On Copositive Matrices

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ABSTRACT

A criterion for copositive matrices is given and for $n = 3$ the set of all copositive matrices is determined in terms of matrix elements. Copositive matrices are applied to the problem of excluding periodic solutions of certain algebraic differential equations.

INTRODUCTION

Since Motzkin [31] introduced the notion of a copositive matrix, the original results have been extended in several directions: characterization of copositive matrices [6, 12, 35], extension to quadratic programming [10, 11, 21, 22, 23, 29] and related combinatorial problems [1, 2, 3, 14, 15, 20], and extension to spaces of infinite dimension [26]. However, it is still difficult to determine whether a given matrix is copositive; and there are only few useful applications. In the following I shall derive some additional criteria for copositivity, and find all copositive matrices for dimension 3. Furthermore the concept of copositivity will be applied to algebraic differential equations.

First I give an account of definitions and earlier results. Let $\mathbb{R}^n$ be the usual coordinate space, and let K be the closed convex cone of nonnegative vectors. Consider the space H of real symmetric matrices $A = (a_{jk})$ of order n. Its dimension is $n(n+1)/2$. Among the many cones in this space the following four are of particular interest (T denotes transpose):

$$P = \{ A : a_{jk} \geq 0 \text{ for } j, k = 1, \ldots, n \},$$
$$S = \{ A : x^T A x \geq 0 \text{ for } x \in \mathbb{R}^n \},$$
$$C = \{ A : x^T A x \geq 0 \text{ for } x \in K \},$$
$$B = \left\{ A : A = \sum_{j=1}^{m} x_j x_j^T, x_j \in K, m \text{ finite} \right\}.$$

P is the cone of positive matrices in the sense of Perron, S are the positive definite matrices, the matrices in C are copositive, and those in B are the completely positive matrices. Each of these cones is convex, closed, pointed, and has nonempty interior. A matrix A with $x^T A x > 0$ for $x \in K$, $x \neq 0$, is called strictly copositive.

A natural inner product in H is given by $\operatorname{tr} XY$. Denote the dual cone by an asterisk. Obviously $P = P^*$. From the identity $\operatorname{tr} A x x^T = x^T A x$ one sees $S = S^*$, $B = C^*$, and thus $B^* = C$. Always $P + S \subset C$; thus by duality, $P \cap S \supset B$. For $n = 2$ one has $P \cup S = C$; for $n = 3, 4$ one has $P + S = C$ (Diananda [9]); for $n = 5$ there are elements in $P \cap S$ which are not in B (examples due to Hall and Horn are given in [14, p. 265 ff.]), and hence $P + S \neq C$. A detailed survey on copositive matrices has been given by M. Hall [14], in particular on the unsolved problem of determining the extremal rays of the cone C (those of P, S, B are easily found). Many results on extremal rays are contained in [1, 2, 3, 4, 14, 15, 20]. An interesting relation between copositivity with respect to a general cone and the Perron property has been shown in [18]. In a series of recent papers (see [29]) quadratic forms with general linear restrictions are considered. In a fundamental paper Cottle, Habetler, and Lemke [6] have given an inductive criterion for copositivity. In the following Theorem 1 I show a more general criterion (actually a whole family of criteria), which also provides a coordinate-free proof of their result (Theorem 2).

The sign $\geqslant$ indicates that a vector or matrix has nonnegative elements; the sign $>$ says that all elements are positive.

DEFINITION 1. Let A be a symmetric matrix, and let B be a strictly copositive matrix of the same order. The pair A, B is called (strictly) codefinite iff $Ax = \lambda Bx$, $x > 0$ implies $\lambda \geqslant 0$ ($\lambda > 0$, respectively).

DEFINITION 2. The symmetric matrix A of order n is called (strictly) copositive of order m, $1 \leqslant m \leqslant n$, iff every principal submatrix of order m is (strictly) copositive.

