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CONSTRUCTING COPOSITIVE MATRICES FROM INTERIOR MATRICES*

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Abstract. Let A be an n by n symmetric matrix with real entries. Using the l_1-norm for vectors and letting $S_1^+ = \{x \in \mathbb{R}^n | ||x||_1 = 1, x \geq 0\}$, the matrix A is said to be *interior* if the quadratic form $x^T Ax$ achieves its minimum on S_1^+ in the interior. Necessary and sufficient conditions are provided for a matrix to be interior. A copositive matrix is referred to as being *exceptional* if it is not the sum of a positive semidefinite matrix and a nonnegative matrix. A method is provided for constructing exceptional copositive matrices by completing a partial copositive matrix that has certain specified overlapping copositive interior principal submatrices.

Key words. Copositive matrix, Interior matrix, Quadratic form, Almost positive semidefinite, Exceptional copositive matrix, Extreme copositive matrix.

AMS subject classifications. 15A18, 15A48, 15A57, 15A63.

1. Introduction.

We will call a vector $v = (v_1, \ldots, v_n)^T \in \mathbb{R}^n$ *nonnegative*, denoted $v \geq 0$, if $v_i \geq 0$, for all i, $1 \leq i \leq n$. Similarly, a matrix $A \in \mathbb{R}^{n\times n}$ will be called *nonnegative*, in the event that all its entries are nonnegative. A symmetric matrix $A \in \mathbb{R}^{n\times n}$ will be called *positive semidefinite* (*positive definite*) if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$ ($x^T Ax > 0$ for all $x \in \mathbb{R}^n, x \neq 0$). A symmetric matrix $A \in \mathbb{R}^{n\times n}$ will be called *copositive* (*strictly copositive*) if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n, x \geq 0$ ($x^T Ax > 0$ for all $x \in \mathbb{R}^n, x \geq 0, x \neq 0$). The vector in $\mathbb{R}^n$ of all ones will be denoted by e, so that $e = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$. The matrix $E_{ij} \in \mathbb{R}^{n\times n}$ denotes the matrix with a 1 in the (i, j) position and zeroes elsewhere, while $e_i \in \mathbb{R}^n$ denotes the vector with a 1 in the ith position and zeroes elsewhere. A symmetric matrix $A \in \mathbb{R}^{n\times n}$ will be called *almost positive semidefinite* (*almost positive definite*) if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$ such that $x^T e = 0$ ($x^T Ax > 0$ for all $x \in \mathbb{R}^n$, $x \neq 0$, such that $x^T e = 0$)[13]. Note that if a matrix is copositive then all its principal submatrices are copositive. We will say that a matrix is *partial copositive* if it has some entries that are specified, and some that are not, and for every principal submatrix which has all its entries specified, this submatrix is copositive. It is easy to show that a 2×2 copositive matrix is

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either positive semidefinite or nonnegative. Diananda [7] showed that every 3×3 or 4×4 copositive matrix is the sum of a positive semidefinite matrix and a nonnegative matrix. We will call a copositive matrix *exceptional* if it is not the sum of a positive semidefinite matrix and a nonnegative matrix. Thus, $n \times n$ exceptional copositive matrices can only occur for $n \geq 5$. Horn [8] gave an example of an exceptional matrix (see Section 3 of this paper). By an *extreme* copositive matrix Q we mean that if $Q = Q_1 + Q_2$, where Q_1 and Q_2 are copositive then $Q_1 = aQ$, and $Q_2 = (1-a)Q$, for some a such that $0 \leq a \leq 1$.

