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Copositive programming: separation and relaxations

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COPOSITIVE PROGRAMMING: SEPARATION AND RELAXATIONS

by

Hongbo Dong

An Abstract

Of a thesis submitted in partial fulfillment of the
requirements for the Doctor of Philosophy
degree in Applied Mathematical and
Computational Sciences in the
Graduate College of The
University of Iowa

December 2011

Thesis Supervisors: Professor Kurt M. Anstreicher
Associate Professor Samuel A. Burer

ABSTRACT

A large portion of research in science and engineering, as well as in business, concerns one similar problem: how to make things "better"? Once properly modeled (often a highly nontrivial task), this kind of question can be approached via a mathematical optimization problem. An optimal solution to a mathematical optimization problem, when interpreted properly, might correspond to new knowledge, effective methodology or good decisions in the corresponding application area. As already proved in many success stories, research in mathematical optimization has a significant impact on numerous aspects of human life.

Recently, it was discovered that a large number of difficult optimization problems can be formulated as copositive programming problems. Famous examples include a large class of quadratic optimization problems as well as many classical combinatorial optimization problems. For some more general optimization problems, copositive programming provides a way to construct tight convex relaxations. Because of this generality, new knowledge of copositive programs has the potential of being uniformly applied to these cases.

While it is provably difficult to design efficient algorithms for general copositive programs, we study copositive programming from two standard aspects, its relaxations and its separation problem. With regard to constructing computationally tractable convex relaxations for copositive programs, we develop direct constructions of two tensor relaxation hierarchies for the completely positive cone, which is a fundamental geometric object in copositive programming. We show the connection of our relaxation hierarchies with known hierarchies. Then we consider the application of these tensor relaxations to the maximum stable set problem.

With regard to the separation problem for copositive programming, we first prove some new results in low dimensions of 5×5 matrices. Then we show how a separation procedure for this low dimensional case can be extended to any symmetric matrix with a certain block structure.

Last but not least, we provide another approach to separation and relaxation for the (generalized) completely positive cone. We prove some generic results, and discuss applications to the completely positive case and another case related to box-constrained quadratic programming. Finally, we conclude the thesis with remarks on some interesting open questions in the field of copositive programming.

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CERTIFICATE OF APPROVAL

PH.D. THESIS

This is to certify that the Ph.D. thesis of

Hongbo Dong

has been approved by the Examining Committee for the thesis requirement for the Doctor of Philosophy degree in Applied Mathematical and Computational Sciences at the December 2011 graduation.

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To my parents and my wife

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A large portion of research in science and engineering, as well as in business, concerns one similar problem: how to make things “better”? Once properly modeled (often a highly nontrivial task), this kind of question can be approached via a mathematical optimization problem. An optimal solution to a mathematical optimization problem, when interpreted properly, might correspond to new knowledge, effective methodology or good decisions in the corresponding application area. As already proved in many success stories, research in mathematical optimization has a significant impact on numerous aspects of human life.

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application of these tensor relaxations to the maximum stable set problem.

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CHAPTER 1
INTRODUCTION TO COPOSITIVE PROGRAMMING

1.1 Copositive Programming: An Outline

The central problem studied in mathematical programming (or mathematical optimization) can be written as:

$$\nu = \inf_{x \in \Re_n} \{f_0(x) : f_i(x) \leq 0, i = 1, ..., m\}, \tag{1.1}$$

where $f_0(\cdot)$ is called the *objection function* and $\{x : f_i(x) \leq 0, i = 1, ..., m\}$ is called the *feasible set*. The main focus is on developing and analyzing computational algorithms that build approximate solutions to (1.1). The field was formally established in 1947, when George Dantzig created the *simplex method* for *Linear Programming*, the first important type of math programs where $f_i(\cdot)$ in (1.1) are all linear functions. In the same year, John von Neumann invented the *duality theory* of linear programming, which is another fundamental concept in mathematical programming. The impact of the simplex method cannot be overstated. It was generally acknowledged to be one of the best algorithms in the 20th century that has changed the world.

Throughout this thesis we focus on a special class of mathematical programs, called *linear conic programs* (LCPs). An LCP has a linear objective function, and its feasible set is the intersection of an affine space with a closed *convex cone*. Formally, let $\Re_n$ denote n-dimensional Euclidean space, associated with standard inner product. A closed convex cone $\mathcal{K}$ is a closed subset of $\Re_n$ such that for any $x, y \in \mathcal{K}$ and nonnegative scalar α, β, $\alpha x + \beta y \in \mathcal{K}$. With provided problem data $c \in \Re_n$, $b \in \Re_m$, and a linear operator $\mathcal{A} : \Re_n \longmapsto \Re_m$, an LCP takes the following form:

$$\nu_* := \inf_x \left\{ c^T x : \mathcal{A}(x) = b,\ x \in \mathcal{K} \right\}. \tag{1.2}$$

Its conic dual problem is

$$\nu^* := \sup_y \left\{ b^T y : c - \mathcal{A}^*(y) \in \mathcal{K}^* \right\}, \tag{1.3}$$

where $\mathcal{A}^* : \Re_m \longmapsto \Re_n$ is the adjoint operator of $\mathcal{A}$, and $\mathcal{K}^* := \{z \in \Re_n : \langle z, x\rangle \geq 0, \forall x \in \mathcal{K}\}$ is called the dual cone of $\mathcal{K}$. First for any $\bar{x}$ feasible in (1.2) and $\bar{y}$ feasible in (1.3), $c^T\bar{x} - b^T\bar{y} = \langle \bar{x}, c\rangle - \langle \mathcal{A}(\bar{x}), \bar{y}\rangle = \langle \bar{x}, c\rangle - \langle \bar{x}, \mathcal{A}^*(\bar{y})\rangle = \langle \bar{x}, c - \mathcal{A}^*(\bar{y})\rangle \geq 0$. Hence $\nu^* \leq \nu_*$, and this is called *weak duality* of LCPs. Further under the assumption of some *constraint qualification*, (1.2) and (1.3) can be shown to have *strong duality*, i.e., $\nu^* = \nu_*$. One frequently used constraint qualification is *strict feasibility*, also called the *Slater condition*, i.e., (1.2) and (1.3) satisfy the Slater condition if $\exists\, \bar{x}, \bar{y}$ such that $\mathcal{A}(\bar{x}) = b$, while $\bar{x} \in \text{relint}(\mathcal{K})$ and $c - \mathcal{A}^*(\bar{y}) \in \text{relint}(\mathcal{K}^*)$, where $\text{relint}(\cdot)$ denotes relative interior points, that is, all interior points of the enclosed set when the set is regarded as a subset of its affinely spanned subspace.

LCP includes three important, and well-studied classes of mathematical programs. These are, (1) when $\mathcal{K} = \Re_n^+$, the nonnegative orthant, LCP amounts to classical Linear Programming (LP), which is a very mature area on its own; (2) when $\mathcal{K}$ is the *Second Order Cone*, $\left\{x \in \Re_n : x_1 \geq \sqrt{x_2^2 + ... + x_n^2}\right\}$, LCP amounts to Second Order Cone Programming (SOCP) [2]; (3) when $\mathcal{K}$ is the cone of all $n \times n$ real symmetric positive semidefinite matrices, it is called Semidefinite Programming (a.k.a SDP, see [1, 75] for an introduction). Much research has been focused on the theory and applications of each of these three cases.

The main topic of this thesis, *copositive programming*, is another type of LCP, where $\mathcal{K}$ is the *completely positive cone*. (We will define this term soon, and impatient readers are directed to (1.4).) The name copositive programming was coined only about one decade ago [12]. Since then, we have seen active and fruitful research in this area. The research on copositive programming has tight connections with combinatorial optimization and polynomial programming and involves machinery not only from traditional continuous optimization and convex analysis, but also, from very unexpected directions such as algebraic geometry.

Copositive programming can be seen as a convexification approach for nonconvex quadratic programs. The general quadratically constrained quadratic programming problem has a copositive relaxation, which is shown to be no weaker, and sometimes strictly tighter, than the relaxation constructed by a convex lower envelop strategy [4]. In many cases, nonconvex optimization problems admit exact copositive formulation (see Section 1.2).

Now we formally define a copositive program. A copositive program is an LCP (1.2) where $\mathcal{K}$ is the *completely positive cone*, defined as follows. Let $\mathcal{S}_n$ be the vector space of all $n \times n$ real symmetric matrices. The completely positive cone $\mathcal{C}_n$ is

$$\mathcal{C}_n := \operatorname{conv}\left\{xx^T : x \in \Re_n^+\right\}, \tag{1.4}$$

where $\operatorname{conv}(\cdot)$ is the convex hull operator, i.e., $\mathcal{C}_n$ is the smallest convex set in $\mathcal{S}_n$ that contains all matrices of form xx^T where $x \in \Re_n^+$. The dual cone of $\mathcal{C}_n^*$ is called the *copositive cone*, defined as,

$$\begin{aligned}\mathcal{C}_n^* &:= \left\{Q \in \mathcal{S}_n : x^T Q x \geq 0, \forall x \in \Re_n^+\right\} \\ &= \left\{Q \in \mathcal{S}_n : \langle Q, X\rangle \geq 0, \forall X \in \mathcal{C}_n\right\}.\end{aligned}$$

Throughout this thesis, whenever the dimension is clear from context or not important for our analysis, we omit the dimension and only write $\mathcal{C}$ and $\mathcal{C}^*$ for simplicity.

Unlike the cases of LP/SOCP/SDP, copositive programming is not polynomially solvable and contains NP-hard instances. (Loosely speaking, a mathematical program is polynomially solvable if there exists an algorithm that computes a "near-optimal" solution within a polynomial number of real arithmetic operations, with respect to the input data size. See, for example, Section 1.2 in [60] for formal definitions and discussion.) This is illustrated by the fact that many NP-hard problems have **exact** copositive programming formulations (we review some such results in Section 1.2). Hence solving the general copositive programs is no easier than solving these NP-hard problems.

However even partial information about $\mathcal{C}$ and $\mathcal{C}^*$ could help solving general copositive programs. One approach is to study computationally tractable approximations for $\mathcal{C}$ and $\mathcal{C}^*$. By replacing $\mathcal{C}$ and $\mathcal{C}^*$ with tractable approximation sets, we obtain efficiently computable LCPs that are approximations for the original copositive programs. Several *hierarchies* of approximation cones exist for $\mathcal{C}$ and $\mathcal{C}^*$. Each hierarchy comprises a sequence of approximation cones, one tighter than the previous and in some sense, exact in the limit. Therefore, from a theoretical point of view, with sufficient computational time and resource, it is possible to solve any copositive program to arbitrary precision. In Section 1.3, we provide a brief review of approximation cones for $\mathcal{C}$ or $\mathcal{C}^*$. Later in Chapter 2, we construct two new approximation hierarchies for $\mathcal{C}$ by using symmetric tensors, and prove duality connections with some known approximation hierarchies.

In practice, one difficulty of applying the full approximation hierarchies for $\mathcal{C}^*$ is that tighter the approximations are computationally more expensive. Usually the cost increases very fast and quickly becomes impractical. A natural alternative is to iteratively add valid linear inequalities (cuts) to improve approximations/relaxations. This kind of approach has been widely employed in the practice of solving mixed-integer linear programs [26]. In order to generate cuts, one would need to repeatedly solve the separation problem for the completely positive cone $\mathcal{C}$, which is stated as follows:

$$\text{Given } \bar{X} \in \mathcal{S}, \text{ either determine } \bar{X} \in \mathcal{C} \text{ or find } M \in \mathcal{S},$$
$$s.t., \ \langle M, \bar{X} \rangle < 0, \text{ and } \forall X \in \mathcal{C}, \langle M, X \rangle \geq 0.$$

Chapter 3 and 4 contain two approaches for this separation problem.

Recently, iterative schemes to solve copositive programs have emerged as an interesting research direction. One such work [21] focuses on the low dimensional case of $n = 5$. Another paper [13] is specific to one particular problem (max-clique), and does not apply to general copositive programs. One promising approach has appeared in polynomial optimization, and the interested reader is directed to a recent PhD thesis [39]. A different approach to dynamically refining an approximation of $\mathcal{C}^*$ is taken in [17].

A disclaimer is that this chapter is not intended to serve as a comprehensive survey. There are absolutely important results that we do not mention. Several surveys for copositive programming have appeared recently [33, 9]. The article [10] contains a bibliography of various aspects of copositive programming.

1.1.1 Basic properties of the completely positive cone and its dual cone

In this subsection we review some basic properties of the completely positive (CP) cone $\mathcal{C}$ and its dual cone $\mathcal{C}^*$. We also review some basic convex analysis concepts whenever necessary. Interested readers are referred to the monograph by Berman and Shaked-Monderer [7] for more algebraic properties of CP matrices. We also suggest a recent article in *SIAM Review* [46] for a survey on copositive matrices.

Other than the definition given in (1.4), the set of $n \times n$ completely positive matrices $\mathcal{C}_n$ is equivalently defined as:

$$\mathcal{C}_n := \left\{ X \in \mathcal{S}_n : \exists \text{ integer } k \geq 0, B \in \mathcal{M}_{n\times k}, B \geq 0, \ s.t. \ X = BB^T \right\}, \qquad (1.5)$$

where $\mathcal{S}_n$ is the set of all symmetric matrices and $\mathcal{M}_{n\times k}$ the set of all real $n \times k$ matrices. $B \geq 0$ means B is elementwise nonnegative. Note that the conditions $x \in \Re_n^+$ in (1.4) and $B \geq 0$ in (1.5) are crucial because without them both definitions reduce to the definition of positive semidefinite matrices.

This definition of $\mathcal{C}_n$ naturally suggests a CP factorization. Given a matrix $X \in \mathcal{C}_n$, the minimum number k such that X admits the factorization in (1.5) is called the *cp-rank* of X. It follows immediately that the cp-rank of X is always greater than or equal to $rank(X)$. The following matrix is an example where its cp-rank is strictly greater than its rank.

Example 1.1.1. [7, Example 3.1] Let

$$X = \begin{pmatrix} 6 & 3 & 3 & 0 \\ 3 & 5 & 1 & 3 \\ 3 & 1 & 5 & 3 \\ 0 & 3 & 3 & 6 \end{pmatrix},$$

where $rank(X) = 3$. However the cp-rank of X is 4. (See [7, Page 140-141] for a proof.)

It is well known that the rank of an $n \times n$ matrix is always no greater than n. Unfortunately this is not the case for cp-rank. Using Carathéodary's theorem, one can show that the cp-rank of an $n \times n$ CP matrix is always finite, and less than or equal to $\frac{n(n+1)}{2} + 1$. (Note that $\mathbf{dim}(\mathcal{S}_n) = \frac{n(n+1)}{2}$.) A slightly tighter general upper bound for cp-rank is $\frac{n(n+1)}{2} - 1$. It is still an open question whether this is the best upper bound in general [7, Section 3.3]. For some subsets of $\mathcal{C}_n$, there exists a better upper bound, $\frac{n^2}{4}$ [32].

Geometrically, $\mathcal{C}_n$ and $\mathcal{C}_n^*$ are both closed, convex cones in $\mathcal{S}_n$. Further, they are both *pointed* (do not contain any linear subspace of $\mathcal{S}_n$), and *full-dimensional* (the smallest linear hyperplane that contains $\mathcal{C}_n$ or $\mathcal{C}_n^*$ is $\mathcal{S}_n$). Without surprise, the set of all extreme rays of $\mathcal{C}_n$ is $\{xx^T : x \in \Re_n^+\}$. An extremal characterization of $\mathcal{C}_n^*$ is generally unknown. Actually, even for low dimension $n = 5$, a full characterization of all extreme rays of $\mathcal{C}_5^*$ has remained unkown until recently [45].

Let $\mathcal{S}_n^+$ denote the cone of $n \times n$ symmetric positive semidefinite matrices and $\mathcal{N}_n$ denote the cone of element-wise nonnegative $n \times n$ real symmetric matrices. We define $\mathcal{D}_n := \mathcal{S}_n^+ \cap \mathcal{N}_n$. This is usually called the cone of *doubly nonnegative (DNN) matrices*, since these matrices are nonnegative in both element-wise and spectral sense. It is easy to see that any CP matrix satisfies these two conditions, hence $\mathcal{C}_n \subseteq \mathcal{D}_n$. In small dimension, these two sets are exactly the same:

Theorem 1.1.1 ([56])**.** *$\mathcal{C}_n = \mathcal{D}_n$ if and only if $n \leq 4$.*

$\mathcal{D}_n$ is also a closed convex cone. On the dual side, we have $\mathcal{D}_n^* = \mathcal{S}_n^+ + \mathcal{N}_n$, i.e., the set of all matrices that can be represented as a summation of a positive semidefinite and elementwise nonnegative matrix. Then $\mathcal{C}_n^* \supseteq \mathcal{D}_n^*$ and equality holds if and only if $n \leq 4$.

It is worth mentioning here that $\mathcal{D}_n$ is an important approximation cone for $\mathcal{C}_n$. By replacing $\mathcal{C}_n$ in a copositive program with $\mathcal{D}_n$, one ends up with the DNN relaxation for the copositive program. Sometimes the structure of $\mathcal{D}_n$ can be exploited to design efficient algorithms to solve the DNN relaxation [20].

Given a matrix $X \in \mathcal{S}_n$, we associate an undirected loopless graph $\mathcal{G}(X)$ with n nodes labeled 1 through n, and edge set $\{(i, j) : i \neq j, X_{ij} \neq 0\}$. A loopless undirected graph G with n nodes is called a *completely positive (CP) graph* if and only if $\forall X \in \mathcal{D}_n$, $\mathcal{G}(X) = G$ implies $X \in \mathcal{C}_n$. In other words, a graph of n nodes, G, is not a CP graph if and only if there exists $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ such that $G = \mathcal{G}(X)$. An interesting theorem provides a characterization for CP graphs [51].

Theorem 1.1.2 ([51])**.** *A loopless, undirected graph on n vertices is a CP graph if and only if it contains no odd cycle of length 5 or greater.*

This theorem has a nice geometric interpretation. For a convex cone $\mathcal{K}$, a *face* $\mathcal{F}$ is a subset of $\mathcal{K}$ such that $\forall x, y \in \mathcal{K}, x + y \in \mathcal{F}$ implies $x, y \in \mathcal{F}$. For a given graph with n nodes, G, two sets defined as:

$$\begin{aligned} \mathcal{F}(G, \mathcal{D}_n) &:= \{X \in \mathcal{D}_n, \mathcal{G}(X) = G\} \\ \mathcal{F}(G, \mathcal{C}_n) &:= \{X \in \mathcal{C}_n, \mathcal{G}(X) = G\} \end{aligned}$$

are faces of $\mathcal{D}_n$ and $\mathcal{C}_n$ respectively, and naturally $\mathcal{F}(G, \mathcal{C}_n) \subseteq \mathcal{F}(G, \mathcal{D}_n)$. Theorem 1.1.2 says these faces match, i.e., $\mathcal{F}(G, \mathcal{C}_n) = \mathcal{F}(G, \mathcal{D}_n)$, if and only if G is a CP graph.

1.1.2 General notation and terminology

Throughout this thesis, capital letters will indicate matrices; lower-case letters will indicate vectors or scalars. We use $\Re_n$ and $\mathcal{M}_{n\times m}$ to denote the Euclidean spaces of n-dimensional column vectors and $n \times m$ real matrices, respectively. $\mathbb{Z}$ is the set of all integers, $\mathbb{Z}_+$ is all nonnegative integers, and $\mathbb{Z}^n_+$ denotes all n-tuples of nonnegative integers. Given a vector $x \in \Re_n$, x_i means the i-th entry of x. For a matrix $M \in \mathcal{M}_{n\times m}$, M_{ij} or $M(i, j)$ is the entry in the i-th row and j-th column. All indices start from 1 unless otherwise stated.

At many places in this thesis we focus on square matrices. We use $\mathcal{M}_n$ to mean $\mathcal{M}_{n\times n}$. $\mathcal{S}_n$ is used to denote all $n \times n$ real symmetric matrices. The n-dimensional Euclidean space $\Re_n$ is endowed with the usual inner product $\langle x, y\rangle :=$

$x^T y$, and $\mathcal{M}_{n\times m}$ is endowed with the trace inner product $\langle X, Y\rangle := \text{trace}(XY^T)$. Sometimes we use $X \bullet Y$ to represent $\langle X, Y\rangle$. $X \circ Y$ is the Hadamard product that has entries $(X \circ Y)_{ij} = X_{ij}Y_{ij}$. In $\mathcal{S}_n$, the inner product reads $\langle X, Y\rangle := \text{trace}(XY^T) = \text{trace}(XY)$. Regarding matrix concatenation, we use the Matlab-style that a comma "," indicates horizontal concatenation, while a semicolon ";" indicates vertical concatentation.

$\mathcal{S}_n^+$ is used to denote the set of all $n \times n$ symmetric positive semidefinite matrices. As in the SDP literature, we use $X \succeq 0$ to represent the condition that $X \in \mathcal{S}_n^+$. $X \geq 0$ and $x \geq 0$ mean that matrix X and vector x are element-wise nonnegative. E and e denote a matrix and a vector with all entries 1, respectively. Also, I denotes the identity matrix. Dimensions of these vectors and matrices will typically be clear from context.

For a vector $v \in \Re_n^+$, $\sqrt{v}$ is the vector whose ith component is $\sqrt{v_i}$. For $x \in \Re^n$ and $X \in \mathcal{M}_n$, $\text{Diag}(x)$ is the diagonal matrix with $\text{Diag}(x)_{ii} = x_i$ and $\text{diag}(X)$ is the vector with $x_i = X_{ii}$. For set $S \subseteq \Re_n$, we use $\text{conv}\{S\} := \{x : x = \sum_i \lambda_i s_i, s_i \in S, \sum_i \lambda_i = 1, \lambda_i \geq 0, \forall i\}$ to denote the convex hull of S. Again the summation in the definition can be assumed to include at most $n + 1$ terms by Carathéodory's theorem. The set $\text{relint}(S)$ is the relative interior of S.

Throughout this thesis, sometimes we use the abbreviation "CP" as "completely positive". Finally, note that some chapter-specific notations will be explained in each chapter separately.

1.2 Copositive Representations of Optimization Problems

Representation results constitute an important part in current copositive programming research. Thanks to these results, new knowledge concerning $\mathcal{C}$ and $\mathcal{C}^*$ has the potential of being uniformly applied to many NP-hard problems. In this section we review some of these representation results. In the first subsection we do so for some specific optimization problems. Then in the second subsection we explain a procedure proposed by Burer [18, 19] for a large class of binary/continous nonconvex quadratic optimization problems.

1.2.1 Some copositive representation results

To the best of the author's knowledge, the very first copositive representation result appeared in [12]. The authors considered the standard quadratic programming problem

$$\nu_* = \min_x \left\{ x^T Q x : \sum_{i=1}^n x_i = 1, x \in \Re_n^+ \right\}, \tag{1.6}$$

where Q is not assumed to be positive semidefinite. Note this problem is NP-hard in general [49]. The authors proved it has the following exact copositive formulation:

$$\nu_* = \min_X \left\{ \langle Q, X \rangle : \langle E, X \rangle = 1, X \in \mathcal{C}_n \right\}, \tag{1.7}$$

then used this formulation to define primal-dual affine-scaling directions in order to escape from local optimal points where a local algorithm for (1.6) got trapped. In a later paper [11], it was shown that by relaxing the constraint $X \in \mathcal{C}_n$ with approximation hierarchies for $\mathcal{C}_n$, one obtains polynomial-time approximation schemes (PTAS) for the standard quadratic programming problem.

