Tractable Subcones and LP-based Algorithms for Testing Copositivity

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December 2015
Revised October 2016

Abstract

The authors in a previous paper devised certain subcones of the copositive cone and showed that one can detect whether a given matrix belongs to each of them by solving linear optimization problems (LPs) with \(O(n)\) variables and \(O(n^2)\) constraints. They also devised LP-based algorithms for testing copositivity using the subcones. In this paper, they investigate the properties of the subcones in more detail and explore larger subcones of the copositive cone whose membership can be detected by solving LPs. They introduce a semidefinite basis (SD basis) that is a basis of the space of \(n \times n\) symmetric matrices consisting of \(n(n + 1)/2\) symmetric semidefinite matrices. Using the SD basis, they devise two new subcones for which detection can be done by solving LPs with \(O(n^2)\) variables and \(O(n^2)\) constraints. The new subcones are larger than the ones in the previous paper and inherit their nice properties. The authors also examine the efficiency of those subcones in numerical experiments. The results show that the subcones are promising for testing copositivity.

Key words. Copositive cone, Doubly nonnegative cone, Matrix decomposition, Linear programming, Semidefinite basis, Maximum clique problem

1 Introduction

Let \(\mathcal{S}_n\) be the set of \(n \times n\) symmetric matrices, and define their inner product as

\[
\langle A, B \rangle = \text{Tr} (B^T A) = \sum_{i,j=1}^{n} a_{ij}b_{ij}.
\]

Bomze et al. [7] coined the term “copositive programming” in relation to the following problem in 2000, on which many studies have since been conducted:

\[
\begin{align*}
\text{Minimize} & \quad \langle C, X \rangle \\
\text{subject to} & \quad \langle A_i, X \rangle = b_i, \quad (i = 1, 2, \ldots, m) \\
& \quad X \in \mathcal{COP}_n.
\end{align*}
\]

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where $\text{COP}_n$ is the set of $n \times n$ copositive matrices, i.e., matrices whose quadratic form takes nonnegative values on the $n$-dimensional nonnegative orthant $\mathbb{R}_+^n$:

$$\text{COP}_n := \{X \in S : d^T X d \geq 0 \text{ for all } d \in \mathbb{R}_+^n\}.$$ 

We call the set $\text{COP}_n$ the copositive cone. A number of studies have focused on the close relationship between copositive programming and quadratic or combinatorial optimization (see, e.g., [7][8][15][32][33][13][14][20]). Interested readers may refer to [21] and [9] for background on and the history of copositive programming.

While copositive programming has the potential of being a useful optimization technique, it still faces challenges. One of these challenges is to develop efficient algorithms for determining whether a given matrix is copositive. It has been shown that the above problem is co-NP-complete [31][19][20] and many algorithms have been proposed to solve it (see, e.g., [6][12][30][29][38][35][10][16][22][36][11]). Here, we are interested in numerical algorithms which (a) apply to general symmetric matrices without any structural assumptions or dimensional restrictions; (b) are not merely recursive, i.e., do not rely on information taken from all principal submatrices, but rather focus on generating subproblems in a somehow data-driven way, as described in [10]. There are few such algorithms, but they often use tractable subcones $\mathcal{M}_n$ of the copositive cone $\text{COP}_n$ for detecting copositivity (see, e.g., [12][35][10][36]). As described in Section 5, these algorithms require one to check whether $A \in \mathcal{M}_n$ or $A \notin \mathcal{M}_n$ repeatedly over simplicial partitions. The desirable properties of the subcones $\mathcal{M}_n \subseteq \text{COP}_n$ used by these algorithms can be summarized as follows:

P1 For any given $n \times n$ symmetric matrix $A \in S_n$, we can check whether $A \in \mathcal{M}_n$ within a reasonable computation time, and

P2 $\mathcal{M}_n$ is a subset of the copositive cone $\text{COP}_n$ that at least includes the $n \times n$ nonnegative cone $\mathcal{N}_n$ and contains as many elements $\text{COP}_n$ as possible.

The authors, in [36], devised certain subcones $\mathcal{M}_n$ and showed that one can detect whether a given matrix belongs to one of them by solving linear optimization problems (LPs) with $O(n)$ variables and $O(n^2)$ constraints. They also created an LP-based algorithm that uses these subcones for testing copositivity.

The aim of this paper is twofold. First, we investigate the properties of the subcones in more detail, especially in terms of their convex hulls. Second, we search for subcones of $\text{COP}_n$ that have properties P1 and P2. To address the second aim, we introduce a semidefinite basis (SD basis) that is a basis of the space $S_n$ consisting of $n(n + 1)/2$ symmetric semidefinite matrices. Using the SD basis, we devise two new types of subcones for which detection can be done by solving LPs with $O(n^2)$ variables and $O(n^3)$ constraints. As we will show in Corollary 3.4, these subcones are larger than the ones proposed in [36] and inherit their nice properties. We also examine the efficiency of those subcones in numerical experiments.

This paper is organized as follows: In Section 2, we show several tractable subcones of $\text{COP}_n$ that are receiving much attention in the field of copositive programming and investigate their properties, the results of which are summarized in Figures 1 and 2. In Section 3, we propose new subcones of $\text{COP}_n$ having properties P1 and P2. We define SD bases using Definitions 3.2 and 3.3 and construct new LPs for detecting whether a given matrix belongs to the subcones.

Our study is motivated by the desire to develop efficient algorithms for testing copositivity. However, as we will see in Sections 2 and 3, all of the subcones appearing in this paper are merely contained in the Minkowski sum $S_n^+ + N_n \subseteq \text{COP}_n$ of the $n \times n$ positive semidefinite cone $S_n$ and $n \times n$ nonnegative cone $N_n$. Based on this fact, in Section 4, we perform numerical experiments in which the new subcones are used for identifying the given matrices $A \in S_n^+ + N_n$. As our main purpose, Section 5 describes
experiments for testing copositivity of matrices arising from the maximum clique problems. The results of these experiments show that the new subcones are quite promising not only for identification of $A \in S_n^+ + \mathcal{N}_n$ but also for testing copositivity. We give concluding remarks in Section 6.

2 Some tractable subcones of the copositive cone and related work

The following cones are attracting a lot of attention in the context of the relationship between combinatorial optimization and conic optimization (see, e.g., [21][9]).

- The nonnegative cone $\mathcal{N}_n := \{X \in \mathcal{S}_n \mid x_{ij} \geq 0 \text{ for all } i, j \in \{1, 2, \ldots, n\}\}$.
- The semidefinite cone $\mathcal{S}_n^+ := \{X \in \mathcal{S}_n \mid d^T X d \geq 0 \text{ for all } d \in \mathbb{R}^n\}$.
- The copositive cone $\mathcal{COP}_n := \{X \in \mathcal{S}_n \mid d^T X d \geq 0 \text{ for all } d \in \mathbb{R}_+^n\}$.
- The Minkowski sum $\mathcal{S}_n^+ + \mathcal{N}_n$ of $\mathcal{S}_n^+$ and $\mathcal{N}_n$.
- The union $\mathcal{S}_n^+ \cup \mathcal{N}_n$ of $\mathcal{S}_n^+$ and $\mathcal{N}_n$.
- The doubly nonnegative cone $\mathcal{S}_n^+ \cap \mathcal{N}_n$, i.e., the set of positive semidefinite and componentwise non-negative matrices.
- The completely positive cone $\mathcal{CP}_n := \text{conv}\left(\{xx^T \mid x \in \mathbb{R}_+^n\}\right)$, where conv $(S)$ denotes the convex hull of the set $S$.

