Tractable Subcones and LP-based Algorithms for Testing Copositivity

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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 better subcones of the copositive cone having desirable properties. 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 $S_n$ be the set of $n \times n$ symmetric matrices and define their inner product as

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

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

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

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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 $\mathbb{R}_+^n$:

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

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, 31, 32, 13, 14, 19]). Interested readers may refer to [20] 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 [30, 18, 19] and many algorithms have been proposed to solve it (see, e.g., [6, 12, 29, 28, 37, 34, 10, 16, 21, 35, 11]).

Here, we are interested in algorithms that use tractable subcones $\mathcal{M}_n$ of the copositive cone $\text{COP}_n$ for detecting copositivity (see, e.g., [12, 34, 35]). 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 easily check whether $A \in \mathcal{M}_n$, and

**P2** $\mathcal{M}_n$ is a subset of the copositive cone $\text{COP}_n$ that is as large as possible.

The authors, in [35], 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 aims of this paper are 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 $O(n^2)$ constraints. As we will show in Corollary 3.6, these subcones are larger than the ones proposed in [35] 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 3.1 and 3.3 and construct new LPs for detecting whether a given matrix belongs to the subcones. Note that the subcones are also subcones of 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 $N_n$. Section 4 describes numerical experiments in which the new subcones are used for identifying the given matrices $A \in S_n^+ + N_n$, and 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 $A \in S_n^+ + N_n$ but also for testing copositivity. We give concluding remarks in Section 6.
2 Some tractable subcones of the copositive cone

The following cones are attracting a lot of attention in a context of the relationship between combinatorial optimization and conic optimization (see, e.g., [20, 9]).

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

Except the set $S_n^+ \cup N_n$, 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:

$$\operatorname{COP}_n \supseteq S_n^+ + N_n \supseteq S_n^+ \cup N_n \supseteq S_n^+ \supseteq S_n^+ \cap N_n \supseteq \operatorname{CP}_n.$$ (2)

It is known that the following proposition holds by defining the inner product as in (1).

**Proposition 2.1** (Properties of the copositive cone). (i) The dual cone of the copositive cone $\operatorname{COP}_n$ with respect to the inner product (1) is the completely positive cone $\operatorname{CP}_n$ and vice versa (see p.57 of [4] and Theorem 2.3 of [5]).

(ii) If $n \leq 4$, then $\operatorname{COP}_n = S_n^+ + N_n$ (see [17] and Proposition 1.23 of [5]).

(iii) The dual cone of the doubly nonnegative cone $S_n^+ \cap N_n$ with respect to the inner product (1) is the Minkowski sum $S_n^+ + N_n$ of the positive semidefinite cone $S_n^+$ and the nonnegative cone $N_n$, and vice versa (see Remark 2.2).

**Remark 2.2.** Proposition 2.1 (iii): The equality $(S_n^+ \cap N_n)^* = \operatorname{cl}(S_n^+ + N_n)$ follows from a well-known result that $(K_1 \cap K_2)^* = \operatorname{cl}(K_1 + K_2)$ holds for any closed convex cones $K_1$ and $K_2$ (see, e.g., p. 11 of [23] or Corollary 2.2 of [4]). The closedness of the set $S_n^+ + N_n$ follows from a result presented in [33]. See also Proposition 4.1 of [36], where the authors showed this property within a more general framework.

As mentioned in Section 1, the problem of testing copositivity, i.e., deciding whether a given symmetric matrix $A$ is in the cone $\operatorname{COP}_n$ or not, is co-NP-complete [30, 18, 19]. On the other hand, the problem of testing whether or not $A \in S_n^+ + N_n$ can be solved by solving the following doubly nonnegative program (which can be expressed as a semidefinite program)

$$\begin{align*}
\text{Minimize} & \quad \langle A, X \rangle \\
\text{subject to} & \quad \langle I_n, X \rangle = 1, \ X \in S_n^+ \cap N_n
\end{align*}$$

where $I_n$ denotes the $n \times n$ identity matrix. Thus, the set $S_n^+ + N_n$ is a rather large and tractable convex subcone of $\operatorname{COP}_n$. However, solving the doubly nonnegative problem takes an awful lot of time [34, 36].
and does not make for a practical implementation. To overcome this drawback, more easily tractable subcones of the copositive cone have been proposed.

For any given matrix $A \in \mathcal{S}_n$, we define

$$N(A)_{ij} := \begin{cases} A_{ij} & \text{if } A_{ij} > 0 \text{ and } i \neq j \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad S(A) := A - N(A). \tag{3}$$

In [34], the authors defined the following set:

$$\mathcal{H}_n := \{ A \in \mathcal{S}_n \mid S(A) \in \mathcal{S}_n^+ \}. \tag{4}$$

Note that $A = S(A) + N(A) \in \mathcal{S}_n^+ + \mathcal{N}_n$ if $A \in \mathcal{H}_n$. Also, for any $A \in \mathcal{N}_n$, $S(A)$ is a nonnegative diagonal matrix, and hence, $\mathcal{N}_n \subseteq \mathcal{H}_n$. The determination of $A \in \mathcal{H}_n$ is easy and can be done by checking the positivity of $A_{ij}(i \neq j)$ and by performing a Cholesky factorization of $S(A)$ (cf. Algorithm 4.2.4 in [25]).

Thus, from the inclusion relation (2), we see that the set $\mathcal{H}_n$ has the desirable \textbf{P1} property. However, $S(A)$ is not necessarily positive semidefinite even if $A \in \mathcal{S}_n^+ + \mathcal{N}_n$ or $A \in \mathcal{S}_n^+$. The following theorem summarizes the properties of the set $\mathcal{H}_n$.

**Theorem 2.3** ([24] and Theorem 4.2 of [34]). $\mathcal{H}_n$ is a convex cone and $\mathcal{N}_n \subseteq \mathcal{H}_n \subseteq \mathcal{S}_n^+ + \mathcal{N}_n$. If $n \geq 3$, these inclusions are strict and $\mathcal{S}_n^+ \not\subseteq \mathcal{H}_n$. For $n = 2$, we have $\mathcal{H}_n = \mathcal{S}_n^+ \cup \mathcal{N}_n = \mathcal{S}_n^+ + \mathcal{N}_n = \text{COP}_n$.