We will denote the vector l_1-norm [12] by $||x||_1 = \sum_{i=1}^n |x_i|$, and by S_1^+ the portion of the unit 1-sphere $S_1 = \{x \in \mathbb{R}^n |\ ||x||_1 = 1\}$ in the nonnegative orthant, thus $S_1^+ = \{x \in \mathbb{R}^n |||x||_1 = 1, x \geq 0\}$. Let $A \in \mathbb{R}^{n\times n}$ be symmetric. The set S_1^+ is compact so a minimum for x^TAx is achieved on this set. We will say that A is *interior* if such a minimum, namely $\min_{x\in S_1^+} x^TAx$, is achieved in the interior of S_1^+. Note that A is not necessarily copositive in this definition, although A being copositive is our primary interest. This definition does not preclude the possibility that the minimum is also achieved on the boundary, just that it will be achieved in the interior in any case. For example, with $n = 3$ and

$$A = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix},$$

the matrix A is interior, since the minimum of the quadratic form x^TAx is achieved in the interior of S_1^+ at the vector $\frac{1}{4}(1,2,1)^T$. Although the minimum is also achieved on the boundary at $\frac{1}{2}(1,1,0)^T$. For a symmetric matrix $A \in \mathbb{R}^{n\times n}$, if the minimum of x^TAx is not achieved in the interior of S_1^+ then the minimum is achieved at a vector u with some zero components. Let us call $u' \in \mathbb{R}^k$, where $1 \leq k < n$, the vector consisting of the positive components of u, so that u' is of the form $u' = (u_{i_1}, \ldots, u_{i_k})^T$, and is in the interior of $S_1^{+'} = \{x' \in \mathbb{R}^k |\ ||x'||_p = 1, x' \geq 0\}$, and where $i_1, \ldots, i_k$ are determined by deleting the zero components of the minimizer u. Then $\min_{x\in S_1^+} x^TAx = \min_{x'\in S_1^{+'}} x'^TA'x'$, where A' is the principal submatrix of A obtained by deleting the ith row and column of A, for every i such that $i \notin \{i_1, \ldots, i_k\}$. Thus A' is an interior matrix.

To be consistent with when $n = 1$ we will say that the matrix $A = (a)$ is interior, even though $S_1^+ = \{1\}$ has no interior or boundary. In this case, $\min_{x\in S_1^+} x^TAx = \min_{x=1} ax^2 = a$. Note that for a 1×1 matrix A, being copositive and not strictly copositive implies that $A = (0)$. For another example, this time with $n = 2$, take $A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}$. Then with $x = [\,x_1 \quad x_2\,]^T$ we have $x^TAx = x_1^2 + (x_1 + x_2)^2$, so $\min_{x\in S_1^+} x^TAx = 1$ and the minimum is achieved at $u = [\,0 \quad 1\,]^T$ (in the notation of the preceding paragraph) and $A' = (1)$ is an interior matrix and $u' = 1$.

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In Section 2 we provide necessary and sufficient conditions for a matrix to be interior. In Section 3 we employ interior principal submatrices to construct copositive matrices that are exceptional. In particular, we will show how to construct an exceptional copositive matrix by performing a completion of a matrix that has certain overlapping principal submatrices specified, which are copositive and interior. Section 4 contains examples that demonstrate this method of construction.

2. Interior matrices. Theorem 1 below minimizes the quadratic form on S_1^+. A variation of Theorem 1 in which the quadratic form is maximized on S_1^+, and x^TAx has no maxima on the boundary, was proved by Sidorenko in [17], whose proof relies on [5] and [6]. Our interest lies in minimizing the quadratic form because with copositive matrices, which are not strictly copositive, the value of that minimum on the nonnegative orthant is zero. We are also interested in the location of the minimizer, which may move from the boundary to the interior, or vice versa, on changing from maximizing to minimizing. Our proofs are self-contained and different than Sidorenko's.

THEOREM 1. *Let $A \in \mathbb{R}^{n\times n}$ be symmetric. Then A is interior if and only if (i) and (ii) hold.*

(i) There exists $u > 0$, $||u||_1 = 1$, and $\mu \in \mathbb{R}$ such that $Au = \mu e$;

(ii) $y^TAy \geq 0$ for all $y \in \mathbb{R}^n$ such that $y^Te = 0$ (i.e. A is almost positive semidefinite).

If A is interior then $\mu = \min_{x\in S_1^+} x^TAx = u^TAu$.