Except the set $\mathcal{S}_n^+ \cup \mathcal{N}_n$, all of the above cones are proper (see Section 1.6 of [5], where a proper cone is called a full cone), and we can easily see from the definitions that the following inclusions hold:

$$\mathcal{COP}_n \supseteq \mathcal{S}_n^+ + \mathcal{N}_n \supseteq \mathcal{S}_n^+ \cup \mathcal{N}_n \supseteq \mathcal{S}_n^+ \supseteq \mathcal{S}_n^+ \cap \mathcal{N}_n \supseteq \mathcal{CP}_n.$$ (2)

As mentioned in Section 1, the problem of testing copositivity, i.e., deciding whether a given symmetric matrix $A$ is in the cone $\mathcal{COP}_n$ or not, is co-NP-complete [31][19][20]. On the other hand, since we know that $\mathcal{S}_n^+ + \mathcal{N}_n$ is the dual cone of the doubly nonnegative cone $\mathcal{S}_n^+ \cap \mathcal{N}_n$, we see that

$$\mathcal{S}_n^+ + \mathcal{N}_n = \{A \in \mathcal{S}_n \mid \langle A, X \rangle \geq 0 \text{ for any } X \in \mathcal{S}_n^+ \cap \mathcal{N}_n\}$$

and that the problem of testing whether or not $A \in \mathcal{S}_n^+ + \mathcal{N}_n$ can be solved (to an accuracy of $\epsilon$) by solving the following doubly nonnegative program (which can be expressed as a semidefinite program of size $O(n^2)$)

$$\begin{align*}
\text{Minimize} & \quad \langle A, X \rangle \\
\text{subject to} & \quad \langle I_n, X \rangle = 1, \; X \in \mathcal{S}_n^+ \cap \mathcal{N}_n
\end{align*}$$ (3)

where $I_n$ denotes then $\times n$ identity matrix Thus, the set $\mathcal{S}_n^+ + \mathcal{N}_n$ is a rather large and tractable convex subcone of $\mathcal{COP}_n$. However, solving the problem takes a lot of time [35], [37] and does not make for a practical implementation in general. To overcome this drawback, more easily tractable subcones of the copositive cone have been proposed.
For any given matrix $A \in S_n$, we define

$$N(A)_{ij} := \begin{cases} A_{ij} & (A_{ij} > 0 \text{ and } i \neq j) \\ 0 & \text{(otherwise)} \end{cases} \quad \text{and} \quad S(A) := A - N(A). \quad (4)$$

In [35], the authors defined the following set:

$$H_n := \{ A \in S_n \mid S(A) \in S_n^+ \}. \quad (5)$$

Note that $A = S(A) + N(A) \in S_n^+ + N_n$ if $A \in H_n$. Also, for any $A \in N_n$, $S(A)$ is a nonnegative diagonal matrix, and hence, $N_n \subseteq H_n$. The determination of $A \in H_n$ is easy and can be done by extracting the positive elements $A_{ij} > 0$ ($i \neq j$) as $(N(A))_{ij}$ and by performing a Cholesky factorization of $S(A)$ (cf. Algorithm 4.2.4 in [26]). Thus, from the inclusion relation (2), we see that the set $H_n$ has the desirable $\textbf{P1}$ property. However, $S(A)$ is not necessarily positive semidefinite even if $A \in S_n^+ + N_n$ or $A \in S_n^+$. The following theorem summarizes the properties of the set $H_n$.

**Theorem 2.1** ([25] and Theorem 4.2 of [35]). $H_n$ is a convex cone and $N_n \subseteq H_n \subseteq S_n^+ + N_n$. If $n \geq 3$, these inclusions are strict and $S_n^+ \not\subseteq H_n$. For $n = 2$, we have $H_n = S_n^+ \setminus N_n = S_n^+ + N_n = \text{COP}_n$.

The construction of the subcone $H_n$ is based on the idea of “nonnegativity-checking first and positive semidefiniteness-checking second.” In [36], another subcone is provided that is based on the idea of “positive semidefiniteness-checking first and nonnegativity-checking second.”

For a given symmetric matrix $A \in S_n$, let $P = [p_1, p_2, \ldots, p_n]$ be an orthonormal matrix and $\Lambda = \text{Diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ be a diagonal matrix satisfying

$$A = P\Lambda P^T = \sum_{i=1}^{n} \lambda_i p_i p_i^T \quad (6)$$

By introducing another diagonal matrix $\Omega = \text{Diag}(\omega_1, \omega_2, \ldots, \omega_n)$, we can make the following decomposition:

$$A = P(\Lambda - \Omega) P^T + P\Omega P^T \quad (7)$$

If $A - \Omega \in N_n$, i.e., if $\lambda_i \geq \omega_i$ ($i = 1, 2, \ldots, n$), then the matrix $P(\Lambda - \Omega) P^T$ is positive semidefinite. Thus, if we can find a suitable diagonal matrix $\Omega$ satisfying

$$\lambda_i \geq \omega_i \quad (i = 1, 2, \ldots, n), \quad [P\Omega P^T]_{ij} \geq 0 \quad (1 \leq i \leq j \leq n) \quad (8)$$

then (7) and (2) imply

$$A = P(\Lambda - \Omega) P^T + P\Omega P^T \in S_n^+ + N_n \subseteq \text{COP}_n. \quad (9)$$

We can determine whether such a matrix exists or not by solving the following linear optimization problem with variables $\omega_i$ ($i = 1, 2, \ldots, n$) and $\alpha$:

$$\text{(LP)}_{\alpha, \lambda} \quad \begin{array}{lll} \text{Maximize} & \alpha \\ \text{subject to} & \omega_i \leq \lambda_i \\ & \omega_k p_k p_k^T \geq \alpha \\ \end{array} \quad (i = 1, 2, \ldots, n) \quad \sum_{k=1}^{n} \omega_k p_k p_k^T \geq \alpha \\

(10)$$

Here, for a given matrix $A$, $[A]_{ij}$ denotes the $(i, j)$th element of $A$.

The problem $(\text{LP})_{\alpha, \lambda}$ has a feasible solution at which $\omega_i = \lambda_i$ ($i = 1, 2, \ldots, n$) and

$$\alpha = \min \left\{ [P\Lambda P^T]_{ij} \mid 1 \leq i \leq j \leq n \right\} = \min \left\{ \sum_{k=1}^{n} \lambda_k [p_k]_i [p_k]_j \mid 1 \leq i \leq j \leq n \right\}$$
For each \( i = 1, 2, \ldots, n \), the constraints

\[
[P\Omega P^T]_{ii} = \left[ \sum_{k=1}^{n} \omega_k p_k p_k^T \right]_{ii} = \sum_{k=1}^{n} \omega_k |p_k|^2 \geq \alpha
\]

and \( \omega_k \leq \lambda_k \) (\( k = 1, 2, \ldots, n \)) imply the bound \( \alpha \leq \min \left\{ \sum_{k=1}^{n} \lambda_k |p_k|^2 \mid 1 \leq i \leq n \right\} \). Thus, \((LP)_{P,\Lambda}\) has an optimal solution with optimal value \( \alpha_x(P, \Lambda) \). If \( \alpha_x(P, \Lambda) \geq 0 \), there exists a matrix \( \Omega \) for which the decomposition (8) holds. The following set \( \mathcal{G}_n^a \) of \( \mathcal{M}_n \) is based on the above observations and was proposed in [36].

\[
\mathcal{G}_n^a := \left\{ A \in \mathcal{S}_n \mid \alpha_x(P, \Lambda) \geq 0 \text{ for some orthonormal matrix } P \text{ satisfying (6)} \right\}.
\] (11)

In [36], the authors described other sets \( \mathcal{G}_n^o \) and \( \mathcal{G}_n^s \) that are closely related to \( \mathcal{G}_n^a \).

\[
\begin{align*}
\mathcal{G}_n^o & := \left\{ A \in \mathcal{S}_n \mid \alpha_x(P, \Lambda) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (6)} \right\}, \\
\mathcal{G}_n^s & := \left\{ A \in \mathcal{S}_n \mid \alpha_x(P, \Lambda) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (6)} \right\}.
\end{align*}
\] (12)

Note that we use the word “arbitrary” as a counter concept of “orthonormal.” If (8) holds for any arbitrary (not necessarily orthonormal) matrix \( P \), then (9) also holds, which implies the following inclusions:

\[
\mathcal{G}_n^a \subseteq \mathcal{G}_n^o \subseteq \mathcal{G}_n^s \subseteq \mathcal{S}_n^+ + \mathcal{N}_n.
\] (13)

Before describing the properties of the sets \( \mathcal{G}_n^a \), \( \mathcal{G}_n^o \) and \( \mathcal{G}_n^s \), we will prove a preliminary lemma.

