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INDEFINITE COPOSITIVE MATRICES WITH EXACTLY ONE POSITIVE EIGENVALUE OR EXACTLY ONE NEGATIVE EIGENVALUE*

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Abstract. Checking copositivity of a matrix is a co-NP-complete problem. This paper studies copositive matrices with certain spectral properties. It shows that an indefinite matrix with exactly one *positive* eigenvalue is copositive if and only if the matrix is nonnegative. Moreover, it shows that finding out if a matrix with exactly one *negative* eigenvalue is strictly copositive or not can be formulated as a combination of two convex quadratic programming problems which can be solved efficiently.

Key words. Copositive matrices, Perron-Frobenius property.

AMS subject classifications. 15B48, 15A63.

1. Introduction.

Let $\mathcal{S}$ be the space of $n \times n$ symmetric matrices. Given $A \in \mathcal{S}$, we say that A is copositive if

$$x^T Ax \geq 0 \text{ for all } x \in \mathbb{R}^n_+,$$

where $\mathbb{R}^n_+$ is the nonnegative orthant. We say that A is strictly copositive if

$$x^T Ax > 0 \text{ for all } x \in \mathbb{R}^n_+ \setminus \{0\}.$$

The set of copositive matrices forms a closed convex cone, the copositive cone

$$\mathcal{C} = \{A \in \mathcal{S} \mid x^T Ax \geq 0 \text{ for all } x \in \mathbb{R}^n_+\}.$$

Many combinatorial optimization problems such as the clique number, stability number and chromatic number can be formulated as linear optimization problems over the copositive cone. For further details, see [4].

It is known in [7] that checking copositivity is a co-NP-complete decision problem. Therefore, in general it is not likely that the copositive cone can be described explicitly. In this paper, we study some subsets of the copositive cone which can be characterized easily, depending on the number of negative eigenvalues of the matrix.

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Clearly, checking copositivity of a matrix A is equivalent to verifying if the quadratic form $x^T Ax$ is nonnegative over the standard simplex, $\{x \in \mathbb{R}^n_+ \mid \sum\limits_{i=1}^{n} x_i = 1\}$. Note that the quadratic form given by a matrix A can be simplified by transforming it into diagonal form.

To this end, let the eigenvalues of A be ordered as $\lambda_1 \leq \cdots \leq \lambda_{n-1} \leq \lambda_n$. Since $A \in \mathcal{S}$, we can decompose A into $A = Q\Lambda Q^T$, where $\Lambda = \mathrm{Diag}(\lambda_1, \ldots, \lambda_n)$ and Q is an orthogonal matrix whose columns are the corresponding eigenvectors. Denote the linearly independent rows of Q as $q^1, \ldots, q^n \in \mathbb{R}^n$, and define the convex hull $\mathcal{Q} := \mathrm{conv}\{q^1, \ldots, q^n\}$ and $y := Q^T x$. With these notations, we have

$$A \in \mathcal{C} \quad \Leftrightarrow \quad y^T \Lambda y \geq 0 \text{ for all } y \in \mathcal{Q}. \tag{1.1}$$

Note that $\mathcal{Q}$ is a polytope. Actually, $\mathcal{Q}$ is the image of the standard simplex, which is a base of $\mathbb{R}^n_+$, under the linear mapping $x \mapsto Q^T x$, whence $\mathcal{Q}$ is also a simplex.

Definition 1.1. We say that the Perron-Frobenius property holds for a matrix $A \in \mathcal{S}$ if there is a $z \in \mathbb{R}^n_+ \setminus \{0\}$ such that $Az = \lambda_n z$, where λ_n is the largest eigenvalue.

The Perron-Frobenius property of copositive matrices was studied in [1], [5] and [6]. In particular, it is known (e.g. [6, Theorem 11]) that if an indefinite matrix with exactly one positive eigenvalue is copositive, then it has the Perron-Frobenius property. In this paper, we show that the converse is true for matrices with nonnegative diagonal elements. We also give a simple characterization of indefinite copositive matrices with exactly one positive eigenvalue.

Furthermore, we show that we can check whether or not a matrix with exactly one negative eigenvalue is strictly copositive by solving two convex quadratic problems. Thus, checking strict copositivity of matrices in this subset turns out to be "easy".

Throughout the paper, $\mathrm{bd}(S)$ and $\mathrm{int}(S)$ denote the boundary of the set S and the interior of the set S, respectively.