The construction of the subcone $\mathcal{H}_n$ is based on the idea of “nonnegativity-checking first and positive semidefiniteness-checking second.” In [35], another subcone is provided that is based on the idea of “positive semidefiniteness-checking first and nonnegativity-checking second.”

For a given symmetric matrix $A \in \mathcal{S}_n$, 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

$$A = PP^T = \sum_{i=1}^{n} \lambda_i p_i p_i^T \tag{5}$$

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

$$A = P(\Lambda - \Omega)P^T + P\Omega P^T \tag{6}$$

If $\Lambda - \Omega \in \mathcal{N}_n$, 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

$$\lambda_i \geq \omega_i \quad (i = 1, 2, \ldots, n), \quad [P\Omega P^T]_{ij} \geq 0 \quad (1 \leq i \leq j \leq n) \tag{7}$$

then (6) and (2) imply

$$A = P(\Lambda - \Omega)P^T + P\Omega P^T \in \mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \text{COP}_n. \tag{8}$$

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 $\alpha$:

$$\begin{align*}
\text{(LP)}_{P, \Lambda} \\
\text{Maximize} & \quad \alpha \\
\text{subject to} & \quad \omega_i \leq \lambda_i \quad (i = 1, 2, \ldots, n) \\
& \quad [P\Omega P^T]_{ij} = \sum_{k=1}^{n} \omega_k p_k p_k^T \geq \alpha \quad (1 \leq i \leq j \leq n)
\end{align*} \tag{9}$$
The problem \((LP)_{P,A}\) has a feasible solution at which \(\omega_i = \lambda_i\) \((i = 1, 2, \ldots, n)\) and

\[
\alpha = \min \left\{ \sum_{k=1}^{n} \omega_k p_k p_k^T \right\} = \min \left\{ \sum_{k=1}^{n} \omega_k [p_k]_i [p_k]_j \right\}
\]

For each \(i = 1, 2, \ldots, n\), the constraints

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

and \(\omega_k \leq \lambda_k\) \((k = 1, 2, \ldots, n)\) imply the bound \(\alpha \leq \min \left\{ \sum_{k=1}^{n} \lambda_k [p_k]_i^2 \right\}\). Thus, \((LP)_{P,A}\) has an optimal solution with optimal value \(\alpha_* (P,A) \geq 0\). If \(\alpha_* (P,A) \geq 0\), there exists a matrix \(\Omega\) for which the decomposition (7) holds. The following set \(G_*^a\) of \(M_n\) is based on the above observations and was proposed in [35].

\[
G_*^a := \{ A \in S_n \mid \alpha_* (P,A) \geq 0 \text{ for some orthonormal matrix } P \text{ satisfying (5)} \}.
\]

As stated above, if \(\alpha_* (P,A) \geq 0\) for a given decomposition \(A = P\Lambda P^T\), we can determine \(A \in G_*^a\). In this case, we just need to compute a matrix decomposition and solve a linear optimization problem with \(n + 1\) variables and \(O(n^2)\) constraints, which implies that it is rather practical to use the set \(G_*^a\) as an alternative to using \(M_n\). Suppose that \(A \in S_n\) has \(n\) different eigenvalues. Then the possible orthonormal matrices \(P = [p_1, p_2, \ldots, p_n]\) are identifiable, except for the permutation and sign inversion of \([p_1, p_2, \ldots, p_n]\), and by representing (5) as

\[
A = \sum_{i=1}^{n} \lambda_i p_i p_i^T,
\]

we can see that the problem \((LP)_{P,A}\) is unique for any possible \(P\). In this case, \(\alpha_* (P,A) < 0\) with a specific \(P\) implies \(A \not\in G_*^a\). However, if this is not the case (i.e., an eigenspace of \(A\) has at least dimension 2), \(\alpha_* (P,A) < 0\) with a specific \(P\) does not necessarily guarantee that \(A \not\in G_*^a\). Thus, we cannot say that the set \(G_*^a\) has the desirable \(\text{P}1\) property. However, as we will see in Theorem 2.5 below, \(G_*^a\) may possess the other desirable property, \(\text{P}2\).

In [35], the authors described other sets \(G_*^a\) and \(\tilde{G}_*^a\) that are closely related to \(G_*^a\).

\[
G_*^a := \{ A \in S_n \mid \alpha_* (P,A) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (5)} \},
\tilde{G}_*^a := \{ A \in S_n \mid \alpha_* (P,A) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (5)} \}.
\]

Note that if (7) holds for any arbitrary (not necessarily orthonormal) matrix \(P\), then (8) also holds, which implies the following inclusions:

\[
G_*^a \subseteq G_*^a \subseteq \tilde{G}_*^a \subseteq S_n^+ + N_n.
\]

Before describing the properties of the sets \(G_*^a\), \(G_*^a\) and \(\tilde{G}_*^a\), we will prove a preliminary lemma.

**Lemma 2.4.** Let \(K_1\) and \(K_2\) be two convex cones. Then \(\text{conv} (K_1 \cup K_2) = K_1 + K_2\).

**Proof.** Since \(K_1\) and \(K_2\) are convex cones, we can easily see that the inclusion \(K_1 + K_2 \subseteq \text{conv} (K_1 \cup K_2)\) holds. The converse inclusion also follows from the fact that \(K_1\) and \(K_2\) are convex cones. Since \(K_1\) 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

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

\[\square\]

The following theorem shows some of the properties of \( \mathcal{G}_n^\alpha \), \( \mathcal{G}_n^n \), and \( \widetilde{\mathcal{G}}_n^n \). Here, we give a complete proof of the theorem, although we have already proven (i), (ii), and (iii) in Theorem 3.2 of [35] and its proof.

**Theorem 2.5.** (i) The sets \( \mathcal{G}_n^\alpha \), \( \mathcal{G}_n^n \) and \( \widetilde{\mathcal{G}}_n^n \) are subcones of \( \mathcal{S}_n^+ + \mathcal{N}_n \)

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

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

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

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

(v) \( \mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^n \subseteq \mathcal{G}_n^\alpha = \text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) \subseteq \mathcal{G}_n^n \subseteq \mathcal{COP}_n \).