**Lemma 2.2.** Let \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) be two convex cones satisfying \( \{ \alpha x \mid \alpha \in \mathbb{R}_+, \ x \in \mathcal{K} \} \subseteq \mathcal{K} \). Then \( \text{conv} (\mathcal{K}_1 \cup \mathcal{K}_2) = \mathcal{K}_1 + \mathcal{K}_2 \).

**Proof.** Since \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) are convex cones, we can easily see that the inclusion \( \mathcal{K}_1 + \mathcal{K}_2 \subseteq \text{conv} (\mathcal{K}_1 \cup \mathcal{K}_2) \) holds. The converse inclusion also follows from the fact that \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) are convex cones. Since \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \) contain the origin, we see that the inclusion \( \mathcal{K}_1 \cup \mathcal{K}_2 \subseteq \mathcal{K}_1 + \mathcal{K}_2 \) holds. From this inclusion and the convexity of the sets \( \mathcal{K}_1 \) and \( \mathcal{K}_2 \), we can conclude that

\[
\text{conv} (\mathcal{K}_1 \cup \mathcal{K}_2) \subseteq \text{conv} (\mathcal{K}_1 + \mathcal{K}_2) = \mathcal{K}_1 + \mathcal{K}_2.
\]

The following theorem shows some of the properties of \( \mathcal{G}_n^a \), \( \mathcal{G}_n^o \), and \( \mathcal{G}_n^s \). Assertions (i)-(iii) were proved in Theorem 3.2 of [36]. Assertion (iv) comes from the fact that \( \mathcal{S}_n^+ \) and \( \mathcal{N}_n \) are convex cones and from Lemma 2.2. Assertions (v)-(vii) follow from (ii)-(v), the inclusion (13) and Theorem 2.1.

**Theorem 2.3.** (i) The sets \( \mathcal{G}_n^a \), \( \mathcal{G}_n^o \) and \( \mathcal{G}_n^s \) are subcones of \( \mathcal{S}_n^+ + \mathcal{N}_n \)

(ii) \( \mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^a \)

(iii) \( \mathcal{G}_n^a = \text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) \), where the set \( \text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) \) is defined by

\[
\text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) := \left\{ S + N \mid S \in \mathcal{S}_n^+, \ N \in \mathcal{N}_n, \ S \text{ and } N \text{ commute} \right\}.
\]

(iv) \( \text{conv} (\mathcal{S}_n^+ + \mathcal{N}_n) = \mathcal{S}_n^+ + \mathcal{N}_n \).

(v) \( \mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^o \subseteq \mathcal{G}_n^s = \text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) \subseteq \mathcal{G}_n^s \subseteq \mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{COP}_n \).
(vi) If \( n = 2 \), then \( S^+_n \cup N_n = \mathcal{G}^n = \mathcal{G}^n_s = \text{com}(S^+_n + N_n) = \widehat{\mathcal{G}}^n = S^+_n + N_n = \mathcal{COP}_n \).

(vii) \( \text{conv}(S^+_n \cup N_n) = \text{conv}(\mathcal{G}^n) = \text{conv}(\mathcal{G}^n_s) = \text{conv}((\text{com}(S^+_n + N_n))) = \text{conv}(\widehat{\mathcal{G}}^n) = S^+_n + N_n \).

A number of examples provided in [36] illustrate the differences between \( \mathcal{H}_n \), \( \mathcal{G}^n_s \), and \( \mathcal{G}^n \). Figure 1 draws those examples and (ii) of Theorem 2.3. Moreover, Figure 2 follows from (vii) of Theorem 2.3 and the convexity of the sets \( N_n \), \( S_n \) and \( \mathcal{H}_n \) (see Theorem 2.1).

![Figure 1: The inclusion relations among the subcones of \( \mathcal{COP}_1 \)](image)

![Figure 2: The inclusion relations among the subcones of \( \mathcal{COP}_n \)](image)
At present, it is not clear whether the set $G_n^+ = \text{com}(S_n^+ + N_n)$ is convex or not. As we will mention on page 17, our numerical results suggest that the set might be not convex.

Before closing this discussion, we should point out another interesting subset of $\mathcal{COP}_n$ proposed by Bomze and Eichfelder [10]. Suppose that a given matrix $A \in S_n$ can be decomposed as (6), and define the diagonal matrix $\Lambda_+ := PA_+ P^T$ and $A_- := A_+ - A$. Then, we can easily see that $A_+$ and $A_-$ are positive semidefinite. Using this decomposition $A = A_+ - A_-$, Bomze and Eichfelder derived the following LP-based sufficient condition for $A \in \mathcal{COP}_n$ in [10].

**Theorem 2.4** (Theorem 2.6 of [10]). Let $x \in \mathbb{R}_+^n$ be such that $A_+ x$ has only positive coordinates. If

$$(x^T A_+ x)(A_-)_{ii} \leq [(A_+ x)_i]^2 \quad (i = 1, 2, \ldots, n)$$

then $A \in \mathcal{COP}_n$.

Consider the following LP with $O(n)$ variables and $O(n)$ constraints,

$$\inf \{ f^T x \mid A_+ x \geq e, \; x \in \mathbb{R}_+^n \} \quad (14)$$

where $f$ is an arbitrary vector and $e$ denotes the vector of all ones. Define the set $L_n^* := \{ A \in S_n \mid (x^T A_+ x)(A_-)_{ii} \leq [(A_+ x)_i]^2 \; (i = 1, 2, \ldots, n) \text{ for some feasible solution } x \text{ of } (14) \}$. Then Theorem 2.4 ensures that $L_n^* \subseteq \mathcal{COP}_n$. The following proposition gives a characterization when the feasible set of the LP of (14) is empty.

**Proposition 2.5** (Proposition 2.7 of [10]). The condition $\ker A_+ \cap \{ x \in \mathbb{R}_+^n \mid e^T x = 1 \} \neq \emptyset$ is equivalent to $\{ x \in \mathbb{R}_+^n \mid A_+ x \geq e \} = \emptyset$.

Consider the matrix,

$$A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \in S_2^+.$$  

Thus, $A_+ = A$ and the set $\ker A_+ \cap \{ x \in \mathbb{R}_+^n \mid e^T x = 1 \} \neq \emptyset$. Proposition 2.5 ensures that $A \notin L_2^*$, and hence, $S_n^+ \not\subseteq L_n^*$ for $n \geq 2$, similarly to the set $H_n$ for $n \geq 3$ (see Theorem 2.1).

### 3 Semidefinite bases

In this section, we improve the subcone $G_n^+$ in terms of $\mathbf{P2}$. For a given matrix $A$ of (6), the linear optimization problem (LP)$_{P,A}$ in (10) can be solved in order to find a nonnegative matrix that is a linear combination

$$\sum_{i=1}^{n} \omega_ip_ip_i^T$$

of $n$ linearly independent positive semidefinite matrices $p_ip_i^T \in S_n^+$ ($i = 1, 2, \ldots, n$). This is done by decomposing $A \in S_n$ into two parts:

$$A = \sum_{i=1}^{n} (\lambda_i - \omega_i)p_ip_i^T + \sum_{i=1}^{n} \omega_ip_ip_i^T \quad (15)$$
such that the first part
\[ \sum_{i=1}^{n} (\lambda_i - \omega_i) p_i p_i^T \]
is positive semidefinite. Since \( p_i p_i^T \in S_n^+ \) \((i = 1, 2, \ldots, n)\) are just only \(n\) linearly independent matrices in \(n(n + 1)/2\) dimensional space \(S_n\), the intersection of the set of linear combinations of \(p_i p_i^T\) and the nonnegative cone \(N_n\) may not have a volume even if it is nonempty. On the other hand, if we have a set of positive semidefinite matrices \(p_i p_i^T \in S_n^+ \) \((i = 1, 2, \ldots, n(n + 1)/2)\) that gives a basis of \(S_n\), then the corresponding intersection becomes the nonnegative cone \(N_n\) itself, and we may expect a higher chance of finding a nonnegative matrix by enlarging the feasible region of \((LP)_{P, \Lambda}\). In fact, we can easily find a basis of \(S_n\) consisting of \(n(n + 1)/2\) semidefinite matrices from \(n\) given orthonormal vectors \(p_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\) based on the following result from [18].

