LP-based algorithms for hard conic optimization problems

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Abstract

This thesis deal with copositive programming. A symmetric matrix A is said to be copositive if the quadratic form takes no negative value on the nonnegative orthant and the set of copositive matrices is called the copositive cone. Copositive programing leads to equivalent reformulation of NP-hard combinatorial and quadratic optimization. This makes copositive programming NP-hard itself and unfortunately it is known that even checking whether a given matrix belongs to the copositive cone is co-NP-complete. This thesis devotes particular attention to findinig desirable subcones $\mathcal{M}_n$ to providing practical algorithms for testing copositivity. A new type of subcones $\mathcal{M}_n$ is devised for which one can detect whether a given matrix belongs to one of them by solving linear optimization problems with $O(n)$ variables and $O(n^2)$ constraints. An LP-based algorithm using these subcones is also provided. The properties of the subcones are investigated in more detail, especially in terms of their convex hulls. Second, they swarch for subcones of $\mathcal{COP}_n$. From these observations, a new basis, the *semidefinite basis (SD basis)*, is introduced; it is a basis of the space $\mathcal{S}_n$ consisting of $n(n+1)/2$ symmetric semidefinite matrices. Using the SD basis two other new types of subcones are devised for which the detection can be done by solving linear optimization problems with $O(n^2)$ variables and $O(n^2)$ constraints. As we will show in Corollary 3.2.6, these subcones are larger than the subcones of the first type and inherit their nice properties. Numerical experiments are conducted to evaluate the efficiency of these subcones for testing copositivity.

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Chapter 1

Introduction

An optimization problem is defined as an objective function to maximize and the constraints that it will be maximized over. There are many applications of optimization in economics, electrical engineering, computational finance, control engineering, management science, etc. Optimization problems can be divided into two classes by whether their variables are continuous or discrete, i.e., the class of continuous optimization problems and the class of combinatorial optimization problmes. Most basic continuous optimization problem is to minimize a linear function with linear constraints, the so-called linear optimization problem. It is formulated as

$$\begin{array}{ll} \text{Minimize} & \langle c, x \rangle \\ \text{subject to} & Ax = b \\ & x \in \mathbb{R}^n_+ \end{array}$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$,$c \in \mathbb{R}^n$ and $\mathbb{R}^n_+$ is the n-dimensional nonegative orthant,

$$\mathbb{R}^n_+ := \{x \in \mathbb{R}^n \mid x \geq 0\}.$$

In 1947, Dantzig[19] formulated general linear programming and developed the simplex method to solve its problems. The simplex method starts at a vertex of a polytope corresponding to the feasible region and moves to an adjacent vertex to reduce the objective value until it reaches a vertex of an optimal solution. It is known that the algorithm works very well in practice for linear optimization problems. However, Klee and Minty[41] introduced an example for which the simplex method takes an exponential number of iterations. They proved that the simplex method with the most negative reduced cost pivot rule visits all $2^n - 1$ vertices of the problem. It was shown that the linear programming problem is solvable in polynomial time by using Khachiyan's[40] ellipsoid method, but it is too slow to be of practical interest. In 1984, Karmarkar[39] introduced a new algorithm, called the interior-point method, to solve linear programming problems in polynomial time; this method is efficient in practice. The simplex method moves on the polytope of the feasible region, while the interior point method goes through the interior of the polytope. After Karmarkar's interior point method, a large number of studies on interior point methods appeared. Among these methods, Kojima, Mizuno, and Yoshise[42] developed the primal dual interior point method; this method has wide usage for soving linear optimization problems and conic optimization problems, which are generalizations of linear programming as described below.

As generalizations of linear optimization problems, conic optimization problems have attracted much attention in the field of continuous optimization. A set $\mathcal{K}_n$ is called a cone if for any $X \in \mathcal{K}_n$ and for any $\alpha \geq 0$, αX belongs to $\mathcal{K}_n$. A conic optimization problem consists of a linear objective function to minimize over the intersection of an affine subspace and proper cone $\mathcal{K}_n$, where a cone $\mathcal{K}$ is called a proper cone if it has nonempty interior and is closed convex, and pointed. Nesterov and Nemirocskii[47] introduced the conic optimization of the form:

$$\begin{array}{ll} \text{Minimize} & \langle c, x \rangle \\ \text{subject to} & \langle a_i, x \rangle = b_i \quad (i = 1, \dots m) \\ & x \in \mathcal{K}_n \end{array}$$

where $\langle a, b \rangle$ denotes the inner product of a and b. They showed theory of polynomial time interior point algorithm for a conic optimization problem. A typical conic optimization problem is positive semidefinite programming in which the variable matrices are in the positive semidefinite cone. It is formulated as

$$\begin{array}{ll} \text{Minimize} & \langle C, X \rangle \\ \text{subject to} & \langle A_i, X \rangle = b_i \quad (i = 1, \dots m) \\ & X \in \mathcal{S}_n^+ \end{array}$$

where $\langle A, B \rangle = \mathrm{Tr}(A^T B) = \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij}$ denotes the inner product on the space of n dimensional symmetric matrices $\mathcal{S}_n$. $\mathcal{S}_n^+$ is the positive semidefinite cone defined by

$$\mathcal{S}_n^+ = \{X \in \mathcal{S}_n \mid d^T X d \geq 0 \text{ for all } x \in \mathbb{R}^n\}$$

Alizadeh[2] showed that the primal dual interior point method for linear programming can be extended to positive semidefinite programming. Since then, many software packages have veen developed, e.g., SDPA[53], SeDuMi[52] and SDPT3[54]. Positive semidefinite programming has many applications in which an approximation to an NP-hard combinatorial optimization is sought. Here, we review the MAX-CUT and the Lov́asz ϑ-function as important applications of positive semidefinite programming for combinatorial optimization problems.

1.1 MAX-CUT

The MAX-CUT is an NP-hard combinatorial optimization problem. Let G be an undirected graph with node set $V = 1, \ldots, n$ and edge set E. Let $w_{ij} = w_{ji} \geq 0$ be the weight on edge $(i,j) \in E$. The MAX-CUT problem is to determine a subset S of V in such a way that the sum of the weights w_{ij} of edges (i,j) such that $i \in S$ and $j \in V \setminus S$ is maximized.

We can formulate the MAX-CUT problem as an integer programming as follows. Let us assign a variable x_i to each vertex of E and define $x_i = 1$ for $j \in S$ and $x_j = -1$ for $j \in V \setminus S$. The MAX-CUT problem is modeled as

$$\begin{array}{lll} \text{Maximize} & \frac{1}{2}\sum_{i<j} w_{ij}(1 - x_i x_j) & \\ \text{subject to} & x_i \in \{-1, 1\}, & (i = 1, \ldots n) \end{array} \tag{1.1}$$

Any feasible solution of (1.1) is obviously a cut, and $(1 - x_i x_j)$ is 0 if vertices i and j are in the same subset of E, and 2 otherwise. (1.1) can be equivalently translated as

$$\begin{array}{lll} \text{Maximize} & \frac{1}{2}\left(\sum_{i<j} w_{ij} - \langle W, X\rangle\right) & \\ \text{subject to} & x_i \in \{-1, 1\}, & (i = 1, \ldots n) \\ & X = xx^T & \end{array} \tag{1.2}$$

Note that $x_i \in \{-1, 1\}$ $(i = 1, \dots n)$ are equivalent to $X_{ii} = 1$ $(i = 1, \dots n)$ and $X = xx^T$ is equivalent to $X \in \mathcal{S}_n^+$ and $\mathrm{rank}(X) = 1$. We can obtain the following relaxation problem of (1.2) by removing the rank-1 restriction.

$$\begin{array}{lll} \text{Maximize} & \frac{1}{2}\left(\sum_{i<j} w_{ij} - \langle W, X \rangle\right) & \\ \text{subject to} & X_{ii} = 1, & (i = 1, \dots n) \\ & X \in \mathcal{S}_n^+ & \end{array} \tag{1.3}$$

Goemans and Williamson[30] first used (1.3) to formulate an approximation algorithm that produces a MAX-CUT solution that is within a factor of 0.878 of the optimal value of (1.1).

1.2 Lov́asz ϑ-function

The Lov́asz ϑ-function $\vartheta(G)$ of a graph G, as introduced by Lov́asz[43], is given as the optimal value of the following positive semidefinite programming problem;

$$\begin{array}{lll} \text{Maximize} & e^T X e & \\ \text{subject to} & X_{ij} = 0, & (i \neq j \ , \ (i, j) \in E) \\ & \mathrm{Tr}(X) = 1 & \\ & X \in \mathcal{S}_n^+ & \end{array} \tag{1.4}$$

with e denoting the all-ones vector. The ϑ-function plays an important role in relation with the clique number and chromatic number of a graph $G = (V, E)$. A subset $S \subseteq V$ is called a clique if there is an edge for any vertices $i, j \in S$, while the cardinality of the maximum clique of G is called the clique number and is denoted by $\omega(G)$. The chromatic number of G, denoted by $\chi(G)$, is the minimum number of colors to color all vertices so that any two adjacent vertices have different colors. The relationship between these three numbers, called the sandwich theorem is

$$\omega(G) \leq \vartheta(\bar{G}) \leq \chi(G)$$

where $\bar{G}$ denotes the complement graph of G. Thus, the Lov́asz ϑ-function of $\bar{G}$ gives an upper bound and a lower bound of the clique number and chromatic number of G.

1.3 Copositive programming

More recently, the copositive cone $\mathcal{COP}_n$ and the completely positive cone $\mathcal{CP}_n$ have attracted much attention in the field of conic optimization as generalization of positive semidefinite programming. A symmetric matrix is copositive if the quadratic form is nonegative on the nonnegative orthant,

$$\mathcal{COP}_n = \left\{ X \in \mathcal{S}_n \mid d^T X d \geq 0 \ \text{ for all } d \in \mathbb{R}^n_+ \right\}$$

where $\mathbb{R}^n_+$ is the set of $n-$dimensional nonnegative vectors. Its dual cone $\mathcal{CP}_n$ is defined as

$$\mathcal{CP}_n = \text{conv } \left(\left\{ xx^T \mid x \in \mathbb{R}^n_+ \right\} \right)$$

The copositive cone and the completely positive cone also have a close relationship with combinatorial optimization problems and (not necessarily convex) quadratic optimization problems. As we previously mentioned, the Lovász ϑ-function of $\bar{G}$ gives an upper and a lower bound of the clique number and chromatic number of G, while these problems can be equivalently reformulated as copositive programming problems. The standard quadratic problem, the stable set problem, the quadratic assignment problem, and certain graph-partitioning problems can also be equivalently reformulated as copositive problems. More generally, Burer[18] showed that the optimal value of every quadratic problem with linear and binary constraints can be equivalently reformulated as a copositive programming problem. However, the equivalence makes copositive programming NP-hard, and unfortunately, it is known that even checking whether a given matrix belongs to the copositive cone is co-NP-complete[46]. Copositivity first arose in 1950s, and numerous conditions for copositivity have been proposed[5, 9, 10, 37, 59]. Most of them require checking principal submatrices, and they are only of use when the number of dimensions is small. However, Bundfuss and Dür[16] proposed a radically new algorithm to test copositivity. This algorithm requires investigating the nonnegativity of a quadratic form over the standard simplex and iteratively divides up the standard simplex into smaller and smaller parts to indicate the copositivity of a matrix. After the introduction of the algorithm, researchers developed numerical algorithm to test copositivity; most of them follow somewhat related ideas. Sponsel, Bundfuss and

Dür[55] proposed improved versions of the algorithm. The algorithms use tractable subcones $\mathcal{M}_n$ of the copositive cone $\mathcal{COP}_n$ for detecting copositivity. As described in Chapter 4, they require one to check whether a $A \in \mathcal{M}_n$ or not repeatedly over simplicial partitions. The desirable properties of the subcones $\mathcal{M}_n \subseteq \mathcal{COP}_n$ used by these algorithms can be summarized as follows:

P1 For any given $n \times n$ symmetric matrix $A \in \mathcal{S}_n$, 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 $\mathcal{COP}_n$ that at least includes the $n \times n$ nonnegative cone $\mathcal{N}_n$ and contains as many elements $\mathcal{COP}_n$ as possible.