RESULTS

THEOREM 1. *Let A of order n be (strictly) copositive of order $n - 1$. The following statements are equivalent:*

(1) *A is (strictly) copositive.*

(2) *There is a strictly copositive matrix B of order n such that the pair A, B is (strictly) codefinite.*

(3) *For every strictly copositive matrix B of order n the pair A, B is (strictly) codefinite.*

Proof. (1) → (3): Let B be strictly copositive of order n. Suppose $Ax = \lambda Bx$, $x > 0$. Then $x^T A x = \lambda x^T B x$, and thus $\lambda \geqslant 0$ (or $\lambda > 0$, respectively). Since (3) → (2) is obvious, it remains to show (2) → (1). Suppose the form $x^T A x$ assumes negative (nonpositive, respectively) values for certain $x \geqslant 0$, $x \neq 0$. Since A is (strictly) copositive of order $n - 1$, such x are necessarily positive. Consider the form $x^T A x$ on the set $D = \{x \geqslant 0, x^T B x = 1\}$. It assumes its minimum at a point $\bar{x}$ of the relative interior of D. The minimum is negative (nonpositive). From the necessary condition for a minimum of $x^T A x$ on D it follows that $A\bar{x} = \lambda B\bar{x}$ with $\lambda = \bar{x}^T A \bar{x}$. In view of statement (2), $\lambda \geqslant 0$ (or $\lambda > 0$), which leads to a contradiction.   ∎

From Theorem 1 one can easily proceed to Theorem 2, which is essentially the result of Cottle, Habetler, and Lemke [6]. For convenience the theorem is stated in a negative form.

THEOREM 2. *Let A of order n be copositive of order $n - 1$. Then the following statements are equivalent*:

(1) *A is not copositive.*
(2) *For every $b > 0$ there is an $x > 0$ such that $Ax = \lambda b$, $\lambda < 0$.*
(3) *The matrix $-A^{-1}$ exists and is nonnegative.*
(4) $\det A < 0$ *and* $\operatorname{adj} A \geqslant 0$.

Here $\det A$ is the determinant and $\operatorname{adj} A$ is the adjugate, i.e. the matrix of signed cofactors, such that $A \operatorname{adj} A = (\det A) I$.

Proof. For the matrix B in Theorem 1 one can choose the identity or matrices $B = bb^T$ of rank 1, where $b > 0$ is a positive vector. Then the equivalence of (1) and (2) follows from Theorem 1 by contraposition. Assume (2), and suppose there is y with $Ay = 0$. Since $Ax = b$ has a solution for $b > 0$, it follows $y^T b = 0$ for $b > 0$; thus $y = 0$. Hence A^{-1} exists. For every $b > 0$ the vector $x = A^{-1} b$ is elementwise negative. Thus $-A^{-1}$ is a nonnegative matrix, which shows (3). Of course from (3) follows (2).

From Theorem 1, choosing $B = I$, it follows that there is $x > 0$ such that $Ax = \lambda x$, $\lambda < 0$. Suppose A has a second negative eigenvalue, $Ay = \mu y$, $y^T x = 0$, $y \neq 0$, $\mu < 0$. The vector y has positive and negative components in view of $x > 0$, $y^T x = 0$. Choose $\alpha > 0$ such that $x + \alpha y \geqslant 0$, and $x + \alpha y$ has at least one zero component. Since A is copositive of order $n - 1$,

$$0 \leqslant (x + \alpha y)^T A (x + \alpha y) = \lambda x^T x + \mu \alpha^2 y^T y < 0.$$

Thus A has exactly one negative eigenvalue, and $\det A < 0$, which shows the equivalence with (4).   ∎

For completeness I include the corresponding result on strictly copositive matrices. The proof basically follows [6], but is somewhat shorter.

THEOREM 3.   *Let A of order n be strictly copositive of order $n - 1$. Then the following statements are equivalent:*

(1) *A is not strictly copositive.*
(2) *For every $b > 0$ there is an $x > 0$ such that $Ax = \lambda b$, $\lambda \leqslant 0$.*
(3) *det $A \leqslant 0$ and adj $A > 0$.*

Proof.   The equivalence of (1) and (2) follows from Theorem 1. Now assume (1) and (2).

Case 1: A is not copositive.   Then $\det A < 0$ and $-A^{-1} \geqslant 0$ in view of Theorem 2. For any vector u and $v = (\operatorname{adj} A)u$,

$$v^T A v = (\det A) u^T (\operatorname{adj} A) u \qquad\qquad (*)$$

If adj A is not elementwise positive, then there is a vector $u \geqslant 0$, $u \neq 0$ such that $v \geqslant 0$, $v \neq 0$ is not positive. By strict copositivity of order $n - 1$ it follows that $v^T A v > 0$, whereas $(\det A) u^T (\operatorname{adj} A) u \leqslant 0$.