A related problem arising from graph theory is the *maximum stable set* problem. Given a loopless undirected graph $\mathcal{G}$ with n nodes, a *stable set* is a subset of

$\mathcal{V}(\mathcal{G})$, the vertex set of $\mathcal{G}$, that induces a subgraph with no edge. The maximum stable set problem asks for the largest cardinality of a stable set in $\mathcal{G}$. This cardinality is usually called the *stability number* of $\mathcal{G}$ and denoted by $\alpha(\mathcal{G})$. It is well known that determining $\alpha(\mathcal{G})$ is an NP-complete problem [38] and can be formulated as a standard quadratic programming problem [57]:

$$\frac{1}{\alpha(\mathcal{G})} = \min_x \left\{ x^T(I + A_{\mathcal{G}})x : \sum_{i=1}^n x_i = 1, x \in \Re_n^+ \right\},$$

where $A_{\mathcal{G}}$ is the incidence matrix of graph $\mathcal{G}$, i.e., $A_{\mathcal{G}}(i,j) = 1$ if $(i,j) \in \mathcal{E}(\mathcal{G})$, the edge set of $\mathcal{G}$, otherwise $A_{\mathcal{G}}(i,j) = 0$. By using the previous result, it can be exactly formulated as a copositive program in the form of (1.7), and a PTAS is available for computing $\frac{1}{\alpha(\mathcal{G})}$. (However this scheme is not a PTAS for computing $\alpha(\mathcal{G})$.)

A different copositive formulation for computing $\alpha(\mathcal{G})$ is the following [27]:

$$\alpha(\mathcal{G}) = \max_X \left\{ \langle E, X \rangle : X_{ij} = 0, \forall (i,j) \in \mathcal{E}(\mathcal{G}), \mathrm{trace}(X) = 1, X \in \mathcal{C}_n \right\}.$$

Again by replacing $\mathcal{C}_n$ with its approximation hierarchies, de Klerk and Pasechnik [27] constructed a sequence of lifted optimization problems whose optimal values reach the exact $\alpha(\mathcal{G})$ after at most $\alpha(\mathcal{G})^2$ number of liftings. Compared to Lovász and Schrijver's lift-and-project procedure [55], this approach requires fewer liftings when $\alpha(\mathcal{G}) < O(\sqrt{n})$.

Another combinatorial NP-complete problem that admits an exact copositive programming formulation is the Min-cut tri-partitioning problem [64]. Given an undirected graph $\mathcal{G}$ with node set $\mathcal{V}(\mathcal{G})$ and positively weighted edges $a_{ij} > 0$, $\forall (i,j) \in \mathcal{E}(\mathcal{G})$, the problem asks for a partition $\{S_1, S_2, S_3\}$ of $\mathcal{V}(\mathcal{G})$, with fixed cardinalities $m_1 + m_2 + m_3 = n$, such that the weight of edges across S_1 and S_2, $\sum_{i \in S_1, j \in S_2} a_{ij}$, is minimal. This problem is a special case of the general graph partitioning problem, and closely related with *bandwidth minimization* and *vertex separator* problems (see [44] and reference therein). Povh and Rendl [64] proved an exact copositive programming formulation for the Min-cut tri-partitioning problem, and by relaxing the completely positive constraint, obtained a sequence of semidefinite relaxations. The authors also proved one associated semidefinite relaxation is equivalent to the spectral relaxation introduced by Helmberg [44].

In [65], the notoriously difficult and heavily-studied Quadratic Assignment Problem (QAP) was also proved to admit a copositive formulation. Two other examples without a combinatorial nature are: Fractional Quadratic Optimization [3], and a mixed binary linear programs with stochastic objective function [59].

1.2.2 A procedure for nonconvex quadratic programming problems

In this section we briefly review a general procedure proposed by Burer [18] that constructs exact copositive formulations for linear equality constrained nonconvex quadratic programs, with binary/continuous variables, and (possibly) linear complementarity constraints. This subsection is based on two of Burer's papers [18, 19]. However, we postpone the discussion of the generalized copositivity/completely positivity in [19] to Section 1.4.

Consider the following linear constrained nonconvex quadratic program:

$$\nu_* = \min_x \left\{ x^T Q x + 2c^T x : Ax = b, x \in \Re^+_n \right\}, \tag{1.8}$$

where $Q \in \mathcal{S}_n$ is not positive semidefinite, $A \in \mathcal{M}_{n\times m}$ and $b \in \Re_n$. The author proved it is equivalent to the following copositive program:

$$\nu^* = \min_Y \left\{ \left\langle \begin{pmatrix} 0 & q^T \\ q & Q \end{pmatrix}, \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \right\rangle : \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}_{n+1}, \begin{array}{c} Ax = b, \\ \operatorname{diag}(AXA^T) = b \circ b \end{array} \right\}. \tag{1.9}$$

Additionally, the author proved that, under certain conditions, one can incorporate some quadratic equality constraints into (1.8) while maintaining the exact copositive representation. Specifically, consider problem (1.8) with a finite number of additional constraints: $\{x^T H_i x + 2h_i^T x = \phi_i (i = 1, ..., r)\}$. As long as the following three conditions are satisfied, to obtain an exact copositive formulation for this augmented problem it suffices to add linear constraints $\left\{\langle H_i, X\rangle + 2h_i^T x = \phi_i (i = 1, ..., r)\right\}$ into (1.9). These three key conditions are:

1. $\exists\, \bar{x}$ that is feasible in (1.8), satisfies all quadratic constraints $\{\bar{x}^T H_i \bar{x} + 2h_i^T \bar{x} = \phi_i (i = 1, ..., r)\}$ and satisfies $(H_i \bar{x} + h_i)^T d = 0$ for all i and $d \in \{d \in \Re_n^+ : Ad = 0\}$;

2. For $i = 1, ..., r,\ \phi_i = \min_x \{x^T H_i x + 2h_i^T x : Ax = b, x \in \Re_n^+\}$;

3. For $i = 1, ..., r,\ \max_x \{x^T H_i x + 2h_i^T x : Ax = b, x \in \Re_n^+\} < +\infty$.

These conditions may seem artificial, however, they do incorporate some important cases. If the feasible region of (1.8) is bounded, then the first condition is trivial to satisfy. One successful story of employing these three conditions is to deal with binary constraints $x_i^2 - x_i = 0 \Leftrightarrow x_i \in \{0, 1\}$ and linear complementarity constraints $x_i x_j = 0$ for some $1 \leq i \neq j \leq n$. The influential paper by Burer [18] contains the details of these two cases.

1.3 Approximation Hierarchies

Since $\mathcal{C}$ and $\mathcal{C}^*$ are computationally intractable in general, it is natural to study their tractable inner/outer approximations. Perhaps the most well known (and frequently used) hierarchies are sequences of inner approximations for $\mathcal{C}^*$, constructed in light of Pólya's Theorem [43, Section 2.24]. In this section, we review three such hierarchies. Later in Chapter 2, we propose two new outer approximation hierarchies for $\mathcal{C}$, and show that they are closely related with some approximation hierarchies reviewed in this section.

A polynomial $P(x)$, where x is a vector of variables $x = [x_1, ..., x_n]^T$, is said to be *nonnegative* if $P(x) \geq 0$ for all $x \in \mathbb{R}_n$. Throughout this section, we focus on *homogeneous* polynomials, which are polynomials with terms of the same degree. A necessary condition for a polynomial to be nonnegative is that it has even degree. Following the common notations used in literature (for example [53]), we use $\mathbb{R}[x]_d$ to denote the set of all n-variate homogeneous polynomials of degree d, and $\mathcal{P}_{2d}$ to denote the set of all n-variate nonnegative polynomials in $\mathbb{R}[x]_{2d}$. In this section we assume n is fixed, and avoid using n in our notation whenever appropriate. The topology on $\mathbb{R}[x]_d$ is defined by treating coefficients of each polynomial as a real vector, with a fixed ordering of all the monomials. $\mathbb{I}(d)$ is used to denote the set of vectors that represent exponents of a monomial in $\mathbb{R}[x]_d$, i.e., $\mathbb{I}(d) := \{\beta \in \mathbb{Z}_n^+ : \sum_{i=1}^n \beta_i = d\}$.

The starting point for constructing approximations for $\mathcal{C}^*$ is usually the following observation, where one represents the copositivity of a matrix in terms of nonnegativity of a homogeneous polynomial. For given M, let

$$P^{(0)}(x) := (x \circ x)^T M(x \circ x) = \sum_i M_{ij} x_i^2 x_j^2 \tag{1.10}$$

Observation. A symmetric $n \times n$ matrix M is copositive if and only if $P^{(0)}(x)$ is in $\mathcal{P}_4$.

One sufficient condition for $P^{(0)}(x)$ to be nonnegative is that all its coefficients are nonnegative. This leads to an inner approximation for the copositive cone $\mathcal{C}^*$, the set of all real symmetric elementwise nonnegative matrices:

$$\begin{aligned} \mathcal{L}^0 &:= \left\{M \mid P^{(0)}(x) \textit{ as in } (1.10) \textit{ has nonnegative coefficients}\right\} \\ &= \{M \mid M(i,j) \geq 0, \forall i,j\} = \mathcal{N} \subseteq \mathcal{C}^*. \end{aligned}$$

A weaker sufficient condition for a homogeneous polynomial $p(x) \in \mathbb{R}[x]_{2d}$ to be nonnegative is to be a sum of squares (s.o.s), i.e., $\exists$ polynomials $h_i(x)$, $i = 1, ..., l$ such that $p(x) = \sum_{i=1}^{l} h_i(x)^2$. It is known that we can assume without loss of generality that $h_i(x) \in \mathbb{R}[x]_d$ and homogeneous [14, Lemma 2.1]. We use Σ_{2d} to denote all s.o.s. polynomials in $\mathbb{R}[x]_{2d}$. Then Σ_{2d} is a closed convex cone for fixed d [66, 69, 53]. By using this s.o.s. sufficient condition, another inner approximation of the copositive cone $\mathcal{C}^*$ can be defined as follows:

$$\mathcal{K}^0 := \left\{ M \mid P^{(0)}(x) \in \Sigma_4,\ \textit{where } P^{(0)}(x) \textit{ is defined in } (1.10) \right\} \subseteq \mathcal{C}^*.$$

It was proved by Parrilo [62] that $\mathcal{K}^0$ is exactly the dual of the doubly nonnegative cone $\mathcal{D}$:

$$\mathcal{K}^0 = \mathcal{D}^* = \mathcal{S}^+ + \mathcal{N}.$$

To obtain a full approximation hierarchy, for $r \in \mathbb{Z}_+$, define the polynomial $P^{(r)}(x)$ as follows:

$$P^{(r)}(x) := P^{(0)}(x) \left(\sum_{i=1}^{n} x_i^2 \right)^r = \sum_{i,j=1}^{n} M_{ij} x_i^2 x_j^2 \left(\sum_{i=1}^{n} x_i^2 \right)^r . \tag{1.11}$$

Then two sequence of sets are defined as [62, 27]:

$$\begin{aligned} \mathcal{L}^r &:= \left\{ M \mid P^{(r)}(x) \textit{ has nonnegative coefficients} \right\}, \\ \mathcal{K}^r &:= \left\{ M \mid P^{(r)}(x) \in \Sigma_{2r+4} \right\}. \end{aligned}$$

It is easy to see by definition that $\mathcal{L}^r \subseteq \mathcal{K}^r$, $\forall r \in \mathbb{Z}_+$. Further this gives two inner approximation hierarchies of $\mathcal{C}^*$:

$$\mathcal{N} = \mathcal{L}^0 \subseteq \mathcal{L}^1 \subseteq \cdots \subseteq \mathcal{L}^r \subseteq \mathcal{L}^{r+1} \subseteq \cdots \subseteq \mathcal{C}^*,$$

$$\mathcal{D}^* = \mathcal{K}^0 \subseteq \mathcal{K}^1 \subseteq \cdots \subseteq \mathcal{K}^r \subseteq \mathcal{K}^{r+1} \subseteq \cdots \subseteq \mathcal{C}^*.$$

Obviously $\mathcal{K}^r$ is a convex cone, and in fact it is also closed. To see this, first let $\mathcal{F}^{(r)} : \mathcal{S}_n \longmapsto \mathbb{R}[x]_{2r+4}$ denote the linear operator that maps M to $P^{(r)}(x)$ as in (1.11). Its image is a (finite dimensional) linear subspace of $\mathbb{R}[x]_{2r+4}$. Now since Σ_{2r+4} is closed in $\mathbb{R}[x]_{2r+4}$, $\mathcal{K}^r$ is the preimage of a closed set in $\mathbb{R}[x]_{2r+4}$, hence closed.

In [63], the authors introduced a new class of semidefinite inner approximations $\{\mathcal{Q}^r\}_{r=0}^{\infty}$ of the copositive cone $\mathcal{C}^*$. To simplify notation we use z to represent the vector $(x \circ x)$, i.e., for $\beta \in \mathbb{I}_n(r)$, $z^\beta = x^{2\beta}$. A set of polynomials $\mathcal{E}^r \subseteq \mathbb{R}[z]_{r+2}$ is defined as:

$$\mathcal{E}^r := \left\{ \sum_{\beta \in \mathbb{I}_n(r), |\beta| = r} z^\beta z^T (P_\beta + N_\beta) x : P_\beta \in \mathcal{S}^+, N_\beta \in \mathcal{N} \right\},$$

Then $\forall r \in \mathbb{Z}_+$, the approximation cone $\mathcal{Q}^r$ is:

$$\mathcal{Q}^r := \left\{ M \,\middle|\, \left(\sum_{i=1}^n z_i \right)^r z^T M z \in \mathcal{E}^r \right\}. \tag{1.12}$$

$\mathcal{Q}^r$ is a convex cone, and in fact also closed. In [63] the authors mentioned that the closedness of $\mathcal{Q}^r$ follows an easy limit argument. However, after some private communication with one of the authors, it appears the proof is actually a little less straightforward. We provide another proof here by using a theorem in convex analysis.

The key step is to show that $\mathcal{E}^r$ is a closed subset of $\mathbb{R}[z]_{r+2}$. Once that is established, $\mathcal{Q}^r$ is the preimage of $\mathcal{E}^r$ under a linear operator defined similarly in the case of $\mathcal{K}^r$, and the closedness of $\mathcal{Q}^r$ follows. To see that $\mathcal{E}^r$ is closed, we need the following theorem.

Theorem 1.3.1. *[67, Corollary 9.1.3] Let $K_1, ..., K_m$ be non-empty convex cones in a Euclidean space satisfying the following condition: if $\tau_i \in \mathbf{cl}(K_i)$ for $i = 1, ..., m$ and $\tau_1 + ... + \tau_m = 0$ then τ_i belongs to the lineality space of $\mathbf{cl}(K_i)$ for $i = 1, ..., m$. Then*

$$\mathbf{cl}(K_1 + ... + K_m) = \mathbf{cl}(K_1) + ... + \mathbf{cl}(K_m).$$

To apply this theorem, we let $K_\beta = \left\{ z^\beta z^T (P_\beta + N_\beta) z : P_\beta \in \mathcal{S}^+, N_\beta \in \mathcal{N} \right\}$, then $\mathcal{E}^r = \sum_{\beta \in \mathbb{I}(r+2)} K_\beta$. K_β is isomorphic to $\mathcal{D}^*$, hence is a closed convex cone with lineality space $\{0\}$. Now we verify the condition in Theorem 1.3.1 is satisfied. Take

$\tau_\beta = z^\beta z^T(P_\beta + N_\beta)z \in K_\beta$, if

$$\sum_{\beta \in \mathbb{I}(r+2)} z^\beta z^T(P_\beta + N_\beta)z = 0$$

then for *any* positive vector $z > 0$, $z^T(P_\beta + N_\beta)z = 0$, $\forall\beta$. Further by continuity and convexity, $\langle P_\beta + N_\beta, X\rangle = 0, \forall X \in \mathcal{C}, \forall\beta$. However $\mathcal{C}$ is full-dimensional in $\mathcal{S}$. Therefore $P_\beta + N_\beta = 0, \forall\beta$. This concludes the proof.

It is straightforward to check by definition that for any $r \in \mathbb{Z}_+$,

$$\mathcal{L}^r \subseteq \mathcal{Q}^r \subseteq \mathcal{K}^r. \tag{1.13}$$

Furthermore, as shown in [62] and [27] by using a theorem of Pólya ([43, Section 2.24]), the linear programming approximation hierarchy is "almost exact" in the limit:

Theorem 1.3.2 ([62],[27])**.** *Let M be a strictly copositive matrix, i.e., $y^T My > 0$ for all $y \in \mathbb{R}_n, y \geq 0, e^T y = 1$. Then there exists a finite $R \in \mathbb{Z}_+$ such that $M \in \mathcal{L}_n^R$.*

It then follows from (1.13) and Theorem 1.3.2 that the hierarchies $\{Q^r\}_{r\in\mathbb{Z}_+}$ and $\{\mathcal{K}^r\}_{r\in\mathbb{Z}_+}$ are also "almost exact" in the limit.

We remark that there exists some other approximation hierarchies for $\mathcal{C}$ and $\mathcal{C}^*$. For example, outer approximations for $\mathcal{C}^*$ can be constructed by approximating the standard simplex with rational lattice [11, 79], and inner approximations for $\mathcal{C}^*$ can be constructed via simplicial partitioning [34]. Lasserre [52] provides another approach to build semidefinite outer (inner) approximations for $\mathcal{C}^*$ ($\mathcal{C}$).

1.4 Generalized Completely Positive and Copositive Matrices

In this section we generalize the concept of completely positivity and copositivity. Recall the definition of $\mathcal{C} = \text{conv}\{xx^T : x \in \Re_n^+\}$ and $\mathcal{C}^* = \{Q \in \mathcal{S}_n :$

$x^TQx \geq 0, \forall x \in \Re_n^+\}$. If we replace $\Re_n^+$ by an arbitrary closed convex cone $\mathcal{K} \subseteq \Re_n$, we obtain the *generalized completely positive cone* and the *generalized copositive cone*:

$$\begin{aligned} \mathcal{C}(\mathcal{K}) &:= \text{conv}\{xx^T : x \in \mathcal{K}\}, \\ \mathcal{C}(\mathcal{K})^* &:= \left\{Q \in \mathcal{S}_n : x^TQx \geq 0, \forall x \in \mathcal{K}\right\}. \end{aligned}$$

Both $\mathcal{C}(\mathcal{K})$ and $\mathcal{C}(\mathcal{K})^*$ are closed convex cones and they are dual cones of each other [72].

This generalization naturally arises from quadratic programming. For example, consider the class of NP-hard, nonconvex quadratic programming problem with linear constraints:

$$\nu_* := \inf\{\langle \tilde{x}, \tilde{H}\tilde{x}\rangle + 2\langle \tilde{c}, \tilde{x}\rangle : \tilde{A}\tilde{x} = \tilde{a},\ \tilde{B}\tilde{x} \geq \tilde{b}\}. \tag{1.14}$$

It can be cast as the following two problems (see Theorem 1.4.1 for proof):

$$\begin{aligned} \nu_* &= \inf\left\{\ x^THx : X \in \mathcal{K},\ x_1 = 1\ \right\}, &(1.15)\\ &= \inf\{\ \langle H, X\rangle : X \in \mathcal{C}(\mathcal{K}),\ X_{11} = 1\ \}, &(1.16)\end{aligned}$$

where $\mathcal{K} = \{x : Ax = 0, Bx \geq 0\}$, and

$$x = \begin{pmatrix} 1 \\ \tilde{x} \end{pmatrix}, \quad H = \begin{pmatrix} 0 & \tilde{c}^T \\ \tilde{c} & \tilde{H} \end{pmatrix}, \quad A = \begin{pmatrix} -\tilde{a} & \tilde{A} \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ -\tilde{b} & \tilde{B} \end{pmatrix}.$$

Many local and global methods exist for solving (1.14) [37, 40], and BARON [68] provides a general-purpose software.

The equivalence between (1.14) and (1.15) is straightforward by definition. We provide a proof of the lifting-linearization procedure, i.e., the equivalence of (1.15) and (1.16). Actually the proof does not assume any structure of $\mathcal{K}$ except that it is a closed convex cone and the feasible region of (1.15) is non-empty. (Therefore this procedure is valid for more general problems, for example, quadratically constrained quadratic programs. See the end of this section for a result in this case.)

Theorem 1.4.1. *Let ν_* be defined as in (1.14), and $\mathcal{K}$, x, H, A, B defined in previous dicussion. Then* $\nu_* = \inf\{\langle H, X\rangle : X \in \mathcal{C}(\mathcal{K}), X_{11} = 1\}$.

Proof. Let ρ_* be the optimal value of the right-hand side optimization problem. By standard techniques, the right-hand side is a relaxation of (1.15), and so $\nu_* \geq \rho_*$. If $\nu_* = -\infty$, then $\rho_* = -\infty$, and the result follows.

So assume ν_* is finite. Then $\langle x, Hx\rangle \geq 0$ for all $x \in \mathcal{K}$ with $x_1 = 0$. Otherwise, any $x \in P$ with $x_1 = 0$ and $\langle x, Hx\rangle = \langle H, xx^T\rangle < 0$ would be a negative recession direction for (1.15).

Now, to prove $\nu_* \leq \rho_*$, let X be any feasible solution of the right-hand side. Because $X \in \mathcal{C}(\mathcal{K})$, there exists a finite set $\{x_k\} \subset \mathcal{K}$ such that $X = \sum_k x_k x_k^T$. We further break $\{x_k\}$ into two groups: those for which $[x_k]_1 > 0$ and those for which $[x_k]_1 = 0$. By scaling and the fact that $X_{11} = 1$, we may write

$$X = \sum_{k\,:\,[x_k]_1>0} \lambda_k \begin{pmatrix} 1 \\ \tilde{x}_k \end{pmatrix} \begin{pmatrix} 1 \\ \tilde{x}_k \end{pmatrix}^T + \sum_{k\,:\,[x_k]_1=0} x_k x_k^T,$$

where $\tilde{x_k} = [x_k]_{2:n}$, $\lambda_k > 0$ and $\sum_{k\,:\,[x_k]_1>0} \lambda_k = 1$. So, by the definition of ν_* and the preceding paragraph,

$$\langle H, X\rangle \geq \sum_{k\,:\,[x_k]_1>0} \lambda_k \nu_* + \sum_{k\,:\,[x_k]_1=0} 0 = \nu_*.$$

This implies $\rho_* \geq \nu_*$, as desired. □

Burer [19] showed that the representation results in [18] can be generalized by replacing the nonnegative orthant $\Re_n^+$ with any closed convex cone $\mathcal{K}$ (see also [36]). Specifically, if in Section 1.2.2, $\Re_n^+$ in (1.8) is replaced by $\mathcal{K}$, and $\mathcal{C}_{n+1}$ in (1.9) is replaced by $\mathcal{C}(\Re^+ \times \mathcal{K})$, all the results follow analogously. Furthermore, the procedure of including quadratic equalities also generalizes. We call linear optimizations over these generalized completely positive (copositive) cones *generalized copositive programs.*

Recently, Burer and Dong [22] proved that, any quadratically constrained quadratic program (QCQP) with a nonempty bounded feasible region can be equivalently reformulated as a generalized copositive program. While it is not very surprising if we are allowed to use arbitrary $\mathcal{K}$, interestingly, they provide two representations using two specific cones: $\mathcal{K}$ being a direct product of multiple second order cones and $\mathcal{K}$ being a positive semidefinite cone. Their analysis is based on the assumption that the QCQP has a nonempty and bounded feasible region, and heavily uses the machinery developed in [19]. This representation result motivates further research on generalized completely positive cone with $\mathcal{K}$ being direct product of nonnegative orthant, second order cones and semidefinite cones.