1.4 Contribution and structure of this thesis

This thesis devotes particular attention to findinig desirable subcones $\mathcal{M}_n$ satisfying the above properties **P1** and **P2** and to providing practical algorithms for testing copositivity. A new type of subcones $\mathcal{M}_n$ is devised for which one can detect whether a given matrix belongs to one of them by solving linear optimization problems with $O(n)$ variables and $O(n^2)$ constraints. An LP-based algorithm using these subcones is also provided. The properties of the subcones are investigated in more detail, especially in terms of their convex hulls. Second, they swarch for subcones of $\mathcal{COP}_n$ that have properties **P1** and **P2**. From these observations, a new basis, the *semidefinite basis (SD basis)*, is introduced; it is a basis of the space $\mathcal{S}_n$ consisting of $n(n+1)/2$ symmetric semidefinite matrices. Using the SD basis two other new types of subcones are devised for which the detection can be done by solving linear optimization problems with $O(n^2)$ variables and $O(n^2)$ constraints. As we will show in Corollary 3.2.6, these subcones are larger than the subcones of the first type and inherit their nice properties. Numerical experiments are conduced to evaluate the efficiency of these subbcones for testing copositivity.

The remainder of this thesis is structured as follows. In Chapter 2, we review the copositive cone and completely positive cone and describe their properties. As we previously mentioned, there is a close relationship between copositive programming and combinatorial and quadratic optimization problems. In Chapter 3, we show several tractable subcones of $\mathcal{COP}_n$ having properties **P1** and **P2**.

These studies were motivated by the desire to develop efficient algorithms for testing copositivity. However, as we will see in Chapter 3, all of the subcones appearing in this paper are merely contained in the Minkowski sum $\mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{COP}_n$ of the $n \times n$ positive semidefinite cone $\mathcal{S}_n$ and $n \times n$ nonnegative cone $\mathcal{N}_n$. In light of this fact, in Chapter 4, we review numerical experiments in which the new subcones are used for identifying the given matrices $A \in \mathcal{S}_n^+ + \mathcal{N}_n$. Chapter 4 describes experiments for testing the 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 $A \in \mathcal{S}_n^+ + \mathcal{N}_n$, but also for testing copositivity. Chapter 5 is devoted to concluding remarks.

Chapter 2

Copositive cone and completely positive cone

2.1 Theoretical properties

In this section, we study theoretical properties of copositive cone. As we mentioned in Chapter 1, the copositive cone and completely positive cone are defined as

$$\begin{aligned} \mathcal{COP}_n &= \left\{X \in \mathcal{S}_n \mid d^T X d \geq 0 \text{ for all } d \in \mathbb{R}^n_+\right\} \\ \mathcal{CP}_n &= \operatorname{conv}\left(\left\{xx^T \mid x \in \mathbb{R}^n_+\right\}\right) \end{aligned}$$

We define the dual cone $\mathcal{K}_n^*$ of a cone $\mathcal{K}_n \subseteq \mathcal{S}_n$ by

$$\mathcal{K}_n^* = \{X \in \mathcal{S}_n \mid \langle X, Y \rangle \geq 0 \text{ for all } Y \in \mathcal{K}_n\}$$

We define the nonnegative cone denoted by $\mathcal{N}_n$.

$$\mathcal{N}_n := \{X \in \mathcal{S}_n \mid x_{ij} \geq 0 \text{ for all } i, j \in \{1, 2, \dots, n\}\}$$

All of the above cones are proper (see Section 1.6 of [7] where the proper cone is called a *full cone*), and we can easily see from the definitions that the following inclusions hold:

$$\mathcal{COP}_n \supseteq \mathcal{S}_n^+ \supseteq \mathcal{S}_n^+ \cap \mathcal{N}_n \supseteq \mathcal{CP}_n. \tag{2.1}$$

It is known that the following proposition holds by defining an inner product between X and Y as

$$\langle X, Y\rangle := \mathrm{Tr}\,(Y^T X). \tag{2.2}$$

Proposition 2.1.1 (Properties of the copositive cone). **(i)** *The dual cone of the copositive cone $\mathcal{COP}_n$ with respect to the inner product (2.2) is the completely positive cone $\mathcal{CP}_n$ and vice versa (see p.57 of [6] and Theorem 2.3 of [7]).*

(ii) *If $n \le 4$ then $\mathcal{COP}_n = \mathcal{S}_n^+ + \mathcal{N}_n$ (see [22] and Proposition 1.23 of [7]).*

(iii) *The dual cone of the doubly nonnegative cone $\mathcal{S}_n^+ \cap \mathcal{N}_n$ with respect to the inner product (2.2) is the Minkowski sum $\mathcal{S}_n^+ + \mathcal{N}_n$ of the positive semidefinite cone $\mathcal{S}_n^+$ and the nonnegative cone $\mathcal{N}_n$ and vice versa (see Remark 2.1.2).*

Remark 2.1.2. *Proposition 2.1.1, (iii): The equality $(\mathcal{S}_n^+ \cap \mathcal{N}_n)^* = \mathrm{cl}\,(\mathcal{S}_n^+ + \mathcal{N}_n)$ follows from a well-known result that $(\mathcal{K}_1 \cap \mathcal{K}_2)^* = \mathrm{cl}\,(\mathcal{K}_1 + K_2)$ holds for any closed convex cones $\mathcal{K}_1$ and $\mathcal{K}_2$ (see, e.g., p.11 of [27] or Corollary 2.2 of [6]. The closedness of the set $\mathcal{S}_n^+ + \mathcal{N}_n$ follows from a result in [51]. See also Proposition 4.1 of [60] where the authors showed the property in a little more general framework.*

The following inclusions follow from (2.1) and the above proposition

$$\mathcal{COP}_n \supseteq \mathcal{S}_n^+ + \mathcal{N}_n \supseteq \mathcal{S}_n^+ \supseteq \mathcal{S}_n^+ \cap \mathcal{N}_n \supseteq \mathcal{CP}_n \tag{2.3}$$

and specially, if $n \le 4$ then we have

$$\mathcal{COP}_n = \mathcal{S}_n^+ + \mathcal{N}_n \supseteq \mathcal{S}_n^+ \supseteq \mathcal{S}_n^+ \cap \mathcal{N}_n = \mathcal{CP}_n. \tag{2.4}$$

An example that $\mathcal{S}_5^+ + \mathcal{N}_5 \ne \mathcal{COP}_5$ is the so-called Horn-matrix[32]

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

For $x \in \mathbb{R}^n_+$,

$$\begin{aligned} x^T H x &= (x_1 - x_2 + x_3 + x_4 - x_5)^2 + 4x_2x_4 + 4x_3(x_5 - x_4) \\ &= (x_1 - x_2 + x_3 - x_4 + x_5)^2 + 4x_2x_5 + 4x_1(x_4 - x_5). \end{aligned}$$

If $x_5 \geq x_4$, by the first expression, $x^T H x$ is nonnegative. If $x_5 \leq x_4$, second expression shows the nonnegativity of $x^T H x$. Hall and Newman proved that H is extremal for $\mathcal{COP}_5$ therefore $H \notin \mathcal{S}^+_n + \mathcal{N}_n$.

Note that the four cones, $\mathcal{COP}_n$, $\mathcal{CP}_n$, $\mathcal{S}^+_n \cap \mathcal{N}_n$ and $\mathcal{S}^+_n + \mathcal{N}_n$ lack the self-duality and hence are not symmetric. Since about 2000, there have been many studies conducted on the above four cones as a new research direction in the field of conic optimization [11, 12, 21, 56, 48, 16, 49, 18, 35, 17, 60, 55, 44], and they are called studies on *copositive programming* [11].

A growing research interest in the field is to provide efficient algorithms to determine whether a given matrix belongs to $\mathcal{COP}_n$ (or $\mathcal{CP}_n$, or $\mathcal{S}^+_n + \mathcal{N}_n$). It is known that the problem of testing copositivity, i.e., deciding $A \in \mathcal{COP}_n$ or not, is co-NP-complete [46, 24].

2.2 relationship between copositive cone and quadratic or combinatorial optimization

2.2.1 Standard quadratic optimization

Bomze et al. formulated an NP-hard problem called the standard quadratic optimization as a copositive programming problem. The standard quadratic problem has a quadratic objective function and nonnegative variable vector satisfies one linear constraint

$$\begin{aligned} \text{Minimize} \quad & x^T A x \\ \text{subject to} \quad & e^T x = 1 \\ & x \in \mathbb{R}^n_+ \end{aligned}$$

where e denotes the all-ones vector and $A \in \mathcal{S}^n$. A is not necessarily positive semidefinite i.e. the objective function is not necessarily convex. The objective function $x^T Ax$ transforms to $\langle A, xx^T \rangle$ and $e^T x = 1$ to $\langle E, xx^T \rangle = 1$ with $E = ee^T$ The problem reformulated as

$$\begin{array}{ll} \text{Minimize} & \langle A, X \rangle \\ \text{subject to} & \langle E, X \rangle = 1 \\ & X = xx^T \\ & x \in \mathbb{R}^n_+ \end{array}$$

We get a relaxation problem by replacing $X = xx^T$ with $X \in \mathcal{CP}_n$ as

$$\begin{array}{ll} \text{Minimize} & \langle A, X \rangle \\ \text{subject to} & \langle E, X \rangle = 1 \\ & X \in \mathcal{CP}_n. \end{array}$$

Bomze et al. showed the extremal points of the feasible set of the problem are exactly the rank-one matrices $X = xx^T$. The objective function is linear so there is an optimal solution at an extremal points of the feasible set. Hence, The problem is not relaxation but an exact reformulation.

2.2.2 Clique number and stability number

The clique problem also can be reformulated as copositive programming. A subset of vertices of an undirected graph G called clique if there is an edge for any pare of vertices of the set. The clique number of a graph G, denoted $\omega(G)$, is the number of vertices in a maximum clique of G. Motzking and Staus showed that $\frac{1}{\omega(G)}$ is given as the optimal value of the following optimization problem:

$$\begin{array}{lll} \frac{1}{\omega(G)} = & \text{Minimize} & x^T(E - A_G)x \\ & \text{subject to} & e^T x = 1 \\ & & x \in \mathbb{R}^n_+. \end{array}$$

This problem is a standard quadratic optimization problem and we can equivalently reformulated as a completely positive optimization problem:

$$
\begin{array}{rll}
\frac{1}{\omega(G)} = & \text{Minimize} & \langle E - A_G, X\rangle \\
& \text{subject to} & \langle E, X\rangle = 1 \\
& & X \in \mathcal{CP}_n.
\end{array} \tag{2.5}
$$

It is well-known that taking the dual problem of (2.5), we get a copositive formulation of the clique problem[11].

$$
\begin{array}{rll}
\frac{1}{\omega(G)} = & \text{Maximize} & \gamma \\
& \text{subject to} & \gamma(E - A_G) - E \in \mathcal{COP}_n.
\end{array} \tag{2.6}
$$

The problem (2.6) can be reformulated as

$$
\begin{array}{rll}
\omega(G) = & \text{Minimize} & \gamma \\
& \text{subject to} & \gamma(E - A_G) - E \in \mathcal{COP}_n.
\end{array} \tag{2.7}
$$

Since $\omega(G)$ is a natural number, we only have to whether $\gamma(E-A_G)-E \in \mathcal{COP}_n$ or not at most n times to determine the clique number of G by using this formulation.