Case 2: A is copositive.   By Theorem 1, $Ax = \lambda b$, $b > 0$, $x > 0$ implies $\lambda \geqslant 0$. At least for one $x > 0$ it must occur that $\lambda = 0$ (thus $\det A = 0$); otherwise A would be strictly copositive. Suppose there is a second nonpositive eigenvalue, $Ay = \mu y$, $\mu \leqslant 0$, $y \neq 0$, $y^T x = 0$. Choose α such that $x + \alpha y \geqslant 0$ with at least one zero component. Then

$$0 < (x + \alpha y)^T A (x + \alpha y) = \lambda x^T x + \mu \alpha^2 y^T y \leqslant 0.$$

Thus A is positive semidefinite of rank $n - 1$. For any semidefinite matrix A of rank $n - 1$ the adjugate is adj $A = xx^T$, where x is a (normalized) eigenvector for $\lambda = 0$. Thus adj $A > 0$.

These arguments yield statement (3). Now suppose (3) and that A is strictly copositive. Then from $(*)$ a contradiction immediately follows.   ∎

In [6] it has been observed that the determinant criteria of Motzkin [32, 33] and Garsia [13] can be derived from Theorems 2 and 3.

From Theorem 2 it would appear that, among the matrices which are copositive of order $n - 1$, the copositive matrices are characterized by a large set of inequalities, corresponding to the cofactors. In the cases $n = 2$ and $n = 3$ there is in fact only one inequality in addition to $\det A \geqslant 0$. The result for $n = 2$ is well known. The matrix $A = (a_{jk})$ is copositive iff $a_{11} \geqslant 0$, $a_{22} \geqslant 0$,

and

$$a_{11}a_{22} - a_{12}^2 \geq 0 \quad \text{or} \quad a_{12} \geq 0.$$

It is strictly copositive iff $a_{11} > 0$, $a_{22} > 0$, and

$$a_{11}a_{22} - a_{12}^2 > 0 \quad \text{or} \quad a_{12} \geq 0.$$

The case $n = 3$ is covered in the following theorem.

THEOREM 4.   *Let $n = 3$. The matrix A is copositive if and only if the conditions*

(1) $a_{11} \geq 0$, $a_{22} \geq 0$, $a_{33} \geq 0$,
(2) $a_{12} \geq -\sqrt{a_{11}a_{22}}$, $a_{23} \geq -\sqrt{a_{22}a_{33}}$, $a_{31} \geq -\sqrt{a_{33}a_{11}}$

are satisfied, as well as at least one of the following conditions:

(3a) $a_{12}\sqrt{a_{33}} + a_{23}\sqrt{a_{11}} + a_{31}\sqrt{a_{22}} + \sqrt{a_{11}a_{22}a_{33}} \geq 0.$
(3b) $\det A \geq 0.$

The matrix is strictly copositive if and only if these conditions are satisfied with strict inequality in (1), (2), (3b).

Proof.   First assume $a_{11} > 0$, $a_{22} > 0$, $a_{33} > 0$. By diagonal scaling we can put the matrix into the form

$$A = \begin{pmatrix} 1 & \alpha & \beta \\ \alpha & 1 & \gamma \\ \beta & \gamma & 1 \end{pmatrix}. \tag{1}$$

Now the necessary and sufficient conditions for copositivity of order two are

$$\alpha \geq -1, \qquad \beta \geq -1, \qquad \gamma \geq -1. \tag{2}$$

Under this hypothesis the necessary and sufficient condition for A *not* to be copositive is

$$\det A < 0 \quad \text{and} \quad \operatorname{adj} A \geq 0,$$

i.e.,

$$1 + 2\alpha\beta\gamma < \alpha^2 + \beta^2 + \gamma^2 \tag{3}$$

and

$$\alpha^2 \leqslant 1, \qquad \beta^2 \leqslant 1, \qquad \gamma^2 \leqslant 1, \tag{4a}$$

$$\alpha\beta \geqslant \gamma, \qquad \beta\gamma \geqslant \alpha, \qquad \alpha\gamma \geqslant \beta. \tag{4b}$$

The assertion of Theorem 4 claims that A is *not* copositive iff (3) is satisfied and

$$\alpha + \beta + \gamma + 1 < 0. \tag{5}$$

One has to show that, under the hypothesis of (2), (3), the conditions (4) and (5) are equivalent.