1.5 Structure of the Rest of the Thesis

The remaining chapters contain original research conducted by the author during his PhD study. Chapter 2 proposes a new approach for constructing outer approximation hierarchies for $\mathcal{C}$ based on symmetric tensors and explores connections with known inner approximation hierarchies for $\mathcal{C}^*$. This chapter is based on [29]. Chapter 3 provides an approach for solving the separation problem for $\mathcal{C}$ using sparsity. Chapter 4 introduces the concept of "boundary cone" and uses it to approach the separation problem as well as the construction of relaxations for $\mathcal{C}$. These two chapters are based on papers [31] and [23] submitted to academic journals.

CHAPTER 2
RELAXATIONS FOR THE COMPLETELY POSITIVE CONE: A TENSOR APPROACH

2.1 Introduction

As the general intractability of $\mathcal{C}$ and $\mathcal{C}^*$, one natural approach is to study their computationally tractable approximations. In this chapter, we present a new approach of constructing relaxations hierarchies for the $n \times n$ completely positive cone $\mathcal{C}_n$. We refer the reader to Section 1.3 for a review of some known inner approximation hierarchies for the copositive cone $\mathcal{C}_n^*$. In Section 2.2, we construct two relaxation hierarchies for $\mathcal{C}_n$. One is a sequence of polyhedral cones and the other is a sequence of cones with semidefinite constraints. In section 2.3, we derive alternative characterizations for several hierarchies, and then establish the duality relations between our approximation hierarchies (which are outer-approximations of $\mathcal{C}_n$), and two known inner-approximation hierarchies for $\mathcal{C}_n^*$: $\{\mathcal{L}_n^r\}_{r\in\mathbb{Z}^+}$ and $\{\mathcal{Q}_n^r\}_{r\in\mathbb{Z}^+}$. Although the explicit characterization of the polyhedral approximation hierarchy first appeared in [14], our tensor characterization is new. As a Corollary, we show that any matrix not in $\mathcal{C}_n$ is excluded by our outer approximation hierarchies with sufficiently large order (the super-script r in $\mathcal{L}_n^r$ and $\mathcal{Q}_n^r$). As an application, in Section 2.4 we apply our results to the linear programming bounds of the stability number of a graph. We give a new combinatorial proof of a known result in [63]. We also give an explicit construction of a primal optimal solution with its tensor lifting corresponding to each of these approximations.

2.1.1 Some specific notation and terminology

To simplify our later analysis using polynomials, we use a pair of vectors, one as a superscript of the other, to represent a monomial; for example, x^m. Usually we use x to denote a vector of variables used in a polynomial, whose dimension is usually n, and $m \in \mathbb{Z}_+^n$ is a vector of the same dimension used to represent the multiplicity of each variable. For example, if $x = [x_1, x_2, x_3]^T$ and $m = [0, 4, 2]^T$, then x^m means the monomial $x_2^4 x_3^2$. The *degree* of a monomial is the summation of the multiplicities of all variables. In the previous example, the degree of x^m (also denoted by $|m|$) is $4 + 2 = 6$. The degree of a polynomial is the degree of its monomial term of highest degree. We say a polynomial is *homogeneous* if each of its monomial terms has the same degree. In this chapter, unless otherwise stated, all polynomials we use are homogeneous, and n-variate (with variables $x_1, ..., x_n$).

We use $\mathbb{I}_n(r)$ to denote all the integral vectors used to represent exponents of monomials of degree r, i.e.,

$$\mathbb{I}_n(r) := \left\{ m \in \mathbb{Z}_+^n \;\middle|\; |m| = \sum_{i=1}^{n} m_i = r \right\}.$$

Usually we use the letter lower case letters m and p to denote elements in $\mathbb{I}_n(r)$.

The term "tensor" we use throughout this paper really means hyper-matrix, especially that of same length n in each *dimension*. In a tensor of *order* r, one needs r indices to specify one entry, where each index takes an integral value in $\{1, 2, ..., n\}$. In particular, a tensor of order 1 is a vector of length n, and a tensor of order 2 is a $n \times n$ square matrix. We use $\mathcal{M}_n^r$ to denote all tensors of order r. Note that for $r = 2$, the square matrix case, we have $\mathcal{M}_n^2 = \mathcal{M}_n$.

As we use a vector of nonnegative integers to represent the exponents of a monomial, for tensors we introduce another kind of multi-index notation to index entries in a tensor. In later analysis we will heavily use these two kinds of multi-index notations. It is important to understand the difference and connection between these notations.

For a tensor $T \in \mathcal{M}_n^r$, we use an r-dimension row vector whose coordinates are all nonnegative integers between 1 and n, enclosed in a pair of box brackets, to specify an entry in T. For example, for $T \in \mathcal{M}_n^3$, $T[1, 3, 2]$ is the entry at position 1 in the first dimension, position 3 in the second dimension, and position 2 in the last dimension. We use $\mathbb{N}_r(n)$ to denote all such indexing vectors. Formally,

$$\mathbb{N}_r(n) := \{\alpha \in \mathbb{Z}_+^r \mid 1 \le \alpha_i \le n, i = 1, ..., r\}.$$

Lower-case Greek letters are used to refer to elements in $\mathbb{N}_r(n)$. For example if $T \in \mathcal{M}_n^r$ and $\alpha \in \mathbb{N}_r(n)$, we use $T[\alpha]$ to refer an entry in T.

We say a tensor is *symmetric* if the values of its entries are independent of **permutation** of its indices. For example, a symmetric tensor of order 2 is simply a symmetric matrix. If T is a symmetric tensor of order 3, and $a, b, c \in \{1, ..., n\}$, then $T[a, b, c] = T[a, c, b] = T[b, a, c] = \cdots = T[c, b, a]$. $\mathcal{S}_n^r$ is used to denote the set of all symmetric tensors of order r.

The inner product over M_n^r (similarly in $\mathcal{S}_n^r$) is defined as

$$\langle T, Z \rangle = \sum_{\alpha \in \mathbb{N}_r(n)} T[\alpha] Z[\alpha]. \quad \forall T, Z \in \mathcal{M}_n^r.$$

For $r > 2$, and $\beta \in \mathbb{N}_{r-2}(n)$, $T[\beta, :, :]$ means an ordinary matrix obtained by fixing the first $r - 2$ indices of T as β. Since often the last two indices are special in our analysis, sometimes we use T^β for shorter notation, and T_{ij}^β means $T[\beta, i, j]$, for $1 \le i, j \le n$.

For a symmetric tensor $T \in \mathcal{S}_n^r$, $T[\alpha] = T[\beta]$ if there exists a permutation τ such that $\tau(\alpha) = \beta$. So we can define (permutational) equivalence classes in $\mathbb{N}_r(n)$ in this way. We use $[\![\alpha]\!]$ to denote the equivalence class that includes α. One can define a bijection between all equivalence classes in $\mathbb{N}_r(n)$ and all elements in

$\mathbb{I}_n(r)$. By abuse of notation, we represent this bijection by $[\![\cdot]\!] : \mathbb{N}_r(n) \longrightarrow \mathbb{I}_n(r)$. For $\alpha \in \mathbb{N}_r(n)$ and $m \in \mathbb{I}_n(r)$, we say $[\![\alpha]\!] = m$ if α has m_1 number of 1's, m_2 number of 2's, etc. For example, if $r = 4$ and $n = 5$, $\alpha = [3, 3, 1, 5] \in \mathbb{N}_r(n)$, then $[\![\alpha]\!] = [1, 0, 2, 0, 1] \in \mathbb{I}_n(r)$, because in α, we have one entry equal to 1, zero entry equal to 2, one entry equal to 3, two entry equal to 4 and none entry equal to 5.

Remark 2.1.1. It is beneficial to remember that vectors in $\mathbb{N}_r(n)$ has length r, bounds n, while vectors in $\mathbb{I}_n(r)$ has length n, sum r.

We next define several tensor operators that are convenient in our later analysis. First, given a tensor $T \in \mathcal{M}_n^{r+2}$, we define $\mathbf{Slices}(T)$ to be the set of $n \times n$ matrices which are "slices" of T obtained by fixing its first r indices, i.e., a matrix $P \in \mathbf{Slices}(T)$ iff $\exists \beta \in \mathbb{N}_r(n)$ such that $P = T^\beta = T[\beta, :, :]$.

Next we define an operator $\mathbf{Collapse} : \mathcal{M}_n^{r+2} \longrightarrow \mathcal{M}_n^2$ as:

$$\mathbf{Collapse}(T)[i, j] = \sum_{P \in \mathbf{Slices}(T)} P_{ij} = \sum_{\beta \in \mathbb{N}_r(n)} T[\beta, i, j] = \sum_{\beta \in \mathbb{N}_r(n)} T^\beta_{ij}.$$

Given a matrix $P \in \mathcal{M}_n^2$, $\mathbf{Stack}_r(P)$ is a tensor constructed by "stacking" P for n layers along r dimensions; precisely, $\mathbf{Stack}_r(P) \in \mathcal{M}_n^{r+2}$ and

$$\mathbf{Stack}_r(P)[\beta, i, j] = P_{ij}, \quad \forall \beta \in \mathbb{N}_r(n).$$

When the value r associated with the operator is clear in context, we omit it and write $\mathbf{Stack}(\cdot)$ instead of $\mathbf{Stack}_r(\cdot)$.

Actually, $\mathbf{Collapse}(\cdot)$ and $\mathbf{Stack}(\cdot)$ are a pair of adjoint operators, i.e., $\forall T \in \mathcal{M}_n^{r+2}$, $\forall P \in \mathcal{M}_n^2$,

$$\langle \mathbf{Collapse}(T), P \rangle = \sum_{\beta \in \mathbb{N}_r(n)} \langle T[\beta, :, :], P \rangle = \langle T, \mathbf{Stack}(P) \rangle,$$

where the inner product in $\mathcal{M}_n^{r+2}$ is defined in the standard way: for $T, \tilde{T} \in \mathcal{M}_n^{r+2}$,

$$\left\langle T, \tilde{T} \right\rangle := \sum_{\alpha \in \mathbb{N}_{r+2}(n)} T[\alpha] \tilde{T}[\alpha].$$

For a square matrix $P \in \mathcal{M}_n^2$, one may symmetrize it via $\mathbf{Sym}(P) = \frac{P + P^T}{2}$.

One can similarly symmetrize a tensor. The symmetrization operator **Sym** : $\mathcal{M}_n^r \longrightarrow \mathcal{S}^r$ is defined as follows:

$$\mathbf{Sym}(T)[\beta] = \sum_{[\![\alpha]\!]=[\![\beta]\!]} T[\alpha] \Big/ c([\![\beta]\!]), \quad \forall \beta \in \mathbb{N}_r(n),$$

where $c(\cdot)$ is the multinomial coefficient defined as:

$$c(m) := \begin{cases} \frac{|m|!}{\prod_{i=1}^n (m_i)!} \ , & m \in \mathbb{I}_n(r); \\ 0 \ , & \textit{otherwise}. \end{cases}$$

Sometimes we use $T \simeq_{Sym} \tilde{T}$ to mean that $\mathbf{Sym}(T) = \mathbf{Sym}(\tilde{T})$. It is worth mentioning that if $T \simeq_{Sym} \tilde{T}$ and $Z \in \mathcal{S}^r$, then $\langle T, Z\rangle = \langle \tilde{T}, Z\rangle$.

For $m \in \mathbb{I}_n(r+2)$, we define $m(i,j) = m - e_i - e_j$, where e_i is a vector with 1 at the i-th position and 0's elsewhere, and similarly for e_j.

Remark 2.1.2. It is worth mentioning that given $m \in \mathbb{I}_n(r+2)$, $m(i,j)$ is not always in $\mathbb{I}_n(r)$, since $m(i,j)$ might contain negative entries. If so, $c(m(i,j)) = 0$ by definition.

There are many ways to interpret $c(m)$. One way related to our later discussion is the following:

$$\left(\sum_{i=1}^n x_i^2\right)^r = \sum_{m\in\mathbb{I}_n(r)} c(m) x^{2m}.$$

Another interpretation of $c(m)$, which sheds light on the connection of polynomial terminology and tensor terminology, is that for $m \in \mathbb{I}_n(r)$,

$$c(m) = |\{\alpha \in \mathbb{N}_r(n) : [\![\alpha]\!] = m\}|\,,$$

i.e., $c(m)$ equals the number of elements in the equivalence class corresponding to m.

2.2 Symmetric Tensor Approximations for the Completely Positive Cone

We first construct a polyhedral outer approximation hierarchy $\{\mathcal{T}_n^r\}_{r=1}^{\infty}$ for the completely positive cone $\mathcal{C}_n$. Then by adding positive semidefinite conditions we obtain a semidefinite approximation hierarchy $\{\mathcal{TD}_n^r\}_{r=1}^{\infty}$. In the next section, we prove duality relations between these outer approximations and the inner approximations of $\mathcal{C}_n^*$ described in Section 1.3. Before the construction, we describe some specialized tensor notations.

First consider the standard simplex in $\mathbb{R}^n$: $\Delta_n := \{x \in \mathbb{R}_n : e^T x = 1, x \geq 0\}$. For fixed $x \in \Delta$, we can construct an "outer-product" tensor $Z \in \mathcal{S}_n^{r+2}$ as:

$$Z[i_1, i_2, i_3, ..., i_{r+2}] := x_{i_1} x_{i_2} \cdots x_{i_{r+2}}. \tag{2.1}$$

Then it is easy to see that every matrix in **Slices**(Z) is a positive scaling of the matrix xx^T, hence a completely positive matrix, and collapsing Z yields the matrix xx^T:

$$\textbf{Collapse}(Z) = \sum_{i_1,\ldots,i_r=1}^{n} x_{i_1} \cdots x_{i_r} xx^T = \left(e^T x\right)^r xx^T = xx^T. \tag{2.2}$$

For the sake of computational tractability, we relax the complete positivity of each slice of the tensor Z to either nonnegativity or double nonnegativity. These relaxations motivate us to define the following two sets for integer $r \geq 1$:

$$\mathcal{T}_n^r := \left\{X \mid \exists Z \in \mathcal{S}_n^{r+2}, Z \geq 0, X = \textbf{Collapse}(Z)\right\}, \tag{2.3}$$

$$\mathcal{TD}_n^r := \left\{X \,\middle|\, \exists Z \in \mathcal{S}_n^{r+2}, \textbf{Slices}(Z) \subseteq \mathcal{D}_n, X = \textbf{Collapse}(Z)\right\}. \tag{2.4}$$

For convenience, we define: $\mathcal{T}_n^0 := \mathcal{N}_n$ and $\mathcal{TD}_n^0 := \mathcal{D}_n$. $\mathcal{T}_n^r$ is a closed convex polyhedron since it is the image of a linear transformation of a polyhedron of higher dimension. Furthermore, we have the following inclusion relation:

Proposition 2.2.1. *For dimension* $n \geq 1$,

$$\mathcal{C}_n \subseteq \cdots \subseteq \mathcal{T}_n^{r+1} \subseteq \mathcal{T}_n^r \subseteq \cdots \subseteq \mathcal{T}_n^1 \subseteq \mathcal{T}_n^0 := \mathcal{N}_n$$

$$\mathcal{C}_n \subseteq \cdots \subseteq \mathcal{TD}_n^{r+1} \subseteq \mathcal{TD}_n^r \subseteq \cdots \subseteq \mathcal{TD}_n^1 \subseteq \mathcal{TD}_n^0 := \mathcal{D}_n$$

Proof. By definition it is obvious that $\mathcal{T}_n^r \subseteq \mathcal{T}_n^0$ and $\mathcal{TD}_n^r \subseteq \mathcal{TD}_n^0$. By (2.1) and (2.2), it is also clear that $xx^T \in \mathcal{T}_n^r$ and $xx^T \in \mathcal{TD}_n^r$, $\forall x \in \Delta_n$. Note that both $\mathcal{T}_n^r$ and $\mathcal{TD}_n^r$ are convex cones, so $\mathcal{C}_n \subseteq \mathcal{T}_n^r$ and $\mathcal{C}_n \subseteq \mathcal{TD}_n^r$.

Now we show that $\mathcal{TD}_n^{r+1} \subseteq \mathcal{TD}_n^r$ for $r > 0$. Suppose $X \in \mathcal{TD}_n^{r+1}$, then by definition $\exists Z \in \mathcal{S}_n^{r+3}$ such that $\mathbf{Slices}(Z) \subseteq \mathcal{D}_n$ and $X = \mathbf{Collapse}(Z)$. Now we define $\tilde{Z}$ by adding all the r-tensors generated by fixing the last index of Z:

$$\tilde{Z}[\alpha] = \sum_{i=1}^{n} Z[\alpha, i], \ \forall \alpha \in \mathbb{N}_{r+2}(n).$$

Since $Z \in \mathcal{S}_n^{r+3}$, it is easy to see $\tilde{Z} \in \mathcal{S}_n^{r+2}$. Further, every matrix in $\mathbf{Slices}(\tilde{Z})$ is a summation of n matrices in $\mathbf{Slices}(Z)$, so $\mathbf{Slices}(\tilde{Z}) \subseteq \mathcal{D}_n$. Finally,

$$\begin{aligned} \mathbf{Collapse}(\tilde{Z}) &= \sum_{\beta \in \mathbb{N}_r(n)} \tilde{Z}[\beta, :, :] = \sum_{\beta \in \mathbb{N}_r(n)} \sum_{i=1}^{n} Z[\beta, :, :, i] \\ &= \sum_{\alpha \in \mathbb{N}_{r+1}(n)} Z[\alpha, :, :] = \mathbf{Collapse}(Z) = X. \end{aligned}$$

Therefore, $X \in \mathcal{TD}_n^r$. The proof of $\mathcal{T}_n^{r+1} \subseteq \mathcal{T}_n^r$ is similar. □

2.3 Duality Relations

The main results in this section are theorems that establish duality relations between two pairs of convex cones:

1. $\mathcal{L}_n^r$ and $\mathcal{T}_n^r$ (Theorem 2.3.1),

2. $\mathcal{Q}_n^r$ and $\mathcal{TD}_n^r$ (Theorem 2.3.2).

First for $\mathcal{T}_n^r$ and $\mathcal{L}_n^r$, we derive explicit characterizations of $\mathcal{T}_n^r$ (Lemma 2.3.1) and $\mathcal{L}_n^r$ (Lemma 2.3.2). Then the duality between $\mathcal{L}_n^r$ and $\mathcal{T}_n^r$ is clear by the following lemmas which say that the extreme rays of $\mathcal{T}_n^r$ define all the facets of $\mathcal{L}_n^r$.

Lemma 2.3.1. *For any nonnegative integer r,*

$$\mathcal{T}_n^r = \left\{ X \,\middle|\, X = \sum_{m \in \mathbb{I}_n(r+2)} \lambda_m F_m, \lambda_m \geq 0, \forall m \in \mathbb{I}_n(r+2) \right\},$$

where $F_m \in \mathcal{S}_n$ and $(F_m)_{ij} = c(m(i,j))$.

Proof. First we define a set of of "elementary tensors" of order $r+2$: for every $m \in \mathbb{I}_n(r+2)$, define $E_m \in \mathcal{S}_n^{r+2}$ as follows:

$$(E_m)[\alpha] = \begin{cases} 1, & \text{if } [\![\alpha]\!] = m \\ 0, & \text{otherwise.} \end{cases}$$

Then it is easy to verify that $F_m = \mathbf{Collapse}(E_m), \forall m \in \mathbb{I}_n(r+2)$. Note $\forall Z \in \mathcal{S}_n^{r+2}$, $Z \geq 0$, Z can be decomposed as a nonnegative combination of these "elementary tensors":

$$Z = \sum_{m \in \mathbb{I}_n(r+2)} \lambda_m E_m, \text{ where } \lambda_m = Z[\alpha] \text{ for } [\![\alpha]\!] = m.$$

Since $\mathbf{Collapse}(\cdot)$ is a linear operator, we have

$$\begin{aligned} \mathcal{T}_n^r &= \left\{ X \,\middle|\, X = \sum_{m \in \mathbb{I}_n(r+2)} \lambda_m \mathbf{Collapse}(E_m), \lambda_m \geq 0, \forall m \in \mathbb{I}_n(r+2) \right\} \\ &= \left\{ X \,\middle|\, X = \sum_{m \in \mathbb{I}_n(r+2)} \lambda_m F_m, \lambda_m \geq 0, \forall m \in \mathbb{I}_n(r+2) \right\}. \end{aligned}$$

□

Remark 2.3.1. Lemma 2.3.1 gives an explicit characterization of the polyhedral cone $\mathcal{T}_n^r$, i.e., every extreme ray of $\mathcal{T}_n^r$ is of form F_m where $m \in \mathbb{I}_n(r+2)$. Note m is a row vector, then an easy computation shows

$$F_m = \frac{c(m)}{(r+2)(r+1)} \left[m^T m - \text{Diag}(m) \right],$$

where $\text{Diag}(m)$ is a diagonal matrix with $\text{Diag}(m)_{ii} = m_i$.

The following explicit characterization of $\mathcal{L}_n^r$ first appeared in [14], we include the derivation here for the sake of completeness.

Lemma 2.3.2. *[14, Theorem 2.4] For any nonnegative integer r,*

$$\mathcal{L}_n^r = \{M \in \mathcal{S}_n \mid \langle F_m, M\rangle \geq 0,\ \forall m \in \mathbb{I}_n(r+2)\}$$

where F_m is defined as in Lemma 2.3.1.

Proof.

$$\begin{aligned} P^{(r)}(x) &= \sum_{i,j=1}^{n} M_{ij}x_i^2x_j^2 \left(\sum_{i=1}^{n} x_i^2\right)^r \\ &= \sum_{i,j=1}^{n} M_{ij}x_i^2x_j^2 \sum_{m\in\mathbb{I}_n(r)} c(m)x^{2m} \\ &= \sum_{\substack{m\in\mathbb{I}_n(r)\\ i,j=1,\dots,n}} c(m)M_{ij}x^{2m+2e_i+2e_j} \\ &= \sum_{m\in\mathbb{I}_n(r+2)} \left(\sum_{i,j=1}^{n} c(m(i,j))M_{ij}\right) x^{2m}. \end{aligned}$$

Hence, by the definition of $\mathcal{L}_n^r$, and $(F_m)_{ij} = c(m(i,j))$,

$$\mathcal{L}_n^r = \{M \in \mathcal{S}_n \,|\langle F_m, M\rangle \geq 0,\ \forall m \in \mathbb{I}_n(r+2)\}\,.$$

□

Now we are ready to state our first main result:

Theorem 2.3.1. *For any nonnegative integer r, the cones $\mathcal{L}_n^r$ and $\mathcal{T}_n^r$ are dual to one another:*

$$(\mathcal{L}_n^r)^* = \mathcal{T}_n^r, \quad (\mathcal{T}_n^r)^* = \mathcal{L}_n^r.$$

Proof. Since both $\mathcal{L}_n^r$ and $\mathcal{T}_n^r$ are finitely generated cones, the result follows immediately from Lemma 2.3.1 and Lemma 2.3.2. □

Next we derive the duality relation between $\mathcal{TD}_n^r$ and $\mathcal{Q}_n^r$. Again we start by deriving a tensor characterization of the cone $\mathcal{Q}_n^r$.

