1. *Suppose $A \in \mathbf{R}^{n\times n}$ is symmetric, invertible, and that A^{-1} is nonnegative and hollow. If A is of the form $A = P + N$, with P positive semidefinite and N nonnegative, then P is zero.*

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Proof The assumption $e_i^T A^{-1} e_i = 0$, for all i, $1 \le i \le n$, can be rewritten $e_i^T A^{-1} A A^{-1} e_i = 0$. Then if $A = P + N$, this implies $0 = e_i^T A^{-1}(P+N)A^{-1}e_i = e_i^T A^{-1} P A^{-1} e_i + e_i^T A^{-1} N A^{-1} e_i$, and so $0 = e_i^T A^{-1} P A^{-1} e_i$, for all i, $1 \le i \le n$. Letting $x_i = A^{-1}e_i$, we have $x_i^T P x_i = 0$, for all i, $1 \le i \le n$, but then $Px_i = 0$, for all i, so $P = 0$. □

The conclusion of Theorem 1, stated as "For P nonzero, then A is not of the form $P + N$", is where our main interest lies. In this contrapositive form, we note that A being copositive is not an assumption of the theorem. Diananda [7] proved that for $n = 3$, and $n = 4$, copositivity coincides with being of the form $P + N$. So from Theorem 1 if A^{-1} is any 3-by-3 or 4-by-4 hollow, nonnegative matrix then A cannot be copositive with P nonzero when written as $P + N$. An example of a matrix meeting the hypotheses of Theorem 1 is $A = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$. If instead A^{-1} is the matrix $\begin{pmatrix} 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & 1 \\ \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 1 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 \end{pmatrix}$, then $A = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}$. Here, not only is A not of the form $P + N$, it is not copositive either (note the central 3-by-3 block).

A copositive matrix, known as the Horn matrix, is

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}, \text{ for which } H^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix}.$$

An example suggesting we cannot improve on Theorem 1 by having $n - 1$ zero diagonal entries, is $A^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$. Then $A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$, which is of the form $P + N$.

It would also appear to be not possible to improve on Theorem 1 by A^{-1} having all zero diagonal entries and not requiring A^{-1} to be nonnegative, by considering $A^{-1} = \frac{1}{2}\begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$, for which $A = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$, and this is also of the form $P + N$.

The following theorem is well-known (See [6], or Lemma 1.1 of [14]).

Theorem 2. *Suppose $A \in \mathbf{R}^{n\times n}$ is invertible. Both A and A^{-1} are nonnegative if and only if A is the product of a permutation matrix and a diagonal matrix with positive diagonal entries.*

Since Theorem 1 is only concerned with symmetric matrices, Theorems 1 and 2 imply that the only way an invertible matrix A of the form $A = P + N$, can have all zeroes on the diagonal of its nonnegative inverse is if $P = 0$, n is even, and A consists of blocks on the diagonal of A, in which each diagonal block is a product of a symmetric permutation matrix and a positive diagonal matrix.

A simple observation is that if P is a positive semidefinite matrix and N is nonnegative, then $A = P+N$ is a copositive matrix. It is well-known (see [7], [8], [10], [12]) that copositive matrices do not have to be of this form, an example of which is the 5-by-5 matrix H (from above) that we called the Horn matrix in [12]. In fact the Horn matrix is extreme [10], i.e. it cannot be written nontrivially as the convex sum of two copositive matrices. In [12] we called copositive matrices *exceptional* if they are not the trivial sum of a positive semidefinite matrix and a nonnegative matrix. Otherwise, we call them *non-exceptional*.

The proof of Theorem 3 will use the property proved in [11] (or see [13], [15]) that for any copositive matrix A, if $x \ge 0$ and $x^T A x = 0$, then $Ax \ge 0$. In [2], [3], Baumert studied copositive matrices that had a weak form of extremity, namely, copositive matrices that are not of the form $C + N$ (nontrivially), in which C is copositive, and N is nonnegative with all zeroes on its diagonal. Baumert gave a characterization for such matrices in

[1], which included an error, later corrected in [5]. In [5], the authors called such matrices *irreducible with respect to the nonnegative cone*. Obviously, if a matrix is not of the form $C+N$, then it is not of the form $P+N$. For Theorem 3 we need the assumption that $n \geq 3$, since in the proof we will write A^{-1} in block form with a specified $(1,2)$ entry, as well as another nonzero column to the right of it.

