Criteria for Copositive Matrices

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ABSTRACT

Some finite criteria for copositive, copositive-plus, and strictly copositive matrices are proposed and compared with existing determinantal tests. The basic mathematical tool is principal pivoting.

1. INTRODUCTION

After reviewing and supplementing the basic theory for copositive matrices, as presented in [3], [4], [8], [10], and [13], we develop some finite criteria for copositive, copositive-plus, and strictly copositive matrices. To determine the copositivity class of a real symmetric matrix, its principal submatrices are searched. There are two kinds of criteria, which we call outer and inner according to whether the decisions are made outside or inside of the principal submatrices in question. The outer criteria, derived and carried out by means of principal pivoting, are more efficient than the inner ones, because in them only the positive definite principal submatrices need to be searched. If an outer criterion indicates that a matrix does not belong to a certain copositivity class, it yields at the same time a ray in the nonnegative orthant, on which the copositivity class in question is broken (i.e., any point on the ray gives an indication that the matrix does not belong to the copositivity class in question). We compare the criteria with existing determinantal tests and propose a determinantal test for copositive-plus matrices. Finally, we give some additional results (for example, we characterize all the 3×3 copositive-plus matrices).

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2. PRELIMINARIES

If $A \in \mathbb{R}^{m \times n}$ (A is a real $m \times n$ matrix), we denote the transpose of A by A^T, column i of A by a_i, the determinant of A by $\det A$ or $|A|$, and the adjoint of A by $\operatorname{adj} A$. Inequalities $A > 0$, $A \geqslant 0$, etc. are to be interpreted elementwise. If $R \subset \{1, \dots, m\}$ and $S \subset \{1, \dots, n\}$, we let A_{RS} stand for the submatrix of A situated in the intersection of rows R and columns S of A, abbreviating $A_{rS} = A_{\{r\}S}$ and $A_{Rs} = A_{R\{s\}}$. If A is square, a submatrix of the form A_{RR} is termed a *principal submatrix* and the determinant of A_{RR} a *principal minor*. By a *principal permutation* of a square matrix we mean equal permutation of the rows and the columns. Nonnegative definite and positive definite are abbreviated as nnd and pd, respectively. A vacuous matrix is defined to be nnd and pd. The nonnegative orthant of $\mathbb{R}^n$ is denoted $\mathbb{R}^n_+$. Any vector $x \in \mathbb{R}^n$ is interpreted as an $n \times 1$ matrix and denoted $x = (x_1, \dots, x_n)$. We let x_S stand for the subvector of x consisting of the components S of x. The ith coordinate vector is denoted e_i. If $s \notin R$, we abbreviate $R + s = R \cup \{s\}$. The cardinality of a set R is denoted $|R|$. The empty set is denoted $\varnothing$.

Letting $A \in \mathbb{R}^{n \times n}$, consider the equation $y = Ax$ in tabular form:

$$A : y = \begin{array}{c} x \\ \boxed{A} \end{array}. \tag{2.1}$$

Here $x_1, \dots, x_n$ are *independent variables*, and $y_1, \dots, y_n$ are *dependent variables*. If $R \subset \{1, \dots, n\}$ and A_{RR} is nonsingular, the *principal pivotal operation* $\mathscr{P}_R$ (with the *pivot* A_{RR}) is defined as the operation under which in (2.1) the variables y_R and x_R are exchanged; see e.g. [7] and [11] (if $R = \varnothing$, $\mathscr{P}_R$ is defined as the identity operation). Let the resulting table be $\hat{A}$. We denote $\hat{A} = \mathscr{P}_R A$, whether A and $\hat{A}$ are tables or matrices. Occasionally we shall denote $A^R = \mathscr{P}_R A$. If $A = [A_{ij}]$ is a block matrix where A_{rr} is a principal submatrix, we let $\mathscr{P}_{(r)}$ stand for the *principal block pivotal operation* with the pivot A_{rr}. Thus, if A_{11} is nonsingular, we may form the following equivalent tables:

$$A : \begin{array}{c} \\ y^1 = \\ y^2 = \end{array} \begin{array}{cc} x^1 & x^2 \\ \hline A_{11} & A_{12} \\ A_{21} & A_{22} \\ \hline \end{array} \overset{\mathscr{P}_{(1)}}{\leftrightarrow} C : \begin{array}{c} \\ x^1 = \\ y^2 = \end{array} \begin{array}{cc} y^1 & x^2 \\ \hline C_{11} & C_{12} \\ C_{21} & C_{22} \\ \hline \end{array}, \tag{2.2}$$

where

$$C_{11}=A_{11}^{-1},\quad C_{12}=-A_{11}^{-1}A_{12},\quad C_{21}=A_{21}A_{11}^{-1},\quad C_{22}=A_{22}-A_{21}A_{11}^{-1}A_{12}.$$

A *single principal pivotal operation* with the pivot a_{rr} is denoted $\mathscr{P}_r$. The general *single pivotal operation* $\mathscr{P}_{rs}$ is defined as the operation under which the variables y_r and x_s in (2.1) are exchanged. If $a_{rr}=0$ or $a_{ss}=0$, and $a_{rs}\neq 0$, $a_{sr}\neq 0$, then $\mathscr{P}_{\{r,s\}}=\mathscr{C}\mathscr{P}_{rs}\mathscr{P}_{sr}$, where $\mathscr{C}$ stands for the principal permutation under which the rows and columns r and s of a square matrix are interchanged.