(vi) If \( n = 2 \), then \( \mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{G}_n^n = \mathcal{G}_n^n = \text{com} (\mathcal{S}_n^+ + \mathcal{N}_n) \).

(vii) \( \text{conv} (\mathcal{S}_n^+ \cup \mathcal{N}_n) = \text{conv} (\mathcal{G}_n^n) = \text{conv} (\mathcal{G}_n^n) = \text{conv} (\text{com} (\mathcal{S}_n^+ + \mathcal{N}_n)) = \text{conv} (\widetilde{\mathcal{G}}_n^n) = \mathcal{S}_n^+ + \mathcal{N}_n \).

**Proof.** Throughout the proof, we will assume that \( A \in \mathcal{S}_n \) is diagonalized as in (5).

(i): Since we have already know that (12) holds, it is sufficient to show that the sets \( \mathcal{G}_n^\alpha \), \( \mathcal{G}_n^n \) and \( \widetilde{\mathcal{G}}_n^n \) are cones. Suppose that the associated linear optimization problem (LP) \( \mathcal{P}_{\alpha} \) has an optimal solution \( (\omega^*, \alpha^*) := (\omega_1^*, \ldots, \omega_n^*, \alpha_n^*) \). Then for any \( \beta \geq 0 \), \( \beta A \) is diagonalized as in \( \beta A = P(\beta \Lambda)P^T \) and \( (\beta \omega^*, \beta \alpha^*) \) is an optimal solution of the problem (LP) \( \mathcal{P}_{\beta \Lambda} \). This implies that \( \beta A \in \mathcal{G}_n^n \) (as well as \( \beta A \in \mathcal{G}_n^\alpha \) and \( \beta A \in \widetilde{\mathcal{G}}_n^n \)) if \( A \in \mathcal{G}_n^n \) (\( A \in \mathcal{G}_n^n \) and \( A \in \widetilde{\mathcal{G}}_n^n \)) and hence \( \mathcal{G}_n^n \), \( \mathcal{G}_n^n \) and \( \widetilde{\mathcal{G}}_n^n \) are cones.

(ii): We show that \( \mathcal{N}_n \subseteq \mathcal{G}_n^n \) and \( \mathcal{S}_n^+ \subseteq \mathcal{G}_n^n \). Suppose that \( A \in \mathcal{N}_n \). Then for all \( \mathcal{P} \), problem (LP) \( \mathcal{P}_{\Lambda} \) has a feasible solution, where \( (\omega, \alpha) = (\lambda_1, \ldots, \lambda_n, 0) \), which implies that \( A \in \mathcal{G}_n^n \). Suppose that \( A \in \mathcal{S}_n^+ \), i.e., \( \lambda_i \geq 0 \) \( (i = 1, 2, \ldots, n) \). Then for all \( \mathcal{P} \), problem (LP) \( \mathcal{P}_{\Lambda} \) has a feasible solution, where \( (\omega, \alpha) = (0, \ldots, 0, 0) \), which implies that \( A \in \mathcal{G}_n^n \). Thus, we have shown \( \mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^n \).

(iii): The inclusion \( \mathcal{G}_n^n \subseteq \text{com}(\mathcal{S}_n^+ + \mathcal{N}_n) \) follows from the construction of the set \( \mathcal{G}_n^n \) as in (10) and (9). The converse inclusion \( \mathcal{G}_n^n \subseteq \text{com}(\mathcal{S}_n^+ + \mathcal{N}_n) \) is also true, since, if \( A \in \text{com}(\mathcal{S}_n^+ + \mathcal{N}_n) \), then there exist an orthonormal matrix \( P \) and diagonal matrices \( \Theta = \text{Diag}(\theta_1, \theta_2, \ldots, \theta_n) \) and \( \Omega = \text{Diag}(\omega_1, \omega_2, \ldots, \omega_n) \) such that

\[
A = P\Theta P^T + \Omega \Omega P^T = \mathcal{S}_n^+ + \mathcal{N}_n
\]

(see Theorem 1.3.12 of [27]) which implies that \( \theta_i \geq 0 \) \( (i = 1, 2, \ldots, n) \) and that the problem (LP) \( \mathcal{P}_{\Lambda} \) with \( \Lambda = \Theta + \Omega \) has a nonnegative objective value at a solution \( (\omega, \alpha) \) where \( \alpha = \min_{ij} \{|P\Omega P^T|_{ij}\} \geq 0 \).

(iv): The assertion follows from the fact that \( \mathcal{S}_n^+ \) and \( \mathcal{N}_n \) are convex cones and from Lemma 2.4.

(v): The assertion follows from (ii) and (iii) above and the inclusion (12).

(vi): The assertion follows from (v) above and Theorem 2.3.

(vii) The assertion follows from (iv) and (v) above.
A number of examples provided in [35] illustrate the differences between $\mathcal{H}_n$, $\mathcal{G}^+_n$, and $\mathcal{G}^n_+$. Figure 1 draws those examples and (ii) of Theorem 2.5. Moreover, Figure 2 follows from (vii) of Theorem 2.5 and the convexity of the sets $\mathcal{N}_n$, $\mathcal{S}_n$ and $\mathcal{H}_n$ (see Theorem 2.3).

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 $A \in \mathcal{S}_n$ can be decomposed as (5), and define the diagonal matrix $\Lambda_+$ by $[\Lambda_+]_{ii} = \max\{0, \lambda_i\}$. Let $A_+ := P\Lambda_+ P^T$ 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 $A \in \text{COP}_n$ in [10].

**Theorem 2.6** (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 $A \in \text{COP}_n$.

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

$$\inf \{ f^T x \mid A_+ x \geq e, \ x \in \mathbb{R}^n_+ \} \quad (13)$$

where $f$ is an arbitrary vector and $e$ denotes the vector of all ones. Define the set

$$L^*_n := \{ A \in S_n \mid (x^T A_+ x)(A_-)_{ii} \leq [(A_+ x)_i]^2 \ (i = 1, 2, \ldots, n) \text{ for some feasible solution } x \text{ of (13)} \}. $$

Then Theorem 2.6 ensures that $L^*_n \subseteq \text{COP}_n$. The following proposition gives a characterization of the feasible set of the LP of (13).