**Proposition 3.1** (Lemma 6.2 of [18]). Let \(v_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\) be \(n\)-dimensional linear independent vectors. Then the set \(V := \{(v_i + v_j)(v_i + v_j)^T \mid 1 \leq i \leq j \leq n\}\) is a set of \(n(n + 1)/2\) linearly independent positive semidefinite matrices. Therefore, the set \(V\) gives a basis of the set \(S_n\) of \(n \times n\) symmetric matrices.

The above proposition ensures that the following set \(\mathcal{B}_+(p_1, p_2, \ldots, p_n)\) is a basis of \(n \times n\) symmetric matrices.

**Definition 3.2** (Semidefinite basis type I). For a given set of \(n\)-dimensional orthonormal vectors \(p_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\), define the map \(\Pi_+ : \mathbb{R}^n \times \mathbb{R}^n \rightarrow S_n^+\) by
\[
\Pi_+(p_i, p_j) := \frac{1}{4}(p_i + p_j)(p_i + p_j)^T.
\]
We call the set
\[
\mathcal{B}_+(p_1, p_2, \ldots, p_n) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq n\}
\]
a semidefinite basis type I induced by \(p_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\).

A variant of the semidefinite basis type I is as follows. Noting that the equivalence
\[
\Pi_+(p_i, p_j) = \frac{1}{2} p_i p_i^T + \frac{1}{2} p_j p_j^T - \Pi_-(p_i, p_j)
\]
holds for any \(i \neq j\), we see that \(\mathcal{B}_-(p_1, p_2, \ldots, p_n)\) is also a basis of \(n \times n\) symmetric matrices.

**Definition 3.3** (Semidefinite basis type II). For a given set of \(n\)-dimensional orthonormal vectors \(p_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\), define the map \(\Pi_- : \mathbb{R}^n \times \mathbb{R}^n \rightarrow S_n^+\) by
\[
\Pi_-(p_i, p_j) := \frac{1}{4}(p_i - p_j)(p_i - p_j)^T.
\]
We call the set
\[
\mathcal{B}_-(p_1, p_2, \ldots, p_n) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq n\} \cup \{\Pi_-(p_i, p_j) \mid 1 \leq i < j \leq n\}
\]
a semidefinite basis type II induced by \(p_i \in \mathbb{R}^n \) \((i = 1, 2, \ldots, n)\).

Using the map \(\Pi_+\) in (16), the linear optimization problem \((LP)_{P, \Lambda}\) in (10) can be equivalently written as
\[
(LP)_{P, \Lambda} \quad \text{Maximize} \quad \alpha \quad \text{subject to} \quad \omega_{ii}^+ \leq \lambda_i \quad \left(\sum_{k=1}^{n} \omega_{kk}^+ \Pi_+(p_k, p_k)\right)_{ij} \geq \alpha \quad (1 \leq i \leq j \leq n).\]
The problem \((LP)_{P,A}^+\) is based on the decomposition (15). Starting with (15), the matrix \(A\) can be decomposed using \(\Pi_+ (p_i, p_j)\) in (16) and \(\Pi_-(p_i, p_j)\) in (18) as

\[
A = \sum_{i=1}^{n} (\lambda_i - \omega_{ii}^+) \Pi_+ (p_i, p_i) + \sum_{i=1}^{n} \omega_{ii}^+ \Pi_+ (p_i, p_i) + \sum_{1 \leq i < j \leq n} (\omega_{ij}^+ + \omega_{ji}^+) \Pi_+ (p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^+ \Pi_+ (p_i, p_j)
\]

\[
A = \sum_{i=1}^{n} (\lambda_i - \omega_{ii}^+) \Pi_+ (p_i, p_i) + \sum_{i=1}^{n} \omega_{ii}^+ \Pi_+ (p_i, p_i) + \sum_{1 \leq i < j \leq n} (\omega_{ij}^+ + \omega_{ji}^+) \Pi_+ (p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^+ \Pi_+ (p_i, p_j)
\]

On the basis of the decomposition (20) and (21), we devise the following two linear optimization problems as extensions of \((LP)_{P,A}^+\):

\[
(LP)_{P,A}^+ \begin{array}{l}
\text{Maximize } \alpha \\
\text{subject to } \\
\omega_{ii}^+ \leq \lambda_i \\
\omega_{ij}^+ \leq 0 \\
\sum_{1 \leq k \leq l \leq n} \omega_{kl}^+ \Pi_+ (p_k, p_l) \geq \alpha \\
(1 \leq i \leq j \leq n)
\end{array}
\]

\[
(LP)_{P,A}^- \begin{array}{l}
\text{Maximize } \alpha \\
\text{subject to } \\
\omega_{ii}^- \leq \lambda_i \\
\omega_{ij}^- \leq 0 \\
\sum_{1 \leq k \leq l \leq n} \omega_{kl}^- \Pi_-(p_k, p_l) \geq \alpha \\
(1 \leq i \leq j \leq n)
\end{array}
\]

Problem \((LP)_{P,A}^+\) has \(n(n+1)/2 + 1\) variables and \(n(n+1)\) constraints, and problem \((LP)_{P,A}^-\) has \(n^2 + 1\) variables and \(n(3n+1)/2\) constraints (see Table 1). Since \([PQPT]_{ij}\) in (10) is given by \(\sum_{k=1}^{n} \omega_{kk} \Pi_+ (p_k, p_k)\), we can prove that both linear optimization problems \((LP)_{P,A}^+\) and \((LP)_{P,A}^-\) are feasible and bounded by making arguments similar to the one for \((LP)_{P,A}^+\) on page 5. Thus, \((LP)_{P,A}^+\) and \((LP)_{P,A}^-\) have optimal solutions with corresponding optimal values \(\alpha^+_+(P,A)\) and \(\alpha^-_+(P,A)\).

If the optimal value \(\alpha^+_+(P,A)\) of \((LP)_{P,A}^+\) is nonnegative, then, by rearranging (20), the optimal solution \(\omega_{ij}^{++} (1 \leq i \leq j \leq n)\) can be made to give the following decomposition:

\[
A = \sum_{i=1}^{n} (\lambda_i - \omega_{ii}^{++}) \Pi_+ (p_i, p_i) + \sum_{1 \leq i < j \leq n} (\omega_{ij}^{++}) \Pi_+ (p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^{++} \Pi_+ (p_i, p_j) \in S^n + N_n.
\]
In the same way, if the optimal value $\alpha^\pm(P, \Lambda)$ of (LP)${}^\pm_{P, \Lambda}$ is nonnegative, then, by rearranging (21), the optimal solution $\omega_{ij}^+ (1 \leq i, j \leq n)$, $\omega_{ij}^- (1 \leq i < j \leq n)$ can be made to give the following decomposition:

$$
A = \left[ \sum_{i=1}^{n} (\lambda_i - \omega_{ii}^+ \Pi_+ (p_i, p_i)) + \sum_{1 \leq i < j \leq n} (-\omega_{ij}^+) \Pi_+ (p_i, p_j) + \sum_{1 \leq i < j \leq n} (-\omega_{ij}^-) \Pi_- (p_i, p_j) \right]
$$

$$
+ \left[ \sum_{1 \leq i < j \leq n} \omega_{ij}^+ \Pi_+ (p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^- \Pi_- (p_i, p_j) \right] \in S^+_n + N_n.
$$

On the basis of the above observations, we can define new subcones of $S^+_n + N_n$ in a similar manner as (11) and (12):

$$
\mathcal{F}^{+, s}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for some orthonormal matrix } P \text{ satisfying (6) } \},
$$

$$
\mathcal{F}^{+, a}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (6) } \},
$$

$$
\mathcal{F}^{\pm, a}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (6) } \},
$$

$$
\mathcal{F}^{\pm, s}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for some orthonormal matrix } P \text{ satisfying (6) } \},
$$

$$
\mathcal{F}^{\pm, a}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (6) } \},
$$

$$
\mathcal{F}^{\pm, s}_n := \{ A \in S_n | \alpha^+_n(P, \Lambda) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (6) } \}
$$

where $\alpha^+_n(P, \Lambda)$ and $\alpha^\pm_n(P, \Lambda)$ are optimal values of (LP)$_{P, \Lambda}$ and (LP)${}^\pm_{P, \Lambda}$, respectively. From the construction of problems (LP)${}^+_{P, \Lambda}$, (LP)${}^\pm_{P, \Lambda}$ and (LP)${}^\pm_{P, \Lambda}$, we can easily see that

$$
\mathcal{G}^+_n \subseteq \mathcal{F}^{+, s}_n \subseteq \mathcal{F}^{+, a}_n, \quad \mathcal{G}^+_n \subseteq \mathcal{F}^{+ a}_n \subseteq \mathcal{F}^{+ s}_n, \quad \mathcal{G}^{+ s}_n \subseteq \mathcal{F}^{+ s}_n \subseteq \mathcal{F}^{+ a}_n
$$

hold. The following corollary follows from (v)-(vii) of Theorem 2.3 and the above inclusions.