The stability number of a graph also can be reformulated as a copositive optimization problem. A subset $S \subseteq V$ is called a stable set if there is no edge for any vertices $i, j \in S$, while the cardinality of the maximum stable set of G is called the stability number and is denoted by $\alpha(G)$. Here, $\alpha(G) = \omega(\bar{G})$, we can get the stability number of G by solving (2.7) for $\bar{G}$ However using somewhat different approach, De Klerk and Pasechnik[21] showed that the stability number of a graph G is given as the optimal value of the following optimization problem:

$$
\begin{array}{rll}
\alpha(G) = & \text{Maximize} & x^T E x \\
& \text{subject to} & e^T x = 1 \\
& & x \in \mathbb{R}^n_+.
\end{array}
$$

2.2.3 Fractional Quadratic optimization

We consider fractional quadratic optimization. Let A be a $n \times n$ matrix. Assume that A the quadratic form $x^T Ax$ does not take zeros over $\mathbb{R}^n_+ \setminus \{0\}$. Preisig[50] showed that the following optimization problem to maximize the quotient of two quadratic forms over standard simplex

$$\begin{array}{ll} \text{Minimize} & \dfrac{x^T Q x}{x^T A x} \\ \text{subject to} & e^T x = 1 \\ & x \in \mathbb{R}^n_+. \end{array}$$

can be equivalently reformulated as

$$\begin{array}{ll} \text{Minimize} & x^T Q x \\ \text{subject to} & x^T A x = 1 \\ & x \in \mathbb{R}^n_+. \end{array} \qquad (2.8)$$

We get a relaxation problem by replacing $X = xx^T$ with $X \in \mathcal{CP}_n$ as

$$\begin{array}{ll} \text{Minimize} & \langle Q, X \rangle \\ \text{subject to} & \langle A, X \rangle = 1 \\ & X \in \mathcal{CP}_n. \end{array} \qquad (2.9)$$

It can be proved that (2.8) and (2.9) are equivalent by using similar argument as used for standard quadratic optimization. Consider an optimal solution of one of these two problems. We can easily construct a feasible solution of the other problem which takes same objective value. More generally, Amaral, Bomze, and Júdice [4] consider the following constrained fractional quadratic problem.

$$\begin{array}{ll} \text{Minimize} & \dfrac{x^T C x + 2c^T x + \gamma}{x^T B x + 2b^T x + \beta} \\ \text{subject to} & Ax = a \\ & x \in \mathbb{R}^n_+. \end{array} \qquad (2.10)$$

with assumption that there are $0 < \delta < \eta < +\infty$ such that the denominator of the objective function of (2.10) belongs to $[\delta, \eta]$ for all feasible solutions. (2.10) can be reformulated as

$$\begin{array}{ll} \text{Minimize} & \dfrac{z^T \bar{C} z}{x^T \bar{B} x} \\ \text{subject to} & z^T \bar{A} z = 0 \\ & z_1 = 1 \\ & z \in \mathbb{R}^{n+1}_+. \end{array} \qquad (2.11)$$

by introducing

$$\bar{A} = \begin{bmatrix} a^T a & -a^T A \\ -A^T a & A^T A \end{bmatrix}, \quad \bar{B} = \begin{bmatrix} \beta & b^T \\ b & B \end{bmatrix}, \quad \bar{C} = \begin{bmatrix} \gamma & c^T \\ c & C \end{bmatrix}.$$

(2.11) is equivalent to the following problem by replacing $zz^T = Z$

$$\begin{array}{ll} \text{Minimize} & \dfrac{\langle \bar{C}, Z \rangle}{\langle \bar{B}, Z \rangle} \\ \text{subject to} & Z_{11} = 1 \\ & \langle \bar{A}, Z \rangle = 0 \\ & \operatorname{rank}(Z) = 1 \\ & Z \in \mathcal{CP}_n. \end{array}$$

Amaral, Bomze, and Júdice [4] showed that the constraint $\operatorname{rank}(Z) = 1$ can equivalently be removed under some assumptions.

2.2.4 Quadratic optimization with 0-1 variables

More generally, Burer showed the optimal value of every quadratic problem with linear and binary constraints can be reformulated as completely positive problem. He dealt with a quadratic problem of the form

$$\begin{array}{lll} \text{Minimize} & x^T Q x + 2c^T x & \\ \text{subject to} & a_i^T x = b_i & (i = 1, \ldots, m) \\ & x \in \mathbb{R}^n_+ & \\ & x_j \in \{0, 1\} & (j \in \mathcal{B}) \end{array} \tag{2.12}$$

where $B \subseteq \{1, \ldots, n\}$. We assume that the feasible set of (2.12) is not empty. This problem include many optimization problems such as standard quadratic problems, quadratic assignment problems. The following completely positive problem can be seen as a relaxation problem of (2.12) by relaxing the rank-1 constraint $X = xx^T$ to

$X \in \mathcal{CP}_n$.

$$\begin{array}{lll} \text{Minimize} & \langle Q, X \rangle + 2c^T x & \\ \text{subject to} & a_i^T x = b_i & (i = 1, \ldots, m) \\ & a_i^T X a_i = b_i^2 & (i = 1, \ldots, m) \\ & x_j = X_{jj} & (j \in \mathcal{B}) \\ & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{CP}_n. & \end{array} \tag{2.13}$$

Burer[18] showed that these two formulations are equivalent.

Chapter 3

Some tools for approximation

In this section, we introduce a basis of the set $\mathcal{S}_n$ of $n \times n$ symmetric matrices and subcones of the copositive cone by using it.

3.1 Subcones of copositive cone

We review the subcones of copsitive cone.

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 [46, 23, 24]. On the other hand, the problem of testing whether or not $A \in \mathcal{S}_n^+ + \mathcal{N}_n$ can be solved by solving the following doubly nonnegative program (which can be expressed as a semidefinite program)

$$\begin{array}{ll} \text{Minimize} & \langle A, X \rangle \\ \text{subject to} & \langle I_n, X \rangle = 1, \\ & X \in \mathcal{S}_n^+ \cap \mathcal{N}_n \end{array}$$

where I_n denotes the $n \times n$ 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 doubly nonnegative problem takes an awful lot of time [55, 60] 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 denote

$$N(A)_{ij} := \begin{cases} A_{ij} & A_{ij} > 0 \text{ and } i \neq j \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad S(A) := A - N(A). \tag{3.1}$$

In [55], the authors defined the following set

$$\mathcal{H}_n := \{A \in \mathcal{S}_n \mid S(A) \in \mathcal{S}_n^+\}. \tag{3.2}$$

Note that $A = S(A) + N(A) \in \mathcal{S}_n^+ + \mathcal{N}_n$ if $A \in \mathcal{H}_n$. Also, for any $A \in \mathcal{N}_n$, $S(A)$ becomes a nonnegative diagonal matrix and hence $\mathcal{N}_n \subseteq \mathcal{H}_n$. The detection whether $A \in \mathcal{H}_n$ is easy and can be done by checking positivity of $A_{ij}(i \neq j)$ and by a Cholesky factorization of $S(A)$ (cf. Algorithm 4.2.4 in [31]). Thus, by the inclusion relation (2.3), we see that the set $\mathcal{H}_n$ satisfies the desirable properties **P1** and **P2** of $\mathcal{M}_n$. 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 several properties of the set $\mathcal{H}_n$.

Theorem 3.1.1 ([28] and Theorem 4.2 of [55])**.** *$\mathcal{H}_n$ 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 $\mathcal{S}_n^+ \nsubseteq \mathcal{H}_n$. For $n = 2$, we have $\mathcal{H}_n = \mathcal{S}_n^+ \cup \mathcal{N}_n = \mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{COP}_n$.*

To prove convexity of $\mathcal{H}_n$, we first show the following lemma.

Lemma 3.1.2 (Lemma 4.3 of [55])**.** *Denote by $\mathcal{Z}_n$ the class of all real square matrices whose off-diagonal entries are nonpositive.*

$$\mathcal{Z}_n = \{A \in \mathcal{S}_n \mid A_{ij} \leq 0 \textit{ for any } i \neq j\}.$$

Let $A, B \in \mathcal{Z}_n$ with $B \geq A$. If A is positive semidefinite, then B is also positive semidefinite.

Proof. Let $A, B \in \mathcal{Z}_n$ with $B \geq A$. The proof is based on contradiction. We assume $A \in \mathcal{S}_n^+$ and $B \notin \mathcal{S}_n^+$. There exist $x \in \mathbb{R}^n$ such that $x^T Bx$ is negative by the definition of $\mathcal{S}_n^+$. We define $\bar{x}$ as follows

$$\bar{x}_i := \begin{cases} -x_i & x_i < 0 \\ x_i & \text{otherwise} \end{cases} \tag{3.3}$$

Clearly, $\bar{x} \in \mathbb{R}^n_+$. $b_{ij}\bar{x}_i\bar{x}_j \leq b_{ij}x_ix_j$ holds since $B \in \mathcal{Z}_n$ then the following inequality holds,

$$\bar{x}^T B\bar{x} \leq x^T Bx < 0.$$

By $B \geq A$ and the nonnegativity of $\bar{x}$, $\bar{x}^T A\bar{x} \leq \bar{x}^T B\bar{x} < 0$ holds but it contradict to positive semidefiniteness of A. It follows that B is positive semidefinite. □

Now we prove Theorem3.1.1.

Proof. It is obvious that $\mathcal{H}_n$ is a cone and inclusions $\mathcal{N}_n \subseteq \mathcal{H}_n \subseteq S^+_n + \mathcal{N}_n$ from the definition. For $n \geq 3$ both enclusions are strict, since

$$A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \in \mathcal{H}_2 \text{ but } A \notin \mathcal{N}_2$$

and

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

Then $B \in \mathcal{S}^+_3$. However,

$$S(B) = B - N(B) = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \notin \mathcal{S}^+_3.$$

For $A \in \mathcal{S}_n$, there are the following two cases:

$$S(A) = \begin{cases} \begin{bmatrix} a_{11} & 0 \\ 0 & a_{22} \end{bmatrix} & (a_{12} > 0) \\ A & (\text{otherwise}). \end{cases}$$

In the first case, $A \in \mathcal{H}_2$ if and only if $a_{11}, a_{22} \geq 0$ which means $A \in \mathcal{N}_2$. In the second case, $A \in \mathcal{H}_2$ if and only if $A \in \mathcal{S}^+_2$. It follows that for $n = 2$, $\mathcal{H}_n = \mathcal{S}^+_n \cup \mathcal{N}_n = \mathcal{S}^+_n + \mathcal{N}_n = \mathcal{COP}_n$.

Finally, we show convexity of $\mathcal{H}_n$. Consider $A, B \in \mathcal{H}_n$, we have to prove $A+B \in \mathcal{H}_n$. $S(A)$ and $S(B)$ belong to $\mathcal{S}^+_n$ by the definition of $\mathcal{H}_n$, and hence $S(A)+S(B) \in \mathcal{S}^+_n$.