**Proposition 2.7** (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 2.7 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 2.3).

### 3 Semidefinite bases

In this section, we improve the subcone $G^*_n$ in terms of $P2$. For a given matrix $A$ of (5), the linear optimization problem (LP)$_{P,A}$ in (9) can be solved in order to find a nonnegative matrix that is a linear combination

$$\sum_{i=1}^{n} \omega_i p_i p_i^T$$

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

$$A = \sum_{i=1}^{n} (\lambda_i - \omega_i) p_i p_i^T + \sum_{i=1}^{n} \omega_i p_i p_i^T \quad (14)$$

such that the first part

$$\sum_{i=1}^{n} (\lambda_i - \omega_i) p_i p_i^T$$

is positive semidefinite. If we have a large number of linearly independent positive semidefinite matrices, there is a higher chance of finding a nonnegative matrix by enlarging the feasible region of (LP)$_{P,A}$. In fact, we will show that we can easily find a basis of $S_n$ consisting of $n(n+1)/2$ semidefinite matrices from a given $n$ orthonormal vectors $p_i \in \mathbb{R}^n$ ($i = 1, 2, \ldots, n$).
Definition 3.1 (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

$$\Pi_+(p_i, p_j) := \frac{1}{4}(p_i + p_j)(p_i + p_j)^T. \quad (15)$$

We call the set

$$B_+(p_1, p_2, \ldots, p_n) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq n\} \quad (16)$$

a semidefinite basis type I induced by $p_i \in \mathbb{R}^n (i = 1, 2, \ldots, n)$.

From (15) and the fact that $p_i$ are orthonormal, we obtain the following:

$$\Pi_+(p_i, p_j)p_k = \begin{cases} p_k & \text{if } i = j = k \\ \frac{1}{4}(p_i + p_j) & \text{if } i \neq j \text{ and } (i = k \text{ or } j = k) \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

The following theorem is the reason why we call the set $B_+(p_1, p_2, \ldots, p_n)$ a semidefinite basis.

**Theorem 3.2.** Let $p_i \in \mathbb{R}^n (i = 1, 2, \ldots, n)$ be $n$-dimensional orthonormal vectors. Then the semidefinite basis $B_+(p_1, p_2, \ldots, p_n)$ defined by Definition 3.1 is a basis of the set $S_n$ of $n \times n$ symmetric matrices.

**Proof.** For $k = 1, 2, \ldots, n$, we will show that the set

$$B_+(p_1, p_2, \ldots, p_k) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq k\}$$

is linearly independent using mathematical induction on $k$. It is clear that $B_+(p_1) = \{p_1p_1^T\}$ is linearly independent. Suppose that $B_+(p_1, p_2, \ldots, p_{k-1})$ is linearly independent and that the following equation holds for $\alpha_{ij} \in \mathbb{R} (1 \leq i \leq j \leq k)$.

$$\sum_{1 \leq i \leq j \leq k} \alpha_{ij}\Pi_+(p_i, p_j) = 0. \quad \text{(16)}$$

By multiplying both sides of the equation with the vector $p_k$, we get

$$0 = \sum_{1 \leq i \leq j \leq k} \alpha_{ij}\Pi_+(p_i, p_j)p_k = \sum_{i=1}^{k} \alpha_{ii}\Pi_+(p_i, p_i)p_k + \sum_{1 \leq i < j \leq k} \alpha_{ij}\Pi_+(p_i, p_j)p_k
$$

$$= \alpha_{kk}p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}(p_i + p_k) \quad \text{(by (17))}$$

$$= \left(\alpha_{kk} + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}\right)p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}p_i = 0 \quad (18)$$

Since $p_i (i = 1, 2, \ldots, k)$ are orthonormal and linearly independent, the above equation implies

$$\alpha_{ik} = 0 \quad (i = 1, 2, \ldots, k - 1) \quad \text{and hence } \alpha_{kk} = 0. \quad (19)$$

Therefore, we have

$$0 = \sum_{1 \leq i \leq j \leq k} \alpha_{ij}\Pi_+(p_i, p_j) = \sum_{1 \leq i \leq j \leq k-1} \alpha_{ij}\Pi_+(p_i, p_j)$$

and the induction hypothesis ensures that

$$\alpha_{ij} = 0 \quad (1 \leq i \leq j \leq k - 1). \quad (20)$$

It follows from (19) and (20) that $B_+(p_1, p_2, \ldots, p_k) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq k\}$ is linearly independent, which completes the proof. \(\square\)
A variant of the semidefinite basis type I is as follows.

**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 \( \Pi_+ : \mathbb{R}^n \times \mathbb{R}^n \to S_n^+ \) by

\[
\Pi_-(p_i, p_j) := \frac{1}{4}(p_i - p_j)(p_i - p_j)^T.
\]

We call the set

\[
\mathcal{B}_-(p_1, p_2, \cdots, p_n) := \{\Pi_+(p_i, p_i) \mid 1 \leq i \leq n\} \cup \{\Pi_-(p_i, p_j) \mid 1 \leq i < j \leq n\}
\]

(22)
a semidefinite basis type II induced by \( p_i \in \mathbb{R}^n (i = 1, 2, \ldots, n) \).

Similarly to the map \( \Pi_+(p_i, p_j) \), it follows from (21) and the orthonormality of \( p_i \) that

\[
\Pi_-(p_i, p_j)p_k = \begin{cases} 
\frac{1}{4}(p_i - p_j) & \text{if } i \neq j \text{ and } (i = k \text{ or } j = k) \\
0 & \text{otherwise}
\end{cases}
\]

(23)

Using the above relations, we obtain the following theorem as a variant of Theorem 3.2.

**Theorem 3.4.** Let \( p_i \in \mathbb{R}^n (i = 1, 2, \ldots, n) \) be \( n \)-dimensional orthonormal vectors. Then the semidefinite basis \( \mathcal{B}_-(p_1, p_2, \cdots, p_n) \) defined by Definition 3.3 is a basis of the set \( S_n \) of \( n \times n \) symmetric matrices.