We shall make use of *Schur's determinantal formula* [6]

$$\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = |A_{11}|\cdot|A_{22}-A_{21}A_{11}^{-1}A_{12}| \qquad (A_{11}\text{ nonsingular}). \quad (2.3)$$

Here $A_{22}-A_{21}A_{11}^{-1}A_{12}$ is a special case of the *Schur complement* [1], obtained from $\mathscr{P}_{(1)}A$ by deleting the first super-row and -column. In addition, from [14] we have the following result.

THEOREM 2.1. *Let $A\in\mathbb{R}^{n\times n}$ be nonsingular, and let $B=A^{-1}$, $R\subset\{1,\dots,n\}$, and $S=\{1,\dots,n\}\setminus R$. Then*

$$\det B_{SS}=(\det A)^{-1}\det A_{RR}.$$

Finally we consider the case that A in (2.2) is symmetric, when $A_{21}=A_{12}^T$ and $C_{21}=-C_{12}^T$. It is easy to see that

$$q=q(x):=x^TAx=y^Tx=y^{1T}C_{11}y^1+x^{2T}C_{22}x^2. \quad (2.4)$$

By the *inertia* of the symmetric matrix A, denoted $\operatorname{In}A$, we mean the triple (k_1,k_2,k_3), where k_1, k_2, and k_3 stand for the numbers of positive, negative, and zero eigenvalues of A, respectively. If A_{11} in (2.2) is nonsingular, we have by [9]

$$\operatorname{In}A=\operatorname{In}A_{11}+\operatorname{In}C_{22}. \quad (2.5)$$

3. BASIC THEORY

DEFINITION 3.1. A matrix $A=A^T\in\mathbb{R}^{n\times n}$ is called *copositive* if $x^TAx\geqslant 0$ for any real n-vector $x\geqslant 0$. A copositive matrix A is termed *copositive-plus* if $x \geqslant 0$ and $x^TAx = 0$ imply $Ax = 0$, and *strictly copositive* if $x \geqslant 0$ and $x^TAx = 0$ imply $x = 0$. A vacuous square matrix is defined to be copositive, copositive-plus, and strictly copositive.

REMARK 3.1. When developing criteria for copositive matrices it suffices to consider symmetric matrices only, because if $A \in \mathbb{R}^{n \times n}$ is not symmetric, it is possible to pass to the symmetric part $\frac{1}{2}(A + A^T)$ of A; cf. [3].

REMARK 3.2. Any strictly copositive matrix is copositive-plus. A copositive-plus matrix is strictly copositive if and only if it is nonsingular or it is singular and has no nonnegative eigenvector associated with the zero eigenvalue. Any nnd (pd) matrix is copositive-plus (strictly copositive).

REMARK 3.3. If A is (strictly) copositive, then $a_{ii} \geqslant 0$ (> 0) for all i. If A is copositive (copositive-plus), then $a_{ii} = 0$ implies $a_{ij} = a_{ji} \geqslant 0$ ($= 0$) for all j; see [5, Lemma 2] and [3, Theorem 6].

REMARK 3.4. If A is copositive (copositive-plus, strictly copositive), so is any positive multiple of A, any principal permutation of A, and any principal submatrix of A.

Next we state a corollary to [13, Propositions 2.4–5].

THEOREM 3.1. *If $a_{ii} = 0$ in $A = A^T \in \mathbb{R}^{n \times n}$, and if $R = \{1, \dots, n\} \setminus \{i\}$, then A is copositive (copositive-plus) if and only if A_{RR} is copositive (copositive-plus) and $a_{ij} = a_{ji} \geqslant 0$ ($= 0$) for all j.*

DEFINITION 3.2. A matrix $A = A^T \in \mathbb{R}^{n \times n}$ is called copositive (copositive-plus, strictly copositive, nnd, pd) of *order* k, $0 \leqslant k \leqslant n$, if every principal submatrix of A of order k belongs to the class in question. A is called copositive (copositive-plus etc.) of *exact order* k if it is copositive (copositive-plus etc.) of order k but not of order $k+1$.

THEOREM 3.2. *If $A = A^T \in \mathbb{R}^{n \times n}$ is copositive, then $x \geqslant 0$ and $x^TAx = 0$ imply $Ax \geqslant 0$.*

Proof. If $q(x) = x^TAx = 0$ with $x \geqslant 0$, then $q'(x) = 2Ax \geqslant 0$, where $q'(x)$ is the gradient of q at x. ∎

For another proof, see [10].

THEOREM 3.3. *Let* $A = A^T \in \mathbb{R}^{n\times n}$. *If* $x \geqslant 0$ *and* $x^TAx = 0$ *imply* $Ax \geqslant 0$ (*respectively* $Ax = 0, x = 0$), *and* $\hat{x}^TA\hat{x} > 0$ *for some* $\hat{x} \geqslant 0$, *then A is copositive* (*respectively copositive-plus, strictly copositive*).