If (i) holds and $y^TAy > 0$ for all $y \neq 0$ such that $y^Te = 0$ (i.e. A is almost positive definite), then $u > 0$ is the only minimizer in S_1^+.

If A is interior and u is not the only minimizer in S_1^+ then A is singular, and $Ay = 0$ for some $y \neq 0$ such that $y^Te = 0$.

Proof. Suppose that A is interior. Since there is a minimizer u for x^TAx in the interior of S_1^+ we may use Lagrange Multipliers and minimize x^TAx subject to $||x||_1 = 1$. Thus $\nabla(x^TAx) = \lambda\nabla(\sum_{i=1}^n x_i)$, when $x = u$, which implies $2(Au)_i = \lambda$, or $Au = \mu e$, where $\mu = \frac{\lambda}{2}$. So (i) holds. Evidently, $\mu = \min_{x\in S_1^+} x^TAx = u^TAu$.

Let $y \in \mathbb{R}^n$ be any $y \neq 0$ be such that $y^Te = 0$. Then for some $c \neq 0$, $u + cy \geq 0$, and since u is a minimizer we have $\frac{(u+cy)^T}{||u+cy||_1}A\frac{(u+cy)}{||u+cy||_1} \geq u^TAu$. But $||u + cy||_1 = (u + cy)^Te = 1$, so we have $u^TAu + 2cy^TAu + c^2y^TAy \geq u^TAu$, or $c^2y^TAy \geq 0$, proving (ii).

Conversely, suppose (i) and (ii) hold. Let z be any vector in S_1^+. Since the vector u together with a basis for $\{y|y^Te = 0\}$ spans $\mathbb{R}^n$ we can write $z = \nu u + y$, where

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$\nu \in \mathbb{R}$ and $y^T e = 0$. Also, $z^T e = 1$ so $\nu = 1$. Then $z^T Az = (u + y)^T A(u + y) = u^T Au + y^T Ay \geq u^T Au$. Thus u is a minimizer in the interior of S_1^+. So A is interior.

Assume (i) and $y^T Ay > 0$ for all $y \neq 0$ such that $y^T e = 0$, and v is another minimizer in S_1^+. Arguing as in the preceding paragraph, we can write $v = \nu u + y$, for some $\nu \in \mathbb{R}$ and some y such that $y^T e = 0$, and again $\nu = 1$. Note that $y \neq 0$ since $v \neq u$. Then $v^T Av = (u + y)^T A(u + y) = u^T Au + 2u^T Ay + y^T Ay = u^T Au$, which implies $y^T Ay = 0$, contradicting our assumption.

To prove the final statement of the theorem suppose v is another minimizer in S_1^+. $w^T Aw \geq \mu$ for all $w \in S_1^+$ implies $w^T Aw \geq \mu(w^T e)^2$ or $w^T (A - \mu ee^T)w \geq 0$ for all $w \geq 0$, i.e. $A - \mu ee^T$ is copositive. Write $v = u + y$, where $y \neq 0$ and $y^T e = 0$. Using the result (for instance, Lemma 1 in [16]) which states that for copositive $B \in \mathbf{R}^{n\times n}$, if $x_0 \geq 0$ and $x_0^T Bx_0 = 0$, then $Bx_0 \geq 0$, we have $(u + y)^T (A - \mu ee^T)(u + y) = 0$, so $(A-\mu ee^T)(u+y) \geq 0$, which implies $A(u+y) \geq \mu ee^T(u+y) = \mu e$. Then $Au+Ay \geq \mu e$ implies $Ay \geq 0$. If $Ay \neq 0$ we would have $u^T Ay > 0$, but then $\mu e^T y > 0$, which is not possible, so $Ay = 0$. □

Corollary 2. *If $A \in \mathbb{R}^{n\times n}$ is copositive interior then A is positive semidefinite.*

Proof. In the notation of the theorem $\mu \geq 0$ and for any $w \in \mathbb{R}^n$, we can write $w = \nu u + y$, where $y^T e = 0$ and $\nu \in \mathbb{R}$, so $w^T Aw = (\nu u + y)^T A(\nu u + y) = \nu^2 u^T Au + y^T Ay \geq 0$. □