**Proof.** The proof is almost the same as that of Theorem 3.2. The only difference is that equation (18) turns out to be

\[
0 = \sum_{i=1}^{k} \alpha_i \Pi_+(p_i, p_i)p_k + \sum_{i<j} \alpha_{ij} \Pi_-(p_i, p_j)p_k
\]

\[
= \alpha_{kk}p_k + \sum_{i=1}^{k-1} \alpha_{ik} \left( \frac{1}{4}(p_i - p_k) \right) (p_k) = \left( \alpha_{kk} - \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} \right) p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} p_i
\]

(by (23))

\[
= \left( \alpha_{kk} - \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} \right) p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} p_i = 0.
\]

\(\square\)

**Remark 3.5** (Difference between the SDP bases and the Peirce decomposition in Jordan algebra). It should be noted that both of the semidefinite bases \( \mathcal{B}_+(p_1, p_2, \cdots, p_n) \) and \( \mathcal{B}_-(p_1, p_2, \cdots, p_n) \) are different from the bases obtained by the Peirce decomposition associated with the idempotent \( C = \sum_{i=1}^{n} p_ip_i^T \) in Jordan algebra (cf. Example 11.15 of [2] and Chapter IV of [22]). To see this, consider the following simple example with \( n = 2 \). Let

\[
p_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad p_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.
\]

Then the semidefinite bases defined by Definitions 3.1 and 3.3 are

\[
\mathcal{B}_+(p_1, p_2) = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1/4 & 1/4 \\ 1/4 & 1/4 \end{bmatrix} \right\} \subseteq S_n^+,
\]

\[
\mathcal{B}_-(p_1, p_2) = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1/4 & -1/4 \\ -1/4 & 1/4 \end{bmatrix} \right\} \subseteq S_n^+.
\]
respectively. On the other hand, the Peirce space associated with the idempotent \( C = p_1p_1^T + p_2p_2^T \) is given by

\[
\begin{align*}
E_1(C) &= \left\{ \begin{bmatrix} \alpha & 0 \\ 0 & 0 \end{bmatrix} \mid \alpha \in \mathbb{R} \right\} \\
E_2(C) &= \left\{ \begin{bmatrix} 0 & 0 \\ 0 & \alpha \end{bmatrix} \mid \alpha \in \mathbb{R} \right\} \\
E_{12}(C) &= \left\{ \begin{bmatrix} 0 & \alpha \\ \alpha & 0 \end{bmatrix} \mid \alpha \in \mathbb{R} \right\}
\end{align*}
\]

and this leads to the basis,

\[
\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right\} \not\subseteq S_n^+
\]

Using the map \( \Pi_+ \) in (15), the linear optimization problem (LP) \( P; \Lambda \) in (9) can be equivalently written as

\[
\begin{align*}
\text{(LP) } P; \Lambda & \quad \text{Maximize } \alpha \\
& \quad \text{subject to } \omega_{ii} \leq \lambda_i \quad (i = 1, 2, \ldots, n) \\
& \quad \quad \sum_{k=1}^n \omega_{kk} \Pi_+(p_k, p_k) \geq \alpha \quad (1 \leq i \leq j \leq n).
\end{align*}
\]

The problem (LP) \( P; \Lambda \) is based on the decomposition (14). Starting with (14), the matrix \( A \) can be decomposed using \( \Pi_+(p_i, p_j) \) in (15) and \( \Pi_-(p_i, p_j) \) in (21) as

\[
\begin{align*}
A &= \sum_{i=1}^n (\lambda_i - \omega_{ii}^+) \Pi_+(p_i, p_i) + \sum_{i=1}^n \omega_{ii}^+ \Pi_+(p_i, p_i) \\
&= \sum_{i=1}^n (\lambda_i - \omega_{ii}^+) \Pi_+(p_i, p_i) + \sum_{i=1}^n \omega_{ii}^+ \Pi_+(p_i, p_i) \\
&\quad + \sum_{1 \leq i < j \leq n} (-\omega_{ij}^+) \Pi_+(p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^+ \Pi_+(p_i, p_j) \\
&= \sum_{i=1}^n (\lambda_i - \omega_{ii}^+) \Pi_+(p_i, p_i) + \sum_{i=1}^n \omega_{ii}^+ \Pi_+(p_i, p_i) \\
&\quad + \sum_{1 \leq i < j \leq n} (-\omega_{ij}^+) \Pi_+(p_i, p_j) + \sum_{1 \leq i < j \leq n} \omega_{ij}^+ \Pi_+(p_i, p_j). \\
\end{align*}
\]

On the basis of the decomposition (24) and (25), we devise the following two linear optimization problems
as extensions of \((LP)_{P,A}^∗\):

\[
\begin{align*}
\text{(LP)}_{P,A}^+ & \quad \text{Maximize } \alpha \quad \text{subject to } \begin{bmatrix} \omega_{ii}^+ \leq \lambda_i \\ \omega_{ij}^+ \leq 0 \end{bmatrix} \\
& \quad \text{for } (i = 1, \ldots, n) \quad (1 \leq i < j \leq n) \\
& \quad \sum_{1 \leq k \leq l \leq n} \omega_{kl}^+ \Pi_+(p_k, p_l) \geq \alpha \quad (1 \leq i \leq j \leq n)
\end{align*}
\]

\[
\begin{align*}
\text{(LP)}_{P,A}^- & \quad \text{Maximize } \alpha \quad \text{subject to } \begin{bmatrix} \omega_{ii}^- \leq \lambda_i \\ \omega_{ij}^- \leq 0, \omega_{ji}^- \leq 0 \end{bmatrix} \\
& \quad \text{for } (i = 1, \ldots, n) \quad (1 \leq i < j \leq n) \\
& \quad \sum_{1 \leq k \leq l \leq n} \omega_{kl}^- \Pi_+(p_k, p_l) + \sum_{1 \leq k < l \leq n} \omega_{kl}^− \Pi_−(p_k, p_l) \geq \alpha \quad (1 \leq i \leq j \leq n)
\end{align*}
\]

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 \([P\Omega P^T]_{ij}\) in (9) is given by \(\sum_{k=1}^{n} k_{ik}^\Lambda (p_k, p_k)\), 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 \((LP)_{P,A}^\star\) on page 5. Thus, \((LP)_{P,A}^+\) and \((LP)_{P,A}^-\) have optimal solutions with corresponding optimal values \(\alpha^+_{ij}(P, A)\) and \(\alpha^-_{ij}(P, A)\).