Lemma 2.3.3. *For any nonnegative integer r, $\mathcal{Q}_n^r$ has the following characterization:*

$$\mathcal{Q}_n^r = \left\{M \,\middle|\, \exists T \in \mathcal{M}_n^{r+2}, \mathbf{Stack}(M) \simeq_{Sym} T, \mathbf{Slices}(T) \subseteq \mathcal{D}_n^*\right\}.$$

Proof. First, we claim the following is an alternative characterization of $\mathcal{Q}_n^r$:

$$\mathcal{Q}_n^r = \left\{ M \,\middle|\, \exists T \in \mathcal{M}_n^{r+2}, \left(\sum_{i=1}^n z_i\right)^r z^T M z = \sum_{\alpha \in \mathbb{N}_r(n)} z^\alpha z^T \left(T^{(\alpha)}\right) z, \mathbf{Slices}(T) \subseteq \mathcal{D}_n^* \right\}. \tag{2.5}$$

Note we change the index sets of $p \in \mathbb{I}_n(r)$ in (1.12) to $\alpha \in \mathbb{N}_r(n)$. To see the equivalence with (1.12), we identify each matrix M_p in (1.12) with the sum of slices of $T \in \mathcal{M}_n^{r+2}$ corresponding to an equivalence class in $\mathbb{N}_r(n)$.

From the matrices $\{M_p\}_{p \in \mathbb{I}_n(r)}$ in (1.12), we construct tensor $T \in \mathcal{M}_n^{r+2}$ in (2.5) as follows:

$$T^\alpha = T[\alpha, :, :] = \frac{1}{c(\llbracket \alpha \rrbracket)} M_{\llbracket \alpha \rrbracket}, \quad \forall \alpha \in \mathbb{N}_r(n).$$

It is obvious that $\mathbf{Slices}(T) \subseteq \mathcal{D}_n^*$ and $M_p = \sum_{\llbracket \alpha \rrbracket = p} T^\alpha$. So T satisfies conditions in (2.5). On the other hand, if we have $T \in \mathcal{M}_n^{r+2}$ with $\mathbf{Slices}(T) \subseteq \mathcal{D}_n^*$, we can construct $M_p = \sum_{\llbracket \alpha \rrbracket = p} T^{(\alpha)} \in \mathcal{D}_n^*$.

Next by comparing the coefficients of the equality in (2.5), it is equivalent to:

$$\sum_{m_i, m_j \geq 1} c(m(i,j)) M_{ij} = \sum_{m_i, m_j \geq 1} \left(\sum_{\llbracket \alpha \rrbracket = m - e_i - e_j} T_{ij}^{(\alpha)} \right), \ \forall m \in \mathbb{I}_n(r+2). \tag{2.6}$$

Further, (2.6) is equivalent to:

$$\mathbf{Stack}(M) \simeq_{Sym} T.$$

Actually, for every $m \in \mathbb{I}_n(r+2)$, the left hand side of (2.6) reads as the summation of all entries in tensor $\mathbf{Stack}(M)$ with multi-index permutationally equivalent to m. Also the right hand side has the same interpretation of tensor T. This proves our lemma. □

We now state a technical lemma which will be useful later in the proof of Theorem 2.3.2.

Lemma 2.3.4. *Let $\mathcal{K} \subseteq \Re^n$ be a convex cone, and $\mathcal{H}$ be a closed convex cone such that $\mathcal{H} \subseteq \mathcal{K}^*$. If for any $X \notin \mathcal{K}$, $\exists H \in \mathcal{H}$, $\langle X, H \rangle < 0$, then $\mathcal{K}$ is closed and*

$\mathcal{K}^* = \mathcal{H}$.

Proof. First by assumption that $\mathcal{H} \subseteq \mathcal{K}^*$, for any $H \in \mathcal{H}$, $\langle X, H\rangle \geq 0$, $\forall X \in \mathcal{K}$. Further each point outside $\mathcal{K}$ is guaranteed to violate at least one of such inequality. So $\mathcal{K}$ is the intersection of (arbitrary many) closed half spaces defined by $\langle \cdot, H\rangle \geq 0$, $H \in \mathcal{H}$. Therefore K is closed.

To show $\mathcal{H} \supseteq \mathcal{K}^*$, suppose otherwise, if there exists $\bar{Y} \in \mathcal{K}^* \setminus \mathcal{H}$, then by a standard separation theorem [67, Corollary 11.4.2], there exists $\bar{X} \in \mathcal{H}^* \setminus \mathcal{K}^{**}$ such that $\langle \bar{X}, \bar{Y}\rangle < 0$ and $\langle \bar{X}, H\rangle > 0$ for all $H \in \mathcal{H}$. Since $\mathcal{K}$ is closed, $\mathcal{K} = \mathcal{K}^{**}$, and $\bar{X} \notin \mathcal{K}$. Then by assumption there exists $\bar{H} \in \mathcal{H}$ such that $\langle \bar{X}, \bar{H}\rangle < 0$. This causes a contradiction. □

Before stating the main theorem, we explain some additional notation. First we use $(\mathcal{D}_n)^{n^r}$ to denote the set of nonsymmetric tensors whose slices are doubly nonnegative matrices:

$$(\mathcal{D}_n)^{n^r} = \{Z \,\big|\, Z \in \mathcal{M}_n^{r+2}, \mathbf{Slices}(Z) \subseteq \mathcal{D}_n\}.$$

Note that the double nonnegativity on slices implies those tensors are symmetric with respect to the last two indices, but generally they are nonsymmetric. Then $\mathcal{S}_n^{r+2} \cap (\mathcal{D}_n)^{n^r}$ is a convex cone and it is essentially the intersection of $\mathcal{S}_n^{r+2}$, which is a linear subspace of $\mathcal{M}_n^{r+2}$, and $(\mathcal{D}_n)^{n^r}$. So it is a closed convex cone and its dual cone in space $\mathcal{M}_n^{r+2}$ is:

$$\left(\mathcal{S}_n^{r+2} \cap (\mathcal{D}_n)^{n^r}\right)^* = \mathbf{cl}\left(\left(\mathcal{S}_n^{r+2}\right)^{\perp} + (\mathcal{D}_n^*)^{n^r}\right).$$

Theorem 2.3.2. *For any nonnegative integer r, $\mathcal{Q}_n^r$ and $\mathcal{TD}_n^r$ have the following duality relation:*

$$(\mathcal{TD}_n^r)^* = \mathcal{Q}_n^r, \quad (\mathcal{Q}_n^r)^* = \mathcal{TD}_n^r.$$

Proof. First we show that $(\mathcal{TD}_n^r)^* \supseteq \mathcal{Q}_n^r$ and $(\mathcal{Q}_n^r)^* \supseteq \mathcal{TD}_n^r$. It suffices to show that for any $M \in \mathcal{Q}_n^r$ and $X \in \mathcal{TD}_n^r$, $\langle M, X\rangle \geq 0$. This holds because

$$\begin{aligned}\langle M, X\rangle &= \sum_{\alpha\in\mathbb{N}_r(n)} \left\langle M, Z^{(\alpha)}\right\rangle = \langle \mathbf{Stack}(M), Z\rangle \\ &= \langle T, Z\rangle = \sum_{\alpha\in\mathbb{N}_r(n)} \left\langle T^{(\alpha)}, Z^{(\alpha)}\right\rangle \geq 0,\end{aligned}$$

where Z is used as in (2.4) and T is defined as in Lemma 2.3.3, and the third equality is because of $Z \in \mathcal{S}_n^r$ and $T \simeq_{Sym} \mathbf{Stack}(M)$. The last inequality is because $T^{(\alpha)} \in \mathcal{D}_n^*$, $Z^{(\alpha)} \in \mathcal{D}_n$.

Next we show $(\mathcal{TD}_n^r)^* \subseteq \mathcal{Q}_n^r$. We use Lemma 2.3.4 and the following alternative system pair to prove this. Given a matrix $X \in \mathcal{M}_n$, we have the following alternative system pair in variables Z and M:

$$\mathbf{Collapse}(Z) = X, \quad Z \in \mathcal{S}_n^{r+2} \cap (\mathcal{D}_n)^{n^r}, \tag{P}$$

$$\langle M, X\rangle < 0, \quad \mathbf{Stack}(M) \in \mathbf{cl}\left(\left(\mathcal{S}_n^{r+2}\right)^{\perp} + (\mathcal{D}_n^*)^{n^r}\right). \tag{D}$$

This pair is an alternative system because $\mathbf{Collapse}(\cdot)$ and $\mathbf{Stack}(\cdot)$ are adjoint operators, and the second condition in system (D) is strictly feasible (for example, let M be a matrix with all entries positive, then $\mathbf{Stack}(M) \in \mathbf{relint}\,(\mathcal{D}_n^*)^{n^r}$) .

For any $X \notin \mathcal{TD}_n^r$, (P) is infeasible, so there exists M such that (D) is feasible. By continuity, we can assume that $\mathbf{Stack}(M) \in (\mathcal{S}_n^{r+2})^{\perp} + (\mathcal{D}_n^*)^{n^r}$. So $\exists\, T \in (\mathcal{D}_n^*)^{n^r}$ such that $\mathbf{Stack}(M) \simeq_{Sym} T$. Hence $M \in \mathcal{Q}_n^r$. Finally by applying Lemma 2.3.4, $(\mathcal{TD}_n^r)^* = \mathcal{Q}_n^r$ and $\mathcal{TD}_n^r$ is closed. Then $(\mathcal{Q}_n^r)^* = (\mathcal{TD}_n^r)^{**} = \mathbf{cl}(\mathcal{TD}_n^r) = \mathcal{TD}_n^r$. This concludes our proof. □

As a Corollary of our main results, any matrix not in $\mathcal{C}_n$ is excluded from $\mathcal{T}_n^r$ for some finite r.

Corollary 2.3.1. *Suppose $Y \notin \mathcal{C}_n$, then there exists finite nonnegative integer R, such that $Y \notin \mathcal{T}_n^R$ and $Y \notin \mathcal{TD}_n^R$.*

Proof. For $Y \notin \mathcal{C}_n$, there exists a strictly copositive $M \in \mathcal{C}_n^*$, such that $\langle M, Y\rangle < 0$.

Then the result follows readily from Theorem 1.3.2, Theorem 2.3.1 and Theorem 2.3.2. □

2.4 An Application

As an application of our results, we examine linear programming bounds of the stability number of a graph. In [63], a closed-form expression for these approximations was given. In this section, we use the tensor structure of $\mathcal{T}_n^r$ to give a new proof of a known sufficient and necessary condition under which these approximations are finite by using the pigeon-hole principle. Then we give an explicit primal optimal solution as well as its tensor lifting for each of these tensor approximations.

Given a graph $\mathcal{G}$, the Maximum Stable Set problem asks for the cardinality of the largest stable set in $\mathcal{G}$. This cardinality is usually denoted by $\alpha(\mathcal{G})$. It has the following copositive programming formulation [27]:

$$\alpha(\mathcal{G}) = \max_X \left\{E \bullet X : \text{trace}(X) = 1, X_{ij} = 0,\ \forall (i,j) \in \mathcal{G},\ X \in \mathcal{C}_n\right\}, \tag{2.7}$$

with its dual problem

$$\alpha(\mathcal{G}) = \min_\lambda \left\{\lambda : s.t.,\ \lambda(I + A_{\mathcal{G}}) - ee^T \in \mathcal{C}_n^*\right\}. \tag{2.8}$$

Note that strong duality holds because (2.8) is strictly feasible, although (2.7) is not.

By replacing $\mathcal{C}_n$ by its polyhedral relaxations $\{\mathcal{T}_n^r\}$, a class of upper bounds of $\alpha(\mathcal{G})$ are defined as

$$\zeta^{(r)}(\mathcal{G}) := \max_X \left\{E \bullet X : \text{trace}(X) = 1, X_{ij} = 0,\ \forall (i,j) \in \mathcal{G},\ X \in \mathcal{T}_n^r\right\}. \tag{2.9}$$

By Theorem 2.3.1, the dual problem of (2.9) reads:

$$\zeta^{(r)}(\mathcal{G}) = \min_\lambda \left\{\lambda : s.t.,\ \lambda(I + A_{\mathcal{G}}) - ee^T \in \mathcal{L}_n^r\right\}. \tag{2.10}$$

Strong duality holds here because (2.9) and (2.10) are linear programs.

Several properties about $\zeta^{(r)}(\mathcal{G})$ were proved in [63] using the dual form (2.10), where a central result is a closed-form expression of $\zeta^{(r)}(\mathcal{G})$ in terms of $\alpha(\mathcal{G})$ [63, Theorem 1]. Here first we give a combinatorial proof of a corollary in their paper, which is a necessary and sufficient condition for $\zeta^{(r)}(\mathcal{G}) < \infty$. Our proof uses the tensor structure and the pigeon-hole principle.

Proposition 2.4.1. *[63, Corollary 3] $\zeta^{(r)}(\mathcal{G}) < \infty$ if and only if $r + 2 > \alpha(G)$.*

Proof. Let $Z \in \mathcal{S}_n^{r+2}$ be the tensor corresponding to X as in (2.3). Then (2.9) is unbounded if and only if Z has an unbounded variable, or in other words $\exists \beta \in \mathbb{N}_{r+2}(n)$, such that β contains any index at most once, and does not contain any pair $(i, j) \in \mathcal{G}$. This is equivalent to saying β corresponds to a stable set in $\mathcal{G}$. By pigeon-hole principle, this can happen only if $r + 2 \leq \alpha(G)$. Also this must happen when $r + 2 \leq \alpha(\mathcal{G})$, since one may simply choose β to correspond to (a subset of) the maximum stable set. □

It was shown in [63, Theorem 1] that $\zeta^{(r)}(\mathcal{G})$ has the following closed form:

Theorem 2.4.1. *Assume $r + 2 > \alpha(\mathcal{G})$ and $r + 2 = u\alpha(\mathcal{G}) + v$, where u, v are nonnegative integers with $v < \alpha(\mathcal{G})$. Then*

$$\zeta^{(r)}(\mathcal{G}) = \frac{\binom{r+2}{2}}{\binom{u}{2}\alpha(\mathcal{G}) + vu}.$$

In their analysis, the dual formulation (2.10) of $\zeta^{(r)}(\mathcal{G})$ was used. However it is interesting to analyze the structure of a primal optimal solution X in (2.9) since it is directly related with an indicator vector of a max stable set. This is the goal of the rest of the paper.

We define some terminology first. Let $V \subseteq [1, 2, ..., n]$. We say a multi-index $\beta \in \mathbb{N}_s(n)$ is *evenly distributed* over V, denoted by $\beta \curlywedge V$, if each element in V appears in β either $\left\lfloor \frac{s}{|V|} \right\rfloor$ or $\left\lceil \frac{s}{|V|} \right\rceil$ many times. For example, if $s = 5$, and $V = [1, 2, 4]$, then β is evenly distributed over V if β is a permutation of one of the following three cases

$$[1,1,2,2,4]\,,\ [1,2,2,4,4]\,,\ [1,1,2,4,4]\,.$$

Now let us do some counting. Let $u = \left\lfloor \frac{s}{|V|} \right\rfloor$, and $v = s - u|V|$. Then, for any $\beta \curlywedge V$, v elements in V are repeated $u+1$ times in β, and the other $|V| - v$ elements in V are repeated u times in β. In the previous example, $u = 1$, $v = 2$. The number of multi-indices β that are evenly distributed over V is:

$$|\{\beta \in \mathbb{N}_s(n) : \beta \curlywedge V\}| = \binom{|V|}{v} \frac{s!}{[u!]^{|V|-v}\,[(u+1)!]^{v}}.$$

This is calculated by first choosing v elements in V, and then using the multinomial formula. Further for any fixed $\beta \in \mathbb{N}_s(n)$, if we random pick a pair of indices $1 \le i < j \le s$, the probability of $\beta_i = \beta_j$ is:

$$\begin{aligned} P_{pair} &= \left\{\binom{u+1}{2} v + \binom{u}{2} [|V| - v]\right\} \Big/ \binom{s}{2} \\ &= \left\{\binom{u}{2} |V| + uv\right\} \Big/ \binom{s}{2}. \end{aligned}$$

Since the set $\{\beta \in \mathbb{N}_s(n) : \beta \curlywedge V\}$ is closed under permutation, assume $s \ge 2$, the number of β that has **same last two entries** can be calculated by

$$|\{\beta \in \mathbb{N}_s(n) : \beta \curlywedge V, \beta_{s-1} = \beta_s\}| \;\; = \;\; |\{\beta \in \mathbb{N}_s(n) : \beta \curlywedge V\}| \cdot P_{pair}.$$

In the following theorem we construct an optimal solution X for the primal problem (2.9), as well as its corresponding tensor lifting Z. We will use the previous counting results with $s = r+2$, and $|V| = \alpha(\mathcal{G})$.

Theorem 2.4.2. *Assume V_{max} is a maximum stable set of graph $\mathcal{G}$, $\alpha(\mathcal{G}) = |V_{max}|$. Also assume $r + 2 > \alpha(\mathcal{G})$, and $u = \left\lfloor \frac{r+2}{\alpha(\mathcal{G})} \right\rfloor$, $v = r + 2 - \alpha(\mathcal{G})$. Then an optimal solution to (2.9) is given by $X =$ **Collapse**(Z), where $Z \in \mathcal{S}_n^{r+2}$ with entries:*

$$Z[\beta] = \begin{cases} C^{-1} \cdot \zeta^{(r)}(\mathcal{G}) & ; \;\; \textit{if } \beta \curlywedge V_{max}, \beta \in \mathbb{N}_{r+2}(n), \\ 0 & ; \;\; \textit{otherwise}, \end{cases}$$

where $\beta \curlywedge V_{max}$ means β is evenly distributed over V_{max}, i.e., each element in V_{max}

appears in β *either* u *or* $u+1$ *times, and* C *is the the following number*

$$C = \frac{(r+2)!}{[u!]^{\alpha(\mathcal{G})-v}[(u+1)!]^v}\binom{\alpha(\mathcal{G})}{v}.$$

Proof. We verify that X is feasible.

$$\begin{aligned}\text{trace}(X) &= \sum_{i=1}^{n}\sum_{\gamma\in\mathbb{N}_r(n)} Z[\gamma,i,i] = \sum_{\beta\curlywedge V_{max},\beta_{r+1}=\beta_{r+2}} Z[\beta] \\ &= \frac{\zeta^{(r)}(\mathcal{G})}{C}\cdot|\{\beta\in\mathbb{N}_{r+2}(n) : \beta\curlywedge V_{max}, \beta_{r+1}=\beta_{r+2}\}| = 1.\end{aligned}$$

For $(i,j)\in\mathcal{E}$, $X_{ij} = \sum_{\gamma\in\mathbb{N}_r(n)} Z[\gamma,i,j] = 0$. So X is feasible in (2.9). The objective is

$$\begin{aligned}E\bullet X &= \sum_{i,j=1}^{n}\sum_{\gamma\in\mathbb{N}_r(n)} Z[\gamma,i,j] = \sum_{\beta\curlywedge V_{max}} Z[\beta] \\ &= \frac{\zeta^{(r)}(\mathcal{G})}{C}\cdot|\{\beta\in\mathbb{N}_{r+2}(n) : \beta\curlywedge V_{max}\}| = \zeta^{(r)}(\mathcal{G})\end{aligned}$$

□

Remark 2.4.1. Theorem 2.4.1 can also be proved by using the tensor structure and the primal form (2.9). The main idea is that for any feasible tensor lifting Z, one can continuously improve the objective by taking steps towards the direction that emphasizing $Z[\beta]$ with β evenly distributed over some maximal stable set of $\mathcal{G}$.

CHAPTER 3
SEPARATION BASED ON SPARSITY

3.1 Introduction

In this chapter we present an approach for separating any $n \times n$ real symmetric matrix $\bar{X}$ from the CP cone $\mathcal{C}_n$. Again in this chapter, when we do not emphasize the specific dimension, which is usually n, we omit the subscripts in notation $\mathcal{C}_n, \mathcal{C}_n^*, \mathcal{S}_n$ and simply write $\mathcal{C}, \mathcal{C}^*, \mathcal{S}$.

In this section we begin by reviewing some basic facts in standard convex analysis. Let $\mathcal{K}$ be a closed convex cone in $\mathcal{S}$, then $\bar{X} \notin \mathcal{K}$ if and only there exists $V \in \mathcal{S}$, such that $\langle V, \bar{X} \rangle < 0$ while $\langle V, X \rangle \geq 0, \forall X \in \mathcal{K}$. The dual cone of $\mathcal{K}$, $\mathcal{K}^*$, is defined as $\mathcal{K}^* = \{M : \langle M, X \rangle \geq 0, \forall X \in \mathcal{K}\}$. Every element $M \in \mathcal{K}^*$ corresponds to a supporting hyperplane for $\mathcal{K}$: $\langle M, \cdot \rangle \geq 0$. Hence in other words, $\bar{X} \notin \mathcal{K} \Leftrightarrow \exists M \in \mathcal{K}^*, \langle M, \bar{X} \rangle < 0$. The separation problem for $\mathcal{K}$ reads: given $\bar{X} \in \mathcal{S}$, determine whether $\bar{X} \in \mathcal{K}$, if $\bar{X} \notin \mathcal{K}$, find $\bar{M} \in \mathcal{K}^*$ such that $\langle \bar{M}, \bar{X} \rangle < 0$.

We focus on the separation problem for the completely positive cone $\mathcal{C}$. This problem is generally hard, otherwise if there exists an efficient separation oracle for $\mathcal{C}$, in some sense, one can solve any copositive program (with a bounded feasible region) efficiently by employing the ellipsoidal method, which is unlikely to happen unless $P = NP$. See Grötschel, Lovász and Schrijver [41] for a rigorous treatment of ellipsoidal method, and relation between different separation and optimization problems.

Since $\mathcal{C} \subseteq \mathcal{D}$, the cone of doubly nonnegative matrices, given a fixed $\bar{X} \in \mathcal{S}$, in order to solve the separation for $\mathcal{C}$, it is natural to start by testing the membership of $\bar{X} \in \mathcal{D}$. This is easily solvable by simply computing the minimum entry and the minimum eigenvalue of $\bar{X}$. If both values are nonnegative, then $\bar{X} \in \mathcal{D}$. Otherwise if $\bar{X}_{ij} < 0$, then $\frac{E_{ij}+Eji}{2} \in \mathcal{N} \subseteq \mathcal{D}^* \subseteq \mathcal{C}^*$ separates $\bar{X}$ from $\mathcal{D}$ and $\mathcal{C}$, and if $\lambda < 0$ is the minimum eigenvalue of $\bar{X}$ with eigenvector $q \in \Re_n$, then it is straightforward to verify that $qq^T \in \mathcal{S}^+ \subseteq \mathcal{D}^* \subseteq \mathcal{C}^*$ will do the work.

However there exists matrices $\bar{X} \in \mathcal{D} \setminus \mathcal{C}$. The question of interest is given $\bar{X} \in \mathcal{D}$, can we solve the separation problem from $\mathcal{C}$. For small dimensions $n \leq 4$, by Theorem 1.1.1 $\mathcal{C} = \mathcal{D}$, so there is nothing left to separate. A first interesting case is when $n = 5$.

The separation problem for $\mathcal{C}_5$ was first considered in [21]. Following its terminology, we say that a real symmetric matrix is *bad* if $X \in \mathcal{D} \setminus \mathcal{C}$, and *extremely bad* if X is bad, and an extreme ray of $\mathcal{D}$. Burer, Anstreicher and Dür [21] showed that if $X \in \mathcal{D}_5$ is extremely bad, we can construct a "cut" matrix $V \in \mathcal{C}_5^*$ that has $V \bullet X < 0$.