Case 1: *Let* $\alpha, \beta, \gamma \geqslant 0$. From (4a) it follows that $\alpha, \beta, \gamma \in [0,1]$, and from (4b) it follows that $\alpha\beta\gamma \geqslant \alpha^2, \beta^2, \gamma^2$; thus $3\alpha\beta\gamma \geqslant \alpha^2 + \beta^2 + \gamma^2$. From (3) it follows that $1 + 2\alpha\beta\gamma < 3\alpha\beta\gamma$; thus $\alpha\beta\gamma > 1$, in contradiction to $\alpha, \beta, \gamma \in [0,1]$. Hence (4) is empty. Of course (5) is empty.

Case 2: $\alpha, \beta \geqslant 0, \gamma < 0$. From (4b) follows $0 \geqslant \beta\gamma \geqslant \alpha \geqslant 0$, thus $\alpha = \beta = 0$. From (3) it follows that $\gamma > 1$, which contradicts (4a). Hence (4) is empty. But (5) is also empty in view of $1 \leqslant 1 + \alpha + \beta < -\gamma$, in contradiction to (2).

Case 3: $\alpha > 0, \beta, \gamma \leqslant 0$. Then $\beta, \gamma \in [-1,0]$. First we show $(4) \rightarrow (5)$. We add the inequality (3) and the inequality $2(1 + \alpha)(\alpha - \beta\gamma) \leqslant 0$ from (4b) to obtain $(1 + \alpha)^2 < (\beta + \gamma)^2$, from which follows $1 + \alpha < -(\beta + \gamma)$. Now assume (2), (3), (5). From $\alpha < -\beta - \gamma - 1 \leqslant -\beta$ and $\beta, \gamma \in [-1,0]$ it follows that $\alpha \leqslant 1$ and $\alpha\gamma \geqslant \beta$. Similarly $\alpha\beta \geqslant \gamma$. It remains to show $\alpha \leqslant \beta\gamma$. Suppose $\alpha > \beta\gamma$. Then from (3) it follows that $\alpha > \beta\gamma + \sqrt{(1 - \beta^2)(1 - \gamma^2)}$ $=: \alpha_0$. From (5), $\alpha < -\beta - \gamma - 1 =: \alpha_1$. But $\alpha_1 \leqslant \alpha_0$ in view of $-(1 + \beta)(1 + \gamma) \leqslant \sqrt{(1 - \beta^2)(1 - \gamma^2)}$. Thus (4) is proved.

Case 4: $\alpha, \beta, \gamma \leqslant 0$. From (2) it follows that $\alpha, \beta, \gamma \in [-1,0]$, and (4) is trivial. It remains to show that (5) is a consequence of (3). Suppose $\alpha + \beta + \gamma \geqslant -1$. Then $(\alpha + \beta + \gamma)^2 \leqslant 1$; thus $1 - (\alpha^2 + \beta^2 + \gamma^2) \geqslant 2(\alpha\beta + \beta\gamma + \gamma\alpha) \geqslant -2\alpha\beta\gamma$, which contradicts (3). ∎

If some of the diagonal elements are zero, then the matrix can be diagonally scaled as in (1) with some of the 1's replaced by 0's. Then the proof of equivalence is very simple.

The proof of the assertion on strict copositivity is verbally the same; one has to pay careful attention to equality signs.