Corollary 3. *Let $A \in \mathbb{R}^{n\times n}$ be symmetric. Then A has an almost positive semidefinite principal submatrix $A' \in \mathbb{R}^{k\times k}$, for some k, with $1 \leq k \leq n$.*

Proof. If A is not interior, as discussed in the introduction, it follows from Theorem 1 that A has a principal submatrix A' for which (i) and (ii) hold. □

It is worth noting that in the event that the interior matrix A' of Corollary 3 is a 1×1 matrix, then this corollary is vacuous. Again using

$$A = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}$$

as given in the introduction, this copositive matrix is an example of an interior matrix which has minimizers $\frac{1}{4}(1, 2, 1)^T$ and $\frac{1}{6}(1, 3, 2)^T$ in the interior of S_1^+, and on the boundary has minimizers $\frac{1}{2}(1, 1, 0)^T$ and $\frac{1}{2}(0, 1, 1)^T$. The $n \times n$ matrix $A = I - ee^T$ is also an example of a matrix that is interior, since for $x \geq 0$ we have $x^T Ax = x^T x - (x^T e)^2 \geq (x^T e)^2(\frac{1}{n} - 1)$ with equality if and only if x is a multiple of e.

3. Constructing copositive matrices. Examples of copositive matrices are most easily constructed by forming the sum of a positive semidefinite matrix and a

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nonnegative matrix. We will provide a method for constructing copositive matrices not of this form, that is, exceptional copositive matrices. The Horn matrix, which corresponds to the Horn quadratic form in [8],

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}, \tag{3.1}$$

is an example of an exceptional copositive matrix. In fact, as is shown in [7], [8], H is extreme in the set of all copositive matrices. The positive semidefinite extreme copositive matrices are described in [4], [8], [9], as are the nonnegative extreme copositive matrices, and that leaves the exceptional extreme copositive matrices. Effectively characterizing all extreme copositive matrices is a long-standing unsolved problem [4]. In Theorem 4.1 of [9] Hall and Newman provide a necessary condition for the construction of an extreme copositive matrix. In [2] Baumert constructs $n \times n$ extreme copositive matrices by bordering an $(n-1) \times (n-1)$ extreme matrix in a certain way, and in [3] Baumert constructs extreme copositive 5×5 matrices for which not all entries are ± 1. In [1] Baston constructs extreme copositive $n \times n$ matrices with all entries equal to ± 1, when $n \geq 8$.

Corollary 2 along with the remarks in the introduction (about the minimum of the quadratic form when not achieved in the interior being achieved on the boundary) imply Theorem 4, which is essentially part (i) of Lemma 7 in [7]. Theorem 4 places a necessary condition on any method devised for constructing copositive matrices which are not strictly copositive.

Theorem 4. (Diananda)*) Let $A \in \mathbb{R}^{n \times n}$ be copositive, and not strictly copositive. Then A has a copositive interior principal submatrix A' with*

$$\min_{x \in S_1^+} x^T A x = \min_{x' \in S_1^{+\prime}} x'^T A' x' = 0,$$

and A' is positive semidefinite.

Lemma 5 provides a sufficient condition for a copositive matrix to be not writable as a sum of a positive semidefinite matrix and a nonzero nonnegative matrix (Note we do not say exceptional). Note that the Horn matrix is not interior, since if it was then from Theorem 1 we would have $Hu = 0$ for some $u > 0$, because $\mu = 0$. But this is not possible since H is nonsingular. The Horn matrix is an example of a matrix that cannot be expressed as the sum of a positive semidefinite matrix and a nonnegative matrix. Thus the fact that a matrix cannot be expressed as the sum of a positive semidefinite matrix and a nonnegative matrix does not imply that the matrix is interior.