Proof. Clearly it suffices to prove the copositive case. Suppose that $\bar{x}^TA\bar{x} < 0$ for some $\bar{x} \geqslant 0$. Then there is an $\alpha \in (0,1)$ such that $x_\alpha := (1-\alpha)\bar{x} + \alpha\hat{x} \geqslant 0$ is a zero of $q(x) = x^TAx$. Because $Ax_\alpha \geqslant 0$, we find

$$0 = x_\alpha^TAx_\alpha = (1-\alpha)^2\bar{x}^TA\bar{x} + 2\alpha(1-\alpha)\bar{x}^TA\hat{x} + \alpha^2\hat{x}^TA\hat{x}$$

$$= 2(1-\alpha)\bar{x}^T(Ax_\alpha) + \alpha^2\hat{x}^TA\hat{x} - (1-\alpha)^2\bar{x}^TA\bar{x} > 0,$$

a contradiction. ∎

For another proof of the copositive (copositive-plus) case, see [13, Theorem 3.1] ([3, Theorems 2 and 5]).

THEOREM 3.4. *If* $A = A^T \in \mathbb{R}^{n\times n}$ *is nonsingular and copositive, then* A^{-1} *contains no nonpositive column.*

Proof. Let $B := A^{-1}$, and suppose that there is a $b_i \leqslant 0$. Take $x = -b_i \geqslant 0$; then $y := -Ab_i = -e_i$ and $q = y^Tx = b_{ii} \leqslant 0$. If $b_{ii} < 0$, there is a contradiction, and if $b_{ii} = 0$, the result is contrary to Theorem 3.2. ∎

THEOREM 3.5. *If* $A = A^T \in \mathbb{R}^{n\times n}$ *is nonsingular and copositive-plus* (*and thus strictly copositive*), *then* A^{-1} *contains no nonnegative column with a zero diagonal element.*

Proof. Let $B := A^{-1}$, and suppose there is a $b_i \geqslant 0$ with $b_{ii} = 0$. Take $0 \neq x = b_i \geqslant 0$, when $y := Ax = e_i \neq 0$ and $q = y^Tx = 0$, a contradiction. ∎

THEOREM 3.6 [4,8]. *If* $A = A^T \in \mathbb{R}^{n\times n}$ *is copositive of exact order* $n-1$, *then*

(i) In $A = (n-1, 1, 0)$, *and there is a positive eigenvector associated with the negative eigenvalue;*

(ii) *A is nonsingular and nnd of order* $n-1$, det $A < 0$, *and* $A^{-1} \leqslant 0$;

(iii) *if A is strictly copositive of order* $n-1$, *then it is pd of order* $n-1$ *and* $A^{-1} < 0$.

The following result is a sharpening of Theorem 3.6.

THEOREM 3.7. *If* $A = A^T \in \mathbb{R}^{n \times n}$ *is copositive of exact order* $n-1$, *then*

(i) A *is pd of order* $n-2$;
(ii) *all the principal minors of order* $\geqslant 2$ *of* A^{-1} *are negative*;
(iii) $A^{-1} \leqslant 0$ *with negative off-diagonal elements.*

Proof. (i): If A is not pd of order $n-2$, assume, without loss of generality, that the largest pd leading principal submatrix A_{11} of A is of order $k < n-2$. Then, in (2.2), $c_{k+1,k+1} = 0$, since A_{TT} with $T = \{1, \dots, k+1\}$ is nnd, and there must be a $c_{k+1,j} \neq 0$, $j > k+1$, because otherwise $\det A = \det A_{11} \det C_{22}$ would equal zero. But then, with $S = \{1, \dots, k+1, j\}$, $\det A_{SS} < 0$ where $|S| = k+2 < n$, contrary to Theorem 3.6(ii).

(ii): follows from (i) and Theorem 3.6(ii) by using Theorem 2.1.

(iii): If, in $B := A^{-1}(\leqslant 0)$, there is $b_{ij} = b_{ji} = 0$, $i \neq j$, then

$$\begin{vmatrix} b_{ii} & b_{ij} \\ b_{ji} & b_{jj} \end{vmatrix} = b_{ii} b_{jj} \geqslant 0,$$

contrary to (ii). ∎

The following theorem is a consequence of [2, Theorems 3.2, 4.1, 4.4].

THEOREM 3.8. $A = A^T \in \mathbb{R}^{n \times n}$ *is copositive of exact order* $n-1$ *if and only if* $\operatorname{In} A = (n-1, 1, 0)$ *and* $A^{-1} \leqslant 0$.

An equivalent formulation is as follows.

THEOREM 3.9. $A = A^T \in \mathbb{R}^{n \times n}$ *is copositive of exact order* $n-1$ *if and only if* $\det A < 0$, $A^{-1} \leqslant 0$, *and all the leading principal minors of order* $\leqslant n-2$ *of* A *are positive.*

Proof. Necessity is obvious from Theorems 3.6–7. To prove sufficiency let A_{11} in (2.2) be of order $n-2$. Then, in (2.5), $\operatorname{In} A_{11} = (n-2, 0, 0)$ and $\operatorname{In} C_{22} = (1, 1, 0)$ because, from (2.3), $\det C_{22} = \det(A_{22} - A_{21} A_{11}^{-1} A_{12}) < 0$. ∎

REMARK 3.5. Using the concept of a *strictly merely positive subdefinite* matrix [2], we can state the following corollary to Theorem 3.9: A nonsingular matrix $A = A^T \in \mathbb{R}^{n \times n}$ is strictly merely positive subdefinite if and only if

$A \leqslant 0$ and all the leading principal minors of order $\geqslant 2$ of A are negative. This result is a sharpening of [2, Theorem 4.3].