APPLICATION: QUADRATIC DIFFERENTIAL EQUATIONS

A quadratic differential equation is an equation of the form

$$\dot{y} = f(y), \qquad f: \mathbb{R}^n \to \mathbb{R}^n, \tag{6}$$

where

$$f_i(y) = \sum_{j,\,k\,=\,1}^{n} b_{ijk} y_j y_k. \tag{7}$$

Equations of this type occur in many applications, e.g. in population genetics. I assume that the n^3 coefficients are nonnegative. Then the cone K is positively invariant with respect to the equations (6). I introduce relative frequencies by

$$x = y/e^T y, \qquad e^T = (1, \ldots, 1), \tag{8}$$

and obtain, after rescaling the time variable, a differential equation

$$\dot{x} = f(x) - e^T f(x) \cdot x. \tag{9}$$

The cone K as well as the simplex

$$T = \{x \in K, \, e^T x = 1\}$$

is positively invariant with respect to the system (9). The Jacobian of the system (9) on K is

$$J(x) = f'(x) - x e^T f'(x) - e^T f(x) I. \tag{10}$$

For $x \in T$ the Jacobian has the left eigenvector e^T,

$$e^T J(x) = - e^T f(x) \cdot e^T. \tag{11}$$

Thus the divergence of the function $f(x) - e^T f(x) \cdot x$, considered as a vector

field on the simplex T, is

$$D_0(x) = \operatorname{tr} J(x) + e^T f(x)$$

$$= \operatorname{tr} f'(x) - e^T f'(x) x - (n-1) e^T f(x).$$

On the set T the function D_0 coincides with the function $D: K \to R$,

$$D(x) = e^T x \operatorname{tr} f'(x) - e^T f'(x) x - (n-1) e^T f(x). \tag{12}$$

The function D is quadratic in x. It is not the divergence of the vector field (9) on K. In coordinate notation

$$D(x) = \sum_{j,k=1}^{n} \left(\sum_{i=1}^{n} b_{iji} + \sum_{i=1}^{n} b_{iik} - (n+1) \sum_{i=1}^{n} b_{ijk} \right) x_j x_k. \tag{13}$$

Now I consider the case $n = 3$. Then the simplex T is planar. By the criterion of Dulac (or the negative criterion of Bendixson) an autonomous differential system in the plane does not have perodic solutions (except constants) in a given simply connected domain if the divergence does not change sign. Thus $D(x) > 0$ on T [or $D(x) < 0$ on T] excludes the existence of periodic orbits of the system (9).

The function D is a quadratic form on the cone K. One can apply the results of the previous section in order to decide whether D changes sign. In particular, for $n = 3$ Theorem 4 provides the exact conditions on the b_{ijk}.

There are vector fields for which this criterion applies, e.g. $b_{ijk} = 1$, for which $D(x) = -6$. The question whether a system of the form (9) can have periodic solutions at all can be easily answered. Consider a system of high symmetry depending on only 6 parameters (instead of 18):

$$\dot{y}_1 = a y_1^2 + b y_2^2 + c y_3^2 + 2d y_1 y_2 + 2e y_2 y_3 + 2f y_3 y_1,$$

$$\dot{y}_2 = c y_1^2 + a y_2^2 + b y_3^2 + 2f y_1 y_2 + 2d y_2 y_3 + 2e y_3 y_1,$$

$$\dot{y}_3 = b y_1^2 + c y_2^2 + a y_3^2 + 2e y_1 y_2 + 2f y_2 y_3 + 2d y_3 y_1.$$

Straightforward computation shows that the Jacobian at the stationary point

$e/3$ is

$$J = \frac{2}{3} \begin{pmatrix} \alpha & \beta & \gamma \\ \gamma & \alpha & \beta \\ \beta & \gamma & \alpha \end{pmatrix} - \frac{2\varkappa}{9} ee^T - \frac{\varkappa}{3} I,$$

where

$$\alpha = a + d + f, \quad \beta = b + d + c, \quad \gamma = c + e + f, \quad \varkappa = \alpha + \beta + \gamma.$$

The eigenvalues are $\lambda_0 = -\varkappa/3$ with eigenvector e^T and $\lambda_{1,2} = (\alpha - 2\beta - 2\gamma)/3 \pm (\beta - \gamma)i/\sqrt{3}$. Thus for $\beta \neq \gamma$, i.e. $b + d \neq c + f$, and varying α (e.g. a) a Hopf bifurcation occurs. A simple choice is $b = 1$, $c = d = e = f = 0$, $\lambda_{1,2} = (a - 2)/3 \pm i/\sqrt{3}$.

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