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Lemma 5. *Let $A \in \mathbb{R}^{n\times n}$ be copositive and not strictly copositive. If A is interior then A cannot be written as a sum of a positive semidefinite matrix and a nonzero nonnegative matrix.*

Proof. Suppose $A = B+C$, where B is positive semidefinite and C is nonnegative. Then for $u > 0$ we have $0 = u^TAu = u^TBu + u^TCu$. But $u^TCu = 0$ implies $C = 0$. ∎

Consider now the motivating example of

$$A = \begin{bmatrix} 1 & 1 & s \\ 1 & 2 & 1 \\ s & 1 & 1 \end{bmatrix}.$$

If s is a minimum so that A is copositive, then $s = -1$, and in this case A is the sum of a positive semidefinite matrix and a nonzero nonnegative matrix;

$$A = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

However, if s is a minimum so that A is positive semidefinite then $s = 0$. In this case there is a 'gap' between the minimum values of s for which there is a copositive completion versus a positive semidefinite completion. Sometimes, as we are about to show in Theorem 6, there is no such gap.

In Theorem 6 we have a partial positive semidefinite matrix A, where A consists of two overlapping principal blocks (to be described), and one corner entry of A to be specified. See [14] for the general problem of completions of positive semidefinite matrices.

Theorem 6. *Let $A' \in \mathbb{R}^{(n-2)\times(n-2)}$ be copositive, not strictly copositive, and interior. Let*

$$\begin{bmatrix} a & b^T \\ b & A' \end{bmatrix} \in \mathbb{R}^{(n-1)\times(n-1)} \text{ and } \begin{bmatrix} A' & c \\ c^T & d \end{bmatrix} \in \mathbb{R}^{(n-1)\times(n-1)}$$

be positive semidefinite, and

$$A = \begin{bmatrix} a & b^T & s \\ b & A' & c \\ s & c^T & d \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

If s is a minimum among all copositive completions of A, then A is positive semidefinite.

Proof. It was proved in [11] that a copositive completion exists for any partial copositive matrix. Since $\begin{bmatrix} a & b^T \\ b & A' \end{bmatrix}$ is positive semidefinite we have $b = A'u$ for

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some $u \in \mathbb{R}^{n-2}$, from the row and column inclusion property of positive semidefinite matrices (see for instance [15]). The positive semidefiniteness also implies $a - u^T A' u \geq 0$. Similarly, we have $c = A'v$ for $v \in \mathbb{R}^{n-2}$, and $d - v^T A' v \geq 0$. Writing $x = [\, x_1 \quad x' \quad x_n \,]^T$, where $x' \in \mathbb{R}^{n-2}$, we have

$$\begin{aligned}
x^T Ax &= ax_1^2 + x'^T A' x' + dx_n^2 + 2x_1 x'^T A' u + 2x_n x'^T A' v + 2s x_1 x_n, \\
&= (x' + x_1 u + x_n v)^T A' (x' + x_1 u + x_n v) + ax_1^2 + dx_n^2 + 2s x_1 x_n \\
&\qquad\qquad - (x_1 u + x_n v)^T A' (x_1 u + x_n v), \\
&= (x' + x_1 u + x_n v)^T A' (x' + x_1 u + x_n v) + x_1^2 (a - u^T A' u) + x_n^2 (d - v^T A' v) \\
&\qquad\qquad + 2s x_1 x_n - 2 x_1 x_n u^T A' v, \\
&= (x' + x_1 u + x_n v)^T A' (x' + x_1 u + x_n v) + (x_1 \sqrt{a - u^T A' u} - x_n \sqrt{d - v^T A' v})^2 \\
&\qquad\qquad + 2 x_1 x_n (s - u^T A' v + \sqrt{a - u^T A' u} \sqrt{d - v^T A' v}).
\end{aligned}$$

If A is to be copositive we must have the coefficient of $2x_1 x_n$ nonnegative, since if this coefficient were negative we would have $x^T Ax < 0$, with $x \geq 0$, by choosing $x_1, x_n \geq 0$ so that $x_1 \sqrt{a - u^T A' u} - x_n \sqrt{d - v^T A' v} = 0$, which only fixes the ratio of x_1 to x_n, and then choose x_1 and x_n small enough to have $x' = w - x_1 u - x_n v \geq 0$, where $w > 0$ satisfies $w^T A' w = 0$.