THEOREM 3.10 [4,8]. *If the copositive matrix* $A = A^T \in \mathbb{R}^{n \times n}$ *is strictly copositive of exact order* $n-1$, *then*

(i) $\operatorname{In} A = (n-1, 0, 1)$, *and there is a positive eigenvector associated with the zero eigenvalue;*

(ii) A *is nnd, of rank* $n-1$, *and pd of order* $n-1$.

Parallel to Theorem 3.9 we have the following result.

THEOREM 3.11. $A = A^T \in \mathbb{R}^{n \times n}$ *is copositive, and strictly copositive of exact order* $n-1$, *if and only if* $\det A = 0$, *the leading principal minors of order* $\leqslant n-1$ *of* A *are positive, and* A *has a positive eigenvector associated with the zero eigenvalue.*

Proof. Necessity is obvious from Theorem 3.10. To prove sufficiency, note first that A is nnd but not strictly copositive. We shall show that A is pd of order $n-1$. It suffices to verify that all the principal minors of order $n-1$ of A are positive, i.e., that $\operatorname{adj} A$ has a positive diagonal. Now, letting $x > 0$ be a properly normalized eigenvector of A associated with the zero eigenvalue, we have $\operatorname{adj} A = xx^T > 0$; see [8]. ∎

Finally, concerning copositive-plus matrices we have the following result [13, Theorem 4.4].

THEOREM 3.12. *Let* $A = A^T$ *be copositive-plus of order* $n-1$ *but not strictly copositive. Then it is copositive-plus if and only if it is singular.*

4. CRITERIA FOR COPOSITIVITY

The following three theorems are the main results of this study.

THEOREM 4.1. $A = A^T \in \mathbb{R}^{n \times n}$ *is not copositive if and only if for some* $R \subset \{1, \ldots, n\}$ *(possibly for* $R = \varnothing$*), for which* A_{RR} *is pd, there is an* $i \notin R$ *such that*

$$A^R_{i, R+i} \leqslant 0 \quad and \quad a^R_{ii} = 0 \quad \Rightarrow \quad a^R_{ij} < 0 \quad for\ some\ j \notin R, \tag{4.1}$$

where $A^R = \mathscr{P}_R A$.

Proof. *Sufficiency*: Without loss of generality, assume that in (2.2), $A_{11} = A_{RR}$. Take $x = e_i \geqslant 0$, when $q = c_{ii} \leqslant 0$. If $c_{ii} < 0$, A is not copositive. If again $c_{ii} = 0$, then $q = 0$ but $y_j < 0$, indicating the noncopositivity of A; see Theorem 3.2.

Necessity: If A is copositive of exact order k, $0 \leqslant k \leqslant n-1$, assume without loss of generality that the leading principal submatrix A_{11} of order $k+1$ of A is not copositive. By Theorem 3.6 we have, in (2.2), $A_{11}^{-1} = C_{11} \leqslant 0$ (thus, if $A_{11} = [a_{11}]$ is 1×1, then $a_{11} < 0$). If $c_{k+1,k+1} < 0$, then (4.1) holds for $R = \{1,\dots,k\}$, $i = k+1$, because $\mathscr{P}_R A = \mathscr{P}_{k+1} C$. If again $c_{k+1,k+1} = 0$, then $c_{k,k+1} = c_{k+1,k} < 0$ by Theorem 3.7, and (4.1) holds for $R = \{1,\dots,k-1\}$, $i = k$, $j = k+1$, because $\mathscr{P}_R A = \mathscr{P}_{\{k,k+1\}} C$. ■

THEOREM 4.2. *$A = A^T \in \mathbb{R}^{n \times n}$ is not strictly copositive if and only if for some $R \subset \{1,\dots,n\}$ (possibly for $R = \varnothing$) for which A_{RR} is pd, there is an $i \notin R$ such that*

$$A^R_{i,R+i} \leqslant 0, \tag{4.2}$$

where $A^R = \mathscr{P}_R A$.

Proof. *Sufficiency*: Similarly to the sufficiency part of the proof of Theorem 4.1, there is an $0 \neq x \geqslant 0$ for which $q \leqslant 0$, indicating that A is not strictly copositive.