By the construction, we have $S(A+B) \geq S(A) + S(B)$ then $S(A+B) \in \mathcal{S}_n^+$ by Lemma 3.1.2. It follows that $\mathcal{H}_n$ is convex. $\square$

The construction of the set $\mathcal{H}_n$ is based on the idea of "nonnegativity-checking first and positive semidefiniteness-checking second." Now, we provide an alternative choice of $\mathcal{M}_n$ 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 be an orthonormal matrix and $\Lambda = \mathrm{Diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)$ be a diagonal matrix satisfying

$$A = P\Lambda P^T. \tag{3.4}$$

We are interested in decomposing A into a semidefinite matrix and a nonnegative matrix according to the form $A = P\Lambda P^T$. By introducing another diagonal matrix $\Omega = \mathrm{Diag}\,(\omega_1, \omega_2, \ldots, \omega_n)$, consider the following decomposition:

$$A = P(\Lambda - \Omega)P^T + P\Omega P^T \tag{3.5}$$

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

$$\lambda_i \geq \omega_i \ (i = 1, 2, \ldots, n), \quad [P\Omega P^T]_{ij} \geq 0 \ (i, j = 1, 2, \ldots, n, i \leq j) \tag{3.6}$$

then (3.5) and (2.3) imply

$$A = P(\Lambda - \Omega)P^T + P\Omega P^T \in \mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{COP}_n. \tag{3.7}$$

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

$$\begin{array}{llll} & \text{Maximize} & \alpha & \\ (\mathrm{LP})_{P,\Lambda} & \text{subject to} & \omega_i \leq \lambda_i & (i = 1, 2, \ldots, n) \\ & & [P\Omega P^T]_{i,j} = \sum_{k=1}^n \omega_k p_{ik} p_{jk} \geq \alpha & (i, j = 1, 2, \ldots, n, i \leq j) \end{array} \tag{3.8}$$

Note that $(\mathrm{LP})_{P,\Lambda}$ has the feasible solution at which $\omega_i = \lambda_i$ $(i = 1, 2, \ldots, n)$ and $\alpha = \min_{ij} \sum_{k=1}^n \lambda_k p_{ik} p_{jk}$ and hence has an optimal solution with optimal value

$\alpha^*(P,\Lambda)$. If $\alpha^*(P,\Lambda) \geq 0$ then there exists a matrix Ω for which the decomposition (3.6) holds. Based on these observations, we provide another alternate $\mathcal{G}_n^s$ of $\mathcal{M}_n$ as follows:

$$\mathcal{G}_n^s := \{A \in \mathcal{S}_n \mid \alpha^*(P,\Lambda) \geq 0 \text{ for } \textit{some} \text{ orthonormal matrix } P \text{ satisfying (3.4) } \}. \tag{3.9}$$

As stated above, if $\alpha^*(P,\Lambda) \geq 0$ for a given decomposition $A = P\Lambda P^T$ then we can determine $A \in \mathcal{G}_n^s$. In this case, we just need to compute a matrix decomposition and to 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 $\mathcal{G}_n^s$ as an alternate of $\mathcal{M}_n$ Suppose that $A \in \mathcal{S}_n$ has n different eigenvalues. Then the possible orthonormal matrices $P = [p_1, p_2, \cdots, p_n]$ are identifiable except for permutation and sign inversion of $\{p_1, p_2, \cdots, p_n\}$ and by the representation

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

of (3.4), we see that the problem $(\mathrm{LP})_{P,\Lambda}$ is unique for any possible P. In this case, $\alpha^*(P,\Lambda) < 0$ with a specific P implies $A \notin \mathcal{G}_n^s$. However, otherwise (i.e., an eigenspace of A has at least dimension 2), $\alpha^*(P,\Lambda) < 0$ with a specific P does not necessarily guarantee that $A \notin \mathcal{G}_n^s$. So we cannot say that the set $\mathcal{G}_n^s$ satisfies the desirable property **P1** of $\mathcal{M}_n$. However, as we see in Theorem 3.1.3 below, $\mathcal{G}_n^s$ may satisfy the other desirable property **P2**.

Let us introduce other new sets $\mathcal{G}_n^a$ and $\widehat{\mathcal{G}_n^s}$ which are closely related to the set $\mathcal{G}_n^s$ and they might be useful to clarify some theoretical properties or to improve our algorithm:

$$\mathcal{G}_n^a := \{A \in \mathcal{S}_n \mid \alpha^*(P,\Lambda) \geq 0 \text{ for } \textit{any} \text{ orthonormal matrix } P \text{ satisfying (3.4) } \}, \tag{3.10}$$

$$\widehat{\mathcal{G}_n^s} := \{A \in \mathcal{S}_n \mid \alpha^*(P,\Lambda) \geq 0 \text{ for } \textit{some arbitrary} \text{ matrix } P \text{ satisfying (3.4) } \}. \tag{3.11}$$

Note that if (3.6) holds for any arbitrary (not necessarily orthonormal) matrix P then (3.7) also holds, which implies the following inclusions:

$$\mathcal{G}_n^a \subseteq \mathcal{G}_n^s \subseteq \widehat{\mathcal{G}_n^s} \subseteq \mathcal{S}_n^+ + \mathcal{N}_n. \tag{3.12}$$

More precisely, the sets $\mathcal{G}_n^s$, $\mathcal{G}_n^a$ and $\widehat{\mathcal{G}}_n^s$ have the following properties.

Theorem 3.1.3. *The sets $\mathcal{G}_n^s$, $\mathcal{G}_n^a$ and $\widehat{\mathcal{G}}_n^s$ are cones and*

$$\mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^a \subseteq \mathcal{G}_n^s = \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n) \subseteq \widehat{\mathcal{G}_n^s} \subseteq \mathcal{S}_n^+ + \mathcal{N}_n \subseteq \mathcal{COP}_n$$

where the set $\mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$ *is defined by*

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

For $n = 2$, we have

$$\mathcal{S}_n^+ \cup \mathcal{N}_n = \mathcal{G}_n^a = \mathcal{G}_n^s = \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n) = \widehat{\mathcal{G}_n^s} = \mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{COP}_n.$$

Proof. We assume that $A \in \mathcal{S}_n$ is diagonalized as in (3.4) throughout the proof.

Suppose that the associated linear optimization problem $(\mathrm{LP})_{P,\Lambda}$ has an optimal solution $(\omega^*, \alpha^*) := (\omega_1^*, \ldots, \omega_n^*, \alpha^*)$. Then for any $\beta \geq 0$, βA is diagonalized as in $\beta A = P(\beta\Lambda)P^T$ and $(\beta\omega^*, \beta\alpha^*)$ is an optimal solution of the associated linear optimization problem $(\mathrm{LP})_{P,\beta\Lambda}$. This implies that $\beta A \in \mathcal{G}_n^s$ (respectively $\beta A \in \mathcal{G}_n^a$, respectively $\beta A \in \widehat{\mathcal{G}_n^s}$) if $A \in \mathcal{G}_n^s$ (respectively $A \in \mathcal{G}_n^a$, respectively $A \in \widehat{\mathcal{G}_n^s}$) and hence $\mathcal{G}_n^s$, $\mathcal{G}_n^a$ and $\widehat{\mathcal{G}_n^s}$ are cones.

We have already seen that (3.12) holds. So it is sufficient to show that (i) $\mathcal{S}_n^+ \cup \mathcal{N}_n \subseteq \mathcal{G}_n^a$ and (ii) $\mathcal{G}_n^s = \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$.

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

(ii) $\mathcal{G}_n^s = \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$: The inclusion $\mathcal{G}_n^s \subseteq \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$ follows from the construction of the set $\mathcal{G}_n^s$ as in (3.9) and (3.8). The converse inclusion $\mathcal{G}_n^s \supseteq \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$ is also true since if $A \in \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n)$ then there exist an orthonormal matrix P and diagonal matrices $\Theta = \mathrm{Diag}\,(\theta_1, \theta_2, \ldots, \theta_n)$ and $\Omega = \mathrm{Diag}\,(\omega_1, \omega_2, \ldots, \omega_n)$ such that

$$A = P\Theta P^T + P\Omega P^T,\ P\Theta P^T \in \mathcal{S}_n^+,\ P\Omega P^T \in \mathcal{N}_n$$

(see Theorem 1.3.12 of [34]) which implies that $\theta_i \geq 0$ $(i = 1, 2, \ldots, n)$ and that the problem $(\mathrm{LP})_{P,\Lambda}$ with $\Lambda = \Theta + \Omega$ has a nonnegative objective value at a solution (ω, α) where $\alpha = \min_{i,j}\{[P\Omega P^T]_{ij}\} \geq 0$.

The results for $n = 2$ follow from Theorem 3.1.1. $\square$

As we have seen in Theorem 3.1.1, $\mathcal{N}_n \subseteq \mathcal{H}_n$ but $\mathcal{S}_n^+ \not\subseteq \mathcal{H}_n$ for $n \geq 3$. Theorem 3.1.3 suggests that the set $\mathcal{G}_n^s$ might be better than the set $\mathcal{H}_n$ in the sense of the desirable property **(P2)** of $\mathcal{M}_n$. The following examples show some contrasts between $\mathcal{H}_n$, $\mathcal{G}_n^s$ and $\mathcal{G}_n^a$.

Example 3.1.4. *Consider*

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

Then, by the definition (3.1),

$$S(A) = A - N(A) = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & -1 \\ 1 & -1 & 2 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \in \mathcal{S}_3^+$$

which implies that $A \in \mathcal{H}_3$. Moreover,

$$N(A)S(A) = S(A)N(A) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

which implies that $A = S(A) + N(A) \in \mathrm{com}(\mathcal{S}_3^+ + \mathcal{N}_3)$, and by Theorem 3.1.3, $A \in \mathcal{G}_3^s$ holds. Thus $\mathcal{H}_3 \cap \mathcal{G}_3^s \neq \emptyset$.

Example 3.1.5 (cf. Proof of Theorem 4.2 in [55])**.** *Consider*

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

Then $A \in \mathcal{S}_3^+$ and by Theorem 3.1.3, we see that $A \in \mathcal{G}_3^s$. However,

$$S(A) = A - N(A) = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \notin \mathcal{S}_3^+$$

which implies that $A \notin \mathcal{H}_3$. Thus $\mathcal{G}_3^s \setminus \mathcal{H}_3 \neq \emptyset$.

Example 3.1.6. *Consider*

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

and let

$$S = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ and } N = A - S = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

Then $S \in \mathcal{S}_3^+, N \in \mathcal{N}_3$ and

$$SN = NS = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

holds which implies that $A \in \mathrm{com}(\mathcal{S}_3^+ + \mathcal{N}_3) \subseteq \mathcal{G}_3^s$. Moreover, if we set

$$P := \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{14}} & \frac{5}{\sqrt{42}} \\ \frac{1}{\sqrt{3}} & -\frac{3}{\sqrt{14}} & -\frac{1}{\sqrt{42}} \\ -\frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{14}} & \frac{4}{\sqrt{42}} \end{bmatrix}, \Lambda := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

then P and Λ satisfy (3.4) and the corresponding problem $(\mathrm{LP})_{P,\Lambda}$ is given as follows:

$$\begin{array}{ll} \text{Maximize} & \alpha \\ \text{subject to} & \omega_1 \leq -1, \omega_2 \leq 2, \omega_3 \leq 2 \\ & \omega_1 \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{bmatrix} + \omega_2 \begin{bmatrix} \frac{1}{14} & -\frac{3}{14} & -\frac{1}{7} \\ -\frac{3}{14} & \frac{9}{14} & \frac{3}{7} \\ -\frac{1}{7} & \frac{3}{7} & \frac{2}{7} \end{bmatrix} + \omega_3 \begin{bmatrix} \frac{25}{42} & -\frac{5}{42} & \frac{10}{21} \\ -\frac{5}{42} & \frac{1}{42} & -\frac{2}{21} \\ \frac{10}{21} & -\frac{2}{21} & \frac{8}{21} \end{bmatrix} \geq \alpha E. \end{array}$$

By solving this problem, we know that $\alpha^*(P, \Lambda) < 0$. Thus the matrix A lies on $\mathcal{G}_3^s$ but not on $\mathcal{G}_3^a$. Thus $\mathcal{G}_3^s \setminus \mathcal{G}_3^a \neq \emptyset$.