Thus if we want s to be a minimum so that A is copositive, we will have that the coefficient of $2x_1 x_n$ is zero. But in this event, A will be positive semidefinite. $\square$

Diananda [7] defined the notion of $A^*(n)$ for an $n \times n$ copositive matrix A, which means that for any $\epsilon > 0$ the matrix $A - \epsilon(E_{ij} + E_{ji})$ is not copositive, for any i, j, $1 \leq i, j \leq n$. Evidently being $A^*(n)$ is a weaker condition than being extreme copositive, and being exceptional is weaker that being $A^*(n)$. Baumert [2] improved on Theorem 4 which we state as Theorem 7.

THEOREM 7. (Baumert)*) Let $A \in \mathbb{R}^{n \times n}$ be $A^*(n)$. Then for each i, $1 \leq i \leq n$, the (i, i) diagonal entry of A lies in a copositive, not strictly copositive, interior principal submatrix of A.*

Theorem 7 tells us that when attempting to construct an exceptional matrix, if it is to be $A^*(n)$ then we should arrange that some copositive interior principal submatrices cover all the diagonal entries. For our next theorem we make some simplifying assumptions about the form of these copositive interior principal submatrices.

In Theorem 8 we again start with a partial positive semidefinite matrix, but this time with A consisting of three overlapping principal blocks, and three corner entries of A to be specified. Without loss of generality we will assume that the diagonal entries of A are all equal to 1. Since every 2×2 principal submatrix of a copositive matrix is copositive, and every 2×2 copositive matrix is either positive semidefinite

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or nonnegative, it follows that every off-diagonal entry is at least -1. From [11] we can also assume without loss of generality that all entries of A are at most 1.

THEOREM 8. *Let $A' \in \mathbb{R}^{(n-2)\times(n-2)}$ have all diagonal entries equal to 1, and be copositive, not strictly copositive, and interior. Let $A \in \mathbb{R}^{n\times n}$ have all diagonal entries equal to 1, all off-diagonal entries between -1 and 1, and consist of three overlapping principal blocks each of which are copositive, not strictly copositive, and interior with central principal block A', thus*

$$A = \begin{bmatrix} 1 & b^T & r & s \\ b & & & t \\ r & A' & & c \\ s & t & c^T & 1 \end{bmatrix},$$

where the upper left $(n-2)\times(n-2)$ principal block of A, and the lower right $(n-2)\times(n-2)$ principal block of A are also copositive and interior. If s is a minimum among all copositive completions (r, s, t) of A, then with s in the $(1, n)$ and $(n, 1)$ corners of A either there is a positive semidefinite completion of A or else all copositive completions of A are exceptional.

Proof. Since the graph of the specified entries is chordal we know that there is a positive semidefinite completion [14]. Using Theorem 1 in [11] about the existence of a copositive completion, since all diagonal entries of A are equal to 1, if $r = s = t = 1$ then A is copositive. Now choose s to be a minimum among all copositive completions (r, s, t) such that $-1 \le r, s, t \le 1$. It is worth noting that s is fixed for the remainder of the proof.