In this chapter we describe new separation procedures that apply to bad matrices. In Section 3.2, we generalize the separation procedure from [21] to apply to a broader class of matrices $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ than the extremely bad matrices considered in [21]. As in [21], the cut matrix constructed has the form of a transformed Horn matrix, where the Horn matrix is in $\mathcal{C}_5^* \setminus \mathcal{D}_5^*$. We also show that these "transformed Horn cuts" induce 10-dimensional faces of the 15-dimensional cone $\mathcal{C}_5$. In Section 3.3 we describe an even more general separation procedure that applies to any matrix $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ that is not componentwise strictly positive. The cut generation procedure in this case relies on the solution of a conic optimization problem. In Section 3.4 we describe separation procedures motivated by the procedure of Section 3.3 that apply to matrices in $\mathcal{D}_n \setminus \mathcal{C}_n$, $n > 5$ with a block structure. In Section

3.5 we numerically apply the separation procedures developed in Sections 2-4 to selected test problems.

To date, most of the literature concerning the use of CP matrices in optimization has involved schemes for approximating the copositive cones $\mathcal{C}_n^*$. A different approach to dynamically refining an approximation of $\mathcal{C}_n^*$ is taken in [17]. To our knowledge, the only paper other than [21] that considers strengthening the DNN relaxation of a problem posed over CP matrices by generating cuts corresponding to copositve matrices is [13]. However, the methodology described in [13] is specific to one particular problem (max-clique), while our approach is independent of the underlying problem and assumes only that the goal is to obtain a CP solution.

3.2 Separation via the Horn Matrix

In this section we describe a procedure for separating a bad 5×5 matrix from $\mathcal{C}_5$ that generalizes the separation procedure for extremely bad matrices in [21]. Recall that from [21], the class of extremely bad matrices (extreme rays of $\mathcal{D}_5$ that are not in $\mathcal{C}_5$) is

$$\mathcal{E}_5 := \{X \in \mathcal{D}_5 : \text{rank}(X) = 3 \text{ and } \mathcal{G}(X) \text{ is a 5-cycle}\}.$$

where $\mathcal{G}(X)$ is the undirected graph with vertex set $\{1, 2, \ldots, n\}$ and edge set $\{\{i \neq j\} : x_{ij} \neq 0\}$.

Note that when $\mathcal{G}(X)$ is a 5-cycle, every vertex has degree equal to two. We will generalize the procedure of [21] to apply to the case where $\text{rank}(X) = 3$ and $\mathcal{G}(X)$ has *at least one* vertex with degree two.

Our construction utilizes several results from [8] regarding matrices in $\mathcal{D}_5 \setminus \mathcal{C}_5$

of the form

$$X = \begin{pmatrix} X_{11} & \alpha_1 & \alpha_2 \\ \alpha_1^T & 1 & 0 \\ \alpha_2^T & 0 & 1 \end{pmatrix}, \tag{3.1}$$

where $X_{11} \in \mathcal{D}_3$. Note that the assumption of an off-diagonal zero in X is equivalent to assuming that $\mathcal{G}(X)$ is not a complete graph. Following the notation of [8], for a matrix $X \in \mathcal{D}_5$ of the form (3.1), let C denote the Schur complement $C = X_{11} - \alpha_1\alpha_1^T - \alpha_2\alpha_2^T$. Let $\mu(C)$ denote the number of negative components above the diagonal in C, and if $\mu(C) > 0$ define

$$\lambda_4 = \min_{1\le i<j\le 3} \left\{ \frac{x_{i4}x_{j4}}{-c_{ij}} \middle| c_{ij} < 0 \right\}, \quad \lambda_5 = \min_{1\le i<j\le 3} \left\{ \frac{x_{i5}x_{j5}}{-c_{ij}} \middle| c_{ij} < 0 \right\}. \tag{3.2}$$

It is shown in [8, Theorem 2.5] that $X \in \mathcal{C}_5$ if $\mu(C) > 1$ and $\lambda_4 + \lambda_5 \ge 1$, and in [8, Theorem 3.1] that $X \in \mathcal{C}_5$ if $\mu(C) \ne 2$. Thus for a matrix $X \in \mathcal{D}_5$ of the form (3.1), $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ implies that $\mu(C) = 2$ and $\lambda_4 + \lambda_5 < 1$. Finally, when $\operatorname{rank}(X) = 3$, it is shown in [8, Theorem 4.2] that these conditions are also sufficient to have $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$. For convenience we repeat this result here.

Theorem 3.2.1. [8, Theorem 4.2] *Assume that* $X \in \mathcal{D}_5$ *has the form* (3.1)*, with* $\operatorname{rank}(X) = 3$*. Then* $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ *if and only if* $\mu(C) = 2$ *and* $\lambda_4 + \lambda_5 < 1$*, where* λ_4 *and* λ_5 *are given by* (3.2)*.*

As in [21], the separation procedure developed here is based on a transformation of the well-known Horn matrix [42],

$$H := \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix} \in \mathcal{C}_5^* \setminus \mathcal{D}_5^*.$$

Theorem 3.2.2. *Suppose that* $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ *has* $\operatorname{rank}(X) = 3$*, and* $\mathcal{G}(X)$ *has a vertex* *of degree two. Then there exists a permutation matrix P and a diagonal matrix Λ with* $\mathrm{diag}(\Lambda) > 0$ *such that*

$$P\Lambda H\Lambda P^T \bullet X < 0.$$

Proof. To begin, consider a transformation of X of the form

$$\tilde{X} = \Sigma Q X Q^T \Sigma, \tag{3.3}$$

where Σ is a diagonal matrix with $\mathrm{diag}(\Sigma) > 0$ and Q is a permutation matrix. Then X satisfies the conditions of the theorem if and only if $\tilde{X}$ does. Moreover,

$$\begin{aligned} P\Lambda H\Lambda P^T \bullet \tilde{X} &= P\Lambda H\Lambda P^T \bullet \Sigma Q X Q^T \Sigma \\ &= P\Lambda H\Lambda P^T \bullet \Sigma(PP^T)QXQ^T(PP^T)\Sigma \\ &= Q^T P(P^T\Sigma P)\Lambda H\Lambda(P^T\Sigma P)P^T Q \bullet X \\ &= \tilde{P}\tilde{\Lambda}H\tilde{\Lambda}\tilde{P}^T \bullet X, \end{aligned}$$

where $\tilde{P} = Q^T P$ and $\tilde{\Lambda} = (P^T\Sigma P)\Lambda$. It follows that if we apply an initial transformation of the form (3.3) and show that the theorem holds for $\tilde{X}$, then it also holds for X. Below we will continue to refer to such a transformed matrix as X rather than $\tilde{X}$ to reduce notation.

Note that $\mathrm{diag}(X) > 0$, because otherwise $X \succeq 0$ implies that the only nonzero block in X is a 4×4 DNN matrix, and therefore $X \in \mathcal{C}_5$. Since $\mathcal{G}(X)$ has a vertex of degree 2, after applying a suitable permutation we may assume that $x_{45} = x_{15} = 0$, $x_{25} > 0$, $x_{35} > 0$. The assumption that $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ then implies that $x_{14} > 0$, since otherwise it is easy to see that $\mathcal{G}(X)$ would contain no 5-cycle, implying $X \in \mathcal{C}_5$ [7]. Let C denote the Schur complement $C = X_{11} - \alpha_1\alpha_1^T - \alpha_2\alpha_2^T$. By Theorem 3.2.1, C has exactly two negative entries above the diagonal, so at least one of c_{13} and c_{23} must be negative. If necessary interchanging row/column 2 and 3, we can assume that $c_{13} < 0$. After applying a suitable diagonal scaling we may therefore assume that X has the form (3.1), with $\alpha_1 = (1, u, v)^T$ and $\alpha_2 = (0, 1, 1)^T$.

The fact that $\text{rank}(X) = 3$ implies that $\text{rank}(C) = 1$, and $X \succeq 0$ implies that $C \succeq 0$. Since $c_{13} < 0$, it follows that there are scalars $x > 0$, $y > 0$, $z > 0$ so that C has one of the following forms:

$$C = \begin{pmatrix} x \\ y \\ -z \end{pmatrix} \begin{pmatrix} x \\ y \\ -z \end{pmatrix}^T \quad \text{or} \quad C = \begin{pmatrix} x \\ -y \\ -z \end{pmatrix} \begin{pmatrix} x \\ -y \\ -z \end{pmatrix}^T .$$

We next show that in fact the second case is impossible under the assumptions of the theorem. Assume that

$$C = \begin{pmatrix} x \\ -y \\ -z \end{pmatrix} \begin{pmatrix} x \\ -y \\ -z \end{pmatrix}^T , \quad \text{so} \quad X_{11} = \begin{pmatrix} x^2+1 & u-xy & v-xz \\ u-xy & y^2+u^2+1 & yz+uv+1 \\ v-xz & yz+uv+1 & z^2+v^2+1 \end{pmatrix} . \tag{3.4}$$

By Theorem 3.2.1, $\lambda_4 + \lambda_5 < 1$, where λ_4 and λ_5 are defined as in (3.2). Obviously $\lambda_5 = 0$, and $\lambda_4 = \min\{\frac{u}{xy}, \frac{v}{xz}\}$. But $\lambda_4 = \frac{u}{xy} < 1 \Rightarrow -xy + u < 0 \Rightarrow x_{12} < 0$, which is impossible since $X \in \mathcal{D}_5$. Assuming that $\lambda_4 = \frac{v}{xy} < 1$ leads to a similar contradiction $x_{13} < 0$, and therefore (3.4) cannot occur. We may therefore conclude that

$$C = \begin{pmatrix} x \\ y \\ -z \end{pmatrix} \begin{pmatrix} x \\ y \\ -z \end{pmatrix}^T , \quad \text{so} \quad X_{11} = \begin{pmatrix} x^2+1 & xy+u & v-xz \\ xy+u & y^2+u^2+1 & uv-yz+1 \\ v-xz & uv-yz+1 & z^2+v^2+1 \end{pmatrix} . \tag{3.5}$$

Again $\lambda_5 = 0$, and now $\lambda_4 = \min\{\frac{v}{xz}, \frac{uv}{yz}\}$. Then $\lambda_4 = \frac{v}{xz} < 1 \Rightarrow x_{13} < 0$, which is impossible, so we must have $\lambda_4 = \frac{uv}{yz} < 1$.

Let T be the permuted Horn matrix

$$T := PHP^T = \begin{pmatrix} 1 & -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{pmatrix}, \quad \text{where} \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Computation using symbolic mathematical software yields

$$\text{Det}\,(X \circ T) = -4x^2(yz - uv)^2 < 0.$$

Thus $X \circ T$ is nonsingular, and symbolic software obtains $(X \circ T)^{-1} = \frac{1}{2(uv-yz)} D_x M D_x$, where $D_x = \text{Diag}((\frac{1}{x}, 1, 1, \frac{1}{x}, 1)^T)$ and

$$M = \begin{pmatrix} 2uv & z & y & vxy - uxz + 2uv & y + z \\ z & 0 & 1 & z + vx & 1 \\ y & 1 & 0 & y - ux & 1 \\ vxy - uxz + 2uv & z + vx & y - ux & 2(u + xy)(v - xz) & y + z + vx - ux \\ y + z & 1 & 1 & y + z + vx - ux & 2(1 + uv - yz) \end{pmatrix}.$$

By using the inequalities $x_{13} = v - xz \geq 0$, $x_{23} = uv - yz + 1 \geq 0$ and an implied inequality $\lambda_4 < 1 \Rightarrow yz > uv \geq uxz \Rightarrow y > ux$, one can easily verify that $M \geq 0$ and therefore $(X \circ T)^{-1} \leq 0$, with at least one strictly negative component in each row.

Finally, define $w = -(X \circ T)^{-1}e > 0$, $V = \text{Diag}(w)T\,\text{Diag}(w) = P\Lambda H \Lambda P^T$ where $\Lambda = P^T\,\text{Diag}(w)P$. Then

$$\begin{aligned} V \bullet X &= \text{Diag}(w)T\,\text{Diag}(w) \bullet X = (T \circ ww^T) \bullet X = ww^T \bullet (X \circ T) \\ &= w^T(X \circ T)w = e^T(X \circ T)^{-1}(X \circ T)(X \circ T)^{-1}e = e^T w < 0. \end{aligned}$$

□

When X is extremely bad, it can be shown that the matrix $X \circ T$ in the proof of Theorem 3.2.2 is almost copositive[1], which implies the facts that $X \circ T$ is nonsingular and $(X \circ T)^{-1} \leq 0$ [74, Theorem 4.1]. However, we have been unable to show that $X \circ T$ is almost copositive under the more general assumptions of Theorem 3.2.2.

Let $V \in \mathcal{C}_5^*$, and consider a cut of the form $V \bullet X \geq 0$ that is valid for any $X \in \mathcal{C}_5$. From the standpoint of eliminating elements of $\mathcal{D}_5 \setminus \mathcal{C}_5$, it is desirable for the face

$$\mathcal{F}(\mathcal{C}_5, V) = \{X \in \mathcal{C}_5 : V \bullet X = 0\}$$

to have high dimension. We next show that the cut based on a transformed Horn matrix from Theorem 3.2.2 induces a 10-dimensional face of the 15-dimensional cone $\mathcal{C}_5$. (It is known [35] that $\mathcal{C}_n$ has an interior in the $n(n+1)/2$-dimensional space corresponding to $\mathcal{S}_n$.)

Theorem 3.2.3. *Let $V = P\Lambda H \Lambda P^T$, where P is a permutation matrix and Λ is a diagonal matrix with* $\operatorname{diag}(\Lambda) > 0$. *Then* $\dim \mathcal{F}(\mathcal{C}_5, V) = 10$.

Proof. Without loss of generality we may take $P = \Lambda = I$, so $V = H$. The extreme rays of $\mathcal{F}(\mathcal{C}_5, H)$ are then matrices of the form $X = xx^T$, where $x \geq 0$ and $x^T H x = 0$, and any element of $\mathcal{F}(\mathcal{C}_5, H)$ can be written as a nonnegative combination of such extreme rays. To determine $\dim \mathcal{F}(\mathcal{C}_5, H)$ we must therefore determine the maximum number of such extreme rays that are linearly independent.

For any $X = xx^T$, $x \geq 0$ let $\mathcal{I}(x) = \{i : x(i) > 0\}$. We first consider which sets $\mathcal{I}(x)$ are possible for $X = xx^T \in \mathcal{F}(\mathcal{C}_5, H)$. It is easy to show that

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

[1] An $n \times n$ matrix is almost copositive if it is not copositive, but all of its $(n-1) \times (n-1)$ principal submatrices are copositive.

The fact that $H \in \mathcal{C}_5^*$ then follows from the fact that for any $x \geq 0$, either $x_4 \geq x_5$ or $x_5 \geq x_4$. Moreover, $x > 0$ and $x^T Hx = 0$ would imply $x_4 = x_5 > 0$, and therefore $x_2 = 0$, a contradiction, so $|\mathcal{I}(x)| = 5$ is impossible. Similarly $|\mathcal{I}(x)| = 4$ implies that $x_4 = x_5 > 0$, and therefore $x_2 = 0$, so $(x_1 - x_2 + x_3 + x_4 - x_5)^2 = (x_1 + x_3)^2 > 0$, and $xx^T \notin \mathcal{F}(\mathcal{C}_5, H)$. Thus $|\mathcal{I}(x)| = 4$ is impossible. Finally $|\mathcal{I}(x)| = 1$ is impossible since $\operatorname{diag}(H) = e > 0$, so the only possibilities are $|\mathcal{I}(x)| = 2$ and $|\mathcal{I}(x)| = 3$.

Let H^+ and X^+ be the principal submatrices of H and $X = xx^T$, respectively, corresponding to the positive components of x. For $|\mathcal{I}(x)| = 2$, H^+ has the form

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

and obviously $x^T Hx = 0$ is only possible in the first case. It follows that if $|\mathcal{I}(x)| = 2$, then $\mathcal{I}(x)$ is either $\{1, 2\}$, $\{2, 3\}$, $\{3, 4\}$, $\{4, 5\}$ or $\{5, 1\}$, and in each case X^+ is a positive multiple of ee^T.

Next assume that $|\mathcal{I}(x)| = 3$. Clearly H^+ cannot have a row equal to $(1, 1, 1)$, and the 3×3 principal submatrices of H that do not contain such a row correspond to $\mathcal{I}(x)$ equal to $\{1, 2, 3\}$, $\{2, 3, 4\}$, $\{3, 4, 5\}$, $\{4, 5, 1\}$ and $\{5, 1, 2\}$. Consider $\mathcal{I}(x) = \{1, 2, 3\}$, so

$$H^+ = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}.$$

Since $H^+ \succeq 0$, $x^T Hx = 0 \iff H^+ x^+ = 0$, where $x^+ = (x_1, x_2, x_3)^T$. It is then obvious that $x^+ = x_2(u, 1, 1 - u)^T$ for some $0 < u < 1$. The vector t corresponding to the upper triangle of $x^+(x^+)^T$ then has the form

$$t = (x_{11}, x_{12}, x_{13}, x_{22}, x_{23}, x_{33})^T = x_2^2(u^2, u, u(1 - u), 1, (1 - u), (1 - u)^2)^T. \quad (3.6)$$

Any vector of the form (3.6) satisfies the equations

$$\begin{aligned} t_1 - 2t_2 + t_4 - t_6 &= 0 \\ t_1 - t_2 + t_3 &= 0 \\ t_2 - t_4 + t_5 &= 0. \end{aligned}$$

These equations are linearly independent, so there can be at most 3 linearly independent vectors of the form (3.6). However, the values $u = 0$ and $u = 1$ correspond to two of the matrices $X = xx^T$ with $|\mathcal{I}(x) = 2|$, so only one matrix with $0 < u < 1$ can be added while maintaining a linearly independent set. The same argument applies for all of the other possibilities having $|\mathcal{I}(x) = 3|$, so the maximum possible dimension for $\mathcal{F}(\mathcal{C}_5, H)$ is ten. Finally it can be verified numerically that the five $X = xx^T$ with distinct $|\mathcal{I}(x) = 2|$, and five with distinct $|\mathcal{I}(x) = 3|$, are in fact linearly independent. $\square$

As mentioned above, Theorem 3.2.2 can be viewed as a generalization of the separation result for extremely bad 5×5 matrices in [21, Theorem 8]. To make this connection more explicit, we can use the fact [21, Section 2] that $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ is extremely bad if and only if X can be written in the form

$$X = P\Lambda \begin{pmatrix} 1 & \beta_1 & 0 & 0 & 1 \\ \beta_1 & \beta_1^2 + \beta_2^2 + 1 & \beta_2 & 0 & 0 \\ 0 & \beta_2 & 1 & 1 & 0 \\ 0 & 0 & 1 & \beta_2^2 + 1 & \beta_1\beta_2 \\ 1 & 0 & 0 & \beta_1\beta_2 & \beta_1^2 + 1 \end{pmatrix} \Lambda P^T,$$

where Λ is a positive diagonal matrix, P is a permutation matrix and $\beta_1, \beta_2 > 0$. With a suitable permutation of rows/columns and a slight modification in Λ, this characterization is equivalent to

$$X = P\Lambda \begin{pmatrix} \beta_1^2+1 & \beta_1\beta_2 & 0 & 1 & 0 \\ \beta_1\beta_2 & \beta_2^2+1 & 0 & 0 & 1 \\ 0 & 0 & \frac{\beta_1^2}{\beta_2^2}+1+\frac{1}{\beta_2^2} & \frac{\beta_1}{\beta_2} & 1 \\ 1 & 0 & \frac{\beta_1}{\beta_2} & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{pmatrix} \Lambda P^T,$$

corresponding to (3.5) with $u = 0$, $v = \frac{\beta_1}{\beta_2}$, $x = \beta_1$, $y = \beta_2$, $z = \frac{1}{\beta_2}$. Another interesting special case where Theorem 3.2.2 applies is as follows. Let H be the Horn matrix and consider the face of $\mathcal{D}_5$,

$$\mathcal{F}(\mathcal{D}_5, H) := \{X \in \mathcal{D}_5 : H \bullet X = 0\}.$$

In the optimization context an element of $\mathcal{F}(\mathcal{D}_5, H)$ could arise naturally via the following sequence. Suppose that an optimization problem posed over $\mathcal{D}_5$ has a solution X that satisfies the assumptions of Theorem 3.2.2 (for example, X is extremely bad). After adding a transformed Horn cut and re-solving, the new solution X' (after diagonal scaling and permutation) would likely be an extreme ray of $\mathcal{F}(\mathcal{D}_5, H)$. Burer (private communication) obtained the following characterization of the extreme rays of $\mathcal{F}(\mathcal{D}_5, H)$.

Theorem 3.2.4. *Let X be an extreme ray of $\mathcal{F}(\mathcal{D}_5, H)$. Then* $\operatorname{rank}(X)$ *equals 1 or 3. Further, if* $\operatorname{rank}(X) = 3$*, then $\mathcal{G}(X)$ is either a 5-cycle, or a 5-cycle with a single additional chord.*

One can characterize the matrices in Theorem 3.2.4 using an argument similar to what is done in [21, Section 2] to characterize extremely bad matrices. The result is that a matrix $X \in \mathcal{D}_5$ satisfies the conditions of Theorem 3.2.4 if and only if there exists a permutation matrix P, a positive diagonal matrix Λ and $\beta_1, \beta_2, \beta_3 > 0$,

$\beta_2 \leq \beta_1\beta_3$, such that

$$X = P\Lambda \begin{pmatrix} \beta_1^2+1 & \beta_1\beta_2 & 0 & 1 & 0 \\ \beta_1\beta_2 & \beta_2^2+1 & 1-\frac{\beta_2}{\beta_1\beta_3} & 0 & 1 \\ 0 & 1-\frac{\beta_2}{\beta_1\beta_3} & \frac{1}{\beta_3^2}+1+\frac{1}{\beta_1^2\beta_3^2} & \frac{1}{\beta_3} & 1 \\ 1 & 0 & \frac{1}{\beta_3} & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{pmatrix} \Lambda P^T,$$

correponding to (3.5) with $u = 0$, $v = \frac{1}{\beta_3}$, $x = \beta_1$, $y = \beta_2$, $z = \frac{1}{\beta_1\beta_3}$. Note that such an X is extremely bad if and only if $\beta_2 = \beta_1\beta_3$.

3.3 Separation via Conic Programming

In this section we describe a separation procedure that applies to a broader class of matrices $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ than the procedure of the previous section. Let $X \in \mathcal{D}_5$, with at least one off-diagonal zero, and assume that $\mathrm{diag}(X) > 0$ since otherwise $X \in \mathcal{C}_5$ is immediate. After a permutation and diagonal scaling, X may be assumed to have the form (3.1). For such a matrix a useful characterization of $X \in \mathcal{C}_5$ is given by the following theorem from [8].

Theorem 3.3.1. [8, Theorem 2.1] *Let $X \in \mathcal{D}_5$ have the form* (3.1)*. Then $X \in \mathcal{C}_5$ if and only if there are matrices A_{11} and A_{22} such that $X_{11} = A_{11} + A_{22}$, and*

$$\begin{pmatrix} A_{ii} & \alpha_i \\ \alpha_i^T & 1 \end{pmatrix} \in \mathcal{D}_4, \quad i = 1, 2.$$

In [8], Theorem 3.3.1 is utilized only as a proof mechanism, but we now show that it has algorithmic consequences as well.