**Corollary 3.4. (i)**

$$
S^+_n \cup N_n \subseteq \mathcal{G}^+_n \subseteq \mathcal{G}^+_n = \text{com}(S^+_n + N_n) \subseteq \mathcal{F}^{+, s}_n \subseteq S^+_n + N_n
$$

$$
S^+_n \cup N_n \subseteq \mathcal{F}^{+ a}_n \subseteq \mathcal{F}^{+ s}_n \subseteq \mathcal{F}^{+ s}_n \subseteq \mathcal{F}^{+ a}_n \subseteq S^+_n + N_n
$$

$$
S^+_n \cup N_n \subseteq \mathcal{F}^{+ a}_n \subseteq \mathcal{F}^{+ s}_n \subseteq \mathcal{F}^{+ s}_n \subseteq \mathcal{F}^{+ a}_n \subseteq S^+_n + N_n
$$

**Corollary 3.4. (ii)** If $n = 2$, then each of the sets $\mathcal{F}^{+, s}_n$, $\mathcal{F}^{+, a}_n$, $\mathcal{F}^{+ s}_n$, $\mathcal{F}^{+ a}_n$, $\mathcal{F}^\pm_n$ and $\mathcal{F}^\pm_n$ coincides with $S^+_n + N_n$.

**Corollary 3.4. (iii)** The convex hull of each of the sets $\mathcal{F}^{+, s}_n$, $\mathcal{F}^{+, a}_n$, $\mathcal{F}^{+ s}_n$, $\mathcal{F}^{+ a}_n$, $\mathcal{F}^\pm_n$ and $\mathcal{F}^\pm_n$ is $S^+_n + N_n$.

The following table summarizes the sizes of LPs (10), (22), and (23) that we have to solve in order to identify, respectively, $A \in \mathcal{G}^+_n$ (or $A \in \mathcal{G}^+_n$), $A \in \mathcal{F}^{+, s}_n$ (or $A \in \overline{\mathcal{F}^{+, s}_n}$), and $A \in \mathcal{F}^\pm_n$ (or $A \in \mathcal{F}^\pm_n$).

## 4 Identification of $A \in S^+_n + N_n$

In this section, we investigate the effect of using the sets $\mathcal{F}^{+, s}_n$, $\mathcal{F}^{+, a}_n$, $\mathcal{F}^{+ s}_n$, and $\mathcal{F}^\pm_n$ for identification of the fact $A \in S^+_n + N_n$. 

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We generated random instances of $A \in S_n^+ + N_n$ based on the method described in Section 2 of [10]. For an $n \times n$ matrix $B$ with entries independently drawn from a standard normal distribution, we obtained a random positive semidefinite matrix $S = BB^T$. An $n \times n$ random nonnegative matrix $N$ was constructed using $N = C - c_{\min} I_n$ with $C = F + F^T$ for a random matrix $F$ with entries uniformly distributed in $[0, 1]$ and $c_{\min}$ being the minimal diagonal entry of $C$. We set $A = S + N \in S_n^+ + N_n$. The construction was designed so as to maintain nonnegativity of $N$ while increasing the chance that $S + N$ would be indefinite and thereby avoid instances that are too easy.

For each instance $A \in S_n^+ + N_n$, we checked whether $A \in G_s^n$ ($A \in F_{n}^{+s}$ and $A \in F_{n}^{-s}$) by solving (LP)$_{P,A}$ in (10) ((LP)$_{P,A}$ in (22) and (LP)$_{P,A}$ in (23)), where $P$ and $A$ were obtained using the MATLAB command "[P,A] = eig(A)."

Table 2 shows the number of matrices that were identified as $A \in G_s^n$ ($A \in F_{n}^{+s}$ and $A \in F_{n}^{-s}$) and the average CPU time, where 1000 matrices were generated for each $n$. The table yields the following observations:

- All of the matrices were identified as $A \in S_n^+ + N_n$ by checking $A \in F_{n}^{\pm s}$. The result is comparable to the one in Section 2 of [10].
- For any $n$, the number of identified matrices increases in the order of the set inclusion relation: $G_s^n \subseteq F_n^{+s} \subseteq F_n^{\pm s}$.
- For the sets $G_s^n$ and $F_n^{+s}$, the number of identified matrices decreases as the size of $n$ increases.
- Comparing the results for $F_n^{+s}$ and $F_n^{\pm s}$, the average CPU time is approximately proportional to the number of identified matrices.

Table 2: Results of identification of $A \in S_n^+ + N_n$; 1000 matrices were generated for each $n

<table>
<thead>
<tr>
<th>$n$</th>
<th>$G_s^n$</th>
<th>$F_n^{+s}$</th>
<th>$F_n^{\pm s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td># of $A$</td>
<td>Ave. time(s)</td>
<td># of $A$</td>
<td>Ave. time(s)</td>
</tr>
<tr>
<td>10</td>
<td>247</td>
<td>4.707</td>
<td>856</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>12.860</td>
<td>719</td>
</tr>
<tr>
<td>50</td>
<td>0</td>
<td>2373.744</td>
<td>440</td>
</tr>
</tbody>
</table>
5 LP-based algorithms for testing $A \in \mathcal{COP}_n$

In this section, we investigate the effect of using the sets $\mathcal{F}^+_n$, $\widetilde{\mathcal{F}}^+_n$, $\mathcal{F}^\times_n$ and $\widetilde{\mathcal{F}}^\times_n$ for testing whether a given matrix $A$ is copositive by using Sponsel, Bundfuss and Dür’s algorithm [35].

5.1 Outline of the algorithms

By defining the standard simplex $\Delta^S$ by $\Delta^S = \{x \in \mathbb{R}^n_+ \mid e^T x = 1\}$, we can see that a given $n \times n$ symmetric matrix $A$ is copositive if and only if

$$x^T A x \geq 0 \quad \text{for all} \quad x \in \Delta^S$$

(see Lemma 1 of [12]). For an arbitrary simplex $\Delta$, a family of simplices $\mathcal{P} = \{\Delta^1, \ldots, \Delta^m\}$ is called a simplicial partition of $\Delta$ if it satisfies

$$\Delta = \bigcup_{i=1}^m \Delta^i \text{ and } \text{int}(\Delta^i) \cap \text{int}(\Delta^j) \neq \emptyset \text{ for all } i \neq j.$$ 

Such a partition can be generated by successively bisecting simplices in the partition. For a given simplex $\Delta = \text{conv}\{v_1, \ldots, v_n\}$, consider the midpoint $v_{n+1} = \frac{1}{2}(v_i + v_j)$ of the edge $[v_i, v_j]$. Then the subdivision $\Delta^1 = \{v_1, \ldots, v_{i-1}, v_{n+1}, v_{i+1}, \ldots, v_n\}$ and $\Delta^2 = \{v_1, \ldots, v_{j-1}, v_{n+1}, v_{j+1}, \ldots, v_n\}$ of $\Delta$ satisfies the above conditions for simplicial partitions. See [27] for a detailed description of simplicial partitions.