If there is an (r, s, t) providing a positive semidefinite completion of A we're done. Suppose now, for the sake of obtaining a contradiction, that A does not have a positive semidefinite completion with the $(1, n)$ and $(n, 1)$ entries equal to s, and that there is a copositive completion (r, s, t) with $A = B + C$, where B is positive semidefinite and C is nonnegative. Since A' is interior, there exists $u \in \mathbb{R}^{n-2}$, $u > 0$, such that $[0 \quad u^T \quad 0]\, A \begin{bmatrix} 0 \\ u \\ 0 \end{bmatrix} = 0$. Then reasoning as in the proof of Lemma 5 this implies that the central $(n-2)\times(n-2)$ principal block of C is zero. Similarly, for the upper left and lower right $(n-2)\times(n-2)$ principal blocks of C. Thus the only candidates for nonzero entries in C are the $(1, n-1)$, $(1, n)$, and $(2, n)$ entries $c_{1(n-1)} = c_{(n-1)1}$, $c_{1n} = c_{n1}$, and $c_{2n} = c_{n2}$, respectively. Now $s = b_{1n} + c_{1n}$. If $c_{1n} > 0$ we would have $s > b_{1n}$, which is not possible, since b_{1n} would give a smaller value than s for a copositive completion of A with $(r, s, t) = (b_{1(n-1)} + c_{1(n-1)}, b_{1n}, b_{2n} + c_{2n})$. So we must have $c_{1n} = 0$. But now the equation $A = B + C$ implies there is a positive semidefinite completion of A with $(r, s, t) = (b_{1(n-1)}, s, b_{2n})$, which we assumed not be the case. $\square$

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Theorem 8 and its proof are readily modified to other sizes and numbers of copositive, not strictly copositive, interior overlapping principal blocks along the diagonal of A, and corner entry s a minimum among all copositive completions (There isn't even a requirement that the overlapping blocks be the same size). We explore examples of such completions in the next section.

4. Examples of exceptional matrices. If $n = 4$ and we follow the construction of Theorem 8, the 2×2 principal blocks being copositive, not strictly copositive, and interior means they must equal $\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$. Thus

$$A = \begin{bmatrix} 1 & -1 & r & s \\ -1 & 1 & -1 & t \\ r & -1 & 1 & -1 \\ s & t & -1 & 1 \end{bmatrix}.$$

The minimum s for which A is copositive is evidently $s = -1$, when $r = t = 1$, so A has a positive semidefinite completion.

If we try to construct a 5×5 matrix with four overlapping 2×2 copositive interior principal blocks, we will have

$$A = \begin{bmatrix} 1 & -1 & a_{13} & a_{14} & a_{15} \\ -1 & 1 & -1 & a_{24} & a_{25} \\ a_{13} & -1 & 1 & -1 & a_{35} \\ a_{14} & a_{24} & -1 & 1 & -1 \\ a_{15} & a_{25} & a_{35} & -1 & 1 \end{bmatrix}.$$

Since each 3×3 principal overlapping diagonal block has to be copositive, and no entry is greater than 1, we have from Theorem 6 applied to the 3×3 blocks, that

$$A = \begin{bmatrix} 1 & -1 & 1 & a_{14} & a_{15} \\ -1 & 1 & -1 & 1 & a_{25} \\ 1 & -1 & 1 & -1 & 1 \\ a_{14} & 1 & -1 & 1 & -1 \\ a_{15} & a_{25} & 1 & -1 & 1 \end{bmatrix},$$

which when completed with a_{15} minimal becomes the Horn matrix H (see below).

If A is an $n \times n$ copositive matrix with $n-2$ overlapping copositive, not strictly copositive, interior principal diagonal blocks of the form

$$\begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix},$$

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so that A conforms to a modified form of Theorem 8, easy to see that for n even the minimum value for s is -1 since with $A = ww^T$, where w is the alternating signs vector $w = (1, -1, 1, \cdots, -1)^T$, we have a positive semidefinite completion as with the 4×4 example above.

For general odd $n \geq 5$, the construction of the preceding paragraph starting with the same $n-2$ overlapping copositive interior principal diagonal blocks provides a natural extension of the Horn matrix. The Horn matrix is the matrix of the quadratic form $x^T Hx = (x_1 + x_2 + \cdots + x_n)^2 - 4x_1x_2 - 4x_2x_3 - \cdots - 4x_{n-1}x_n - 4x_nx_1$, when $n = 5$. The matrix for odd $n \geq 5$ is

$$A = \begin{bmatrix} 1 & -1 & 1 & 1 & \cdots & \cdots & 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & \ddots & & \ddots & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & & & \ddots & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & \ddots & & & \ddots & 1 \\ \vdots & \ddots & 1 & -1 & 1 & \ddots & & & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 1 & \ddots & & & & \ddots & 1 & -1 & 1 & 1 \\ 1 & 1 & \ddots & & & \ddots & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & \ddots & & & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & \cdots & \cdots & 1 & 1 & -1 & 1 \end{bmatrix},$$