Necessity: If A has a nonpositive diagonal element a_{ii}, take $R = \varnothing$. Otherwise, let A be strictly copositive of exact order k, $1 \leqslant k \leqslant n-1$, and assume without loss of generality that the leading principal submatrix D of order $k+1$ of A is not strictly copositive. If D is not copositive, then $D^{-1} < 0$, and we proceed in the same way as in the necessity part of the proof of Theorem 4.1, noting that no diagonal element of D^{-1} is zero. If again D is copositive, it is of rank k and pd of order k; see Theorem 3.10. Consider the tables

$$D: \begin{array}{r} \\ y^1 = \\ y^2 = \end{array} \begin{array}{c} \begin{array}{cc} x^1 & x^2 \end{array} \\ \boxed{\begin{array}{cc} D_{11} & D_{12} \\ D_{12}^T & D_{22} \end{array}} \end{array} \xrightarrow{\mathscr{P}_{(1)}} E: \begin{array}{r} \\ x^1 = \\ y^2 = \end{array} \begin{array}{c} \begin{array}{cc} y^1 & x^2 \end{array} \\ \boxed{\begin{array}{cc} E_{11} & E_{12} \\ -E_{12}^T & 0 \end{array}} \end{array},$$

where $x^1, y^1 \in \mathbb{R}^k$ and $x^2, y^2 \in \mathbb{R}$. (Since D is of rank k and the $k \times k$ block D_{11} is nonsingular, E_{22} is zero as the Schur complement of D_{11} in D.) The equation $Dx = 0$ has the solution $x^1 = E_{12} x^2$, where x^2 is arbitrary. So $\begin{bmatrix} E_{12} \\ 1 \end{bmatrix}$

is an eigenvector of D, associated with the zero eigenvalue. By Theorem 3.10, $E_{12} > 0$. Thus (4.2) holds for $R = \{1,\dots,k\}$ and $i = k+1$. ∎

THEOREM 4.3. *$A = A^T \in \mathbb{R}^{n\times n}$ is not copositive-plus if and only if for some $R \subset \{1,\dots,n\}$ (possibly for $R = \varnothing$) for which A_{RR} is pd, there is an $i \notin R$ such that*

$$A^R_{i,R+i} \leqslant 0 \text{ and } a^R_{ii} = 0 \quad \Rightarrow \quad a^R_{ij} \neq 0 \quad \text{for some } j \notin R, \tag{4.3}$$

where $A^R = \mathscr{P}_R A$.

Proof. *Sufficiency*: Similarly to the sufficiency part of the proof of Theorem 4.1, there is an $0 \neq x \geqslant 0$ for which $q = c_{ii} \leqslant 0$. If $c_{ii} < 0$, A is not copositive. If again $c_{ii} = 0$, then $q = 0$ but $y_j \neq 0$, indicating that A is not copositive-plus.

Necessity: If A has a negative diagonal element a_{ii}, take $R = \varnothing$. Otherwise, let A be copositive-plus of exact order k, $1 \leqslant k \leqslant n-1$, and assume without loss of generality that the leading principal submatrix D of order $k+1$ of A is not copositive-plus. If D is not copositive, we continue in the same way as in the necessity part of the proof of Theorem 4.1. If again D is copositive, let it be strictly copositive of exact order h, where necessarily $h < k$; see Theorem 3.10. Without loss of generality assume that the leading $(h+1)\times(h+1)$ principal submatrix of D is not strictly copositive. Because it is copositive, it is of rank h and pd of order h. Consider the tables

$$D:\ \begin{array}{r} \\ y^1 = \\ y^2 = \\ y^3 = \\ y^4 = \end{array}\!\!\begin{array}{cccc} x^1 & x^2 & x^3 & x^4 \\ \hline D_{11} & D_{12} & D_{13} & D_{14} \\ D_{21} & D_{22} & D_{23} & D_{24} \\ D_{31} & D_{32} & D_{33} & D_{34} \\ D_{41} & D_{42} & D_{43} & D_{44} \end{array} \ \xrightarrow{\mathscr{P}_{(1)}} E:\ \begin{array}{r} \\ x^1 = \\ y^2 = \\ y^3 = \\ y^4 = \end{array}\!\!\begin{array}{cccc} y^1 & x^2 & x^3 & x^4 \\ \hline E_{11} & E_{12} & E_{13} & E_{14} \\ E_{21} & E_{22} & E_{23} & E_{24} \\ E_{31} & E_{32} & E_{33} & E_{34} \\ E_{41} & E_{42} & E_{43} & E_{44} \end{array}, \tag{4.4}$$

where $x^1, y^1 \in \mathbb{R}^h$ and $x^2, x^4, y^2, y^4 \in \mathbb{R}$, and x^3, y^3 may be vacuous. Here $E_{12} > 0$ and $E_{22} = 0$; cf. the necessity part of the proof of Theorem 4.2. Because D, omitting the last row and column, is copositive-plus, there is $E_{32} = 0$ (unless it is vacuous), and because D is copositive, $E_{42} \geqslant 0$. In fact, $E_{42} > 0$, because D must be nonsingular by Theorem 3.12, and so (4.3) holds for $R = \{1,\dots,h\}$, $i = h+1$, $j = k+1$. ∎

REMARK 4.1. Remark 3.3 is a special case (with $R = \varnothing$) of the sufficiency parts of Theorems 4.1–3.

As for Theorems 4.1–3, it is, in principle, rather easy to enumerate all the pd principal submatrices of A by using single principal pivotal operations with positive pivots only. Of course, much computational effort may be required if A is of large order.