If the optimal value \(\alpha^+_{ij}(P, A)\) of \((LP)_{P,A}^+\) is nonnegative, then, by rearranging (24), 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 \(\alpha^-_{ij}(P, A)\) of \((LP)_{P,A}^-\) is nonnegative, then, by rearranging (25), the optimal solution \(\omega^-_{ij}\) (1 \(\leq i \leq j \leq n\), \(\omega^-_{ij}\) (1 \(\leq i < j \leq n\)) can be made to give the following decomposition:

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

On the basis of the above observations, we can define new subcones of \(S_n^+ + N_n\) in a similar manner as (10) and (11):

\[
\begin{align*}
& F_{n,s}^+ := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for some orthonormal matrix } P \text{ satisfying (5)} \}, \\
& F_{n,a}^+ := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (5)} \}, \\
& F_{n,s}^- := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (5)} \}, \\
& F_{n,a}^- := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (5)} \}, \\
& F_{n,s}^\star := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for some arbitrary matrix } P \text{ satisfying (5)} \}.
\]

\[
\begin{align*}
& F_{n,a}^\star := \{A \in S_n \mid \alpha^+_{ij}(P, A) \geq 0 \text{ for any orthonormal matrix } P \text{ satisfying (5)} \},
\end{align*}
\]

12
where $\alpha^+(P, \Lambda)$ and $\alpha^\pm(P, \Lambda)$ are optimal values of $(\text{LP})^+_\Lambda$ and $(\text{LP})^\pm_\Lambda$, respectively. From the construction of problems $(\text{LP})^-_\Lambda$, $(\text{LP})^+_\Lambda$ and $(\text{LP})^\pm_\Lambda$, we can easily see that

$$G^+_n \subseteq F^{+s}_n \subseteq F^{s}_{+n}, \quad G^0_n \subseteq F^+_n \subseteq F^{s+}_n, \quad \widehat{G}^+_n \subseteq F^+_{n} \subseteq \widehat{F}^{s+}_{n}$$

hold. The following corollary follows from (v)-(vii) of Theorem 2.5 and the above inclusions.

**Corollary 3.6.** (i)

$$S^+_n \cup \mathcal{N}_n \subseteq G^+_n \subseteq G^0_n = \text{com}(S^+_n + \mathcal{N}_n) \subseteq \widehat{G}^+_n \subseteq S^+_n + \mathcal{N}_n$$

$$S^+_n \cup \mathcal{N}_n \subseteq F^+_n \subseteq F^{s+}_n \subseteq \widehat{F}^{s+}_{n} \subseteq S^+_n + \mathcal{N}_n$$

$$S^+_n \cup \mathcal{N}_n \subseteq F^+_n \subseteq F^{s+}_n \subseteq \widehat{F}^{s+}_{n} \subseteq S^+_n + \mathcal{N}_n$$

(ii) If $n = 2$, then each of the sets $F^{a+}_n$, $F^{s+}_n$, $\widehat{F}^{a+}_{n}$, $\widehat{F}^{s+}_{n}$ and $\widehat{F}^{s+}_{n}$ coincides with $S^+_n + \mathcal{N}_n$.

(iii) The convex hull of each of the sets $F^{a+}_n$, $F^{s+}_n$, $\widehat{F}^{a+}_{n}$, $\widehat{F}^{s+}_{n}$ and $\widehat{F}^{s+}_{n}$ is $S^+_n + \mathcal{N}_n$.

The following table summarizes the sizes of LPs (9), (26), and (27) that we have to solve in order to identify, respectively, $A \in G^+_n$ (or $A \in \widehat{G}^+_n$), $A \in F^{a+}_n$ (or $A \in \widehat{F}^{a+}_{n}$) and $A \in F^{s+}_n$ (or $A \in \widehat{F}^{s+}_{n}$).

<table>
<thead>
<tr>
<th>Identification</th>
<th>$A \in G^+_n$ (or $A \in \widehat{G}^+_n$)</th>
<th>$A \in F^{a+}<em>n$ (or $A \in \widehat{F}^{a+}</em>{n}$)</th>
<th>$A \in F^{s+}<em>n$ (or $A \in \widehat{F}^{s+}</em>{n}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td># of variables</td>
<td>$n+1$</td>
<td>$n(n+1)/2 + 1$</td>
<td>$n^2 + 1$</td>
</tr>
<tr>
<td># of constraints</td>
<td>$n(n+3)/2$</td>
<td>$n(n+1)$</td>
<td>$n(3n+1)/2$</td>
</tr>
</tbody>
</table>

4 Identification of $A \in S^+_n + \mathcal{N}_n$

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

We generated random instances of $A \in S^+_n + \mathcal{N}_n$ 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 $N = C - c_{\text{min}} I_n$ with $C = F + F^T$ for a random matrix $F$ with entries uniformly distributed in $[0, 1]$ and $c_{\text{min}}$ being the minimal diagonal entry of $C$. We set $A = S + N \in S^+_n + \mathcal{N}_n$. 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 $A \in S^+_n + \mathcal{N}_n$, we checked whether $A \in G^+_n$ (or $A \in \widehat{G}^+_n$) by solving $(\text{LP})^+_\Lambda$ in (9) (LP$^+_\Lambda$ in (26) and (LP$^\pm_\Lambda$ in (27)), where $P$ and $\Lambda$ were obtained using the MATLAB command “$[P, \Lambda] = \text{eig}(A)$.”
Table 2 shows the number of matrices that were identified as $A \in G_s^n$, or $A \in F^{+s}_n$, or $A \in F_{-s}^n$, 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 $A \in F_{-s}^n$. 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: $G_s^n \subseteq F^{+s}_n \subseteq F_{-s}^n$.
- For the sets $G_s^n$ and $F^{+s}_n$, the number of identified matrices decreases as the size of $n$ increases.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$G_s^n$</th>
<th>$F^{+s}_n$</th>
<th>$F_{-s}^n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>247</td>
<td>856</td>
<td>1000</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>719</td>
<td>1000</td>
</tr>
<tr>
<td>50</td>
<td>0</td>
<td>440</td>
<td>1000</td>
</tr>
</tbody>
</table>

5 LP-based algorithms for testing $A \in COP_n$

In this section, we investigate the effect of using the sets $F^{+s}_n$, $F^{+s}_n$, $F_{-s}^n$ and $F_{-s}^n$ for testing whether a given matrix $A$ is copositive by using Sponsel, Bundfuss and Dür’s algorithm [34].

