Sufficient conditions to be exceptional

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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 $A \in \mathbb{R}^{n \times n}$ is **positive semidefinite** (positive definite) if $x^T Ax \geq 0$ (or $x^T Ax > 0$) for all $x \in \mathbb{R}^n$, $x \neq 0$. A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called **copositive** (strictly copositive) if $x^T Ax \geq 0$ (or $x^T Ax > 0$) for all $x \in \mathbb{R}^n$, $x \geq 0$, $x \neq 0$. We will let $e_i \in \mathbb{R}^n$ denote the vector with $i$th 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 be **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 $A \in \mathbb{R}^{n \times n}$ 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 $i$, $1 \leq i \leq n$, can be rewritten $e_i^T A^{-1} A A^{-1} e_i = 0$. Then if $A = P + N$, this implies $0 = e_i^T A^{-1} (P + N) A e_i = e_i^T A^{-1} P A^{-1} e_i + e_i^T A^{-1} N A^{-1} e_i$, and so $0 = e_i^T A^{-1} P A^{-1} e_i$, for all $i$, $1 \leq i \leq n$. Letting $x_i = A^{-1} e_i$, we have $x_i^T P x_i = 0$, for all $i$, $1 \leq i \leq n$, but then $P x_i = 0$, 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 $\begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 1 & 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \end{pmatrix}$, then $A = \begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$.

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

An example suggesting we cannot improve on Theorem 1 by having $n - 1$ zero diagonal entries, is $A^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$. 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 $x \succeq 0$ and $x^T Ax = 0$, then $Ax \succeq 0$. 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 \( A \in \mathbb{R}^{n \times n} \) 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

\[
Q^T A^{-1} Q = Q^T \begin{pmatrix} B_1 & B_2 \\ B_2^T & B_3 \end{pmatrix} Q = \begin{pmatrix} B_1 & B_2 Q_1 \\ Q_1 B_2^T & Q_1 B_3 Q_1 \end{pmatrix},
\]

has a nonzero last column in the top right 2-by-\((n - 2)\) block matrix \( B_2 Q_1 \). 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 \( Q^T A \) in block form as \( Q^T A = \begin{pmatrix} C_1 + N_1 & a \\ a^T & a_{nn} \end{pmatrix} \), 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 \( Q^T A^{-1} Q \) in block form, although in a different way than earlier, as \( Q^T A^{-1} Q = \begin{pmatrix} D & b \\ b^T & 0 \end{pmatrix} \), 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 \( C_1 b = -N_1 b \), and then since \( N_1 \) and \( b \) are nonnegative we have \( b^T C_1 b = -b^T N_1 b \leq 0 \). But this implies \( b^T C_1 b = 0 \). Then \( C_1 b \geq 0 \), from the property mentioned in the paragraph before the theorem, and so \( N_1 b = 0 \).

However, \( N_1 b \) 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 $A \in \mathbb{R}^{n \times n}$ be symmetric and invertible. Suppose there exists an invertible matrix $B \in \mathbb{R}^{n \times n}$ 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 $i$, $1 \leq i \leq n$, $0 = e_i^T B^T A^{-1}B e_i = e_i^T C^T A e_i = e_i^T C^T (P + N) e_i = e_i^T C^T P e_i + e_i^T C^T N e_i$. This implies for each $i$, $0 = e_i^T C^T P e_i$. Then $P e_i = 0$ for all $i$, so $P = 0$.

For the “Moreover” part of the statement of the theorem, since for each $i$ we have $e_i^T C^T A e_i = 0$, and $A$ is copositive, then $A e_i \geq 0$, from the property of copositive matrices stated in Section 2. Therefore $B = A e_i \geq 0$.

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

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

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

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

and

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

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

$$
A = \begin{pmatrix}
1 & -1 & 1 & 1 & 1 & 1 & -1 \\
-1 & 1 & -1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & 1 & -1 \\
-1 & 1 & 1 & 1 & 1 & -1 & 1
\end{pmatrix}, \quad A^{-1} = \frac{1}{6} \begin{pmatrix}
2 & -1 & -1 & 2 & 2 & -1 & -1 \\
-1 & 2 & -1 & -1 & 2 & 2 & -1 \\
-1 & -1 & 2 & -1 & -1 & 2 & 2 \\
2 & -1 & -1 & 2 & -1 & -1 & 2 \\
-1 & 2 & 2 & -1 & -1 & 2 & -1 \\
-1 & -1 & 2 & 2 & -1 & -1 & 2
\end{pmatrix}.
$$
for which
\[ B = \begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 1 & 0 & 0 & 0 \\
0 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 & 1
\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}
0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 & 0
\end{pmatrix} \]
\[ A^{-1}B = \frac{1}{2} \]
\[ B^T A^{-1}B = \frac{1}{2} \]

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

**Theorem 5.** For \( n \geq 3 \), let \( A \in \mathbb{R}^{n \times n} \) 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 \( 0 = e_i^T A^{-1} N A^{-1} e_1 \), 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 \( N = 0 \).

\[ \square \]

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

Theorem 6 appears at the end of [5], where they use \( \mathcal{O}^5 \), \( \mathcal{S}^5 \) and \( \mathcal{N}^5 \), respectively, to denote the copositive, positive semidefinite, and nonnegative matrices, in \( \mathbb{R}^{5 \times 5} \).

**Theorem 6.** Let \( A \in \mathcal{O}^5 \setminus (\mathcal{S}^5 + \mathcal{N}^5) \). 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 $\theta_i$’s, for $1 \leq i \leq 5$, that ensure $S$ has a hollow inverse. In effect, we will show that the $\theta_i$’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 be used to show that the top left 4-by-4 principal minor of $S$, namely

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

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

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