Figure 3.1 draws those examples and (ii) of Theorem 3.1.3. Moreover, Figure 3.2 follows from (vii) of Theorem 3.1.3 and the convexity of the sets $\mathcal{N}_n$, $\mathcal{S}_n$ and $\mathcal{H}_n$ (see Theorem 3.1.1).

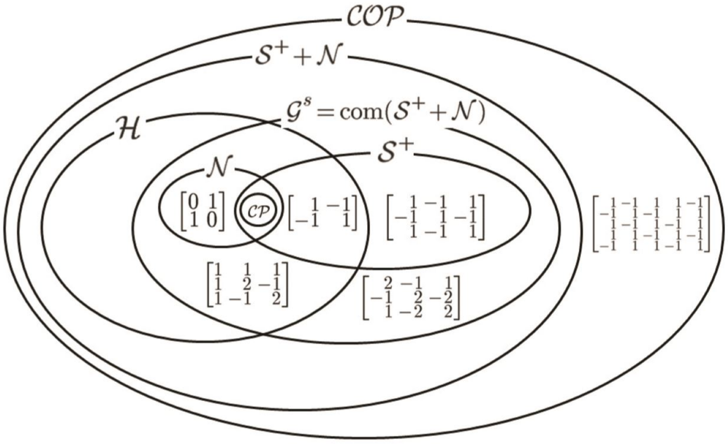

Figure 3.1: The inclusion relations among the subcones of $\mathcal{COP}$ I

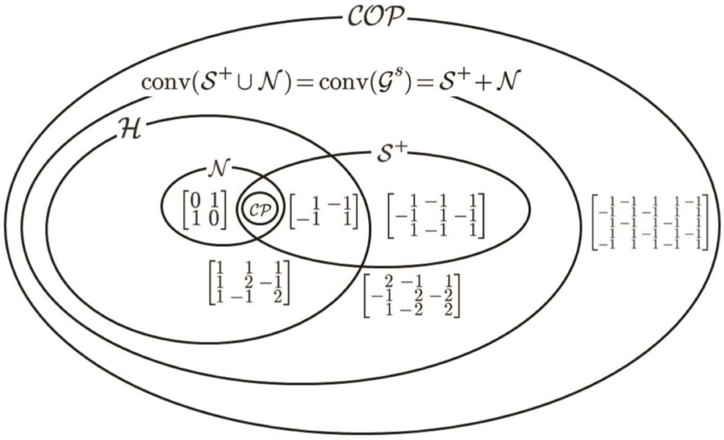

Figure 3.2: The inclusion relations among the subcones of $\mathcal{COP}_n$ II

3.2 SDbasis and sub cones of copositive cone

We improve the subcone $\mathcal{G}_n^s$ in terms of **P2**. For a given matrix A of (3.4), the linear optimization problem $(\mathrm{LP})_{P,\Lambda}$ in (3.8) 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 $p_i p_i^T \in \mathcal{S}_n^+$ $(i = 1, 2, \ldots, n)$. This is done by decomposing $A \in \mathcal{S}_n$ into two parts:

$$A = \sum_{i=1}^{n} (\lambda_i - \omega_i) p_i p_i^T + \sum_{i=1}^{n} \omega_i p_i p_i^T \tag{3.13}$$

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 $(\mathrm{LP})_{P,\Lambda}$. In fact, we will show that we can easily find a basis of $\mathcal{S}_n$ 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 3.2.1 (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 $\Pi_+ : \mathbb{R}^n \times \mathbb{R}^n \to \mathcal{S}_n^+$ by*

$$\Pi_+(p_i, p_j) := \frac{1}{4}(p_i + p_j)(p_i + p_j)^T. \tag{3.14}$$

We call the set

$$\mathcal{B}_+(p_1, p_2, \ldots, p_n) := \{\Pi_+(p_i, p_j) \mid 1 \le i \le j \le n\} \tag{3.15}$$

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

From (3.14) and the fact that p_i are orthonormal, we obtain the following:

$$\Pi_+(p_i, p_j) p_k = \begin{cases} p_k & \text{if } i = j = k \\ \frac{1}{4}(p_i + p_j) & \text{if } i \neq j \text{ and } (i = k \text{ or } j = k) \\ 0 & \text{otherwise} \end{cases} \tag{3.16}$$

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

Theorem 3.2.2. *Let $p_i \in \mathbb{R}^n (i = 1, 2, \ldots, n)$ be n-dimensional orthonormal vectors. Then the semidefinite basis $\mathcal{B}_+(p_1, p_2, \ldots, p_n)$ defined by Definition 3.2.1 is a basis of the set $\mathcal{S}_n$ of $n \times n$ symmetric matrices.*

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

$$\mathcal{B}_+(p_1, p_2, \cdots, p_k) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq k\}.$$

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

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

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

$$\begin{aligned} 0 = \sum_{1 \leq i \leq j \leq k} \alpha_{ij} \Pi_+(p_i, p_j) p_k &= \sum_{i=1}^{k} \alpha_{ii} \Pi_+(p_i, p_i) p_k + \sum_{1 \leq i < j \leq k} \alpha_{ij} \Pi_+(p_i, p_j) p_k \\ &= \alpha_{kk} p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}(p_i + p_k) \qquad \text{(by (3.16))} \\ &= \left(\alpha_{kk} + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}\right) p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} p_i = 0 \qquad (3.17) \end{aligned}$$

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

$$\alpha_{ik} = 0 \ (i = 1, 2, \ldots, k-1) \text{ and hence } \alpha_{kk} = 0. \qquad (3.18)$$

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

$$\alpha_{ij} = 0 \ \ (1 \leq i \leq j \leq k-1). \qquad (3.19)$$

It follows from (3.18) and (3.19) that $\mathcal{B}_+(p_1, p_2, \cdots, p_k) := \{\Pi_+(p_i, p_j) \mid 1 \leq i \leq j \leq k\}$ is linearly independent, which completes the proof. $\square$

A variant of the semidefinite basis type I is as follows.

Definition 3.2.3 (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 $\Pi_+ : \mathbb{R}^n \times \mathbb{R}^n \to \mathcal{S}_n^+$ by*

$$\Pi_-(p_i, p_j) := \frac{1}{4}(p_i - p_j)(p_i - p_j)^T. \tag{3.20}$$

We call the set

$$\mathcal{B}_-(p_1, p_2, \cdots, p_n) := \{\Pi_+(p_i, p_i) \mid 1 \leq i \leq n\} \cup \{\Pi_-(p_i, p_j) \mid 1 \leq i < j \leq n\} \tag{3.21}$$

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 (3.20) and the orthonormality of p_i that

$$\Pi_-(p_i, p_j)p_k = \begin{cases} \frac{1}{4}(p_i - p_j) & \text{if } i \neq j \text{ and } (i = k \text{ or } j = k) \\ 0 & \text{otherwise} \end{cases} \tag{3.22}$$

Using the above relations, we obtain the following theorem as a variant of Theorem 3.2.2.

Theorem 3.2.4. *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 3.2.3 is a basis of the set $\mathcal{S}_n$ of $n \times n$ symmetric matrices.*

Proof. The proof is almost the same as that of Theorem 3.2.2. The only difference is that equation (3.17) turns out to be

$$\begin{aligned} 0 &= \sum_{i=1}^{k} \alpha_{ii} \Pi_+(p_i, p_i)p_k + \sum_{1 \leq i < j \leq k} \alpha_{ij} \Pi_-(p_i, p_j)p_k \\ &= \alpha_{kk}p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}(p_i - p_k) \qquad \text{(by (3.22))} \\ &= \left(\alpha_{kk} - \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4}\right) p_k + \sum_{i=1}^{k-1} \frac{\alpha_{ik}}{4} p_i = 0. \end{aligned}$$

□

Remark 3.2.5 (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* $C = \sum_{i=1}^n p_i p_i^T$ *in Jordan algebra (cf. Example 11.15 of [3] and Chapter IV of [29]). To see this, consider the following simple example with* $n = 2$*. Let*

$$p_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \; p_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Then the semidefinite bases defined by Definitions 3.2.1 and 3.2.3 are

$$\begin{aligned} \mathcal{B}_+(p_1, p_2) &= \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1/4 & 1/4 \\ 1/4 & 1/4 \end{bmatrix} \right\} \subseteq \mathcal{S}_n^+, \\ \mathcal{B}_-(p_1, p_2) &= \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1/4 & -1/4 \\ -1/4 & 1/4 \end{bmatrix} \right\} \subseteq \mathcal{S}_n^+ \end{aligned}$$

respectively. On the other hand, the Peirce space associated with the idempotent $C = p_1 p_1^T + p_2 p_2^T$ *is given by*

$$\begin{aligned} \mathbb{E}_1(C) &= \left\{ \begin{bmatrix} \alpha & 0 \\ 0 & 0 \end{bmatrix} \mid \alpha \in \mathbb{R} \right\} \\ \mathbb{E}_2(C) &= \left\{ \begin{bmatrix} 0 & 0 \\ 0 & \alpha \end{bmatrix} \mid \alpha \in \mathbb{R} \right\} \\ \mathbb{E}_{12}(C) &= \left\{ \begin{bmatrix} 0 & \alpha \\ \alpha & 0 \end{bmatrix} \mid \alpha \in \mathbb{R} \right\} \end{aligned}$$

and this leads to the basis,

$$\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right\} \not\subseteq \mathcal{S}_n^+$$

Figure 3.3 shows $\mathcal{S}_2^+$ and SDbasis $\mathcal{B}_+(p_1, p_2)$ of Remark 3.2.5. The semidefinite cone for $n = 2$ is representable as

$$\mathcal{S}_2^+ = \left\{ \begin{bmatrix} a & c \\ c & b \end{bmatrix} \mid a \geq 0, \; b \geq 0, \; ab - c^2 \geq 0 \right\}.$$

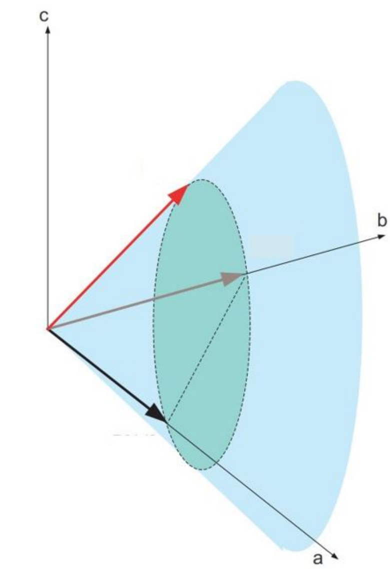

Figure 3.3: The semidefinite cone and $\mathcal{B}_+(p_1, p_2)$ for $n = 2$

The cone in Figure 3.3 is $\mathcal{S}_2^+$ and vectors shows $\mathcal{B}_+(p_1, p_2)$.