2. Copositive matrices with exactly one positive eigenvalue.

As any positive semidefinite matrix is copositive, we may and do assume in the following that A has a negative eigenvalue. Moreover, this section deals with an indefinite matrix with exactly one positive eigenvalue, i.e.,

$$\lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 0 < \lambda_n \quad \text{and} \quad \lambda_1 < 0. \tag{2.1}$$

It is known that $A \in \mathcal{C}$ satisfying (2.1) has the Perron-Frobenius property, see e.g. [6, Theorem 11]. However, in the case $\lambda_1 = 0$, the Perron-Frobenius property might not

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be fulfilled. For instance, consider ([6, p. 280])

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

In this case, $\lambda_1 = 0$ and $\lambda_2 = 2$, and A has a nonnegative eigenvector corresponding to λ_1, but not to λ_2.

We study further copositive matrices satisfying (2.1).

Proposition 2.1. *Let A be an indefinite matrix with exactly one positive eigenvalue. Then A is copositive if and only if the following two conditions both hold:*

(a) $A_{ii} \geq 0$ for all $i = 1, \ldots, n$, and
(b) the Perron-Frobenius property holds for A.

Proof. Let $A \in \mathcal{C}$ satisfy (2.1). Then it is well known that $A_{ii} \geq 0$ for all i and the Perron-Frobenius property holds for A. Thus, one implication is clear.

Now let us consider the other direction. Suppose properties (a) and (b) hold. Define

$$\mathrm{Pos}(A) := \{z \in \mathbb{R}^n \mid z^T \Lambda z \geq 0\}.$$

Obviously, $\mathrm{Pos}(A)$ is a cone. Let

$$\mathrm{Pos}^+(A) := \{z \in \mathbb{R}^n \mid z_n \geq 0,\, z^T \Lambda z \geq 0\} \quad \text{and} \quad \mathrm{Pos}^-(A) := \{z \in \mathbb{R}^n \mid z_n \leq 0,\, z^T \Lambda z \geq 0\}.$$

It is clear that

$$\mathrm{Pos}(A) = \mathrm{Pos}^+(A) \cup \mathrm{Pos}^-(A).$$

We claim that both $\mathrm{Pos}^+(A)$ and $\mathrm{Pos}^-(A)$ are convex cones and prove this for $\mathrm{Pos}^+(A)$. Obviously, $\mathrm{Pos}^+(A)$ is a cone. Define a function of $(n-1)$ variables as

$$f(z_1, \ldots, z_{n-1}) := |\lambda_n|^{-\frac{1}{2}} \left(\sum_{i=1}^{n-1} |\lambda_i| z_i^2 \right)^{\frac{1}{2}}.$$

It is easy to see that f is convex. With this, we have

$$\begin{aligned} \mathrm{Pos}^+(A) &= \{z \in \mathbb{R}^n \mid z_n \geq 0,\, \lambda_n z_n^2 \geq |\lambda_1| z_1^2 + \cdots + |\lambda_{n-1}| z_{n-1}^2\} \\ &= \{z \in \mathbb{R}^n \mid z_n \geq f(z_1, \ldots, z_{n-1})\} = \mathrm{epi}(f). \end{aligned}$$

So, $\mathrm{Pos}^+(A)$ is the epigraph of a convex function, and hence convex. An analogous argument shows that $\mathrm{Pos}^-(A)$ is a convex cone.

From property (a), we have $0 \leq A_{ii} = (q^i)^T \Lambda q^i$, so $q^i \in \mathrm{Pos}(A)$ for all i. Note that the last components of the q^is make up the eigenvector corresponding to the

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largest eigenvalue λ_n. Using property (b), we have that the q_n^i have the same sign for all i. This implies that either $q^i \in \mathrm{Pos}^+(A)$ for all i or $q^i \in \mathrm{Pos}^-(A)$ for all i. If $q^i \in \mathrm{Pos}^+(A)$ for all i, then using convexity of $\mathrm{Pos}^+(A)$ we have that $\mathcal{Q} \subseteq \mathrm{Pos}^+(A)$ and hence $A \in \mathcal{C}$. If $q^i \in \mathrm{Pos}^-(A)$ for all i, then using similar arguments we have that $\mathcal{Q} \subseteq \mathrm{Pos}^-(A)$ which implies $A \in \mathcal{C}$. $\square$

Let us denote the cone of nonnegative matrices as

$$\mathcal{N} := \{M \in \mathcal{S} \mid M_{ij} \geq 0 \text{ for all } i, j\}.$$

It is well known that by the Perron-Frobenius theorem, nonnegative matrices have the Perron-Frobenius property. In our case, the copositive matrices satisfying (2.1) turn out to be nonnegative.