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

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

(see Lemma 1 of [12]). 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 [26] 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 [34]. 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

$$\delta(\mathcal{P}) = \max_{\Delta \in \mathcal{P}} \max_{u, v \in \Delta} ||u - v||.$$ (29)

The above notation was used to show the following necessary and sufficient conditions for copositivity in [34]. The first theorem gives a sufficient condition for copositivity.

**Theorem 5.1** (Theorem 2.1 of [34]). If $A \in \mathcal{S}_n$ satisfies

$$V^T AV \in \text{COP}_n$$

for all $V \in M(\mathcal{P})$ then $A$ is copositive. Hence, for any $\mathcal{M}_n \subseteq \text{COP}_n$, if $A \in \mathcal{S}_n$ satisfies

$$V^T AV \in \mathcal{M}_n$$

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 $V^T AV_\Delta \in \mathcal{N}_n$ holds for any $\Delta \in \mathcal{P}$.

**Theorem 5.2** (Theorem 2.2 of [34]). Let $A \in \mathcal{S}_n$ be strictly copositive, i.e., $A \in \text{int} (\text{COP}_n)$. Then there exists $\varepsilon > 0$ such that for all partitions $\mathcal{P}$ of $\Delta^S$ with $\delta(\mathcal{P}) < \varepsilon$, we have

$$V^T AV \in \mathcal{N}_n$$

for all $V \in M(\mathcal{P})$.

The above theorem ensures that if $A$ is strictly copositive (i.e., $A \in \text{int} (\text{COP}_n)$) then 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 $\delta(\mathcal{P}) \to 0$. A similar result can be obtained for the case $A \notin \text{COP}_n$, as follows.

**Lemma 5.3** (Lemma 2.3 of [34]). The following two statements are equivalent.

1. $A \notin \text{COP}_n$

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

The following algorithm, in [34], is based on the above three results.

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.”
Algorithm 1 Sponsel, Bundfuss and Dür’s algorithm to test copositivity

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

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

1: $\mathcal{P} \leftarrow \{\Delta\}$
2: while $\mathcal{P} \neq \emptyset$ do
3:   Choose $\Delta \in \mathcal{P}$
4:   if $v^TAV < 0$ for some $v \in V(\{\Delta\})$ then
5:     return “$A$ is not copositive”;
6:   end if
7:   if $V_\Delta^TA\Delta \in \mathcal{M}_n$ then
8:     $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$
9:   else
10:   Partition $\Delta$ into $\Delta = \Delta^1 \cup \Delta^2$;
11:   $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\} \cup \{\Delta^1, \Delta^2\}$
12: end if
13: end while
14: Return “$A$ is 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 $\mathcal{M}_n \subseteq \text{COP}_n$.

In this section, we investigate the effect of using the sets $\mathcal{H}_n$ in (4), $\mathcal{G}^*_n$ in (11), and $\mathcal{F}^+_n$ and $\mathcal{F}^-_n$ in (28) as the set $\mathcal{M}_n$ in the above algorithm.

Note that if we choose $\mathcal{M}_n = \mathcal{G}^*_n$ (respectively, $\mathcal{M}_n = \mathcal{F}^+_n$, $\mathcal{M}_n = \mathcal{F}^-_n$), we can improve Algorithm 1 by incorporating the set $\mathcal{M}_n = \mathcal{G}^*_n$ (respectively, $\mathcal{M}_n = \mathcal{F}^+_n$, $\mathcal{M}_n = \mathcal{F}^-_n$), as proposed in [35].

The details of the added steps are as follows. Suppose that we have a diagonalization of the form (5).

At Line 7, we need to solve an additional LP but do not need to diagonalize $V_\Delta^TA\Delta$. Let $P$ and $\Lambda$ be matrices satisfying (5). Then the matrix $V_\Delta^TP$ can be used to diagonalize $V_\Delta^TA\Delta$, i.e.,

$$V_\Delta^TA\Delta = V_\Delta^T(\Lambda \Lambda^TP^T) V_\Delta = (V_\Delta^T P) \Lambda (V_\Delta^T P)^T$$

while $V_\Delta^TP$ is not necessarily orthonormal. Thus, we can test $V_\Delta^TA\Delta \in \mathcal{M}_n$ by solving the corresponding LP, i.e., (LP)$_{V_\Delta^TP}^{\mathcal{M}_n}$ if $\mathcal{M}_n = \mathcal{G}^*_n$, (LP)$_{V_\Delta^TP}^{\mathcal{F}^+_n}$ if $\mathcal{M}_n = \mathcal{F}^+_n$, (LP)$_{V_\Delta^TP}^{\mathcal{F}^-_n}$ if $\mathcal{M}_n = \mathcal{F}^-_n$.

If $V_\Delta^TA\Delta \not\in \mathcal{M}_n$ is not detected at Line 7, we can check whether $V_\Delta^TA\Delta \in \mathcal{M}_n$ 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 $V_\Delta^TA\Delta$ as $V_\Delta^TA\Delta = PA\Lambda^TP$ with an orthonormal matrix $P$ and a diagonal matrix $\Lambda$ and solve the LP.