Theorem 3. *For $n \geq 3$, suppose that $A \in \mathbf{R}^{n\times n}$ is symmetric, irreducible, invertible, and A^{-1} is nonnegative and hollow. If A is of the form $C+N$, in which C is copositive and N is nonnegative and hollow, then N is zero.*

Proof Our method of proof will be to show, with the stated assumptions, that if $A = C+N$, we must have that N is diagonal and therefore $N = 0$.

We proceed now to show that N is diagonal. Choose a permutation matrix R, so that if N has a nonzero off-diagonal entry n_{ij}, we have n_{ij} in the $(1,2)$ position of R^TNR. In other words, we may assume $n_{12} \neq 0$. We know A is irreducible if and only if A^{-1} is irreducible. Write the nonnegative matrix $B = A^{-1}$ partitioned into block form as $A^{-1} = \begin{pmatrix} B_1 & B_2 \\ B_2^T & B_3 \end{pmatrix}$, with B_1 as a 2-by-2 matrix and the other blocks of conforming dimensions. Next, let Q be the permutation matrix given by $Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \oplus Q_1$, in which Q_1 is an $(n-2)$-by-$(n-2)$ permutation matrix chosen so that

$$Q^TA^{-1}Q = Q^T\begin{pmatrix} B_1 & B_2 \\ B_2^T & B_3 \end{pmatrix}Q = \begin{pmatrix} B_1 & B_2Q_1 \\ Q_1^TB_2^T & Q_1^TB_3Q_1 \end{pmatrix},$$

has a nonzero last column in the top right 2-by-$(n-2)$ block matrix B_2Q_1. If it is not possible to choose Q_1 in this way, it would imply A^{-1} was reducible. In other words, with $B = (b_{ij})$, $1 \leq i, j \leq n$, we may assume $b_{1n} \neq 0$ or $b_{2n} \neq 0$ (or both).

Now write Q^TAQ in block form as $Q^TAQ = \begin{pmatrix} C_1+N_1 & a \\ a^T & a_{nn} \end{pmatrix}$, in which C_1 and N_1 are $(n-1)$-by-$(n-1)$ and a is $(n-1)$-by-1, with C_1 copositive, and N_1 a nonnegative matrix. Further, write $Q^TA^{-1}Q$ in block form, although in a different way than earlier, as $Q^TA^{-1}Q = \begin{pmatrix} D & b \\ b^T & 0 \end{pmatrix}$, in which b is $(n-1)$-by-1, and D is $(n-1)$-by-$(n-1)$.

Then

$$\begin{pmatrix} C_1+N_1 & a \\ a^T & a_{nn} \end{pmatrix}\begin{pmatrix} D & b \\ b^T & 0 \end{pmatrix} = \begin{pmatrix} I_{n-1} & 0 \\ 0 & 1 \end{pmatrix},$$

implies $(C_1+N_1)b = 0$. It follows that $C_1b = -N_1b$, and then since N_1 and b are nonnegative we have $b^TC_1b = -b^TN_1b \leq 0$. But this implies $b^TC_1b = 0$. Then $C_1b \geq 0$, from the property mentioned in the paragraph before the theorem, and so $N_1b = 0$.

However, N_1b is the $(n-1)$-by-1 matrix with first two components $n_{11}b_{1n}+n_{12}b_{2n}+\cdots = 0$ and $n_{12}b_{1n}+n_{22}b_{2n}+\cdots = 0$. Since all entries of N_1 and b are nonnegative, this forces $n_{12} = 0$, which is a contradiction. □

Thus, the only way a copositive matrix A can satisfy the assumptions of Theorem 3 is for A to be "irreducible with respect to the nonnegative hollow cone". Again, the Horn matrix provides an example of such a matrix.

3 Extending Theorem 1

Our next theorem (and its proof) reduces to Theorem 1 when the matrix B of Theorem 4 is the identity matrix. Theorem 4 improves on Theorem 1, since the signs of the entries, including the diagonal entries, of A^{-1} are not restricted to being nonnegative. This may be seen from the examples of exceptional matrices from [11] and [12] following the theorem.