Denote the set of vertices of partition $\mathcal{P}$ by

$$V(\mathcal{P}) = \{v \mid v \text{ is a vertex of some } \Delta \in \mathcal{P}\}.$$ 

Each simplex $\Delta$ is determined by its vertices and can be represented by a matrix $V_\Delta$ whose columns are these vertices. Note that $V_\Delta$ is nonsingular and unique up to a permutation of its columns, which does not affect the argument [35]. Define the set of all matrices corresponding to simplices in partition $\mathcal{P}$ as

$$M(\mathcal{P}) = \{V_\Delta : \Delta \in \mathcal{P}\}.$$ 

The “fineness” of a partition $\mathcal{P}$ is quantified by the maximum diameter of a simplex in $\mathcal{P}$, denoted by

$$\delta(\mathcal{P}) = \max_{\Delta \in \mathcal{P}} \max_{u, v \in \Delta} ||u - v||.$$ (25)

The above notation was used to show the following necessary and sufficient conditions for copositivity in [35]. The first theorem gives a sufficient condition for copositivity.

**Theorem 5.1** (Theorem 2.1 of [35]). If $A \in \mathcal{S}_n$ satisfies $V^T A V \in \mathcal{COP}_n$ for all $V \in M(\mathcal{P})$ then $A$ is copositive. Hence, for any $\mathcal{M}_n \subseteq \mathcal{COP}_n$, if $A \in \mathcal{S}_n$ satisfies $V^T A V \in \mathcal{M}_n$ for all $V \in M(\mathcal{P})$,

then $A$ is also copositive.

The above theorem implies that by choosing $\mathcal{M}_n = \mathcal{N}_n$ (see (2)), $A$ is copositive if $V_\Delta^T A V_\Delta \in \mathcal{N}_n$ holds for any $\Delta \in \mathcal{P}$. 

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Theorem 5.2 (Theorem 2.2 of [35]). Let $A \in S_n$ be strictly copositive, i.e., $A \in \text{int}(\text{COP}_n)$. Then there exists $\varepsilon > 0$ such that for all partitions $P$ of $\Delta^S$ with $\delta(P) < \varepsilon$, we have

$$V^T AV \in N_n \text{ for all } V \in M(P).$$

The above theorem ensures that if $A$ is strictly copositive (i.e., $A \in \text{int}(\text{COP}_n)$), the copositivity of $A$ (i.e., $A \in \text{COP}_n$) can be detected in finitely many iterations of an algorithm employing a subdivision rule with $\delta(P) \to 0$. A similar result can be obtained for the case $A \notin \text{COP}_n$, as follows.

Lemma 5.3 (Lemma 2.3 of [35]). The following two statements are equivalent.

1. $A \notin \text{COP}_n$
2. There is an $\varepsilon > 0$ such that for any partition $P$ with $\delta(P) < \varepsilon$, there exists a vertex $v \in V(P)$ such that $v^T Av < 0$.

The following algorithm, in [35], is based on the above three results.

Algorithm 1 Sponsel, Bundfuss and Dür's algorithm to test copositivity

| Input: $A \in S_n, M_n \subseteq \text{COP}_n$ |
| Output: “$A$ is copositive” or “$A$ is not copositive” |

1: $P \leftarrow \{\Delta^S\}$;
2: while $P \neq \emptyset$ do
3: Choose $\Delta \in P$;
4: if $v^T Av < 0$ for some $v \in V(\{\Delta\})$: then
5: return “$A$ is not copositive”;
6: end if
7: if $V_A^T AV_\Delta \in M_n$ then
8: $P \leftarrow P \setminus \{\Delta\}$;
9: else
10: Partition $\Delta$ into $\Delta = \Delta^1 \cup \Delta^2$;
11: $P \leftarrow P \setminus \{\Delta\} \cup \{\Delta^1, \Delta^2\}$;
12: end if
13: end while
14: Return “$A$ is copositive”;

As we have already observed, Theorem 5.2 and Lemma 5.3 imply the following corollary.

Corollary 5.4. 1. If $A$ is strictly copositive, i.e., $A \in \text{int}(\text{COP}_n)$, then Algorithm 1 terminates finitely, returning “$A$ is copositive.”

2. If $A$ is not copositive, i.e., $A \notin \text{COP}_n$, then Algorithm 1 terminates finitely, returning “$A$ is not copositive.”

At Line 8, Algorithm 1 removes the simplex that was determined at Line 7 to be in no further need of exploration by Theorem 5.1. The accuracy and speed of the determination influence the total computational time and depend on the choice of the set $M_n \subseteq \text{COP}_n$.

In this section, we investigate the effect of using the sets $H_n$ in (5), $G_n^s$ in (12), and $F_n^{1+s}$ and $F_n^{2+s}$ in (24) as the set $M_n$ in the above algorithm.
Algorithm 2 Improved version of Algorithm 1

Input: $A \in S_n$, $\mathcal{M}_n \subseteq \overline{\mathcal{M}}_n \subseteq \text{COP}_n$

Output: “$A$ is copositive” or “$A$ is not copositive”

1: $\mathcal{P} \leftarrow \{\Delta^S\}$;
2: while $\mathcal{P} \neq \emptyset$ do
3: \hspace{1em} Choose $\Delta \in \mathcal{P}$;
4: \hspace{1em} if $v^T Av < 0$ for some $v \in V(\{\Delta\})$: then
5: \hspace{2em} \textbf{Return} “$A$ is not copositive”;
6: \hspace{1em} end if
7: \hspace{1em} if $V^T_\Delta AV_\Delta \in \mathcal{M}_n$ then
8: \hspace{2em} $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
9: \hspace{1em} end if
10: \hspace{1em} else
11: \hspace{2em} if $V^T_\Delta AV_\Delta \in \overline{\mathcal{M}}_n$ then
12: \hspace{3em} $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
13: \hspace{2em} end if
14: \hspace{2em} if $V^T_{\Delta_p} AV_{\Delta_p} \in \mathcal{M}_n$ then
15: \hspace{3em} $\Delta \leftarrow \Delta \setminus \{\Delta_p\}$;
16: \hspace{3em} end if
17: \hspace{2em} end if
18: \hspace{2em} end if
19: \hspace{1em} end if
20: \hspace{1em} end if
21: \hspace{1em} end while
22: \textbf{return} “$A$ is copositive”;
Note that if we choose $\mathcal{M}_n = \mathcal{G}_n^*$ (respectively, $\mathcal{M}_n = \mathcal{F}_n^{+,s}, \mathcal{M}_n = \mathcal{F}_n^{+,s}$), we can improve Algorithm 1 by incorporating the set $\overline{\mathcal{M}}_n = \overline{\mathcal{G}}_n^*$ (respectively, $\overline{\mathcal{M}}_n = \overline{\mathcal{F}}_n^{+,s}, \overline{\mathcal{M}}_n = \overline{\mathcal{F}}_n^{+,s}$), as proposed in [36].

The details of the added steps are as follows. Suppose that we have a diagonalization of the form (6).

At Line 7, we need to solve an additional LP but do not need to diagonalize $V_\Delta^T AV_\Delta$. Let $P$ and $\Lambda$ be matrices satisfying (6). Then the matrix $V_\Delta^T P$ can be used to diagonalize $V_\Delta^T AV_\Delta$, i.e.,

$$V_\Delta^T AV_\Delta = V_\Delta^T (P \Lambda P^T) V_\Delta = (V_\Delta^T P) \Lambda (V_\Delta^T P)^T$$

while $V_\Delta^T P$ is not necessarily orthonormal. Thus, we can test $V_\Delta^T AV_\Delta \in \overline{\mathcal{M}}_n$ by solving the corresponding LP, i.e., $(\text{LP})_{V_\Delta^T P, \Lambda}$ if $\mathcal{M}_n = \mathcal{G}_n^*$, $(\text{LP})_{V_\Delta^T P, \Lambda}$ if $\mathcal{M}_n = \mathcal{F}_n^{+,s}$ and $(\text{LP})_{V_\Delta^T P, \Lambda}$ if $\mathcal{M}_n = \mathcal{F}_n^{+,s}$.