Proposition 2.2. *Let A be an indefinite matrix with exactly one positive eigenvalue. Then*

$$A \in \mathcal{C} \quad \Leftrightarrow \quad A \in \mathcal{N}.$$

Proof. Clearly, $\mathcal{N} \subset \mathcal{C}$, so one implication is trivial. To prove the converse, let $A \in \mathcal{C}$ and pick arbitrary indices i, j. We need to show that $0 \leq A_{ij} = (q^i)^T \Lambda q^j$. Since by Proposition 2.1 the Perron-Frobenius property holds for $A = Q\Lambda Q^T$, the last column of Q is nonnegative, so $q_n^i \geq 0$ and $q_n^j \geq 0$.

From Proposition 2.1(a), we have $0 \leq (q^l)^T \Lambda q^l = \sum_{k=1}^{n} \lambda_k (q_k^l)^2$ for $l = i, j$. Using $\lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 0 < \lambda_n$, this implies

$$(\lambda_n)^{\frac{1}{2}} q_n^l \geq \left(\sum_{k=1}^{n-1} |\lambda_k| (q_k^l)^2 \right)^{\frac{1}{2}} \quad \text{for } l = i, j.$$

By multiplying these two inequalities and using Cauchy-Schwarz, we get

$$\lambda_n q_n^i q_n^j \geq \left(\sum_{k=1}^{n-1} |\lambda_k| (q_k^i)^2 \right)^{\frac{1}{2}} \left(\sum_{k=1}^{n-1} |\lambda_k| (q_k^j)^2 \right)^{\frac{1}{2}} \geq |\lambda_1| q_1^i q_1^j + \cdots + |\lambda_{n-1}| q_{n-1}^i q_{n-1}^j.$$

This is equivalent to

$$0 \leq \sum_{k=1}^{n} \lambda_k q_k^i q_k^j = (q^i)^T \Lambda q^j = A_{ij}$$

which shows that $A \in \mathcal{N}$. $\square$

By combining Propositions 2.1 and 2.2, we obtain the following theorem:

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Theorem 2.3. *Let A be an indefinite symmetric matrix with exactly one positive eigenvalue. Then the following are equivalent:*

(a) The Perron-Frobenius property holds for A and $A_{ii} \geq 0$ for all i,
(b) A is nonnegative,
(c) A is copositive.

Furthermore, we can easily identify whether or not the copositive/nonnegative matrices satisfying (2.1) are on the boundary of the copositive cone.

Corollary 2.4. *Let A be an indefinite matrix with exactly one positive eigenvalue. Then $A \in \operatorname{bd}\mathcal{C}$ if and only if $A \in \mathcal{N}$ and there exists an index i such that $A_{ii} = 0$.*

Proof. If $A_{ii} = 0$, then $(e^i)^T A e^i = 0$ where e^i is the i-th unit vector, so $A \in \operatorname{bd}\mathcal{C}$. To show the converse, let $A \in \operatorname{bd}\mathcal{C}$. By Theorem 2.3, we have $A \in \mathcal{N}$. From (1.1), we have that $A \in \operatorname{bd}\mathcal{C}$ if and only if there exists $y \in \mathcal{Q}$ such that $y^T \Lambda y = 0$. Suppose by contradiction that $0 < A_{ii} = (q^i)^T \Lambda q^i$ for all i. Consider an arbitrary $y \in \mathcal{Q}$, i.e., $y = \sum\limits_{i=1}^{n} \alpha_i q^i$ with $\alpha_i \geq 0$ and $\sum\limits_{i=1}^{n} \alpha_i = 1$. From $0 \leq A_{ij} = (q^i)^T \Lambda q^j$ for all i,j and $0 < A_{ii} = (q^i)^T \Lambda q^i$ for all i, we get

$$y^T \Lambda y = \sum_{i,j} \alpha_i \alpha_j [(q^i)^T \Lambda q^j] > 0.$$

Since $y \in \mathcal{Q}$ was arbitrary, this is a contradiction to the fact that there exists $y \in \mathcal{Q}$ such that $y^T \Lambda y = 0$. $\square$