Using the map Π_+ in (3.14), the linear optimization problem $(\mathrm{LP})_{P,\Lambda}$ in (3.8) can be equivalently written as

$$(\mathrm{LP})_{P,\Lambda} \left| \begin{array}{lll} \text{Maximize} & \alpha & \\ \text{subject to} & \omega_{ii} \le \lambda_i & (i = 1, 2, \ldots, n) \\ & \left[\displaystyle\sum_{k=1}^{n} \omega_{kk} \Pi_+(p_k, p_k) \right]_{ij} \ge \alpha & (1 \le i \le j \le n). \end{array} \right.$$

The problem $(\mathrm{LP})_{P,\Lambda}$ is based on the decomposition (3.13). Starting with (3.13), the matrix A can be decomposed using $\Pi_+(p_i, p_j)$ in (3.14) and $\Pi_-(p_i, p_j)$ in (3.20) as

$$
\begin{aligned}
A &= \sum_{i=1}^{n}(\lambda_i - \omega_{ii}^{+})\Pi_{+}(p_i, p_i) + \sum_{i=1}^{n}\omega_{ii}^{+}\Pi_{+}(p_i, p_i) \\
&= \sum_{i=1}^{n}(\lambda_i - \omega_{ii}^{+})\Pi_{+}(p_i, p_i) + \sum_{i=1}^{n}\omega_{ii}^{+}\Pi_{+}(p_i, p_i) \\
&\quad + \sum_{1\le i<j\le n}(-\omega_{ij}^{+})\Pi_{+}(p_i, p_j) + \sum_{1\le i<j\le n}\omega_{ij}^{+}\Pi_{+}(p_i, p_j) \qquad (3.23) \\
&= \sum_{i=1}^{n}(\lambda_i - \omega_{ii}^{+})\Pi_{+}(p_i, p_i) + \sum_{i=1}^{n}\omega_{ii}^{+}\Pi_{+}(p_i, p_i) \\
&\quad + \sum_{1\le i<j\le n}(-\omega_{ij}^{+})\Pi_{+}(p_i, p_j) + \sum_{1\le i<j\le n}\omega_{ij}^{+}\Pi_{+}(p_i, p_j) \\
&\quad + \sum_{1\le i<j\le n}(-\omega_{ij}^{-})\Pi_{-}(p_i, p_j) + \sum_{1\le i<j\le n}\omega_{ij}^{-}\Pi_{+}(p_i, p_j). \qquad (3.24)
\end{aligned}
$$

On the basis of the decomposition (3.23) and (3.24), we devise the following two linear optimization problems as extensions of $(\mathrm{LP})_{P,\Lambda}$:

$$
(\mathrm{LP})_{P,\Lambda}^{+} \quad \left|\begin{array}{lll}
\text{Maximize} & \alpha & \\
\text{subject to} & \omega_{ii}^{+} \le \lambda_i & (i = 1, 2, \ldots, n) \\
& \omega_{ij}^{+} \le 0 & (1 \le i < j \le n) \\
& \left[\displaystyle\sum_{1\le k\le l\le n}\omega_{kl}^{+}\Pi_{+}(p_k, p_l)\right]_{ij} \ge \alpha & (1 \le i \le j \le n)
\end{array}\right. \qquad (3.25)
$$

$$
(\mathrm{LP})_{P,\Lambda}^{\pm} \quad \left|\begin{array}{lll}
\text{Maximize} & \alpha & \\
\text{subject to} & \omega_{ii}^{+} \le \lambda_i & (i = 1, 2, \ldots, n) \\
& \omega_{ij}^{+} \le 0,\ \omega_{ij}^{-} \le 0 & (1 \le i < j \le n) \\
& \left[\displaystyle\sum_{1\le k\le l\le n}\omega_{kl}^{+}\Pi_{+}(p_k, p_l) + \sum_{1\le k<l\le n}\omega_{kl}^{-}\Pi_{-}(p_k, p_l)\right]_{ij} \ge \alpha & (1 \le i \le j \le n)
\end{array}\right. \qquad (3.26)
$$

Problem $(\mathrm{LP})_{P,\Lambda}^{+}$ has $n(n+1)/2+1$ variables and $n(n+1)$ constraints, and problem $(\mathrm{LP})_{P,\Lambda}^{\pm}$ has n^2+1 variables and $n(3n+1)/2$ constraints (see Table 3.1). Since $[P\Omega P^T]_{ij}$ in (3.8) is given by $[\sum_{k=1}^{n}\omega_{kk}\Pi_{+}(p_k, p_k)]_{ij}$, we can prove that both linear optimization problems $(\mathrm{LP})_{P,\Lambda}^{+}$ and $(\mathrm{LP})_{P,\Lambda}^{\pm}$ are feasible and bounded by making arguments similar to the one for $(\mathrm{LP})_{P,\Lambda}$. Thus, $(\mathrm{LP})_{P,\Lambda}^{+}$ and $(\mathrm{LP})_{P,\Lambda}^{\pm}$ have optimal solutions with corresponding optimal values $\alpha_*^{+}(P, \Lambda)$ and $\alpha_*^{\pm}(P, \Lambda)$.

If the optimal value $\alpha_*^+(P,\Lambda)$ of $(\mathrm{LP})^+_{P,\Lambda}$ is nonnegative, then, by rearranging (3.23), the optimal solution ω_{ij}^{+*} $(1 \le i \le j \le n)$ can be made to give the following decomposition:

$$A = \left[\sum_{i=1}^{n}(\lambda_i - \omega_{ii}^{+*})\Pi_+(p_i,p_i) + \sum_{1\le i<j\le n}(-\omega_{ij}^{+*})\Pi_+(p_i,p_j)\right] + \left[\sum_{1\le i\le j\le n}\omega_{ij}^{+*}\Pi_+(p_i,p_j)\right] \in \mathcal{S}_n^n + \mathcal{N}_n.$$

In the same way, if the optimal value $\alpha_*^\pm(P,\Lambda)$ of $(\mathrm{LP})^\pm_{P,\Lambda}$is nonnegative, then, by rearranging (3.24), the optimal solution ω_{ij}^{+*} $(1 \le i \le j \le n)$, ω_{ij}^{-*} $(1 \le i < j \le n)$ can be made to give the following decomposition:

$$\begin{aligned} A &= \left[\sum_{i=1}^{n}(\lambda_i - \omega_{ii}^{+*})\Pi_+(p_i,p_i) + \sum_{1\le i<j\le n}(-\omega_{ij}^{+*})\Pi_+(p_i,p_j) + \sum_{1\le i<j\le n}(-\omega_{ij}^{-*})\Pi_-(p_i,p_j)\right] \\ &\quad + \left[\sum_{1\le i\le j\le n}\omega_{ij}^{+*}\Pi_+(p_i,p_j) + \sum_{1\le i<j\le n}\omega_{ij}^{-*}\Pi_-(p_i,p_j)\right] \in \mathcal{S}_n^n + \mathcal{N}_n. \end{aligned}$$

On the basis of the above observations, we can define new subcones of $\mathcal{S}_n^n + \mathcal{N}_n$ in a similar manner as (3.9):

$$\begin{aligned}
\mathcal{F}_n^{+s} &:= \{A \in \mathcal{S}_n \mid \alpha_*^+(P,\Lambda) \ge 0 \text{ for } \textit{some} \text{ orthonormal matrix } P \text{ satisfying (3.4) }\},\\
\mathcal{F}_n^{+a} &:= \{A \in \mathcal{S}_n \mid \alpha_*^+(P,\Lambda) \ge 0 \text{ for } \textit{any} \text{ orthonormal matrix } P \text{ satisfying (3.4) }\},\\
\widehat{\mathcal{F}_n^{+s}} &:= \{A \in \mathcal{S}_n \mid \alpha_*^+(P,\Lambda) \ge 0 \text{ for } \textit{some arbitrary} \text{ matrix } P \text{ satisfying (3.4) }\},\\
\mathcal{F}_n^{\pm s} &:= \{A \in \mathcal{S}_n \mid \alpha_*^\pm(P,\Lambda) \ge 0 \text{ for } \textit{some} \text{ orthonormal matrix } P \text{ satisfying (3.4) }\},\\
\mathcal{F}_n^{\pm a} &:= \{A \in \mathcal{S}_n \mid \alpha_*^\pm(P,\Lambda) \ge 0 \text{ for } \textit{any} \text{ orthonormal matrix } P \text{ satisfying (3.4) }\},\\
\widehat{\mathcal{F}_n^{\pm s}} &:= \{A \in \mathcal{S}_n \mid \alpha_*^\pm(P,\Lambda) \ge 0 \text{ for } \textit{some arbitrary} \text{ matrix } P \text{ satisfying (3.4) }\}
\end{aligned} \tag{3.27}$$

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

$$\mathcal{G}_n^s \subseteq \mathcal{F}_n^{+s} \subseteq \mathcal{F}_n^{\pm s}, \qquad \mathcal{G}_n^a \subseteq \mathcal{F}_n^{+a} \subseteq \mathcal{F}_n^{\pm a}, \qquad \widehat{\mathcal{G}_n^{+s}} \subseteq \widehat{\mathcal{F}_n^{+s}} \subseteq \widehat{\mathcal{F}_n^{\pm s}}$$

hold. The following corollary follows from (v)-(vii) of Theorem 3.1.3 and the above inclusions.

Corollary 3.2.6. **(i)**

$$
\begin{array}{ccccccccc}
\mathcal{S}_n^+ \cup \mathcal{N}_n & \subseteq & \mathcal{G}_n^a & \subseteq & \mathcal{G}_n^s = \mathrm{com}(\mathcal{S}_n^+ + \mathcal{N}_n) & \subseteq & \widehat{\mathcal{G}_n^s} & \subseteq & \mathcal{S}_n^+ + \mathcal{N}_n \\
 & & \rotatebox{-90}{$\subseteq$} & & \rotatebox{-90}{$\subseteq$} & & \rotatebox{-90}{$\subseteq$} & & \\
\mathcal{S}_n^+ \cup \mathcal{N}_n & \subseteq & \mathcal{F}_n^{+a} & \subseteq & \mathcal{F}_n^{+s} & \subseteq & \widehat{\mathcal{F}_n^{+s}} & \subseteq & \mathcal{S}_n^+ + \mathcal{N}_n \\
 & & \rotatebox{-90}{$\subseteq$} & & \rotatebox{-90}{$\subseteq$} & & \rotatebox{-90}{$\subseteq$} & & \\
\mathcal{S}_n^+ \cup \mathcal{N}_n & \subseteq & \mathcal{F}_n^{\pm a} & \subseteq & \mathcal{F}_n^{\pm s} & \subseteq & \widehat{\mathcal{F}_n^{\pm s}} & \subseteq & \mathcal{S}_n^+ + \mathcal{N}_n
\end{array}
$$

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

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

The following table summarizes the sizes of LPs (3.8), (3.25), and (3.26) that we have to solve in order to identify, respectively, $A \in \mathcal{G}_n^s$ (or $A \in \widehat{\mathcal{G}_n^s}$), $A \in \mathcal{F}_n^{+s}$ (or $A \in \widehat{\mathcal{F}_n^s}$) and $A \in \mathcal{F}_n^{\pm s}$ (or $A \in \widehat{\mathcal{F}_n^s}$).