If $V_\Delta^T AV_\Delta \in \overline{\mathcal{M}}_n$ is not detected at Line 7, we can check whether $V_\Delta^T AV_\Delta \in \mathcal{M}_n$ at Line 10. Similarly to Algorithm 1.2 (where the set $\mathcal{M}_n$ is used at Line 7 of Algorithm 1), we can diagonalize $V_\Delta^T AV_\Delta$ as $V_\Delta^T AV_\Delta = P \Lambda P^T$ with an orthonormal matrix $P$ and a diagonal matrix $\Lambda$ and solve the LP.

At Line 15, we don’t need to diagonalize $V_\Delta^T AV_\Delta$ or to solve any more LPs. Let $\omega^* \in \mathbb{R}^n$ be an optimal solution of the corresponding LP obtained at Line 7 and let $\Omega^* := \text{Diag}(\omega^*)$. Then the feasibility of $\omega^*$ implies the positive semidefiniteness of the matrix $V_\Delta^T \Lambda \Omega^* \Lambda^T V_\Delta$. Thus, if $V_\Delta^T P \Omega^* P^T V_\Delta \in \mathcal{N}_n$, we see that

$$V_\Delta^T P \Omega^* P^T V_\Delta \in \mathcal{N}_n$$

and that $V_\Delta^T P \Omega^* P^T V_\Delta \in \overline{\mathcal{M}}_n$.

### 5.2 Numerical results

We implemented Algorithms 1 and 2 in MATLAB R2015a on a 3.07GHz Core i7 machine with 12 GB of RAM, using Gurobi 6.5 for solving LPs.

As test instances, we used the following matrix,

$$B_\gamma := \gamma (E - A_G) - E \quad (26)$$

where $E \in \mathcal{S}_n$ is the matrix whose elements are all ones and the matrix $A_G \in \mathcal{S}_n$ is the adjacency matrix of a given undirected graph $G$ with $n$ nodes. The matrix $B_\gamma$ comes from the maximal clique problem. The maximum clique problem is to find a clique (complete subgraph) of maximum cardinality in $G$. It has been shown (in [15]) that the maximum cardinality, the so-called clique number $\omega(G)$, is equal to the optimal value of

$$\omega(G) = \min \{ \gamma \in \mathbb{N} \mid B_\gamma \in \text{COP}_n \}.$$

Thus, the clique number can be found by checking the copositivity of $B_\gamma$ for at most $\gamma = n, n - 1, \ldots, 1$.

Figure 3 on page 20 shows the instances of $G$ that were used in [35]. We know the clique numbers of $G_8$ and $G_{12}$ are $\omega(G_8) = 3$ and $\omega(G_{12}) = 4$, respectively.

The aim of the implementation is to explore the differences in behavior when using $\mathcal{H}_n$, $\mathcal{G}_n^*$, $\mathcal{F}_n^{+,s}$, $\overline{\mathcal{F}}_n^{+,s}$, $\mathcal{F}_n^{+,s}$ or $\overline{\mathcal{F}}_n^{+,s}$ as the set $\mathcal{M}_n$ rather than to compute the clique number efficiently. Hence, the experiment examined $B_\gamma$ for various values of $\gamma$ at intervals of 0.1 around the value $\omega(G)$ (see Tables 3 and 4 on page 21).
As already mentioned, \( \alpha_\ast(P, \Lambda) < 0 \) (\( \alpha_\ast^+(P, \Lambda) < 0 \) and \( \alpha_\ast^-(P, \Lambda) < 0 \)) with a specific \( P \) does not necessarily guarantee that \( A \notin G_n \) or \( A \notin \overline{G_n} \) (\( A \notin \mathcal{F}^{+\times}_n \) or \( A \notin \mathcal{F}^{-\times}_n \), \( A \notin \mathcal{F}^{+\times}_n \) or \( A \notin \mathcal{F}^{-\times}_n \)). Thus, it not strictly accurate to say that we can use those sets for \( M_n \), and the algorithms may miss some of the \( \Delta \)'s that could otherwise have been removed. However, although this may have some effect on speed, it does not affect the termination of the algorithm, as it is guaranteed by the subdivision rule satisfying \( \delta(P) \to 0 \), where \( \delta(P) \) is defined by (25).

Tables 3 and 4 show the numerical results for \( G_8 \) and \( G_{12} \), respectively. Both tables compare the results of the following six algorithms in terms of the number of iterations (the column “Iter.”) and the total computational time (the column “Time (s)”):

- **Algorithm 1.1**: Algorithm 1 with \( M_n = H_n \).
- **Algorithm 2.1**: Algorithm 2 with \( M_n = \mathcal{G}^+_n \) and \( \overline{M}_n = \overline{G}^+_n \).
- **Algorithm 1.2**: Algorithm 1 with \( M_n = \mathcal{F}^{+\times}_n \).
- **Algorithm 2.2**: Algorithm 2 with \( M_n = \mathcal{F}^{+\times}_n \) and \( \overline{M}_n = \overline{F}^{+\times}_n \).
- **Algorithm 2.3**: Algorithm 2 with \( M_n = \mathcal{F}^{-\times}_n \) and \( \overline{M}_n = \overline{F}^{-\times}_n \).
- **Algorithm 1.3**: Algorithm 1 with \( M_n = S^+_n + \mathcal{N}_n \).

Note that we performed the last algorithm \( \text{Algorithm 1.3} \) as a reference, while we used SeDuMi 1.3 for solving the semidefinite program (3) with \( A = V^T \Delta AV \) at Line 7 of the algorithm.

The symbol “−” means that the algorithm did not terminate within 6 hours. The reason for the long computation time may come from the fact that for each graph \( G \), the matrix \( B \) lies on the boundary of the copositive cone \( \text{COP}_n \) when \( \gamma = \omega(G) \) (\( \omega(G_8) = 3 \) and \( \omega(G_{12}) = 4 \)).

We can draw the following implications from the results in Table 4 on page 22 for the larger graph \( G_{12} \) (similar implications can be drawn from Tables 3):

- At any \( \gamma \geq 5.2 \), **Algorithms 2.1, 1.2, 2.2, 2.3 and 1.3** terminate in one iteration, and the execution times of **Algorithms 1.2, 2.2 and 2.3** are much shorter than those of **Algorithms 1.1 or 1.3**.
- The lower bound of \( \gamma \) for which the algorithm terminates in one iteration and the one for which the algorithm terminates in 6 hours decrease in going from **Algorithm 1.2** to **Algorithm 1.3**. The reason may be that, as shown in Corollary 3.4, the set inclusion relation \( \mathcal{G}_n \subseteq \mathcal{F}^{+\times}_n \subseteq \mathcal{F}^{-\times}_n \subseteq S^+_n + \mathcal{N}_n \) holds.
- Table 1 on page 11 summarizes the sizes of the LPs for identification. The results here imply that the computational times for solving an LP have the following magnitude relationship for any \( n \geq 3 \):

  **Algorithm 2.1 < Algorithm 1.2 < Algorithm 2.2 < Algorithm 2.3**.

On the other hand, the set inclusion relation \( \mathcal{G}_n \subseteq \mathcal{F}^{+\times}_n \subseteq \mathcal{F}^{-\times}_n \) and the construction of Algorithms 1 and 2 imply that the detection abilities of the algorithms also follow the relationship described above and that the number of iterations has the reverse relationship for any \( \gamma \) in Table 4:

**Algorithm 2.1 > Algorithm 1.2 > Algorithm 2.2 > Algorithm 2.3**.

It seems that the order of the number of iterations has a stronger influence on the total computational time than the order of the computational time for solving an LP.
At each \( \gamma \in [4.1, 4.9] \), the number of iterations of Algorithm 2.3 is much larger than one hundred times those of Algorithm 1.3. This means that the total computational time of Algorithm 2.3 is longer than that of Algorithm 1.3 at each \( \gamma \in [4.1, 4.9] \), while Algorithm 1.3 solves a semidefinite program of size \( O(n^2) \) at each iteration.

At each \( \gamma < 4 \), the algorithms show no significant differences in terms of the number of iterations. The reason may be that they all work to find a \( v \in V(\{\Delta\}) \) such that \( v^T (\gamma (E - AG) - E)v < 0 \), while their computational time depends on the choice of simplex refinement strategy.