If, in Theorems 4.1–3, a table $A^R = \mathscr{P}_R A$ gives an indication that A does not belong to a certain copositivity class, it is possible to determine a ray in $\mathbb{R}^n_+$ on which the copositivity class in question is broken. This can be done as follows. Putting, in table A^R, $\hat{x}_i = 1$ and the other independent variables equal to zero, and calculating $\hat{x}_R$ from the table yields a point $\hat{x} \in \mathbb{R}^n_+$ with $q(\hat{x}) \leqslant 0$. Then $\{x = t\hat{x} \mid t > 0\}$ is a desired ray except in the case $a^R_{ii} = 0$ of Theorem 4.1. In this exceptional case, $q(\hat{x}) = 0$ but $\partial q(\hat{x})/\partial x_j = 2\hat{y}_j < 0$. For $s > 0$, we have $x + se_j \in \mathbb{R}^n_+$. In addition, $q(\hat{x} + se_j) = \hat{x}^T A\hat{x} + 2se_j^T A\hat{x} + s^2 e_j^T Ae_j = s(2\hat{y}_j + sa_{jj}) < 0$ if $s > 0$ is sufficiently small. Choosing $\hat{s} := -\hat{y}_j/a_{jj}$ or $\hat{s} := 1$ according to whether $a_{jj} > 0$ or $a_{jj} \leqslant 0$, we find that $\{x = t(\hat{x} + \hat{s}e_j) \mid t > 0\}$ is a desired ray.

EXAMPLE 4.1. We determine the copositivity class of the matrix

$$A = \begin{bmatrix} 1 & -1 & 1 & 2 \\ -1 & 2 & -3 & -3 \\ 1 & -3 & 5 & 6 \\ 2 & -3 & 6 & 5 \end{bmatrix}.$$

The following sets R yield pd principal submatrices:

$$\varnothing,\ \{1\},\ \{1,2\}^*,\ \{1,3\}^*,\ \{1,4\},\ \{2\},\ \{2,3\}^*,\ \{2,4\},\ \{3\},\ \{4\},$$

the starred sets giving an indication that A is not copositive-plus. For example, in the table

$$C := \mathscr{P}_{\{1,2\}}A: \quad \begin{array}{r|cc:cc|} & y_1 & y_2 & x_3 & x_4 \\ \hline x_1 = & 2 & 1 & 1 & -1 \\ x_2 = & 1 & 1 & 2 & 1 \\ \hdashline y_3 = & -1 & -2 & 0 & 2 \\ y_4 = & 1 & -1 & 2 & 0 \\ \hline \end{array} \quad \text{or} \quad \begin{array}{r|cc|} & y^1 & x^2 \\ \hline x^1 = & C_{11} & C_{12} \\ y^2 = & C_{21} & C_{22} \\ \hline \end{array}$$

this indication is obtained from row 3. Thus A is copositive but not copositive-plus. From table C we see that $\bar{x} = (1,2,1,0) \geqslant 0$ yields $\bar{y} = A\bar{x} =$

$(0,0,0,2) \neq 0$ and $q(\bar{x}) = \bar{x}^T A \bar{x} = 0$. Moreover, we can deduce that $\{x = t\bar{x} \mid t > 0\}$ is the only ray in $\mathbb{R}^n_+$ on which $0 \neq x \geqslant 0$, $Ax \neq 0$, and $q = x^T Ax = 0$. To wit, C_{11} is pd and C_{22} copositive, whence, by (2.4), $q = 0$ implies $y^1 = 0$ and $x_3 x_4 = 0$. Because then $x_1 = x_3 - x_4 \geqslant 0$, the only possibility is that $x_4 = 0$ and $x_3 > 0$.

The criteria contained in Theorems 4.1–3 are in a certain sense "outer" criteria—the decisions are made outside of the principal submatrices A_{RR} in question. In the following three theorems we present the corresponding "inner" criteria, where the decisions are made inside of the principal submatrices. However, the outer criteria are computationally much more efficient than the inner ones, because in them only pd principal submatrices need to be searched.

THEOREM 4.4. *$A = A^T \in \mathbb{R}^{n \times n}$ is not copositive if and only if it contains a nonsingular principal submatrix D such that a column of D^{-1} is nonpositive.*

Proof. *Sufficiency*: By Theorem 3.4, D is not copositive; neither is A.
Necessity: If A is copositive of exact order k, it contains a non-copositive principal submatrix D of order $k+1$. But then $D^{-1} \leqslant 0$. ∎

THEOREM 4.5. *$A = A^T \in \mathbb{R}^{n \times n}$ is not strictly copositive if and only if at least one of the following conditions is satisfied*:

(i) *A contains a nonsingular principal submatrix D such that a column of D^{-1} is nonpositive.*

(ii) *A contains a singular nnd principal submatrix with a nonnegative eigenvector attached to the zero eigenvalue.*

Proof. *Sufficiency*: See Theorem 4.4 and Remark 3.2.
Necessity: If A is strictly copositive of exact order k, it contains a principal submatrix D of order $k+1$ which is not strictly copositive. If D is not copositive, then $D^{-1} < 0$. If again D is copositive, it is singular and nnd, and has a positive eigenvector associated with the zero eigenvalue; see Theorem 3.10. ∎

THEOREM 4.6. *$A = A^T \in \mathbb{R}^{n \times n}$ is not copositive-plus if and only if at least one of the following conditions is satisfied*:

(i) *A contains a nonsingular principal submatrix D such that a column of D^{-1} is nonpositive.*

(ii) *A contains a nonsingular principal submatrix D such that a column of D^{-1} is nonnegative with a zero diagonal element.*

Proof. *Sufficiency*: See Theorems 4.4 and 3.5.