Table 3.1: Sizes of LPs for identification

Identification	$A \in \mathcal{G}_n^s$ (or $A \in \widehat{\mathcal{G}_n^s}$)	$A \in \mathcal{F}_n^{+s}$ (or $A \in \widehat{\mathcal{F}_n^{+s}}$)	$A \in \mathcal{F}_n^{\pm s}$ (or $A \in \widehat{\mathcal{F}_n^{\pm s}}$)
# of variables	$n+1$	$n(n+1)/2+1$	n^2+1
# of constraints	$n(n+3)/2$	$n(n+1)$	$n(3n+1)/2$

We generated random instances of $A \in \mathcal{S}_n^+ + \mathcal{N}_n$ based on the method described in Section 2 of [14]. 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 $A = S + N \in \mathcal{S}_n^+ + \mathcal{N}_n$. 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 $A \in \mathcal{S}_n^+ + \mathcal{N}_n$, we checked whether $A \in \mathcal{G}_n^s$ ($A \in \mathcal{F}_n^{+s}$ and $A \in \mathcal{F}_n^{\pm s}$) by solving $(\mathrm{LP})_{P,\Lambda}$ in (3.8) ($(\mathrm{LP})_{P,\Lambda}^{+}$ in (3.25) and $(\mathrm{LP})_{P,\Lambda}^{\pm}$ in (3.26)), where P and Λ were obtained using the MATLAB command "$[P, \Lambda] = \mathrm{eig}(A)$."

Table 3.2 shows the number of matrices that were identified as $A \in \mathcal{G}_n^s$ ($A \in \mathcal{F}_n^{+s}$ and $A \in \mathcal{F}_n^{\pm s}$) 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 $A \in \mathcal{S}_n^+ + \mathcal{N}_n$ by checking $A \in \mathcal{F}_n^{\pm s}$. The result is comparable to the one in Section 2 of [14].
- For any n, the number of identified matrices increases in the order of the set inclusion relation: $\mathcal{G}_n^s \subseteq \mathcal{F}_n^{+s} \subseteq \mathcal{F}_n^{\pm s}$.
- For the sets $\mathcal{G}_n^s$ and $\mathcal{F}_n^{+s}$, the number of identified matrices decreases as the size of n increases.
- Comparing the results for $\mathcal{F}_n^{+s}$ and $\mathcal{F}_n^{\pm s}$, the average CPU time is approximately proportional to the number of identified matrices.

Table 3.2: Results of identification of $A \in \mathcal{S}_n^+ + \mathcal{N}_n$: 1000 matrices were generated for each n

	$\mathcal{G}_n^s$		$\mathcal{F}_n^{+s}$		$\mathcal{F}_n^{\pm s}$	
n	# of A	Ave. time(s)	# of A	Ave. time(s)	# of A	Ave. time(s)
10	247	4.707	856	8.322	1000	11.003
20	20	12.860	719	120.779	1000	221.889
50	0	2373.744	440	22345.511	1000	50091.542

Chapter 4

LP based algorithms for checking copositivity

In this section, we investigate the effect of using the sets $\mathcal{F}_n^{+s}$, $\widehat{\mathcal{F}_n^{+s}}$, $\mathcal{F}_n^{\pm s}$ and $\widehat{\mathcal{F}_n^{\pm s}}$ for testing whether a given matrix A is copositive by using Sponsel, Bundfuss and Dür's algorithm [55].

4.1 Outline of the algorithms

By defining the standard simplex Δ^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 [16]). A family of simplices $\mathcal{P} = \{\Delta^1, \ldots, \Delta^m\}$ is called a *simplicial partition* of Δ if it satisfies

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

Such a partition can be generated by successively bisecting simplices in the partition. For a given simplex $\Delta = \operatorname{conv}\{v_1, \ldots, v_n\}$, 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 Δ satisfies the above conditions for simplicial partitions. See [33] 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 Δ is determined by its vertices and can be represented by a matrix V_Δ whose columns are these vertices. Note that V_Δ is nonsingular and unique up to a permutation of its columns, which does not affect the argument [55]. 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

$$\delta(\mathcal{P}) = \max_{\Delta \in \mathcal{P}} \max_{u,v \in \Delta} ||u - v||. \tag{4.1}$$

The above notation was used to show the following necessary and sufficient conditions for copositivity in [55]. The first theorem gives a sufficient condition for copositivity.

Theorem 4.1.1 (Theorem 2.1 of [55])**.** *If $A \in \mathcal{S}_n$ satisfies*

$$V^T A V \in \mathcal{COP}_n \textit{ for all } V \in M(\mathcal{P})$$

then A is copositive. Hence, for any $\mathcal{M}_n \subseteq \mathcal{COP}_n$, if $A \in \mathcal{S}^n$ satisfies

$$V^T A V \in \mathcal{M}_n \textit{ for all } V \in M(\mathcal{P}),$$

then A is also copositive.

The above theorem implies that by choosing $\mathcal{M}_n = \mathcal{N}_n$ (see (2.3)), A is copositive if $V_\Delta^T A V_\Delta \in \mathcal{N}_n$ holds for any $\Delta \in \mathcal{P}$.

Theorem 4.1.2 (Theorem 2.2 of [55])**.** *Let $A \in \mathcal{S}_n$ be strictly copositive, i.e., $A \in$ int $(\mathcal{COP}_n)$. Then there exists $\varepsilon > 0$ such that for all partitions $\mathcal{P}$ of Δ^S with $\delta(\mathcal{P}) < \varepsilon$, we have*

$$V^T A V \in \mathcal{N}_n \textit{ for all } V \in M(\mathcal{P}).$$

The above theorem ensures that if A is strictly copositive (i.e., $A \in \operatorname{int}(\mathcal{COP}_n)$) then the copositivity of A (i.e., $A \in \mathcal{COP}_n$) 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 $A \notin \mathcal{COP}_n$, as follows.

Lemma 4.1.3 (Lemma 2.3 of [55]). *The following two statements are equivalent.*

1. $A \notin \mathcal{COP}_n$
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* $v^T A v < 0$

The following algorithm, in [55], is based on the above three results.

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

---

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

Output: "A is copositive" or "A is not copositive"

$\mathcal{P} \leftarrow \{\Delta^S\}$;
while $\mathcal{P} \neq \emptyset$ **do**
  Choose $\Delta \in \mathcal{P}$;
  if $v^T A v < 0$ for some $v \in V(\{\Delta\})$: **then**
    return "A is not copositive";
  end if
  if $V_\Delta^T A V_\Delta \in \mathcal{M}_n$ **then**
    $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
  else
    Partition Δ into $\Delta = \Delta^1 \cup \Delta^2$;
    $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\} \cup \{\Delta^1, \Delta^2\}$;
  end if
end while
Return "A is copositive";

As we have already observed, Theorem 4.1.2 and Lemma 4.1.3 imply the following corollary.

Corollary 4.1.4. *1. If A is strictly copositive, i.e., $A \in \operatorname{int}(\mathcal{COP}_n)$, then Algorithm 1 terminates finitely, returning "A is copositive."*

2. If A is not copositive, i.e., $A \notin \mathcal{COP}_n$ 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 4.1.1. The accuracy and speed of the determination influence the total computational time and depend on the choice of the set $\mathcal{M}_n \subseteq \mathcal{COP}_n$.

In this section, we investigate the effect of using the sets $\mathcal{H}_n$ in (3.2), $\mathcal{G}_n^s$ in (**??**), and $\mathcal{F}_n^{+s}$ and $\mathcal{F}_n^{\pm s}$ in (3.27) as the set $\mathcal{M}_n$ in the above algorithm.

Note that if we choose $\mathcal{M}_n = \mathcal{G}_n^s$ (respectively, $\mathcal{M}_n = \mathcal{F}_n^{+s}$, $\mathcal{M}_n = \mathcal{F}_n^{\pm s}$), we can improve Algorithm 1 by incorporating the set $\widehat{\mathcal{M}_n} = \widehat{\mathcal{G}_n^s}$ (respctively, $\widehat{\mathcal{M}_n} = \widehat{\mathcal{F}_n^{+s}}$, $\widehat{\mathcal{M}_n} = \widehat{\mathcal{F}_n^{\pm s}}$), as proposed in [57].

The details of the added steps are as follows. Suppose that we have a diagonalization of the form (3.4).

At Line 7, we need to solve an additional LP but do not need to diagonalize $V_\Delta^T A V_\Delta$. Let P and Λ be matrices satisfying (3.4). Then the matrix $V_\Delta^T P$ can be used to diagonalize $V_\Delta^T A V_\Delta$, i.e.,,

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

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

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

At Line 15, we do not need to diagonalize $V_{\Delta^p}^T A V_{\Delta^p}$ 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

Algorithm 2 Improved version of Algorithm 1

Input: $A \in \mathcal{S}_n, \mathcal{M}_n \subseteq \widehat{\mathcal{M}_n} \subseteq \mathcal{COP}_n$

Output: "A is copositive" or "A is not copositive"

$\mathcal{P} \leftarrow \{\Delta^S\}$;
while $\mathcal{P} \neq \emptyset$ **do**
    Choose $\Delta \in \mathcal{P}$;
    if $v^T A v < 0$ for some $v \in V(\{\Delta\})$: **then**
        Return "A is not copositive";
    end if
    if $V_\Delta^T A V_\Delta \in \widehat{\mathcal{M}_n}$ **then**
        $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
    else
        if $V_\Delta^T A V_\Delta \in \mathcal{M}_n$ **then**
            $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\}$;
        else
            Partition Δ into $\Delta = \Delta^1 \cup \Delta^2$, and set $\widehat{\Delta} \leftarrow \{\Delta^1, \Delta^2\}$;
            for $p = 1, 2$ **do**
                if $V_{\Delta^p}^T A V_{\Delta^p} \in \widehat{\mathcal{M}_n}$ **then**
                    $\widehat{\Delta} \leftarrow \widehat{\Delta} \setminus \{\Delta^p\}$;
                end if
            end for
            $\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\} \cup \widehat{\Delta}$;
        end if
    end if
end while
return "A is copositive";

$\Omega^* := \mathrm{Diag}\,(\omega^*)$. Then the feasibility of ω^* implies the positive semidefiniteness of the matrix $V_{\Delta^p}^T P(\Lambda - \Omega^*)P^T V_{\Delta^p}$. Thus, if $V_{\Delta^p}^T P\Omega^* P^T V_{\Delta^p} \in \mathcal{N}_n$, we see that

$$V_{\Delta^p}^T A V_{\Delta^p} = V_{\Delta^p}^T P(\Lambda - \Omega^*)P^T V_{\Delta^p} + V_{\Delta^p}^T P\Omega^* P^T V_{\Delta^p} \in \mathcal{S}_n^+ + \mathcal{N}_n$$

and that $V_{\Delta^p}^T A V_{\Delta^p} \in \widehat{\mathcal{M}_n}$.

4.2 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,

$$B_\gamma := \gamma(E - A_G) - E \tag{4.2}$$

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_γ 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 [21]) that the maximum cardinality, the so-called clique number $\omega(G)$, is equal to the optimal value of

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

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

Figure 4.1 on page 43 shows the instances of G that were used in [55]. 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 $\mathcal{H}_n$, $\mathcal{G}_n^s$, $\mathcal{F}_n^{+s}$, $\widehat{\mathcal{F}_n^{+s}}$, $\mathcal{F}_n^{\pm s}$ or $\widehat{\mathcal{F}_n^{\pm s}}$ as the set $\mathcal{M}_n$ rather than to compute the clique number efficiently. Hence, the experiment examined B_γ for various values of γ at intervals of 0.1 around the value $\omega(G)$ (see Tables 4.1 and 4.2 on page 44).