Theorem 4. *Let $A \in \mathbf{R}^{n\times n}$ be symmetric and invertible. Suppose there exists an invertible matrix $B \in \mathbf{R}^{n\times n}$ such that $A^{-1}B$ is nonnegative, and $B^TA^{-1}B$ is hollow. If A is of the form $A = P + N$, with P positive semidefinite and N nonnegative, then P is zero. Moreover, whether or not A is of the form $P + N$, if A is copositive then B is nonnegative.*

Proof Suppose A can be written as $A = P + N$, with P positive semidefinite and N nonnegative. Then, with the assumptions on the matrix B, and letting $A^{-1}B = C$ we have for each i, $1 \le i \le n$, $0 = e_i^TB^TA^{-1}Be_i = e_i^TB^TA^{-1}AA^{-1}Be_i = e_i^TC^TACe_i = e_i^TC^T(P+N)Ce_i = e_i^TC^TPCe_i + e_i^TC^TNCe_i$. This implies for each i, $0 = e_i^TC^TPCe_i$. Then $PCe_i = 0$ for all i, so $P = 0$.

For the "Moreover" part of the statement of the theorem, since for each i we have $e_i^TC^TACe_i = 0$, and A is copositive, then $ACe_i \ge 0$, from the property of copositive matrices stated in Section 2. Therefore $B = AC \ge 0$. □

An example of a matrix A to illustrate Theorem 4 is the Hoffman-Pereira matrix [11], as we called it in [12], which is copositive. This exceptional A along with its inverse is

$$A = \begin{pmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{pmatrix}, A^{-1} = \begin{pmatrix} -1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & -1 \end{pmatrix},$$

and the corresponding B, $A^{-1}B$ and $B^TA^{-1}B$ of Theorem 4 are

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}, \quad A^{-1}B = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

and

$$B^TA^{-1}B = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}.$$

Another illustration of the same theorem is the 7-by-7 extension of the Horn matrix given in [12], which is the exceptional matrix A, along with A^{-1} given by

$$A = \begin{pmatrix} 1 & -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 & -1 & 1 \end{pmatrix}, A^{-1} = \frac{1}{6}\begin{pmatrix} 2 & -1 & -1 & 2 & 2 & -1 & -1 \\ -1 & 2 & -1 & -1 & 2 & 2 & -1 \\ -1 & -1 & 2 & -1 & -1 & 2 & 2 \\ 2 & -1 & -1 & 2 & -1 & -1 & -1 \\ 2 & 2 & -1 & -1 & 2 & -1 & -1 \\ -1 & 2 & 2 & -1 & -1 & 2 & -1 \\ -1 & -1 & 2 & 2 & -1 & -1 & 2 \end{pmatrix},$$

for which

$$B=\begin{pmatrix}1&0&0&0&0&1&1\\1&1&0&0&0&0&1\\1&1&1&0&0&0&0\\0&1&1&1&0&0&0\\0&0&1&1&1&0&0\\0&0&0&1&1&1&0\\0&0&0&0&1&1&1\end{pmatrix},\qquad A^{-1}B=\frac{1}{2}\begin{pmatrix}0&0&1&1&0&0&0\\0&0&0&1&1&0&0\\0&0&0&0&1&1&0\\0&0&0&0&0&1&1\\1&0&0&0&0&0&1\\1&1&0&0&0&0&0\\0&1&1&0&0&0&0\end{pmatrix},$$

and

$$B^TA^{-1}B=\frac{1}{2}\begin{pmatrix}0&0&2&1&1&2&0\\0&0&0&2&1&1&2\\2&0&0&0&2&1&1\\1&2&0&0&0&2&1\\1&1&2&0&0&0&2\\2&1&1&2&0&0&0\\0&2&1&1&2&0&0\end{pmatrix}.$$

Using similar reasoning to that given in Theorem 8 of [12] we also have Theorem 5.

Theorem 5. *For $n \geq 3$, let $A \in \mathbf{R}^{n\times n}$ be symmetric, invertible, with A^{-1} nonnegative, and with A^{-1} having three zero diagonal entries such that all entries are positive in the rows and columns of these three zero diagonal entries. If A is of the form $C + N$, with C copositive and N nonnegative, then N is zero.*

Proof Suppose $0 = e_i^T A^{-1} e_i$, for $i = 1, 2, 3$. Then, as in the proof of Theorem 1, we have when $i = 1$ that $0 = e_1^T A^{-1} N A^{-1} e_1$, which means that the $(n-1)$ -by-$(n-1)$ block of N obtained by deleting row and column 1 is zero. Arguing in the same way for $i = 2$, and $i = 3$, we have that $N = 0$. □

4 The 5-by-5 case

In this section, we will use a theorem from [5], which we state as Theorem 6, to show that the only 5-by-5 exceptional matrix with a hollow nonnegative inverse is the Horn matrix, up to positive diagonal congruence and permutation similarity.