In view of the above observations, we conclude that Algorithm 2.3 with the choices \( \mathcal{M}_n = F_n^{(+)\mathbb{R}}  \) and \( \mathcal{M}_n = F_n^{(+)\mathbb{R}} \) might be a way to check the copositivity of a given matrix \( A \) when \( A \) is strictly copositive.

The above results contrast with those of Bomze and Eichfelder in [10], where the authors show the number of iterations required by their algorithm for testing copositivity of matrices of the form (26). On the contrary to the first observation described above, their algorithm terminates with few iterations when \( \gamma < \omega(G) \), i.e., the corresponding matrix is not copositive, and it requires a huge number of iterations otherwise.

It should be noted that Table 3 shows an interesting result concerning the non-convexity of the set \( G_n^* \), while we know that \( \text{conv} (G_n^*) = S_n + \mathcal{N}_n \) (see Theorem 2.3). Let us look at the result at \( \gamma = 4.0 \) of Algorithm 2.1. The multiple iterations at \( \gamma = 4.0 \) imply that we could not find \( B_4.0 \in G_n^* \) at the first iteration for a certain orthonormal matrix \( P \) satisfying (6). Recall that the matrix \( B_\gamma \) is given by (26). It follows from \( E - AG \in \mathcal{N}_n \subseteq G_n^* \) and from the result at \( \gamma = 3.5 \) in Table 3 that

\[
0.5(E - AG) \in G_n^* \quad \text{and} \quad B_{3.5} = 3.5(E - AG) - E \in G_n^*.
\]

Thus, the fact that we could not determine whether the matrix

\[
B_{4.0} = 4.0(E - AG) - E = 0.5(E - AG) + B_{3.5}
\]

lies in the set \( G_n^* \) suggests that the set \( G_n^* = \text{com}(S_n + \mathcal{N}_n) \) is not convex.

### 6 Concluding remarks

In this paper, we investigated the properties of several tractable subcones of \( \text{COP}_n \) and summarized the results (as Figures 1 and 2). We also devised new subcones of \( \text{COP}_n \) by introducing the semidefinite basis (SD basis) defined as in Definitions 3.2 and 3.3. We conducted numerical experiments using those subcones for identification of given matrices \( A \in \mathcal{S}_n^+ + \mathcal{N}_n \) and for testing the copositivity of matrices arising from the maximum clique problems. We have to solve LPs with \( O(n^2) \) variables and \( O(n^2) \) constraints in order to detect whether a given matrix belongs to those cones, and the computational cost is substantial. However, the numerical results shown in Tables 2, 3, and 4 show that the new subcones are promising not only for identification of \( A \in \mathcal{S}_n^+ + \mathcal{N}_n \) but also for testing copositivity.

Recently, Ahmadi, Dash and Hall [1] developed algorithms for inner approximating the cone of positive semidefinite matrices, wherein they focused on the set \( \mathcal{D}_n \subseteq \mathcal{S}_n^+ \) of \( n \times n \) diagonal dominant matrices. Let \( U_{n,k} \) be the set of vectors in \( \mathbb{R}^n \) that have at most \( k \) nonzero components, each equal to \( \pm 1 \), and define

\[
U_{n,k} := \{ uu^T \mid u \in U_{n,k} \}.
\]

Then, as the authors indicate, the following theorem has already been proven.
Theorem 6.1 (Theorem 3.1 of [1], Barker and Carlson [3]).

\[ D_n = \text{cone} (U_{n,k}) := \left\{ \sum_{i=1}^{\|U_{n,k}\|} \alpha_i U_i \mid U_i \in U_{n,k}, \quad \alpha_i \geq 0 \ (i = 1, \ldots, \|U_{n,k}\|) \right\} \]

From the above theorem, we can see that for the SDP bases \( B_+ (p_1, p_2, \cdots, p_n) \) in (17), \( B_- (p_1, p_2, \cdots, p_n) \) in (19) and \( n \)-dimensional unit vectors \( e_1, e_2, \cdots, e_n \), the following set inclusion relation holds:

\[ B_+ (e_1, e_2, \cdots, e_n) \cup B_- (e_1, e_2, \cdots, e_n) \subseteq D_n = \text{cone} (U_{n,k}) \]

These sets should be investigated in the future.

The motivation of the paper is to create efficient algorithms for testing copositivity using tractable subcones of the copositive cone. In fact, we devised some new subcones for which the identification problems can be formulated in LPs. However, unfortunately, all of the subcones are subsets of \( \mathcal{S}_n + \mathcal{N}_n \) which necessitates heuristics for checking if a matrix is in \( \mathcal{S}_n + \mathcal{N}_n \). A major challenge that we face is to find a tractable subcone outside of the set \( \mathcal{S}_n + \mathcal{N}_n \).

Acknowledgment

The authors would like to sincerely thank the anonymous reviewers for their thoughtful and valuable comments which have significantly improved the paper. Among others, one of the reviewers pointed out that Proposition 3.1 is Lemma 6.2 of [18].

References


Figure 3: The graphs $G_8$ with $\omega(G_8) = 3$ (left) and $G_{12}$ with $\omega(G_{12}) = 4$ (right).
## Table 3: Results for $G_8$

<p>| $\gamma$ | Alg. 1.1 ($H_n$) | Iter. | Time(s) | Alg. 2.1 ($G_n^s$, $G_n^0$) | Iter. | Time(s) | Alg. 1.2 ($F_n^{\pm s}$) | Iter. | Time(s) | Alg. 2.2 ($F_n^{\pm s}$) | Iter. | Time(s) | Alg. 2.3 ($F_n^{\pm s}$) | Iter. | Time(s) | Alg. 1.3 ($S_n^+ + N_n$) | Iter. | Time(s) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2.8 | 2246 | 0.301 | 2463 | 7.197 | 1951 | 4.524 | 1811 | 7.355 | 1635 | 8.731 | 1251 | 448.201 |
| 2.9 | 1606 | 0.191 | 2139 | 6.270 | 1493 | 3.469 | 1393 | 5.458 | 1393 | 6.867 | 1251 | 449.572 |
| 3.0 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 3.1 | 3003 | 0.279 | 5885 | 14.603 | 1827 | 3.864 | 1357 | 4.879 | 503 | 2.394 | 7 | 3.186 |
| 3.2 | 1509 | 0.132 | 3129 | 7.830 | 911 | 1.980 | 377 | 1.347 | 201 | 0.976 | 3 | 1.480 |
| 3.3 | 469 | 0.040 | 2229 | 5.549 | 447 | 0.968 | 249 | 0.918 | 111 | 0.538 | 3 | 1.352 |
| 3.4 | 395 | 0.034 | 1603 | 4.112 | 291 | 0.625 | 167 | 0.650 | 53 | 0.254 | 3 | 1.401 |
| 3.5 | 369 | 0.031 | 1 | 0.003 | 1 | 0.003 | 1 | 0.004 | 1 | 0.004 | 1 | 0.322 |
| 3.6 | 209 | 0.017 | 1 | 0.002 | 1 | 0.003 | 1 | 0.004 | 1 | 0.004 | 1 | 0.362 |
| 3.7 | 115 | 0.009 | 1 | 0.002 | 1 | 0.003 | 1 | 0.004 | 1 | 0.004 | 1 | 0.371 |
| 3.8 | 79 | 0.007 | 1 | 0.002 | 1 | 0.003 | 1 | 0.004 | 1 | 0.004 | 1 | 0.359 |
| 3.9 | 63 | 0.005 | 1 | 0.002 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.322 |
| 4.0 | 47 | 0.004 | 227 | 0.593 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.360 |
| 4.1 | 23 | 0.002 | 1 | 0.003 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.324 |
| 4.2 | 17 | 0.002 | 1 | 0.005 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.330 |
| 4.3 | 17 | 0.002 | 1 | 0.005 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.324 |
| 4.4 | 7 | 0.001 | 1 | 0.005 | 1 | 0.003 | 1 | 0.003 | 1 | 0.005 | 1 | 0.328 |
| 4.5 | 7 | 0.001 | 1 | 0.005 | 1 | 0.003 | 1 | 0.003 | 1 | 0.006 | 1 | 0.258 |</p>
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