3. Copositive matrices with exactly one negative eigenvalue. In this section, we assume that A is an indefinite matrix with exactly one negative eigenvalue, i.e.,

$$\lambda_1 < 0 \leq \lambda_2 \leq \cdots \leq \lambda_n \quad \text{and} \quad 0 < \lambda_n. \tag{3.1}$$

Similar to Section 2, we study copositivity of a matrix A which satisfies (3.1) by transforming its quadratic form into diagonal form. Consider the cone

$$\operatorname{Neg}(A) := \{z \in \mathbb{R}^n \mid z^T \Lambda z \leq 0\}.$$

Clearly, we have $\operatorname{Neg}(A) = \operatorname{Pos}(-A)$. So similarly as in the proof of Proposition 2.1, we can decompose $\operatorname{Neg}(A)$ into two full-dimensional convex cones, i.e.,

$$\operatorname{Neg}(A) = \operatorname{Neg}^+(A) \cup \operatorname{Neg}^-(A)$$

with

$$\operatorname{Neg}^+(A) := \{z \in \mathbb{R}^n \mid z_1 \geq 0,\ z^T \Lambda z \leq 0\} \ \text{ and } \ \operatorname{Neg}^-(A) := \{z \in \mathbb{R}^n \mid z_1 \leq 0,\ z^T \Lambda z \leq 0\}.$$

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From (1.1), it is clear that

$$A \in \mathcal{C} \quad \Leftrightarrow \quad \mathcal{Q} \cap \operatorname{int} \operatorname{Neg}(A) = \emptyset. \tag{3.2}$$

Using $\lambda_1 < 0 < \lambda_n$ and $\operatorname{Neg}^+(A) \cap \operatorname{Neg}^-(A) = \{z \in \mathbb{R}^n \mid z_i = 0 \text{ if } \lambda_i \neq 0\}$, we have

$$\operatorname{int} \operatorname{Neg}^+(A) \cap \operatorname{int} \operatorname{Neg}^-(A) = \emptyset. \tag{3.3}$$

Combining (3.2) and (3.3), we have

$$A \in \mathcal{C} \quad \Leftrightarrow \quad \mathcal{Q} \cap \operatorname{int} \operatorname{Neg}^+(A) = \emptyset \quad \text{and} \quad \mathcal{Q} \cap \operatorname{int} \operatorname{Neg}^-(A) = \emptyset.$$

Hence, we have transformed the problem of checking copositivity into two convex feasibility problems. We can summarize these findings as follows:

Proposition 3.1. *Let A be an indefinite matrix with exactly one negative eigenvalue. Consider the following two convex problems*

$$\begin{aligned} \inf \quad & ||x - z||^2 \\ \text{s.t.} \quad & x \in \mathcal{Q} \\ & z \in \operatorname{int} \operatorname{Neg}(A)^\pm \end{aligned} \tag{3.4}$$

where the set $\operatorname{Neg}(A)^\pm$ is either $\operatorname{Neg}^+(A)$ or $\operatorname{Neg}^-(A)$. If for at least one of the sets $\operatorname{Neg}^+(A)$ and $\operatorname{Neg}^-(A)$, the optimal value of problem (3.4) is zero and the optimal solution is attained, then A is not copositive. Otherwise, A is copositive.

Observe that the feasible set in (3.4) is not closed, which is disadvantageous for practical implementations. Considering the closure of the feasible set, it is easy to see that

$$A \in \operatorname{int} \mathcal{C} \quad \Leftrightarrow \quad \mathcal{Q} \cap \operatorname{Neg}^+(A) = \emptyset \quad \text{and} \quad \mathcal{Q} \cap \operatorname{Neg}^-(A) = \emptyset.$$

Thus, we have the following:

Theorem 3.2. *Let A be an indefinite matrix with exactly one negative eigenvalue. To check if A is strictly copositive, we have to solve the following two convex problems*

$$\begin{aligned} \inf \quad & ||x - z||^2 \\ \text{s.t.} \quad & x \in \mathcal{Q} \\ & z \in \operatorname{Neg}(A)^\pm \end{aligned} \tag{3.5}$$

where the set $\operatorname{Neg}(A)^\pm$ is either $\operatorname{Neg}^+(A)$ or $\operatorname{Neg}^-(A)$. If the optimal value of (3.5) is strictly positive for both problems, then A is strictly copositive. Otherwise, $A \notin \operatorname{int} \mathcal{C}$.