Theorem 3.3.2. *Assume that $X \in \mathcal{D}_5$ has the form* (3.1)*. Then $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ if* *and only if there is a matrix*

$$V = \begin{pmatrix} V_{11} & \beta_1 & \beta_2 \\ \beta_1^T & \gamma_1 & 0 \\ \beta_2^T & 0 & \gamma_2 \end{pmatrix} \quad \textit{such that} \quad \begin{pmatrix} V_{11} & \beta_i \\ \beta_i^T & \gamma_i \end{pmatrix} \in \mathcal{D}_4^*, \quad i = 1, 2,$$

and $V \bullet X < 0$*.*

Proof. Consider the "CP feasibility problem"

$$\begin{aligned} \text{(CPFP)} \quad \min \quad & 2\theta \\ \text{s.t.} \quad & \begin{pmatrix} A_{ii} & \alpha_i \\ \alpha_i^T & 1 \end{pmatrix} + \theta(I+E) \in \mathcal{D}_4, \quad i = 1, 2 \\ & A_{11} + A_{22} = X_{11} \\ & \theta \geq 0, \end{aligned}$$

where by assumption $\alpha_i \geq 0$, $i = 1, 2$ and $X_{11} \in \mathcal{D}_3$. By Theorem 3.3.1, $X \in \mathcal{C}_5$ if and only if the solution value in CPFP is zero. Using conic duality it is straightforward to verify that the dual of CPFP can be written

$$\begin{aligned} \text{(CPDP)} \quad \max \quad & -(V_{11} \bullet X_{11} + 2\alpha_1^T \beta_1 + 2\alpha_2^T \beta_2 + \gamma_1 + \gamma_2) \\ \text{s.t.} \quad & \begin{pmatrix} V_{11} & \beta_i \\ \beta_i^T & \gamma_i \end{pmatrix} \in \mathcal{D}_4^*, \quad i = 1, 2 \\ & (I+E) \bullet V_{11} + e^T \beta_1 + e^T \beta_2 + \gamma_1 + \gamma_2 \leq 1. \end{aligned}$$

Moreover CPFP and CPDP both have feasible interior solutions, so strong duality holds. The proof is completed by noting that the objective in CPDP is exactly $-V \bullet X$. □

Suppose that $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$, and V is a matrix that satisfies the conditions of Theorem 3.3.2. If $\tilde{X} \in \mathcal{C}_5$ is another matrix of the form (3.1), then Theorem 3.3.1 implies that $V \bullet \tilde{X} \geq 0$. However we cannot conclude that $V \in \mathcal{C}_5^*$ because $V \bullet \tilde{X} \geq 0$ only holds for $\tilde{X}$ of the form (3.1), in particular, $\tilde{x}_{45} = 0$. Fortunately, the matrix

V can easily be "completed" to obtain a copositive matrix that still separates X from $\mathcal{C}_5$.

Theorem 3.3.3. *Suppose that $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ has the form* (3.1)*, and V satisfies the conditions of Theorem 3.3.2. Define*

$$V(s) = \begin{pmatrix} V_{11} & \beta_1 & \beta_2 \\ \beta_1^T & \gamma_1 & s \\ \beta_2^T & s & \gamma_2 \end{pmatrix}.$$

Then $V(s) \bullet X < 0$ for any s, and $V(s) \in \mathcal{C}_5^*$ for $s \geq \sqrt{\gamma_1 \gamma_2}$.

Proof. The fact that $V(s) \bullet X = V \bullet X < 0$ is obvious from $x_{45} = 0$, and $V(s) \in \mathcal{C}_5^*$ for $s \geq \sqrt{\gamma_1 \gamma_2}$ follows immediately from [48, Theorem 1]. □

Theorems 3.3.2 and 3.3.3 provide a separation procedure that applies to any $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ that is not componentwise strictly positive. In applying Theorem 6 to separate a given X, one can numerically minimize $X \bullet V$, where V satisfies the conditions in the theorem and is normalized via a condition such as $I \bullet V = 1$ or $(I + E) \bullet V = 1$. In [8, Theorem 6.1] it is claimed that if $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$, $X > 0$, then there is a simple transformation of X that produces another matrix $\tilde{X} \in \mathcal{D}_5 \setminus \mathcal{C}_5$, $\tilde{X} \not> 0$, suggesting that a separation procedure for X could be based on applying the construction of Theorem 3.3.2 to $\tilde{X}$. However it is shown in [30] that in fact [8, Theorem 6.1] is false.

3.4 Separation for Matrices with $n > 5$

Suppose now that $X \in \mathcal{D} \setminus \mathcal{C}$ for $n > 5$. In order to separate X from $\mathcal{C}$, we could attempt to apply the procedure in Section 2 or Section 3 to candidate 5×5 principal submatrices of X. However, it is possible that all such submatrices are in $\mathcal{C}_5$ so that no cut based on a 5×5 principal submatrix can be found. In this section we consider extensions of the separation procedure developed in Section 3 to matrices $X \in \mathcal{D} \setminus \mathcal{C}$, $n > 5$ having block structure. In order to state the separation procedure in its most general form we will utilize the notion of a CP graph. We refer the reader to Section 1.1.1 and Theorem 1.1.2 for definition and main result of CP graph.

Our separation procedure is based on a simple observation for CP matrices in the following form

$$X = \begin{pmatrix} X_{11} & X_{12} & X_{13} & \dots & X_{1k} \\ X_{12}^T & X_{22} & 0 & \dots & 0 \\ X_{13}^T & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ X_{1k}^T & 0 & \dots & 0 & X_{kk} \end{pmatrix}, \tag{3.7}$$

where $k \geq 3$, each X_{ii} is an $n_i \times n_i$ matrix, and $\sum_{i=1}^{k} n_i = n$.

Lemma 3.4.1. *Suppose that $X \in \mathcal{D}_n$ has the form (3.7), $k \geq 3$, and let*

$$X^i = \begin{pmatrix} X_{11} & X_{1i} \\ X_{1i}^T & X_{ii} \end{pmatrix}, i = 2, \dots, k.$$

Then $X \in \mathcal{C}_n$ if and only if there are matrices A_{ii}, $i = 2, \dots, k$ such that $\sum_{i=2}^{k} A_{ii} = X_{11}$, and

$$\begin{pmatrix} A_{ii} & X_{1i} \\ X_{1i}^T & X_{ii} \end{pmatrix} \in \mathcal{C}_{n_1+n_i}, \quad i = 2, \dots, k.$$

Moreover, if $\mathcal{G}(X^i)$ is a CP graph for each $i = 2, \dots, k$, then the above statement remains true with $\mathcal{C}_{n_1+n_i}$ replaced by $\mathcal{D}_{n_1+n_i}$.

Proof. Let $N_1 = 0$, $N_i = N_{i-1} + n_i$, $i = 2, \dots, k$, and $\mathcal{I}_i = \{N_i + 1, \dots, N_i + n_i\}$, $i = 1, \dots, k$. Then $\mathcal{I}_i$ contains the indeces of the rows and columns of X corresponding to X_{ii}. From the structure of X, it is clear that $X \in \mathcal{C}_n$ if and only if there are nonnegative vectors a^{ij} such that

$$X = \sum_{i=2}^{k} \sum_{j=1}^{m_i} a^{ij} (a^{ij})^T,$$

where $a_l^{ij} = 0$ for $l \notin \mathcal{I}_1 \cup \mathcal{I}_i$. The lemma follows by deleting the rows and columns of $\sum_{j=1}^{m_i} a^{ij}(a^{ij})^T$ that are not in $\mathcal{I}_1 \cup \mathcal{I}_i$. That $\mathcal{C}_{n_1+n_i}$ can be replaced by $\mathcal{D}_{n_1+n_i}$ when $\mathcal{G}(X^i)$ is a CP graph follows from definition of CP graph in Section 1.1.1and the fact that $\mathcal{G}(A_{ii})$ must be a subgraph of $\mathcal{G}(X_{11})$ for each i. □

Theorem 3.4.1. *Suppose that $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ has the form* (3.7)*, where $\mathcal{G}(X^i)$ is a CP graph, $i = 2, \ldots, k$. Then there is a matrix*

$$V = \begin{pmatrix} V_{11} & V_{12} & V_{13} & \ldots & V_{1k} \\ V_{12}^T & V_{22} & 0 & \ldots & 0 \\ V_{13}^T & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ V_{1k}^T & 0 & \ldots & 0 & V_{kk} \end{pmatrix}$$

such that

$$\begin{pmatrix} V_{11} & V_{1i} \\ V_{1i}^T & V_{ii} \end{pmatrix} \in \mathcal{D}^*_{n_1+n_i}, \quad i = 2, \ldots, k,$$

and $V \bullet X < 0$. Moreover, the matrix

$$\tilde{V} = \begin{pmatrix} V_{11} & \ldots & V_{1k} \\ \vdots & \ddots & \vdots \\ V_{1k}^T & \ldots & V_{kk} \end{pmatrix},$$

where $V_{ij} = \sqrt{\mathrm{diag}(V_{ii})} \sqrt{\mathrm{diag}(V_{jj})}^T$, $2 \le i \ne j \le k$, has $\tilde{V} \in \mathcal{C}_n^*$ and $\tilde{V} \bullet X = V \bullet X < 0$.

Proof. The proof uses an argument very similar to that used to prove Theorems 3.3.2 and 3.3.3. □

When $n_1 = 2$, a matrix X satisfying the conditions of Theorem 3.4.1 has a book graph with k CP pages, and an algebraic procedure for testing if $X \in \mathcal{C}_n$ is known [6]. There are several situations where we can immediately use Theorem 3.4.1 to separate a matrix of the form (3.7) with $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ from $\mathcal{C}_n$. One case, corresponding to $n_1 = 3$ and $n_i = 1$, $i = 2, \ldots, k$ can be viewed as a generalization of the separation procedure for a matrix of the form (3.1) in the previous section. Assuming that X has no zero diagonal components, after a symmetric permutation and diagonal rescaling, and setting $k \leftarrow k-1$, we may assume that such a matrix X has the form

$$X = \begin{pmatrix} X_{11} & \alpha_1 & \alpha_2 & \ldots & \alpha_k \\ \alpha_1^T & 1 & 0 & \ldots & 0 \\ \alpha_2^T & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \alpha_k^T & 0 & \ldots & 0 & 1 \end{pmatrix}. \tag{3.8}$$

Corollary 3.4.1. *Suppose that $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ has the form (3.8), where $X_{11} \in \mathcal{D}_3$. Then there is a matrix*

$$V = \begin{pmatrix} V_{11} & B \\ B^T & \mathrm{Diag}(\gamma) \end{pmatrix}$$

where $V_{11} \in \mathcal{D}_3^*$, $B = (\beta_1, \beta_2, \ldots, \beta_k)$ and $\gamma \geq 0$ such that

$$\begin{pmatrix} V_{11} & \beta_i \\ \beta_i^T & \gamma_i \end{pmatrix} \in \mathcal{D}_4^*, \quad i = 1, 2, \ldots, k$$

and $V \bullet X < 0$. Moreover, if $s = \sqrt{\gamma}$ then

$$V(s) = \begin{pmatrix} V_{11} & B \\ B^T & ss^T \end{pmatrix} \in \mathcal{C}_n^*.$$

Note that in the case where X has the structure (3.8), the vertices $4, \ldots, k+3$ form a stable set of size k in $\mathcal{G}(X)$. A second case where the structure (3.7) can immediately be used to generate a cut separating a matrix $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ is when $n_i = 2$, $i = 1, \ldots, k$. In this case the subgraph of $\mathcal{G}(X)$ on the vertices $3, \ldots, 2k$ is a matching, and the matrices

$$\begin{pmatrix} V_{11} & V_{1i} \\ V_{1i}^T & V_{ii} \end{pmatrix}$$

in Theorem 3.4.1 are again all in $\mathcal{D}_4^*$.

A second case where block structure can be used to generate cuts for a matrix $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ is when X has the form

$$X = \begin{pmatrix} I & X_{12} & X_{13} & \dots & X_{1k} \\ X_{12}^T & I & X_{23} & \dots & X_{2k} \\ X_{13}^T & X_{23}^T & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & X_{(k-1)k} \\ X_{1k}^T & 0 & \dots & X_{(k-1)k}^T & I \end{pmatrix}, \tag{3.9}$$

where $k \geq 2$, each X_{ij} is an $n_i \times n_j$ matrix, and $\sum_{i=1}^k n_i = n$. The structure in (3.9) corresponds to a partitioning of the vertices $\{1, 2, \dots, n\}$ into k stable sets in $\mathcal{G}(X)$, of size $n_1, \dots, n_k$ (note that $n_i = 1$ is allowed). In order to succinctly characterize when $X \in \mathcal{C}_n$ for such a matrix it is convenient to utilize a multi-index vector $p \in Z^k$, with components $1 \leq p_i \leq n_i$.

Lemma 3.4.2. *Suppose that $X \in \mathcal{D}_n$ has the structure (3.9). For each $p \in Z^k$ with $1 \leq p_i \leq n_i$, $i = 1 \dots, n$, let X^p be the $k \times k$ matrix with components*

$$[X^p]_{ij} = \begin{cases} [X_{ij}]_{p_i p_j} & i \neq j, \\ a_i^p & i = j, \end{cases}$$

where $a^p \in \Re^k$. Then $X \in \mathcal{C}_n$ if and only if there are $a^p \in \Re^k$ so that $X^p \in \mathcal{C}_k$ for each p, and

$$\sum_{p:p_i=j} a_i^p = 1$$

for each $i = 1, \dots, k$ and $1 \leq j \leq n_i$. If in addition $\mathcal{G}(X^p)$ is a CP graph for each p, then the above statement holds with $\mathcal{D}_k$ in place of $\mathcal{C}_k$.

Proof. The proof is similar to that of Lemma 3.4.1, but uses the fact that if X has the form (3.9) and bb^T is a rank-one matrix in the CP-decomposition of X, then for each $i = 1, \ldots, k$, $b_j > 0$ for at most one $j \in \mathcal{I}(i)$. □

Theorem 3.4.2. *Suppose that $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ has the form (3.9), where $\mathcal{G}(X^p)$ is a CP graph for each $p \in Z^k$ with $1 \le p_i \le n_i$, $i = 1, \ldots, k$. Then there is a matrix*

$$V = \begin{pmatrix} \mathrm{Diag}(\gamma^1) & V_{12} & V_{13} & \ldots & V_{1k} \\ V_{12}^T & \mathrm{Diag}(\gamma^2) & V_{23} & \ldots & V_{2k} \\ V_{13}^T & V_{23}^T & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & V_{(k-1)k} \\ V_{1k}^T & 0 & \ldots & V_{(k-1)k}^T & \mathrm{Diag}(\gamma^k) \end{pmatrix},$$

with $V \bullet X < 0$, such that for every $p \in Z^k$ with $1 \le p_i \le n_i$, $i = 1, \ldots, k$, $V^p \in \mathcal{D}_k^*$, where

$$[V^p]_{ij} = \begin{cases} [V_{ij}]_{p_i p_j} & i \neq j, \\ \gamma^i_{p_i} & i = j. \end{cases}$$

Moreover, the matrix

$$\tilde{V} = \begin{pmatrix} V_{11} & \ldots & V_{1k} \\ \vdots & \ddots & \vdots \\ V_{1k}^T & \ldots & V_{kk} \end{pmatrix},$$

where $V_{ii} = \sqrt{\gamma^i}\,\sqrt{\gamma^i}^T$, has $\tilde{V} \in \mathcal{C}_n^*$ and $\tilde{V} \bullet X = V \bullet X < 0$.

Proof. The proof uses an argument very similar to that used to prove Theorems 3.3.2 and 3.3.3. □

To close the section we mention several details regarding the applicability of Lemmas 3.4.1 and 3.4.2 to separate a given $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ from $\mathcal{C}_n$, via the cuts described in Theorems 3.4.1 and 3.4.2. First, in practice a given matrix X may have numerical entries that are small but not exactly zero. In such a case, Lemma 3.4.1 or 3.4.2 can be applied to a perturbed matrix $\tilde{X}$, where entries of X below a specified tolerance are set to zero in $\tilde{X}$. If a cut V separating $\tilde{X}$ from $\mathcal{C}_n$ is found and the zero tolerance is small, then $V \bullet X \approx V \bullet \tilde{X} < 0$, and V is very likely to also separate X from $\mathcal{C}_n$. Second, it is important to recognize that in practice Theorems 3.4.1 and 3.4.2 may provide a cut separating a given $X \in \mathcal{D}_n \setminus \mathcal{C}_n$ even when the sufficient conditions for generating such a cut are not satisfied. In particular, a cut of the form described in Theorem 3.4.1 may be found even when the condition that X^i is a CP graph for each i is not satisfied; similarly a cut of the form described in Theorem 3.4.2 may be found even when the condition that X^p is a CP graph for each p is not satisfied. Finally, the cut matrix $\tilde{V}$ in Theorem 3.4.1 satisfies $\tilde{V} \in \mathcal{C}_n^*$ for any $V_{ij} \geq \sqrt{\operatorname{diag}(V_{ii})}\sqrt{\operatorname{diag}(V_{jj})}^T$, but it is clear that the resulting constraint is tightest for the choice $V_{ij} = \sqrt{\operatorname{diag}(V_{ii})}\sqrt{\operatorname{diag}(V_{jj})}^T$. Similar observations hold for the cut matrices in Corollary 3.4.1 and Theorem 3.4.2.

3.5 Applications

In this section we describe the results of applying the separation procedures developed in the paper to selected test problems. Consider an indefinite quadratic programming problem of the form

$$\begin{aligned} \text{(QP)} \quad \max \quad & x^T Q x + c^T x \\ \text{s.t.} \quad & Ax = b \\ & x \geq 0, \end{aligned}$$

where A is an $m \times n$ matrix. For the case of general Q, (QP) is an NP-Hard problem. Next define the matrices

$$Y = \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix}, \quad \tilde{Q} = \begin{pmatrix} 0 & c^T/2 \\ c/2 & Q \end{pmatrix}, \tag{3.10}$$

and let

$$QP(A,b) = \text{conv}\left\{ \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T : \; Ax = b, \; x \geq 0 \right\}. \tag{3.11}$$

Since the extreme points of $QP(A,b)$ correspond to feasible solutions of (QP), (QP) can be written as the linear optimization problem

$$\begin{aligned} \text{(QP)} \quad \max \quad & \tilde{Q} \bullet Y \\ \text{s.t.} \quad & Y \in QP(A,b). \end{aligned}$$

The connection between (QP) and the topic of the paper is the following result showing that $QP(A,b)$ can be exactly represented using the CP cone.

Theorem 3.5.1. [18] *Assume that* $\{x : Ax = b, \; x \geq 0\}$ *is bounded, and let* $QP(A,b)$ *be defined as in* (3.11). *Then* $QP(A,b) = \{Y \in \mathcal{C}_{n+1} : a_i^T x = b_i, a_i^T X a_i = b_i^2, i = 1, \ldots, m\}$.

One well-studied case of (QP) is the box-constrained quadratic program

$$\begin{aligned} \text{(QPB)} \quad \max \quad & x^T Q x + c^T x \\ \text{s.t.} \quad & 0 \leq x \leq e. \end{aligned}$$

In order to linearize (QPB) one can define Y and $\tilde{Q}$ as in (3.10) and write the objective as $\tilde{Q} \bullet Y$. There are then a number of different constraints that can be imposed on Y. For example, Y should satisfy with the well-known Reformulation-Linearization Technique (RLT) constraints

$$\{0, x_i + x_j - 1\} \leq x_{ij} \leq \{x_i, x_j\}, \quad 1 \leq i,j \leq n, \tag{3.12}$$

as well as the PSD condition $Y \succeq 0$. To apply Theorem 3.5.1 to (QPB), one can add slack variables s and write the constraints as $x + s = e$, $(x,s) \geq 0$. It is then natural to define an augmented matrix

$$Y^+ = \begin{pmatrix} 1 & x^T & s^T \\ x & X & Z \\ s & Z^T & S \end{pmatrix},$$

where S and Z relax ss^T and xs^T, respectively. The "squared constraints" from Theorem 3.5.1 then have the form $\text{diag}(X+2Z+S) = e$, and the CP representation of (QPB) can be written

$$\begin{aligned} (\text{QPB})_{\text{CP}} \quad \max \quad & x^TQx + c^Tx \\ \text{s.t.} \quad & x + s = e, \quad \text{Diag}(X + 2Z + S) = e, \\ & Y^+ \in \mathcal{C}_{2n+1}. \end{aligned}$$

It can also be shown [5, 20] that replacing $\mathcal{C}_{2n+1}$ in $(\text{QPB})_{\text{CP}}$ with $\mathcal{D}_{2n+1}$ is equivalent to solving the relaxation of (QPB) that imposes the PSD condition $Y \succeq 0$ together with the RLT constraints (3.12). Moreover, this relaxation is tight for $n = 2$ but may not be for $n \geq 3$. In [24] it is shown that for (QPB) the off-diagonal components of Y can be constained to be in the Boolean Quadric Polytope (BQP). As a result, valid inequalities for the BQP can be imposed on the off-diagonal components of Y, an approach that was first suggested in [78]. For $n = 3$, the BQP is fully characterized by the RLT constraints and the well-known triangle (TRI) inequalities. However, it is shown in [24] that for $n \geq 3$, the PSD, RLT and TRI constraints on Y are still not sufficient to exactly represent (QPB). This is done by considering the (QPB) instance with $n = 3$ and

$$Q = \begin{pmatrix} -2.25 & -3.00 & -3.00 \\ -3.00 & 0.00 & -0.50 \\ -3.00 & -0.50 & 1.00 \end{pmatrix}, \qquad c = \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix}. \tag{3.13}$$

It is shown in [24] that the solution value for (QPB) with the data (3.13) is 1.0, but the maximum of $\tilde{Q} \bullet Y$ where $Y \succeq 0$ satisfies the RLT and TRI constraints is approximately 1.093.

For the data in (3.13), solving QPB_{CP}, with $\mathcal{D}_7$ in place of $\mathcal{C}_7$ and the triangle inequalities added, results in the 7×7 matrix

$$Y^+ \approx \begin{pmatrix} 1.0000 & 0.1478 & 0.5681 & 0.5681 & 0.8522 & 0.4319 & 0.4319 \\ 0.1478 & 0.0901 & 0.0000 & 0.0000 & 0.0577 & 0.1478 & 0.1478 \\ 0.5681 & 0.0000 & 0.5681 & 0.2841 & 0.5681 & 0.0000 & 0.2840 \\ 0.5681 & 0.0000 & 0.2841 & 0.5681 & 0.5681 & 0.2840 & 0.0000 \\ 0.8522 & 0.0577 & 0.5681 & 0.5681 & 0.7944 & 0.2840 & 0.2840 \\ 0.4319 & 0.1478 & 0.0000 & 0.2840 & 0.2840 & 0.4319 & 0.1478 \\ 0.4319 & 0.1478 & 0.2840 & 0.0000 & 0.2840 & 0.1478 & 0.4319 \end{pmatrix}.$$

It is known [5] that Y^+ is CP if and only if the 6×6 matrix obtained by deleting its first row and column is CP. Further deleting the fifth row and column results in a 5×5 submatrix of Y^+ which is not CP. In fact, this 5×5 matrix meets all the conditions of Theorem 3.2.2, so a transformed Horn cut that separates Y^+ from $\mathcal{C}_7$ can be generated. Alternatively, a cut from Theorem 3.3.3 can be used. In either case imposing the new constraint and re-solving results in a new matrix Y^+ with lower objective value. The same 5×5 principal submatrix again fails to be CP, so another cut can be generated and the process repeated. In Figure 3.1 we show the effect of executing this process using the cuts from Theorem 3.3.3, normalized using $I \bullet V = 1$. After adding 21 cuts, the gap to the true solution value of the problem is reduced below 10^{-8}. (The rank condition in Theorem 3.2.2 fails after 3 cuts are added, but this has no effect on the cuts from Theorem 3.3.3.)