Necessity: Let R be the set for which (4.3) holds. If $a_{ii}^R < 0$, take $D = A_{SS}$ with $S = R + i$, when (i) holds. If again $a_{ii}^R = 0$, take $D = A_{SS}$ with $S = R \cup \{i, j\}$, when (i) or (ii) holds. ∎

We conclude this section by comparing our criteria with existing determinantal tests and by giving a determinantal test for copositive-plus matrices. First we state existing determinantal criteria for copositive and strictly copositive matrices.

THEOREM 4.7. *$A = A^T \in \mathbb{R}^{n \times n}$ is not copositive (strictly copositive) if and only if there is a principal submatrix D of A with* $\det D < 0$ $(\leqslant 0)$ *for which the cofactors of the last column are nonnegative (positive).*

The strictly copositive case of this theorem (related to our Theorem 4.5) is due to Motzkin [12] and proved in another way in [4]. The copositive case (related to our Theorem 4.4) is due to E. Keller and cited, without proof, in [4]. Below, we give a new proof to Theorem 4.7.

Proof of Theorem 4.7. *Sufficiency*: If $\det D < 0$, the last column of D^{-1} is nonpositive (negative), whence A is not copositive; see Theorem 4.4. If again $\det D = 0$, it follows from $D \operatorname{adj} D = 0$ that the last column (say x) of $\operatorname{adj} D$ satisfies $Dx = 0$. But then $x > 0$ and $x^T D x = 0$, whence D (hence A) is not strictly copositive.

Necessity: If A is copositive (strictly copositive) of exact order k, it contains a principal submatrix D of order $k+1$ which is not copositive (strictly copositive). But then $\det D < 0$ and $\operatorname{adj} D \geqslant 0$ ($\det D \leqslant 0$ and $\operatorname{adj} D > 0$); see Theorem 3.1 (3.2) of [4]. ∎

Motzkin [12] has also derived the following version of the strictly copositive case of Theorem 4.7 which is essentially the same as our Theorem 4.2.

THEOREM 4.8. *$A = A^T \in \mathbb{R}^{n \times n}$ is not strictly copositive if and only if there is a principal submatrix D of A with* $\det D \leqslant 0$ *for which all the leading principal minors, except for* $\det D$, *and the cofactors of the last column are positive.*

This theorem can be proved similarly to Theorem 4.7, noting that, in the necessity part, D is pd of order k.

A possible determinantal test for copositive-plus matrices is as follows.

THEOREM 4.9. *A copositive matrix $A = A^T \in \mathbb{R}^{n\times n}$ is not copositive-plus if and only if there is a principal submatrix D of A with* $\det D < 0$ *such that* $\operatorname{adj} D$ *has a nonpositive column with zero diagonal element.*

Proof. Sufficiency is obvious from Theorem 4.6. To prove necessity, note that, by Theorems 4.1 and 4.3, A being copositive but not copositive-plus implies the existence of $R \subset \{1,\dots,n\}$ and $i, j \notin R$ such that A_{RR} is pd, $A^R_{Ri} \geqslant 0$, $a^R_{ii} = 0$, and $a^R_{ij} = a^R_{ji} > 0$. Take $D = A_{SS}$ with $S = R \cup \{i, j\}$. ∎

5. ADDITIONAL RESULTS

The following two theorems are corollaries to Theorems 4.1–3.

THEOREM 5.1. *If a copositive matrix $A = A^T \in \mathbb{R}^{n\times n}$ is copositive-plus of exact order $n-1$, then it is strictly copositive of exact order $n-2$.*

Proof. In the proof of the necessity part of Theorem 4.3, let $k+1 = n$ (here $n \geqslant 2$ because, for $n = 1$, A is copositive-plus if and only if it is copositive). We content that x^3 and y^3 in the tables D and E of (4.4) must be vacuous. If the contrary holds true, then the matrix obtained from D by deleting the third super-row and -column is copositive-plus, implying that $E_{42} = 0$. But this is impossible, as shown in the proof of Theorem 4.3. ∎

THEOREM 5.2. *If $A = A^T \in \mathbb{R}^{n\times n}$ has $p < n$ positive eigenvalues, then it is copositive (copositive-plus, strictly copositive) if and only if it is copositive (copositive-plus, strictly copositive) of order $p+1$.*

Proof. Necessity is obvious. To prove sufficiency, we show that if A is not copositive (copositive-plus, strictly copositive), there is a principal submatrix A_{SS} of order $\leqslant p+1$ of A which is not copositive (copositive-plus, strictly copositive). There are three cases.