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The problems (3.5) can be written as the following two second order cone programming problems (SOCP) with variables $(z, x, \alpha) \in \mathbb{R}^{2n+1}$:

$$\begin{array}{llll} \min & \alpha & \min & \alpha \\ \text{s. t.} & \|x - z\| \le \alpha & \text{s. t.} & \|x - z\| \le \alpha \\ & \|\widetilde{z}\| \le \sqrt{|\lambda_1|} z_1 & & \|\widetilde{z}\| \le -\sqrt{|\lambda_1|} z_1 \\ & x \in \mathcal{Q}, \quad z_1 \ge 0 & & x \in \mathcal{Q}, \quad z_1 \le 0 \end{array} \tag{3.6}$$

where $\widetilde{z} = (\sqrt{\lambda_2}\, z_2, \ldots, \sqrt{\lambda_n}\, z_n) \in \mathbb{R}^{n-1}$. The inequality constraints are so called second order cone constraints. Also recall that $\mathcal{Q}$ is a polytope. Therefore, the constraint $x \in \mathcal{Q}$ can be transformed into a set of linear equations and inequalities as follows: We need one linear equation describing the affine space spanned by $\{q^1, \ldots, q^n\}$, and n linear inequalities obtained computing the span of $\{0, q^1, \ldots, q^n\} \backslash \{q^i\}$ for $i = 1, \ldots, n$. In this format, problems (3.6) can now be solved efficiently using algorithms such as interior point methods. There is standard software for this, for example SeDuMi [8]. We illustrate this approach by a numerical example:

Example 3.3. Consider the following matrix from [2, Example 2.12], which has eigenvalues as studied in this section,

$$A = \begin{bmatrix} 1 & 1.63 & 1 & -0.77 & -0.67 \\ 1.63 & 1 & 0 & 0.32 & -0.82 \\ 1 & 0 & 1 & -0.26 & -0.67 \\ -0.77 & 0.32 & -0.26 & 1 & 0.77 \\ -0.67 & -0.82 & -0.67 & 0.77 & 1 \end{bmatrix}.$$

Solving problems (3.6) for A give $\alpha = 0$ and $z = x = (0.008, 0.315, 0.258, 0.009, 0.41)^T$. Note that x is a negative certificate which means $x^T A x = -0.0052 < 0$, so $A \notin \mathcal{C}$.

We conclude this paper by relating our approach to the one proposed in [9], where the following was shown: If the order of the maximal positive definite principal submatrix is $(n-1)$, then copositivity of the matrix can be checked by a convex quadratic program. The following example shows that an indefinite matrix with exactly one negative eigenvalue does not necessarily contain a maximal positive definite principal submatrix of order $(n-1)$, so the two approaches are complementary.

Example 3.4. Consider the following matrix from [9, Example 4.1],

$$A = \begin{bmatrix} 1 & -1 & 1 & 2 & -3 \\ -1 & 2 & -3 & -3 & 4 \\ 1 & -3 & 5 & 6 & -4 \\ 2 & -3 & 6 & 5 & -8 \\ -3 & 4 & -4 & -8 & 16 \end{bmatrix}.$$

A is indefinite and has exactly one negative eigenvalue, but the maximal positive

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semidefinite submatrix of A is the leading 3×3 principal submatrix. So, in this example, the formulation of [9] is not a convex quadratic problem.

We numerically tested copositivity of A by solving (3.6). There is no negative certificate and the optimal values are very close to zero, so within a given accuracy A is not strictly copositive. This can also be checked directly since $x^T Ax = 0$ for $x = (1, 2, 1, 0, 0)$. In fact, it can be shown that A is copositive by the methods from [3].

4. Conclusion. We studied copositive matrices with certain spectral properties. It turns out that an indefinite matrix with exactly one *positive* eigenvalue is copositive if and only if the matrix is nonnegative. The problem to check if a matrix with exactly one *negative* eigenvalue is strictly copositive can be formulated as a combination of two convex quadratic programming problems.

The proofs were based on the fact that the sets $\mathrm{Pos}(A)$ respectively $\mathrm{Neg}(A)$ have a certain nice structure for matrices with the considered spectral properties. Unfortunately, this structure breaks down in case the single positive (respectively negative) eigenvalue has multiplicity bigger than one. In these situations, checking copositivity remains a difficult problem.

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