Let

$$S=\begin{pmatrix}1&-\cos\theta_1&\cos(\theta_1+\theta_2)&\cos(\theta_4+\theta_5)&-\cos\theta_5\\-\cos\theta_1&1&-\cos\theta_2&\cos(\theta_2+\theta_3)&\cos(\theta_5+\theta_1)\\\cos(\theta_1+\theta_2)&-\cos\theta_2&1&-\cos\theta_3&\cos(\theta_3+\theta_4)\\\cos(\theta_4+\theta_5)&\cos(\theta_2+\theta_3)&-\cos\theta_3&1&-\cos\theta_4\\-\cos\theta_5&\cos(\theta_5+\theta_1)&\cos(\theta_3+\theta_4)&-\cos\theta_4&1\end{pmatrix}.$$

Theorem 6 appears at the end of [5], where they use $\mathcal{C}^5$, $\mathcal{S}^5_+$ and $\mathcal{N}^5$, respectively, to denote the copositive, positive semidefinite, and nonnegative matrices, in $\mathbf{R}^{5\times 5}$.

Theorem 6. *Let $A \in \mathcal{C}^5 - (\mathcal{S}^5_+ + \mathcal{N}^5)$. Then, up to permutation similarity and positive diagonal congruence, A can be written as $A = S + N$, for some hollow $N \in \mathcal{N}^5$, where $\theta_i \geq 0$, for $1 \leq i \leq 5$, and $\sum_{i=1}^5 \theta_i < \pi$.*

Let now A be a 5-by-5 exceptional matrix that has a hollow nonnegative inverse. Theorem 6 implies that, up to permutation similarity and positive diagonal congruence, A can be written as $A = S + N$, where N is hollow and nonnegative. We would like to apply Theorem 3, but we need to first check that A is irreducible. If A is reducible, it is permutation similar to a matrix with irreducible diagonal blocks. We note that if A is reducible this does not necessarily imply S is reducible. If A had a 1-by-1 diagonal block (under permutation similarity), then its inverse could not be hollow. If A had a 2-by-2 diagonal block, then this 2-by-2 block, when inverted, must be nonnegative with both diagonal entries being zero. Then the (not inverted) 2-by-2 block of A would also be nonnegative with both diagonal entries being zero, but S has all ones on the diagonal, in which case we could not have $A = S + N$ (under permutation similarity or positive diagonal congruence). Now applying Theorem 3, since A has a hollow nonnegative inverse, we know that $N = 0$. We next determine the values of the θ_i's, for $1 \le i \le 5$, that ensure S has a hollow inverse. In effect, we will show that the θ_i's are all equal to zero, whereupon S becomes the Horn matrix. Let us examine the 4-by-4 principal minors of S.

A computer algebra system can used to show that the top left 4-by-4 principal minor of S, namely $\det(S[1,2,3,4])$, satisfies

$$\det(S[1,2,3,4]) = -\Big[\cos(\theta_1+\theta_2+\theta_3)+\cos(\theta_4+\theta_5)\Big]^2 \sin^2\theta_2.$$

Suppose now that $\det(S[1,2,3,4]) = 0$. If $0 = \cos(\theta_1+\theta_2+\theta_3)+\cos(\theta_4+\theta_5) = 2\cos(\frac{\theta_1+\theta_2+\theta_3+\theta_4+\theta_5}{2})\cos(\frac{\theta_1+\theta_2+\theta_3-\theta_4-\theta_5}{2})$, then $\cos(\frac{\theta_1+\theta_2+\theta_3-\theta_4-\theta_5}{2}) = 0$, which implies $\theta_1+\theta_2+\theta_3-\theta_4-\theta_5 = m\pi$, for some odd integer m. However, $-\pi < \sum_{i=1}^5 -\theta_i \le \sum_{i=1}^5 \pm\theta_i \le \sum_{i=1}^5 \theta_i < \pi$, so we must have $\theta_2 = 0$.

The other 4-by-4 principal minors can be obtained from $\det(S[1,2,3,4])$ by cyclically permuting the indices appropriately. Then, after setting each of these minors equal to zero, we have $\theta_i = 0$, for $1 \le i \le 5$.

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