At Line 15, we don’t need to diagonalize $V_\Delta^TA\Delta^* p$ 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 $V_\Delta^TP(\Lambda - \Omega^*)P^TV_\Delta^*$. Thus, if $V_\Delta^TP\Omega^*P^TV_\Delta^* \in \mathcal{N}_n$, we see that

$$V_\Delta^TP\Lambda^*P(\Lambda - \Omega^*)P^TV_\Delta^* + V_\Delta^TP\Omega^*P^TV_\Delta^* \in S^+_n + \mathcal{N}_n$$

and that $V_\Delta^TP\Lambda^*P(\Lambda - \Omega^*)P^TV_\Delta^* \in \mathcal{M}_n$. 

16
Algorithm 2 Improved version of Algorithm 1

**Input:** $A \in \mathcal{S}_n$, $\mathcal{M}_n \subseteq \bar{\mathcal{M}}_n \subseteq \text{COP}_n$

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

1: $\mathcal{P} \leftarrow \{\Delta^S\}$
2: while $\mathcal{P} \neq \emptyset$ do
3: Choose $\Delta \in \mathcal{P}$;
4: if $v^T A v < 0$ for some $v \in V(\{\Delta\})$: then
5: Return “$A$ is not copositive”;
6: end if
7: if $V_\Delta^T A V_\Delta \in \bar{\mathcal{M}}_n$ then
8: $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
9: else
10: if $V_\Delta^T A V_\Delta \in \mathcal{M}_n$ then
11: $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
12: else
13: Partition $\Delta$ into $\Delta = \Delta^1 \cup \Delta^2$, and set $\tilde{\Delta} \leftarrow \{\Delta^1, \Delta^2\}$;
14: for $p = 1.2$ do
15: if $V_{\Delta^p}^T A V_{\Delta^p} \in \bar{\mathcal{M}}_n$ then
16: $\tilde{\Delta} \leftarrow \tilde{\Delta} \setminus \{\Delta^p\}$;
17: end if
18: end for
19: $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\} \cup \tilde{\Delta}$;
20: end if
21: end if
22: end while
23: return “$A$ is copositive”;
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,

\[ B_\gamma := \gamma(E - A_G) - E \]  

(30)

where \( E \in S_n \) is the matrix whose elements are all ones and the matrix \( A_G \in S_n \) is the adjacency matrix of a given undirected graph \( G \) with \( n \) nodes. The matrix \( B_\gamma \) comes from the maximum 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

\[ \omega(G) = \min \{ \gamma \in \mathbb{N} | B_\gamma \in \text{COP}_n \} \]

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 22 shows the instances of \( G \) that were used in [34]. 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 \( H_n \), \( G_s n \), \( F^+_s n \), \( dF^+_s n \), \( F_s n \) or \( dF_s n \) as the set \( M_n \) 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 23).

As already mentioned, \( \alpha_+(P, \Lambda) < 0 \) (\( \alpha_+(P, \Lambda) < 0 \) and \( \alpha_-(P, \Lambda) < 0 \)) with a specific \( P \) does not necessarily guarantee that \( A \notin G^+_s n \) or \( A \notin \widehat{G}^+_n \) (\( A \notin F^+_s n \) or \( A \notin \widehat{F}^+_n \)). 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 (29).

Tables 3 and 4 show the numerical results for \( G_8 \) and \( G_{12} \), respectively. Both tables compare the results of the following five algorithms:

**Algorithm 1.1:** Algorithm 1 with \( M_n = H_n \).

**Algorithm 2.1:** Algorithm 2 with \( M_n = G^+_s n \) and \( \widehat{M}_n = \widehat{G}^+_n \).

**Algorithm 1.2:** Algorithm 1 with \( M_n = F^+_s n \).

**Algorithm 2.2:** Algorithm 2 with \( M_n = F^+_s n \) and \( \widehat{M}_n = \widehat{F}^+_n \).

**Algorithm 2.3:** Algorithm 2 with \( M_n = F^+_s n \) and \( \widehat{M}_n = \widehat{F}^+_n \).

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 \( B_\gamma \) 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 make the following observations on the implications of the results in Table 4 on page 24 for the larger graph \( G_{12} \) while similar observations can be made on the ones in Tables 3:
At any $\gamma \geq 5.2$, Algorithms 2.1, 1.2, 2.2, and 2.3 terminate in one iteration, and their execution times are shorter than that of Algorithm 1.1.

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 2.3. The reason may be that, as shown in Corollary 3.6, the set inclusion relation $G_n \subseteq F_n^+ \subseteq F_n^{\pm s}$ holds.

Table 1 on page 13 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 $G_n \subseteq F_n^+ \subseteq F_n^{\pm s}$ 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 $s$ 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 (the column "CPU time (s)" in Table 4) than the order of the computational time for solving an LP.

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 but not on the choice of $M_n$.

In view of the above observations, we conclude that Algorithm 2.3 with the choices $M_n = F_n^{\pm s}$ and $\overline{M}_n = F_n^{\pm s}$ might be a way to check the copositivity of a given matrix $A$ when $A$ is strictly copositive.

It should be noted that Table 3 shows an interesting result concerning the non-convexity of the set $G_n^s$, while we know that $\text{conv}(G_n^s) = S_n + N_n$ (see Theorem 2.5). 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 $B_{4,0} \in G_n^s$ at the first iteration for a certain orthonormal matrix $P$ satisfying (5). Recall that the matrix $B_n$ is given by (30). It follows from $E - AG \in N_n \subseteq G_n^s$ and from the result at $\gamma = 3.5$ in Table 3 that

$$0.5(E - AG) \in G_n^s \text{ and } B_{3,5} = 3.5(E - AG) - E \in G_n^s.$$

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 $G_n^s$ might suggest that the set $G_n^s = \text{com}(S_n + N_n)$ 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 3.1 and 3.3. We conducted numerical experiments using those subcones for identification of given matrices $A \in S_n^+ + N_n$ 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 quite promising not only for identification of $A \in S^+_n + N_n$ 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 $D_n \subseteq S^+_n$ 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]).

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

From the above theorem, we can see that for the SDP bases $B_+(p_1, p_2, \cdots, p_n)$ in (16), $B_-(p_1, p_2, \cdots, p_n)$ in (22) 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.

**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 of testing copositivity: $G_a$

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## Table 4: Results of testing copositivity: $G_{12}$

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