As already mentioned, $\alpha_*(P,\Lambda) < 0$ ($\alpha_*^+(P,\Lambda) < 0$ and $\alpha_*^\pm(P,\Lambda) < 0$) with a specific P does not necessarily guarantee that $A \notin \mathcal{G}_n^s$ or $A \notin \widehat{\mathcal{G}_n^s}$ ($A \notin \mathcal{F}_n^{+s}$ or $A \notin \widehat{\mathcal{F}_n^{+s}}$, $A \notin \mathcal{F}_n^{\pm s}$ or $A \notin \widehat{\mathcal{F}_n^{\pm s}}$). Thus, it not strictly accurate to say that we can use those sets for $\mathcal{M}_n$, and the algorithms may miss some of the Δ'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 $\delta(\mathcal{P}) \to 0$, where $\delta(\mathcal{P})$ is defined by (4.1).

Tables 4.1 and 4.2 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 $\mathcal{M}_n = \mathcal{H}_n$.

Algorithm 2.1: Algorithm 2 with $\mathcal{M}_n = \mathcal{G}_n^s$ and $\widehat{\mathcal{M}_n} = \widehat{\mathcal{G}_n^s}$.

Algorithm 1.2: Algorithm 1 with $\mathcal{M}_n = \mathcal{F}_n^{+s}$.

Algorithm 2.2: Algorithm 2 with $\mathcal{M}_n = \mathcal{F}_n^{+s}$ and $\widehat{\mathcal{M}_n} = \widehat{\mathcal{F}_n^{+s}}$.

Algorithm 2.3: Algorithm 2 with $\mathcal{M}_n = \mathcal{F}_n^{\pm s}$ and $\widehat{\mathcal{M}_n} = \widehat{\mathcal{F}_n^{\pm s}}$.

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_γ lies on the boundary of the copositive cone $\mathcal{COP}_n$ when $\gamma = \omega(G)$ ($\omega(G_8) = 3$ and $\omega(G_{12}) = 4$).

We can draw the following implications from the results in Table 4.2 on page 45 for the larger graph G_{12} (similar implications can be drawn from Tables 4.1):

- 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 γ 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 3.1**. The reason may be that, as shown in Corollary 3.2.6, the set inclusion relation $\mathcal{G}_n \subseteq \mathcal{F}_n^{+s} \subseteq \mathcal{F}_n^{\pm s} \subseteq \mathcal{S}_n^+ + \mathcal{N}_n$ holds.

- Table 3.1 on page 33 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 $\mathcal{G}_n \subseteq \mathcal{F}_n^{+s} \subseteq \mathcal{F}_n^{\pm s}$ 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 γs in Table 4.2:

  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 $v^T(\gamma(E - A_G) - E)v < 0$, 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 $\mathcal{M}_n = \mathcal{F}_n^{\pm s}$ and $\widehat{\mathcal{M}_n} = \widehat{\mathcal{F}_n^{\pm s}}$ 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 [14], where the authors show the number of iterations required by their algorithm for testing copositivity of matrices of the form (4.2). 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 4.1 shows an interesting result concerning the non-convexity of the set $\mathcal{G}_n^s$, while we know that conv $(\mathcal{G}_n^s) = \mathcal{S}_n + \mathcal{N}_n$ (see Theorem 3.1.3). 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 $B_{4.0} \in \mathcal{G}_n^s$ at the first iteration for a certain orthonormal matrix P satisfying (3.4). Recall that the matrix B_γ is given by (4.2). It follows from $E - A_G \in \mathcal{N}_n \subseteq \mathcal{G}_n^s$ and from the result at $\gamma = 3.5$ in Table 4.1 that

$$0.5(E - A_G) \in \mathcal{G}_n^s \text{ and } B_{3,5} = 3.5(E - A_G) - E \in \mathcal{G}_n^s.$$

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

$$B_{4.0} = 4.0(E - A_G) - E = 0.5(E - A_G) + B_{3.5}$$

lies in the set $\mathcal{G}_n^s$ suggests that the set $\mathcal{G}_n^s = \text{com}(\mathcal{S}_n + \mathcal{N}_n)$ is not convex.

Moreover, the numerical results suggest that $\mathcal{F}_n^{\pm s}$ and $\mathcal{S}_n^+ + \mathcal{N}_n$ are different. It appear that $\mathcal{F}_n^{\pm s}$ is not convex since it is known that $\text{conv}(\mathcal{S}_n^+ \cup \mathcal{N}_n) = \mathcal{S}_n^+ + \mathcal{N}_n$ and inclusion relationship of these cones (Corollary 3.2.6).

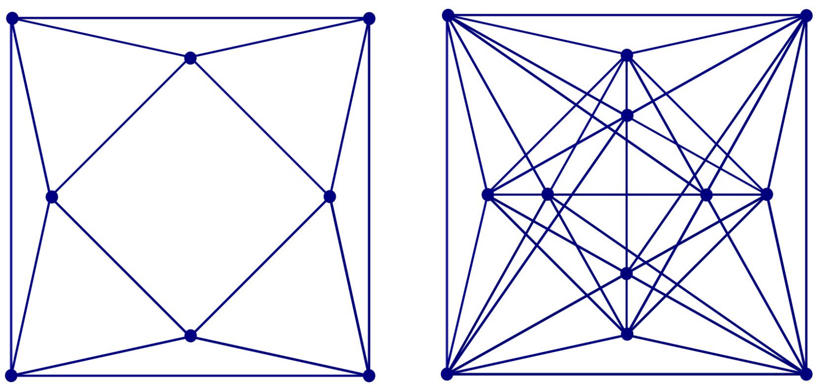

Figure 4.1: The graphs G_8 with $\omega(G_8) = 3$ (left) and G_{12} with $\omega(G_{12}) = 4$ (right).

Table 4.1: Results for G_8

	Alg. 1.1 ($\mathcal{H}_n$)		**Alg. 2.1** ($\mathcal{G}_n^s$, $\widehat{\mathcal{G}_n^s}$)		**Alg. 1.2** ($\mathcal{F}_n^{+s}$)		**Alg. 2.2** ($\mathcal{F}_n^{+s}$, $\widehat{\mathcal{F}_n^{+s}}$)		**Alg. 2.3** ($\mathcal{F}_n^{\pm s}$, $\widehat{\mathcal{F}_n^{\pm s}}$)		**Alg. 1.3** ($\mathcal{S}_n^+ + \mathcal{N}_n$)	
γ	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	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	1309	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

Table 4.2: Results for G_{12}

	Alg. 1.1 ($\mathcal{H}_n$)		**Alg. 2.1** ($\mathcal{G}_n^s$, $\widehat{\mathcal{G}_n^s}$)		**Alg. 1.2** ($\mathcal{F}_n^{+s}$)		**Alg. 2.2** ($\mathcal{F}_n^{+s}$, $\widehat{\mathcal{F}_n^{+s}}$)		**Alg. 2.3** ($\mathcal{F}_n^{\pm s}$, $\widehat{\mathcal{F}_n^{\pm s}}$)		**Alg. 1.3** ($\mathcal{S}_n^+ + \mathcal{N}_n$)	
γ	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)	Iter.	Time(s)
3.8	4084	1.162	4089	17.128	4087	24.831	4085	48.094	4075	85.390	4023	4853.335
3.9	4080	1.187	4089	17.144	4081	24.719	4079	47.219	4051	84.028	4023	5004.118
4.0	-	-	-	-	-	-	-	-	-	-	-	-
4.1	-	-	-	-	-	-	-	-	827717	18054.273	4013	5589.341
4.2	-	-	-	-	-	-	899627	14932.525	296637	5093.561	345	528.262
4.3	-	-	-	-	1024493	15985.310	469665	6007.219	102211	1559.054	39	50.717
4.4	1467851	16744.884	-	-	592539	6657.898	147363	1361.774	36937	545.801	21	26.4293
4.5	1125035	9820.911	-	-	354083	3066.114	66819	559.987	14533	213.376	17	20.961
4.6	762931	5680.756	1107483	14991.047	213485	1506.465	25675	206.767	4603	69.503	7	8.768
4.7	610071	4319.490	793739	8137.410	125747	768.224	22119	180.072	1957	30.490	3	3.809
4.8	569661	3799.361	473137	3413.271	69887	386.279	20997	176.279	645	10.347	3	4.051
4.9	407201	1834.912	232295	1231.091	39091	207.440	1969	16.716	109	1.889	1	1.221
5.0	305627	974.829	190185	859.674	21283	112.276	1213	10.501	1	0.014	1	1.189
5.1	206949	415.090	34641	113.631	12165	64.742	219	2.000	1	0.013	1	1.150
5.2	141383	172.541	1	0.004	1	0.008	1	0.008	1	0.012	1	1.120
5.3	110641	101.475	1	0.003	1	0.008	1	0.007	1	0.012	1	1.040
5.4	90877	67.681	1	0.003	1	0.008	1	0.008	1	0.012	1	1.078
5.5	44731	14.292	1	0.003	1	0.007	1	0.007	1	0.011	1	1.100
5.6	26171	5.910	1	0.004	1	0.007	1	0.007	1	0.012	1	1.000
5.7	15045	2.775	1	0.004	1	0.008	1	0.008	1	0.012	1	1.057
5.8	10239	1.705	1	0.003	1	0.007	1	0.007	1	0.012	1	1.063
5.9	6977	1.042	1	0.003	1	0.007	1	0.007	1	0.011	1	1.051
6.0	4717	0.654	1	0.006	1	0.007	1	0.008	1	0.012	1	1.119

Chapter 5

Concluding remarks

In this thesis, we studied the copositive cone and the completely positive cone. These cones have close relationships between combinatorial or quadratic optimization problems. However, solving copositive or completely positive programming is NP-hard and unfortunately it is known that even checking whether a given matrix belongs to the copositive cone is co-NP-complete. We investigated the properties of several tractable subcones of $\mathcal{COP}_n$ and summarized the results (as Figures 3.1 and 3.2). We also devised new subcones of $\mathcal{COP}_n$ by introducing the *semidefinite basis (SD basis)* defined as in Definitions 3.2.1 and 3.2.3. 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 3.2, 4.1, and 4.2 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 ± 1, and define

$$\mathcal{U}_{n,k} := \{uu^T \mid u \in U_{n,k}\}.$$

Then, as the authors indicate, the following theorem has already been proven.

Theorem 5.0.1 (Theorem 3.1 of [1], Barker and Carlson [8])**.**

$$\mathcal{D}_n = \text{cone}(\mathcal{U}_{n,k}) := \left\{ \sum_{i=1}^{|\mathcal{U}_{n,k}|} \alpha_i U_i \mid U_i \in \mathcal{U}_{n,k}, \quad \alpha_i \geq 0 \ (i = 1, \ldots, |\mathcal{U}_{n,k}|) \right\}$$

From the above theorem, we can see that for the SDP bases $\mathcal{B}_+(p_1, p_2, \cdots, p_n)$ in (3.15), $\mathcal{B}_-(p_1, p_2, \cdots, p_n)$ in (3.21) and n-dimensional unit vectors $e_1, e_2, \cdots, e_n$, the following set inclusion relation holds:

$$\mathcal{B}_+(e_1, e_2, \cdots, e_n) \cup \mathcal{B}_-(e_1, e_2, \cdots, e_n) \subseteq \mathcal{D}_n = \text{cone}(\mathcal{U}_{n,k}).$$

These sets should be investigated in the future.

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