Before continuing, we remark that there are other known approaches that obtain an optimal value for the (QPB) instance (3.13) without branching. For example, in [5] it is shown that for $n = 3$, (QPB) can be exactly represented using

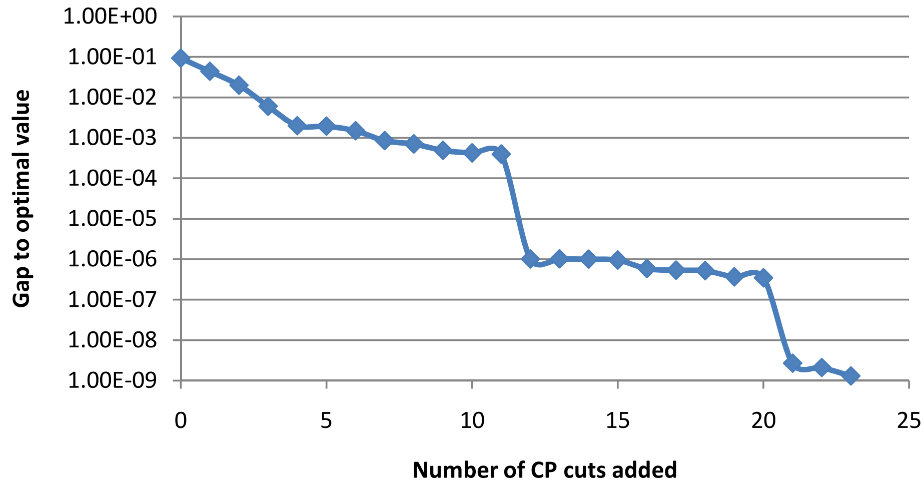

Figure 3.1: Gap to optimal value for Burer-Letchford QPB problem ($n = 3$)

DNN matrices via a triangulation of the 3-cube. This representation provides a tractable formulation that returns the exact optimal solution value for the original problem. A completely different approach is based on using the result of Theorem 3.5.1 and writing a dual for $(\text{QPB})_{\text{CP}}$ that involves the cone $\mathcal{C}^*_{n+1}$. It then turns out that using the cone $\mathcal{K}^1_7$ as an inner approximation of $\mathcal{C}^*_7$ also obtains the exact solution value for the Burer-Letchford instance (3.13). (Recall that $\mathcal{D}^*_7 = \mathcal{K}^*_7 \subset \mathcal{K}^1_7$.) It should be noted, however, that both of these approaches involve "extended variable" formulations of the problem, whereas the procedure based on adding cuts operates in the original problem space.

Next we consider the problem of computing the maximum stable set in a graph. Let A be the adjacency matrix of a graph G on n vertices, and let α be the maximum size of a stable set in G. It is known [27] that

$$\alpha^{-1} = \min\left\{(I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{C}_n\right\}. \tag{3.14}$$

Relaxing $\mathcal{C}_n$ to $\mathcal{D}_n$ results in the Lovász-Schrijver bound

$$(\vartheta')^{-1} = \min\left\{(I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{D}_n\right\}. \tag{3.15}$$

The bound ϑ' was first established (via a different derivation) by Schrijver as a strengthening of Lovász's ϑ number.

For our first example, with $n = 12$, let G_{12} be the complement of the graph corresponding to the vertices of a regular icosahedron [14]. Then $\alpha = 3$ and $\vartheta' \approx 3.24$, a gap of approximately 8%. A notable feature of the stable set problem for G_{12} is that using the cone $\mathcal{K}^1_{12}$ to approximate the dual of (3.14) provides no improvement over $\mathcal{K}^0_{12}$, corresponding to the dual of (3.15) [14]. For the solution matrix X from (3.15), the incidence matrix of $\mathcal{G}(X)$ is

$$\begin{pmatrix} 0&1&1&1&1&1&0&0&0&0&0&0\\ 1&0&1&1&0&0&1&1&0&0&0&0\\ 1&1&0&0&1&0&1&0&1&0&0&0\\ 1&1&0&0&0&1&0&1&0&1&0&0\\ 1&0&1&0&0&1&0&0&1&0&1&0\\ 1&0&0&1&1&0&0&0&0&1&1&0\\ 0&1&1&0&0&0&1&1&0&0&1\\ 0&1&0&1&0&0&1&0&0&1&0&1\\ 0&0&1&0&1&0&1&0&0&0&1&1\\ 0&0&0&1&0&1&0&1&0&0&1&1\\ 0&0&0&0&1&1&0&0&1&1&0&1\\ 0&0&0&0&0&0&1&1&1&1&1&0 \end{pmatrix}. \tag{3.16}$$

It is then easy to see that there are many principal submatrices of the matrix X, up to size 9×9, that meet the conditions of Lemma 3.4.1. For example, consider the principal submatrix formed by omitting rows and columns $\{6, 8, 9\}$, partitioned into the sets $\mathcal{I}_1 = \{1, 2, 3, 10, 11, 12\}$, $\mathcal{I}_2 = \{4\}$, $\mathcal{I}_3 = \{5\}$, $\mathcal{I}_4 = \{7\}$. After a suitable permutation this 9×9 matrix has the form (3.7), with $n_1 = 6$, $n_2 = n_3 = n_4 = 1$, and it is easy to see that $\mathcal{G}(X^i)$ is a CP graph for $i = 2, 3, 4$. However, it turns out that matrices A_{ii} satisfying the DNN feasibility constraints of Lemma 3.4.1 exist, demonstrating that this principal submatrix is in fact CP. This was the case for every principal submatrix satisfying the conditions of Lemma 3.4.1 that we examined.

We next consider applying Lemma 3.4.2. It turns out that the vertices of $\mathcal{G}(X)$ can be partitioned into 4 disjoint stable sets of size 3; one such partition uses the sets $\{1, 7, 10\}$, $\{2, 6, 9\}$, $\{3, 8, 11\}$ and $\{4, 5, 12\}$. Then Lemma 3.4.2 applies, and $\mathcal{G}(X^p)$ is a CP graph for each p since each X^p is a 4×4 matrix. The DNN feasibility system in Lemma 3.4.2 does not have a solution, so Theorem 3.4.2 can be used to generate a cut separating X from $\mathcal{C}_{12}$. Adding this one cut and re-solving, the gap to $1/\alpha = \frac{1}{3}$ is approximately 2×10^{-8}.

Before proceeding, it is worthwhile to note that for the stable set problem for G_{12}, Lemma 3.4.2 could actually be used to *reformulate* the problem (3.14) so that the exact solution value $\alpha = 1/3$ is obtained without adding any cuts. To see this, note that for problem (3.14) on a graph G with adjacency matrix A, it is obvious that $x_{ij} = 1 \implies a_{ij} = 0$, or in other words $\mathcal{G}(X) \subset \overline{G}$, where $\overline{G}$ is the complement of G. For the graph G_{12}, the adjacency matrix for $\overline{G}$ is precisely that of $\mathcal{G}(X)$ in (3.16). Applying Lemma 3.4.2, the condition $X \in \mathcal{C}_{12}$ in (3.14) can be replaced by an equivalent condition involving 81 matrices in $\mathcal{D}_4$, and the problem solved exactly. Compared to the procedure of first solving a relaxation over $\mathcal{D}_{12}$ and then adding a cut based on the solution $\mathcal{G}(X)$, the reformulation has the advantage that only one problem is solved. However, prior knowledge of the underlying problem structure is essential to the reformulation but is unused by the procedure based on adding cuts.

We next consider several stable set problems from [63]. These problems, of sizes $n \in \{8, 11, 14, 17\}$, are specifically constructed to be difficult for SDP-based

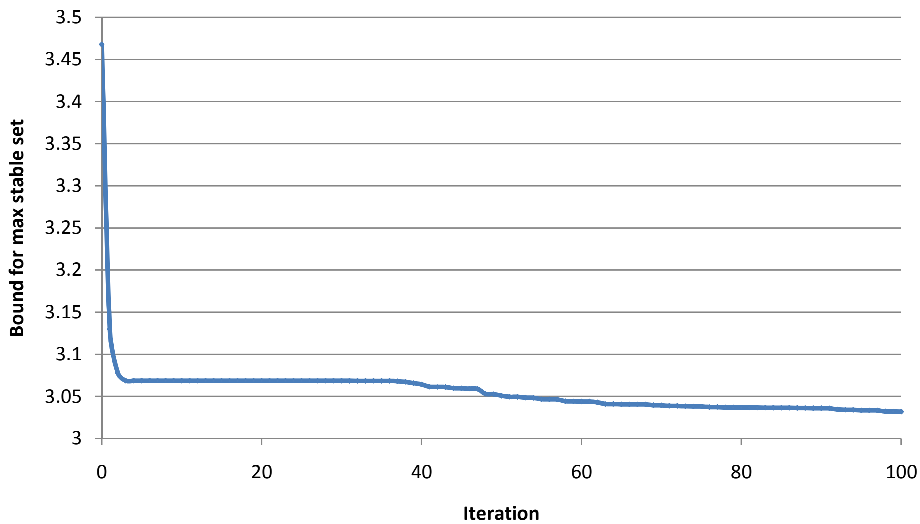

Figure 3.2: Bounds on max stable set for G_8

relaxations such as (3.15). We refer to the underlying graphs as G_8, G_{11}, G_{14} and G_{17}. First consider G_8, for which $\alpha = 3$. The incidence matrix of $\overline{G}_8$ is

$$\begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}. \tag{3.17}$$

It is clear that the vertices of $\overline{G}_8$ can be partitioned into 4 stable sets of size 2. Since we could assume that $\mathcal{G}(X) \subset \overline{G}_8$ (see the discussion above), Lemma 3.4.2 could be used to reformulate the problem (3.14), as described above, so that the exact value of α is obtained. Instead, we apply the methodology of first solving the problem

(3.15), and obtain a solution $X = X^0 \in \mathcal{D}_{12}$ with $\mathcal{G}(X^0)$ as in (3.17). For each partitioning of $\mathcal{G}(X^0)$ into 4 stable sets of size 2 we generate a cut from Theorem 3.4.2, and the augmented problem is then re-solved to obtain a new solution X^1. We then attempt to generate additional cuts based on $\mathcal{G}(X^1)$, re-solve the problem to get a new solution X^2, and continue. On iteration i we generate one cut for each partitioning of $\mathcal{G}(X^i)$ into 4 stable sets of size 2. The resulting bounds on the max stable set obtained for 100 iterations of this procedure are illustrated in Figure 3.2. The bound on $\alpha = 3$ drops to approximately 3.078 on iteration 2, and then decreases slowly on subsequent iterations. The number of cuts generated is 3 on iterations 0 and 1, 1 on iterations 2-30, and 3 or 4 per iteration thereafter. By comparison, in [13] the gap to α for this problem is closed to zero, using copositivity cuts specialized for the max-clique problem posed on the complement graph $\overline{G}_8$.

For the graphs G_n, $n \in \{11, 14, 17\}$, it is not possible to use Lemma 3.7 or Lemma 3.9 to exactly reformulate the condition $X \in \mathcal{C}_n$ in terms of DNN matrices. For these problems we used the following computational approach. We first solved (3.15) to obtain the solution $X = X^0 \in \mathcal{D}_n$ and the bound ϑ'. We then found all possible structures consisting of 4 disjoint stable sets of size 2 in $\mathcal{G}(X)$. (The complement graphs $\overline{G}_i$ for these problems, like $\overline{G}_8$, contain no stable sets of size greater than 3.) We then randomly chose $2n$ of these structures to try to generate cuts based on Lemma 3.9 applied to the corresponding 8×8 principal submatrices of X^0. After adding all of the cuts found, we re-solved the problem to get a new solution X^1 and a new bound on α. We then continue for an additional three rounds of cuts, on each round i using the cuts obtained from $2n$ eligible structures, chosen at random, obtained from the solution of the previous problem X^{i-1}. We performed this entire computational procedure 20 times for each of the 3 problems.

Table 3.1: Results on stable set problems (20 runs for each problem)

					Number of cuts			Bound values		
Graph	α	ϑ'	ϑ^{cop}	Round	min	median	max	min	mean	max
G_{11}	4	4.694	4.280	1	13	16	19	4.342	4.362	4.443
				2	14	18	22	4.244	4.268	4.317
				3	12	17	21	4.237	4.253	4.279
				4	13	17	22	4.234	4.248	4.264
G_{14}	5	5.916	5.485	1	11	15	19	5.530	5.585	5.666
				2	12	17	22	5.441	5.479	5.548
				3	16	20	25	5.413	5.441	5.483
				4	14	17	25	5.405	5.422	5.456
G_{17}	6	7.134	6.657	1	7	12	18	6.731	6.814	6.922
				2	9	17	25	6.594	6.693	6.783
				3	10	15	23	6.571	6.651	6.718
				4	10	16	23	6.565	6.620	6.664

In Table 3.1 we give summary statistics for the results on each problem, including the min, median and max number of cuts found on each round and the min, mean and max bound on α obtained after these cuts were added. For comparison we also give the best bound ϑ^{cop} found in [13]. As can be seen in the table, for problems G_{11} and G_{14}, on each of the 20 runs the bound obtained after 3 rounds of cuts was better than ϑ^{cop}. For problem G_{17}, the bound obtained after 3 rounds of cuts was better than ϑ^{cop} on 11 of the 20 runs, and was better than ϑ^{cop} after 4 rounds of cuts on 19 of the 20 runs. In Figures 3.3, 3.4 and 3.5 we give the distributions of the bounds on α obtained after each round of cuts for the 20 runs on each problem. In addition to the obvious reduction in the bounds after each round of cuts, the figures show that the variation in the bounds is also decreasing.

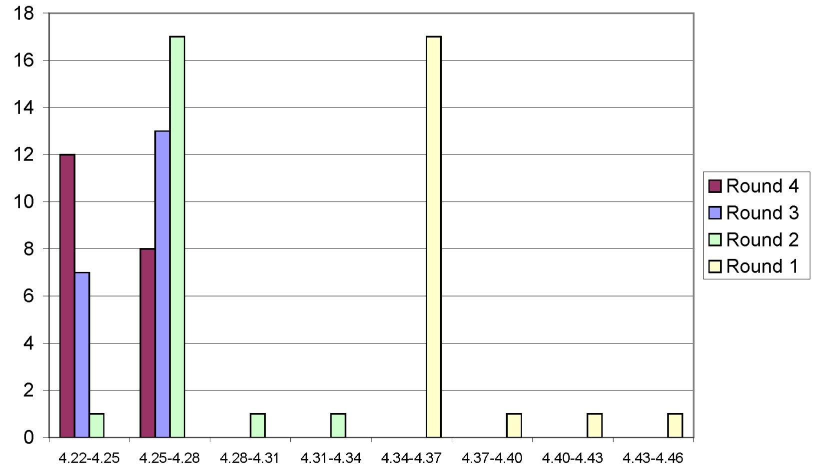

Figure 3.3: Bounds on max stable set for G_{11}

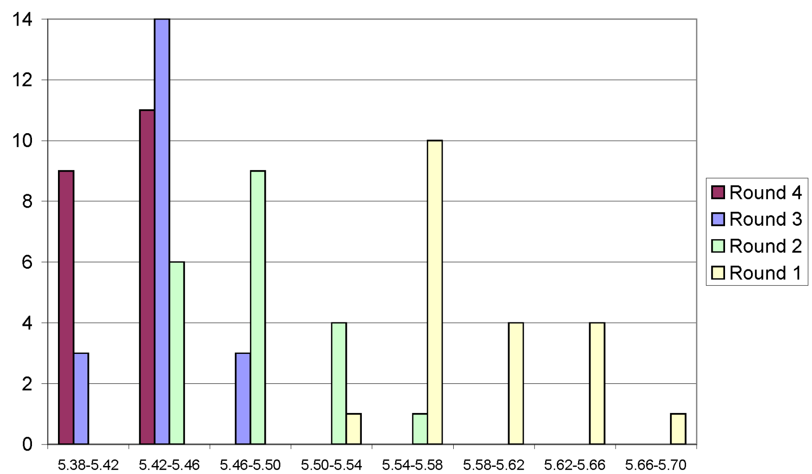

Figure 3.4: Bounds on max stable set for G_{14}

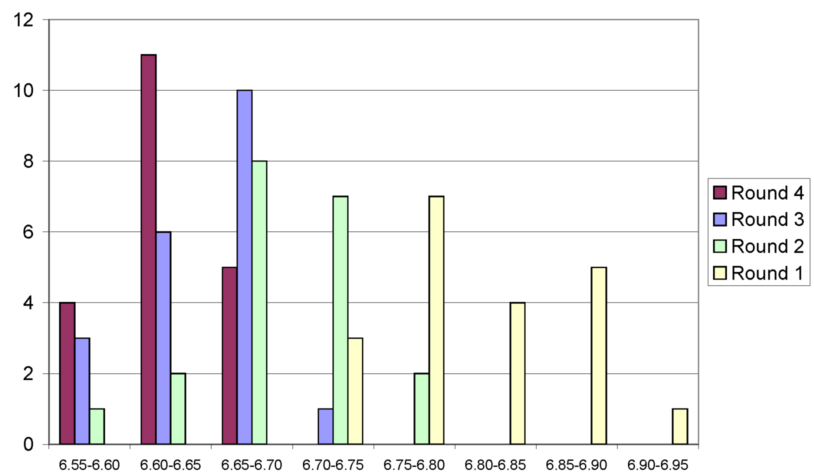

Figure 3.5: Bounds on max stable set for G_{17}

CHAPTER 4
SEPARATION AND RELAXATION BASED ON BOUNDARY CONE

4.1 Introduction

In the last chapter of this thesis, we discuss an approach for the generalized completely positive cone $\mathcal{C}(P)$, where $P := \{x : Ax = 0, Bx \geq 0\} \subseteq \Re_n$ is a pointed, polyhedral cone such that $P \cap \{x : x_1 = 1\}$ is nonempty. We refer the reader to the last part of Section 1.2.2 for motivation and definitions related to this generalization . In this chapter, we will focus on two particular specifications of P in detail: (i) P equals the nonnegative orthant $\Re_n^+ := \{x : x \geq 0\}$, i.e., A is empty and $B = I$; and (ii) P equals the homogenization of the box $\square_{n-1} := \{\tilde{x} : 0 \leq \tilde{x} \leq \tilde{e}\}$, e.g., A is empty and

$$B = \begin{pmatrix} 0 & \tilde{I} \\ \tilde{e} & -\tilde{I} \end{pmatrix},$$

where $\tilde{I}$ is the identity matrix of size $n-1$ and $\tilde{e}$ is the all-ones vector. Another specification of P, which is closely related to (i), is the homogenization of the standard simplex $\Delta_{n-1} := \{\tilde{x} \geq 0 : \tilde{e}^T\tilde{x} = 1\}$, e.g., $A = (-1, \tilde{e}^T)$ and $B = (0, \tilde{I})$.

In this chapter, to minimize notation, we use $\mathcal{C}$ to mean $\mathcal{C}(P)$. When P is in case (i), $\mathcal{C}$ is the completely positive cone. Our main theory in this chapter is independent of P as long as it satisfies the three forthcoming Assumptions 4.2.1–4.2.3.

One standard, tractable relaxation of $\mathcal{C}$ is the following semidefinite relaxation [55, 70], where in addition to enforcing positive semidefiniteness, pairs of constraints defining P are multiplied and linearized to obtain valid constraints for $\mathcal{C}$:

$$\mathcal{D} := \mathcal{D}(P) := \left\{X \succeq 0 : AXA^T = 0,\ AXB^T = 0,\ BXB^T \geq 0\right\}. \tag{4.1}$$

This set can be seen as a generalized version of the doubly nonnegative relaxation. Note again we use $\mathcal{D}$ to be short for $\mathcal{D}(P)$. $\mathcal{D}$ is a strong relaxation of $\mathcal{C}$ in the sense that it incorporates all constraints defining P to the fullest extent possible in the space $\mathcal{S}_n$, e.g., without introducing new variables.

Regarding $\mathcal{C}$, this chapter investigates theoretical properties, algorithmic approaches, and improved convex relaxations. In Section 4.2, we establish some basic facts concerning $\mathcal{C}$, $\mathcal{D}$, and the dual cone $\mathcal{C}^*$. Then, in Section 4.3, we devise a separation procedure for $\mathcal{C}$ based on optimization over the dual cone of $\mathcal{C}_{\text{bd}} := \mathcal{C}(\text{bd}(P)) := \text{cone}\{xx^T : x \in \text{bd}(P)\}$. This separation procedure is especially attractive when $\mathcal{C}_{\text{bd}}^*$ is tractable, e.g., has a representation with lower dimensional matrices. The separation algorithm then leads to a nonlinear formulation of $\mathcal{C}$ in terms of $\mathcal{C}_{\text{bd}}$, which in turn motivates the construction of a new convex relaxation $\mathcal{C}(d)$ of $\mathcal{C}$, which depends on $\mathcal{C}_{\text{bd}}$ and the choice of a "step direction" $d \in P$. We prove that the intersection of such $\mathcal{C}(d)$ over all $d \in P$ captures $\mathcal{C}$ exactly, i.e., $\mathcal{C} = \cap_{d \in P} \mathcal{C}(d)$. Further, one can relax $\mathcal{C}_{\text{bd}}$ in $\mathcal{C}(d)$ to obtain a new tractable relaxation $\mathcal{D}(d)$ of $\mathcal{C}$, which is not weaker than $\mathcal{D}$. In total, we have $\mathcal{C} \subseteq \mathcal{C}(d) \subseteq \mathcal{D}(d) \subseteq \mathcal{D}$. Finally, we extend these ideas to construct a recursive hierarchy of convex relaxations for $\mathcal{C}$, which provides stronger and stronger approximations of $\mathcal{C}$. For a given choice of step directions and fixed recursive depth, each relaxation in the hierarchy is tractable.

In Sections 4.4 and 4.5, we tailor Section 4.3 to the two cases of P mentioned above: the nonnegative orthant $\Re^+_n$ and the homogenization $\text{hom}(\square_{n-1})$ of the box. In the first case, $\mathcal{C}$ is the well-known cone of $n \times n$ completely positive matrices. The monograph [7] provides a recent survey; see also [47, 73, 74]. Recent relevant work includes [21, 31, 35, 50, 46]. In the second case, $\mathcal{C}$ is a fundamental convex cone for quadratic programs over bounded variables for which recent theoretical and computational advances include [5, 24, 25, 76, 77]. In each section, we review the literature on $\mathcal{C}$, focusing on known results in low dimensions. For example, in each of the two cases, respectively, it is known that $\mathcal{C} = \mathcal{D}$ if and only if $n \le 4$ and $n \le 3$. Combining this with the separation procedure of Section 4.3 and the observation that, in each case, $\mathrm{bd}(P)$ decomposes into several lower-dimensional versions of P, we establish separation procedures for the respective dimensions $n = 5$ and $n = 4$. In particular, this gives the first full separation procedure for 5×5 completely positive matrices, which extends the previous separation algorithms of [21, 31] for special classes of matrices in $\mathcal{D} \setminus \mathcal{C}$. Using a result of [5], we also achieve the first separation procedure for $\mathcal{C}(\mathrm{hom}(\square_4))$ when $n = 5$. Through several examples, we also demonstrate the strength of the relaxation hierarchies in these two cases.