Case 1: *A is not copositive and $a^R_{ii} < 0$ in Theorem* 4.1, 4.3 *or* 4.2. Denoting $S = R + i$ and $k = |S|$, it is found that $\operatorname{In} A \geqslant \operatorname{In} A_{SS} = (k-1, 1, 0)$, implying $p \geqslant k-1$ or $k \leqslant p+1$.

Case 2: *A is not copositive (copositive-plus) and $a^R_{ii} = 0$, $a^R_{ij} = a^R_{ji} < 0$ $(\neq 0)$ in Theorem* 4.1 (4.3). Denoting $T = \{i, j\}$, $S = R \cup T$, and $k = |S|$, it is found that $\operatorname{In} A \geqslant \operatorname{In} A_{SS} = \operatorname{In} A_{RR} + \operatorname{In} A^R_{TT} = (k-2, 0, 0) + (1, 1, 0) = (k-1, 1, 0)$, implying $p \geqslant k-1$ or $k \leqslant p+1$.

Case 3: *A is not strictly copositive and* $a_{ii}^R = 0$ *in Theorem* 4.2. Take $S = R + i$, when $|S| = |R| + 1 \leqslant p + 1$. ∎

We note that Pereira [13, Theorems 3.14–15] has proved in another way the copositive and strictly copositive cases of Theorem 5.2.

THEOREM 5.3. *If* $A = A^T \in \mathbb{R}^{n \times n}$ *is of rank* $r < n$, *it is copositive* (*copositive-plus, strictly copositive*) *if and only if it is copositive of order* r (*copositive-plus of order* r, *strictly copositive of order* $r+1$).

Proof. The copositive and copositive-plus cases have been proved in [13, Theorem 3.12, Lemma 4.3]. We prove the strictly copositive case and give a new proof to the copositive case (the same technique cannot here be used for proving the copositive-plus case, because this case has indirectly been applied to establish Theorem 4.3). Necessity is obvious. In proving sufficiency there are two cases (p is as in Theorem 5.2).

Case 1: $r = p$. Then A is nnd and as such copositive. If A is strictly copositive of order $r + 1 = p + 1$, it is strictly copositive by Theorem 5.2.

Case 2: $r \geqslant p + 1$. Then the result follows directly from Theorem 5.2. ∎

Finally, we present two properties of copositive matrices (Theorems 5.4–5) which are valid for orders $\leqslant 3$ but not for orders $\geqslant 4$.

The copositive and strictly copositive matrices of orders 2 and 3 have been characterized in [8]. In the following theorem we characterize the 2×2 and 3×3 copositive-plus matrices.

THEOREM 5.4. $A = A^T \in \mathbb{R}^{n \times n}$, $n \leqslant 3$, *is copositive-plus if and only if it is nnd or, after deleting the possible zero rows and columns, strictly copositive.*

Proof. Sufficiency is obvious, as is necessity for $n = 1$ and for nonsingular 2×2 and 3×3 matrices. We prove then necessity for 2×2 and 3×3 singular matrices with positive diagonal elements. If A is 2×2, it is nnd because $a_{11}, a_{22} > 0$. For $n = 3$, it suffices to consider the scaled matrix

$$A = \begin{bmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{bmatrix}. \tag{5.1}$$

Here $a, b, c \geqslant -1$ because A is copositive; see [8]. If $|a| < 1$, $|b| < 1$, or $|c| < 1$, then A is nnd, and if $a, b, c \geqslant 0$, then A is strictly copositive. It remains to consider the case where at least one of a, b, c equals -1. Without loss of generality, assume that $a = -1$. Then it follows from the singularity of A that $c = -b$, whence $b \leqslant 1$. But if $a = -1$ and $-1 \leqslant b = -c \leqslant 1$, then A is nnd. ∎

The preceding theorem does not hold for $n \geqslant 4$, as is seen e.g. from the matrix

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \left[\begin{array}{rr|rr} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & 1 \end{array}\right].$$

Here A_{11} is nnd but not strictly copositive, and A_{22} is strictly copositive but not nnd. Thus A is copositive-plus but neither nnd nor strictly copositive.

THEOREM 5.5. *If $A = A^T \in \mathbb{R}^{n \times n}$, $n \leqslant 3$, is a nonsingular strictly copositive matrix, then all the diagonal elements of A^{-1} cannot be zero.*

Proof. The cases $n = 1$ and $n = 2$ being trivial, consider the A of (5.1). For the cofactors of all the diagonal elements in A to be zero, there must be $|a| = |b| = |c| = 1$. The strict copositivity of A implies, $a, b, c > -1$ (see [8]), whence $a = b = c = 1$. But such an A is singular, a contradiction. ∎

For $n \geqslant 4$, the preceding theorem does not hold. As a counterexample we give the matrix

$$A = \begin{bmatrix} 1 & 0 & -1 & 1 \\ 0 & 1 & 1 & -1 \\ -1 & 1 & 2 & 0 \\ 1 & -1 & 0 & 2 \end{bmatrix} \quad \text{with} \quad A^{-1} = \frac{1}{2}\begin{bmatrix} 0 & 2 & -1 & 1 \\ 2 & 0 & 1 & -1 \\ -1 & 1 & 0 & 1 \\ 1 & -1 & 1 & 0 \end{bmatrix}.$$

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