which is copositive because we can write it as a sum of three matrices in two ways as $A = B_i + C_i + D_i$, for $i = 1, 2$, where B_i is positive semidefinite, C_i is nonnegative, for $i = 1, 2$, and there exists a vector $w \in \mathbb{R}^n$ such that D_1 satisfies $x^T D_1 x \geq 0$ for all $x \geq 0$ such that $x^T w \geq 0$, and D_2 satisfies $x^T D_2 x \geq 0$ for all $x \geq 0$ such that $x^T w \leq 0$. In fact, let $u = (1, -1, 1, -1, \cdots, -1, 1)^T \in \mathbb{R}^{n-2}$, $v = (-1, 1)^T$, $w_1 = (u, v)^T$, $B_1 = w_1 w_1^T$ and $D_1 = -2(e_1(0, v)^T + \begin{bmatrix} 0 \\ v \end{bmatrix} e_1^T)$, so that $x^T D_1 x \geq 0$, when $x \geq 0$ and $x^T \begin{bmatrix} 0 \\ v \end{bmatrix} \leq 0$. Then $A = B_1 + C_1 + D_1$, where C_1 is a nonnegative matrix with 2's in various positions but not on the diagonal, 1st or 2nd subdiagonal, nor the 1st or 2nd superdiagonal. If we let $w_2 = (u, -v)^T$, $B_2 = w_2 w_2^T$ and $D_2 = 2(e_{n-2}(0, v)^T + \begin{bmatrix} 0 \\ v \end{bmatrix} e_{n-2}^T)$, so that $x^T D_2 x \geq 0$, when $x \geq 0$ and $x^T \begin{bmatrix} 0 \\ v \end{bmatrix} \geq 0$, then $A = B_2 + C_2 + D_2$, where C_2 is a nonnegative matrix with 2's in the $(n-3, n-1)$ and $(n-1, n-3)$ positions, and in various other positions not on the diagonal, the 1st or 2nd subdiagonal, nor the 1st or 2nd superdiagonal. Since s cannot be any smaller, and A is copositive, we know $s = -1$ is the minimum. However, the matrix A with overlapping 3×3 principal blocks specified and $s = -1$ cannot be completed to a positive semidefinite matrix, by considering column inclusion with the column vector

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in $\mathbb{R}^2$ whose first component is $s = -1$ and second component the $(2, n)$ entry. If A were completeable to a positive semidefinite matrix, this column vector must be in the range of the 2×2 diagonal block $\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, so this vector has to be $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$. But then arguing similarly with the column vector whose first component is the $(2, n)$ entry 1 and second component is the $(3, n)$ entry, and continuing like this, the last column of A would have to consist of alternating 1's and -1's which is not possible with n odd. The only possibility left to us is that A is exceptional.

If $n = 7$ or $n = 9$ this matrix is exceptional but not extreme, because it is the sum of a nonnegative matrix and an extreme matrix. When $n = 7$ the extreme matrix, which we call the Hoffman-Pereira matrix, is

$$\begin{bmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{bmatrix}$$

as given at the end of [10]. When $n = 9$ the similarly banded matrix with eight diagonal bands of zeroes instead of four can also be shown to be extreme copositive using Theorem 4.1 in [10].

Other examples of nonextreme exceptional copositive matrices may be found by starting with an extreme copositive matrix A, which is of the form described in Theorem 8 (or its modified form), for instance the Horn matrix or the Hoffman-Pereira matrix. Then $A + \epsilon(E_{1n} + E_{n1})$ will be exceptional but not extreme if $0 < \epsilon < s' - s$, where s' is the smallest value of the $(1, n)$ entry for which A has a positive semidefinite completion (Note that conceivably $A + (s' - s)(E_{1n} + E_{n1})$ might not be positive semidefinite).

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