We remark that the completely positive cone $\mathcal{C}(\Re^+_n)$ is actually relevant to any $P \subseteq \Re^+_n$ since then $\mathcal{C}(P) \subseteq \mathcal{C}(\Re^+_n)$. In other words, knowledge of $\mathcal{C}(\Re^+_n)$ can be applied directly to $\mathcal{C}(P)$. In fact, as long as P in any dimension contains n nonnegative variables, $\mathcal{C}(\Re^+_n)$ applies to those variables. For example, the separation procedure for $\mathcal{C}(\Re^+_5)$ can be applied to any subset of five nonnegative variables. In a similar manner, $\mathcal{C}(\mathrm{hom}(\square_{n-1}))$ applies to any P having $n-1$ variables which, prior to homogenization, are in $[0,1]^{n-1}$. Moreover, simple variable scalings allow the application of $\mathcal{C}(\mathrm{hom}(\square_{n-1}))$ to bounded variables generally.

In fact, the completely positive cone has even wider applicability and generality. By splitting free variables and adding slacks, (1.14) can be recast as $\inf\{\langle \hat{x}, \hat{H}\hat{x}\rangle : \hat{x} \in \hat{P}, \hat{x}_1 = 1\}$, where $\hat{P}$ is a polyhedron of the form $\{\hat{x} : \hat{A}\hat{x} = 0, \hat{x} \ge 0\}$ in some larger space $\Re_{\hat{n}}$. Then $\mathcal{C}(\hat{P}) \subseteq \mathcal{C}(\Re^+_{\hat{n}})$. Indeed, the results of Burer [18] imply

$\mathcal{C}(\hat{P}) = \mathcal{C}(\Re^+_{\hat{n}}) \cap \{\hat{X} : \hat{A}\hat{X}\hat{A}^T = 0\}$. There may be, however, specific disadvantages to this general embedding of $\mathcal{C}(P)$ into $\mathcal{C}(\Re^+_{\hat{n}})$. For example, by transforming $\{\tilde{x} : 0 \leq \tilde{x} \leq \tilde{e}\}$ to $\{\binom{\tilde{x}}{\tilde{s}} \geq 0 : \tilde{x} + \tilde{s} = \tilde{e}\}$, $\mathcal{C}(\text{hom}(\square_{n-1}))$ may be embedded into $\mathcal{C}(\Re^+_{2n-1})$, but for $n = 4$, the separation procedure for $\mathcal{C}(\text{hom}(\square_3))$ of this paper is sacrificed since there is no known separation procedure for $\mathcal{C}(\Re^+_7)$. So we do not focus on such embeddings here.

4.2 Properties of the Cone of Quadratic Forms

$\mathcal{C} := \mathcal{C}(P)$ is closed by [72, Lemma 1] and pointed because the positive semidefinite cone contains it. The dual cone of $\mathcal{C}$ is defined as usual:

$$\mathcal{C}^* := \mathcal{C}(P)^* := \{Q : \langle Q, X\rangle \geq 0 \ \forall \ X \in \mathcal{C}\} = \left\{Q : x^T Q x \geq 0 \ \forall \ x \in P\right\}.$$

Generally, even testing whether a matrix is in $\mathcal{C}^*$ is co-NP-complete [58]. Some algorithms have been developed for this aim. For example, see [16] and reference therein.

Since $\mathcal{C}$ is closed and pointed, $\mathcal{C}^*$ has nonempty interior. Note that matrices in $\mathcal{C}^*$ correspond to the homogeneous quadratic functions, which are nonnegative over P. This property is sometimes called *copositivity over* P. $\mathcal{C}^*$ may also be interpreted as the convex cone of all valid inequalities for $\mathcal{C}$. These alternative viewpoints of $\mathcal{C}^*$ will be be used interchangeably throughout Section 4.3.

We make three assumptions on P to simplify the presentation in the paper, the first two of which have been stated in the Introduction:

Assumption 4.2.1. The set $P \cap \{x : x_1 = 1\}$ is nonempty.

Assumption 4.2.2. P is pointed, i.e., $\{x : Ax = 0, Bx = 0\} = \{0\}$

Assumption 4.2.3. The set $\text{relint}_>(P)$ is nonempty, where $\text{relint}_>(P) := \{x : Ax = 0, Bx > 0\}$.

Assumption 4.2.1 ensures feasibility of (1.14). Assumption 4.2.2 implies in particular that $\text{rank}([A; B]) = n$. Together, Assumptions 4.2.2 and 4.2.3 imply that the slice $P \cap \{x : \langle e, Bx \rangle = 1\}$ is nonempty and bounded.

Note that Assumption 4.2.3 can in fact be made without loss of generality. If P does not satisfy Assumption 4.2.3, then we claim there exists a row b_i^T of B such that $\langle b_i, x \rangle = 0$ for all $x \in P$, in which case $\langle b_i, x \rangle \geq 0$ can be moved into $Ax = 0$ and the process repeated until P has interior. The claim is true by the following proof of the contrapositive. Suppose B has m rows, and for each row b_j^T, pick $x^j \in P$ such that $\langle b_j, x^j \rangle > 0$. Then $x^0 := \frac{1}{m} \sum_{j=1}^m x^j$ satisfies $Bx^0 > 0$.

The above assumptions also imply that $\mathcal{C}$ and $\mathcal{D}$ have the same dimension.

Proposition 4.2.1. $\dim(\mathcal{C}) = \dim(\mathcal{D})$. *Furthermore, if* $E \subset P$ *contains the extreme rays of* P*, then* $\dim(\mathcal{C}(E)) = \dim(\mathcal{D})$.

Proof. We first consider the case when A is empty and claim that $\mathcal{C}$ is full-dimensional in $\mathcal{S}_n$. It suffices to find $n(n+1)/2$ linearly independent elements in $\mathcal{C}$. Let $\{r_j\}$ be the normalized extreme rays of P. By Assumptions 4.2.2 and 4.2.3, there are at least n which are linearly independent. We claim that $\{(r_j + r_k)(r_j + r_k)^T : j \leq k\}$ are the desired independent elements. Clearly, all are in $\mathcal{C}$. To see that they are also independent, we first note that, without loss of generality, we may pre- and post-multiply by a change-of-basis matrix to transform to the matrices $\{(e_j + e_k)(e_j + e_k)^T : j \leq k\}$, where e_j is the standard unit vector in $\Re_n$. It is then not difficult to verify that the matrices are linearly indepdendent. Since $\mathcal{C} \subseteq \mathcal{D}$ and $\mathcal{C}$ is full-dimensional, then $\mathcal{D}$ is full-dimensional also.

Now we consider the case when A is non-trivial. Let N be a matrix whose columns span $\{x : Ax = 0\}$, and define $R := \{y : BNy \geq 0\}$. Then $P = NR$, $\mathcal{C} = N\mathcal{C}(R)N^T$, and $\mathcal{D} = N\mathcal{D}(R)N^T$. Moreover, R is pointed and has interior in its own space due to Assumptions 4.2.2 and 4.2.3. Then, by the case when A is empty, $\dim(\mathcal{C}(R)) = \dim(\mathcal{D}(R))$, which implies the result.

The previous argument can be repeated to show $\dim(\mathcal{C}(E)) = \dim(\mathcal{D})$ if $E \subset P$ contains the extreme rays of P. □

For $X \in \mathcal{D}$, the conditions $X \succeq 0$ and $AXA^T = 0$ guarantee $AX = 0$, which clearly implies $AXB^T = 0$. Hence, $\mathcal{D}$ may also be written as

$$\mathcal{D} = \left\{X \succeq 0 : AX = 0,\ BXB^T \geq 0\right\}.$$

Additional properties of $\mathcal{D}$ are established in the following lemmas:

Lemma 4.2.1. *Let $X \in \mathcal{D}$. The following are equivalent: $BXB^T = 0$; $BX = 0$; $X = 0$.*

Proof. Assume $BXB^T = 0$, and let v be any column of XB^T. From $BXB^T = 0$ and $AXB^T = 0$, it clearly holds that $v \in \{x : Ax = 0, Bx = 0\}$, and so $v = 0$ by Assumption 4.2.2. Hence, $XB^T = 0$ or $BX = 0$. Now, since $AX = 0$ and $BX = 0$, the columns of X are in $\{x : Ax = 0, Bx = 0\}$, which implies $X = 0$. The reverse direction $X = 0 \ \Rightarrow\ BX = 0 \ \Rightarrow\ BXB^T = 0$ is obvious. □

Lemma 4.2.2. *Let $X \in \mathcal{D}$, and define $x := XB^Te$. Then $x \in P$, and $X \neq 0$ implies $x \neq 0$. Furthermore, if $\langle B^Tee^TB, X\rangle = 1$, then $X - xx^T \succeq 0$ and $\langle B^Tee^TB, X - xx^T\rangle = 0$.*

Proof. Because $X \in \mathcal{D}$, one readily sees $Ax = AXB^Te = 0$ and $Bx = BXB^Te \geq 0$. So $x \in P$. If $X \neq 0$, then by Lemma 4.2.1, $0 \neq BXB^T \geq 0$. Hence

$$0 < \langle ee^T, BXB^T\rangle = \langle e, BXB^Te\rangle = \langle e, Bx\rangle,$$

which implies $x \neq 0$. Also, the equation

$$\begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} = \begin{pmatrix} 1 & e^TBX \\ XB^Te & X \end{pmatrix} = \begin{pmatrix} e^TB \\ I \end{pmatrix} X \begin{pmatrix} B^Te & I \end{pmatrix}$$

and the Schur-complement theorem imply $X - xx^T \succeq 0$. Next, by using $\langle B^T ee^T B, X\rangle = 1$,

$$\begin{aligned} B^T ee^T B\left(X - xx^T\right) &= B^T ee^T BX - B^T ee^T Bxx^T \\ &= B^T ex^T - \langle e, Bx\rangle B^T ex^T \\ &= (1 - \langle e, Bx\rangle) B^T ex^T \\ &= 0. \end{aligned}$$

So $\langle B^T ee^T B, X - xx^T\rangle = 0$. □

4.3 Separation and Relaxation

In Section 4.3.1, we describe a separation algorithm for $\mathcal{C}$ under the assumption that one can optimize over a cone related to the boundary of P. We call this cone the *boundary cone*. Then in Section 4.3.2, we describe a nonlinear formulation of $\mathcal{C}$ by studying the dual of the optimization problem introduced in the separation algorithm. Finally, in Section 4.3.3, we discuss a new class of related convex relaxations of $\mathcal{C}$, which strengthen $\mathcal{D}$, and in Section 4.3.4, we extend this to a tractable hierarchy of relaxations, which provide even better approximations of $\mathcal{C}$.

4.3.1 A separation algorithm

In this subsection, we establish a separation algorithm for $\mathcal{C}$. The key idea is to consider the boundary cone $\mathcal{C}_{\text{bd}}$, which includes matrices in $\mathcal{C}$ that are generated only from $x \in \text{bd}(P)$, :

$$\mathcal{C}_{\text{bd}} := \mathcal{C}(\text{bd}(P)) \subseteq \mathcal{C}.$$

$\mathcal{C}_{\text{bd}}$ is closed by [72, Lemma 1] and pointed. $\mathcal{C}^*_{\text{bd}}$ denotes the dual cone of $\mathcal{C}_{\text{bd}}$, and $\text{int}(\mathcal{C}^*_{\text{bd}}) \neq \emptyset$. In fact,

$$\text{int}(\mathcal{C}^*_{\text{bd}}) \supseteq \text{int}(\mathcal{C}^*) = \{Q : \langle x, Qx \rangle > 0 \ \ \forall \ \ 0 \neq x \in P\}.$$

We may obtain alternative characterizations of $\mathcal{C}_{\text{bd}}$ and $\mathcal{C}^*_{\text{bd}}$ by breaking $\text{bd}(P)$ into pieces. Let b_i^T denote the i-th row of B, and let B_i denote the matrix gotten from B by deleting b_i^T. Define P_i to be the polyhedron resulting from P when the inequality $\langle b_i, x \rangle \geq 0$ is set to equality, i.e.,

$$P_i := \{x : Ax = 0, \ \langle b_i, x \rangle = 0, \ B_i x \geq 0\}.$$

Then $\text{bd}(P) = \cup_i P_i$. Defining $\mathcal{C}_i := \mathcal{C}(P_i)$ as in Section 1.2.2, we see

$$\mathcal{C}_{\text{bd}} = \sum_i \mathcal{C}_i, \qquad \mathcal{C}^*_{\text{bd}} = \bigcap_i \mathcal{C}^*_i.$$

The inclusion $\mathcal{C}_{\text{bd}} \subseteq \mathcal{C}$ implies $\mathcal{C}^*_{\text{bd}} \supseteq \mathcal{C}^*$. The following important lemma provides conditions under which a matrix in $\mathcal{C}^*_{\text{bd}}$ is actually in $\mathcal{C}^*$.

Lemma 4.3.1. *Let $Q \in \mathcal{C}^*_{\text{bd}}$. If Q is not positive semidefinite on the linear subspace $\{x : Ax = 0, \langle e, Bx \rangle = 0\}$, then $Q \in \mathcal{C}^*$.*

Proof. To show $Q \in \mathcal{C}^*$, we must demonstrate that the quadratic function $q(x) := \langle x, Qx \rangle$ is nonnegative for all $x \in P$. By homogeneity, it suffices to show $q(x)$ is nonnegative over the nonempty, bounded slice $\hat{P} := P \cap \{x : \langle e, Bx \rangle = 1\}$.

We first claim that the minimum value of $q(x)$ over $\hat{P}$ is actually attained on $\text{bd}(\hat{P})$. To see this, let $x \in \text{relint}(\hat{P})$ be arbitrary, and let $d \in \{x : Ax = 0, \langle e, Bx \rangle = 0\}$ satisfy $\langle d, Qd \rangle < 0$, which exists by assumption. Also, ensure that d satisfies $\langle d, Qx \rangle \leq 0$; if not, simply replace d by $-d$. Then, for small $\epsilon > 0$, $x + \epsilon d$ is feasible, and

$$\langle x + \epsilon d, Q(x + \epsilon d) \rangle = \langle x, Qx \rangle + 2\epsilon \langle d, Qx \rangle + \epsilon^2 \langle d, Qd \rangle < \langle x, Qx \rangle.$$

Hence, x is not a global minimum, which proves the claim.

Now, since $Q \in \mathcal{C}^*_{\text{bd}}$, we know $q(x) \geq 0$ for all $x \in \text{bd}(\hat{P})$. By the preceding

Algorithm 1 Separation over $\mathcal{C}$

Input: $\bar{X} \in \mathcal{S}_n$.

Output: YES if $\bar{X} \in \mathcal{C}$; otherwise, NO and $\bar{Q} \in \mathcal{C}^*$ separating $\bar{X}$ from $\mathcal{C}$.

1: If $\bar{X} \notin \mathcal{D}$, then return NO and $\bar{Q} \in \mathcal{D}^*$ separating $\bar{X}$ from $\mathcal{D}$.

2: For chosen $X^0 \in \text{relint}(\mathcal{C}_{\text{bd}})$, calculate the optimal value κ and an optimal solution $\bar{Q}$ of

$$\min_{Q \in \mathcal{S}_n} \left\{ \langle Q, \bar{X} \rangle : \begin{array}{c} Q \in \mathcal{C}^*_{\text{bd}},\ \langle Q, X^0 \rangle \leq 1 \\ \\ \langle \bar{X} B^T e, Q \bar{X} B^T e \rangle \geq 0 \end{array} \right\}. \tag{4.2}$$

3: If $\kappa \geq 0$, then return YES.

4: If $\kappa < 0$, then return NO and $\bar{Q}$.

paragraph, this shows that $q(x)$ is nonnegative for all $x \in \hat{P}$, as desired. □

The separation procedure is stated as Algorithm 1. Since membership in $\mathcal{D}$ is necessary for membership in $\mathcal{C}$, Step 1 first separates $\bar{X}$ over $\mathcal{D}$. Step 2 then constitutes the main work of the algorithm. The idea of the optimization (4.2) is to minimize the inner product $\langle Q, \bar{X} \rangle$ over $Q \in \mathcal{C}^*_{\text{bd}}$ in order to separate based on the sign of κ. We first establish that κ is finite:

Lemma 4.3.2. *If $\bar{X} \in \mathcal{D}$, then the optimal value κ of (4.2) is finite.*

Proof. We show that $\inf\{\langle Q, \bar{X} \rangle : Q \in \mathcal{C}^*_{\text{bd}}, \langle Q, X^0 \rangle \leq 1\}$ is finite or equivalently that the system

$$0 \neq \Delta Q \in \mathcal{C}^*_{\text{bd}}, \quad \langle \Delta Q, X^0 \rangle = 0, \quad \langle \Delta Q, \bar{X} \rangle < 0$$

is inconsistent. Suppose ΔQ satisfies the first two conditions. Since $X^0 \in \text{relint}(\mathcal{C}_{\text{bd}})$, it holds that $\langle \Delta Q, X \rangle = 0$ for all $X \in \text{span}(\mathcal{C}_{\text{bd}})$. By the second half of Proposition 4.2.1, we know $\text{span}(\mathcal{C}_{\text{bd}}) = \text{span}(\mathcal{D})$, and so $\bar{X} \in \text{span}(\mathcal{C}_{\text{bd}})$, which implies $\langle \Delta Q, \bar{X} \rangle = 0$. So the systm is inconsistent. □

It is worth noting that, while κ is finite, the feasible region of (4.2) is not bounded if A is non-trivial. For example, $A^T A$ is a direction of recession. However, by the discussion within Proposition 4.2.1, one can prove that all the unbounded directions are in $\text{span}(\mathcal{D})^\perp$, which equals $\{X \in \mathcal{S}_n : AX = 0\}^\perp$. Hence, those directions do not contribute to the objective $\langle Q, \bar{X}\rangle$ since $\bar{X} \in \mathcal{D}$. So, one could adjust (4.2) to have a bounded feasbile region without affecting the forthcoming proof of correctness of Algorithm 1 by simply constraining Q within the linear subspace $\text{span}(\mathcal{D})$. This equivalence with a bounded problem also shows that the minimum in (4.2) is actually attained, so that $\bar{Q}$ is well-defined.

Because $\mathcal{C}^*_{\text{bd}} \supseteq \mathcal{C}^*$, there is still a danger that Algorithm 1 reaches Step 4 and returns $\bar{Q} \notin \mathcal{C}^*$, rendering the algorithm incorrect. However, the following theorem proves this cannot happen; the critical result is Lemma 4.3.1.

Theorem 4.3.1. *Algorithm 1 correctly solves the separation problem for* $\mathcal{C}$*.*

Proof. If Algorithm 1 terminates in Step 1, then clearly $\bar{X} \notin \mathcal{C}$ and $\bar{Q} \in \mathcal{C}^*$ with $\langle \bar{Q}, \bar{X}\rangle < 0$. So assume the algorithm has reached Step 2. Then $\bar{X} \in \mathcal{D}$, and the optimal value κ in (4.2) is finite by Lemma 4.3.2. Define $\bar{x} := \bar{X}B^T e$; by Lemma 4.2.2, $\bar{x} \in P$.

Suppose $\kappa \geq 0$, causing the algorithm to terminate in Step 3. We claim every (suitably scaled) $Q \in \mathcal{C}^*$ is feasible for (4.2), which will establish $\bar{X} \in \mathcal{C}$. We already know $Q \in \mathcal{C}^*_{\text{bd}}$. We need to show $\langle \bar{x}, Q\bar{x}\rangle \geq 0$, which indeed holds since $\bar{x} \in P$.

Finally suppose $\kappa < 0$, causing termination in Step 4. In particular, $\bar{X} \neq 0$, and so by Lemma 4.2.1, $B\bar{X}B^T \neq 0$. Hence, without loss of generality, we scale $\bar{X}$ so that $\langle B^T ee^T B, \bar{X}\rangle = 1$. By Lemma 4.2.2, this implies also $\bar{X} - \bar{x}\bar{x}^T \succeq 0$ and $\langle B^T ee^T B, \bar{X} - xx^T\rangle = 0$.

We claim $\bar{Q} \in \mathcal{C}^*$, which will complete the proof. By Lemma 4.3.1, it suffices to show $\bar{Q}$ is not positive semidefinite on the linear subspace $\{x : Ax = 0, \langle e, Bx\rangle = 0\}$.

To obtain a contradiction, suppose $\bar{Q}$ is positive semidefinite on this subspace. Then there exists $t \geq 0$ such that $\bar{Q} + t(A^T A + B^T ee^T B) \succeq 0$. We have

$$\begin{aligned}
0 &> \langle \bar{Q}, \bar{X} \rangle = \langle \bar{Q}, \bar{X} - \bar{x}\bar{x}^T \rangle + \langle \bar{x}, \bar{Q}\bar{x} \rangle \\
&= \langle \bar{Q} + t(A^T A + B^T ee^T B), \bar{X} - \bar{x}\bar{x}^T \rangle + \langle \bar{x}, \bar{Q}\bar{x} \rangle - t\langle A^T A + B^T ee^T B, \bar{X} - \bar{x}\bar{x}^T \rangle \\
&\geq \langle \bar{x}, \bar{Q}\bar{x} \rangle - t\langle A^T A + B^T ee^T B, \bar{X} - \bar{x}\bar{x}^T \rangle \\
&= \langle \bar{x}, \bar{Q}\bar{x} \rangle - t\langle B^T ee^T B, \bar{X} - \bar{x}\bar{x}^T \rangle \\
&= \langle \bar{x}, \bar{Q}\bar{x} \rangle,
\end{aligned}$$

which contradicts the feasibility of $\bar{Q}$ in (4.2). □

4.3.2 A nonlinear representation

We now examine the conic dual of the optimization problem (4.2), which appears within Algorithm 1. Defining $\bar{x} := \bar{X} B^T e$, the dual is

$$\begin{aligned}
\max \quad & \rho \\
\text{s.t.} \quad & \bar{X} = \rho X^0 + \lambda\, \bar{x}\bar{x}^T + Z \\
& \rho \leq 0,\ \lambda \geq 0,\ Z \in \mathcal{C}_{\text{bd}}
\end{aligned} \tag{4.3}$$

For non-trivial instances of (4.2) arising within Algorithm 1, i.e., when $0 \neq \bar{X} \in \mathcal{D}$, Lemma 4.2.2 implies $\bar{x} \neq 0$. Also, since $\text{int}(\mathcal{C}^*_{\text{bd}}) \supseteq \text{int}(\mathcal{C}^*) \neq \emptyset$ and $0 \neq \bar{x}\bar{x}^T \in \mathcal{C}$, there exists $Q \in \text{int}(\mathcal{C}^*)$ such that $\langle Q, \bar{x}\bar{x}^T \rangle > 0$ and $\langle Q, X^0 \rangle < 1$. Therefore we know that (4.2) has non-empty interior. Hence, strong duality holds between (4.2) and (4.3), and the dual optimum in (4.3) is always attained.

This provides a nonlinear representation of $\mathcal{C}$:

Proposition 4.3.1. *$X \in \mathcal{C}$ if and only if $X \in \mathcal{D}$ and there exist $\lambda \geq 0$ and $Z \in \mathcal{C}_{\text{bd}}$ such that*

$$X = \lambda(XB^T e)(XB^T e)^T + Z \tag{4.4}$$

Proof. ($\Rightarrow$) Let $\bar{X}$ in (4.3) be the given X. Since Algorithm 1 terminates with $\kappa \geq 0$, by strong duality (4.3) has a feasible solution (ρ, λ, Z) with $\rho = 0$. This gives (4.4).

($\Leftarrow$) Since $X \in \mathcal{D}$, $XB^T e \in P$ by Lemma 4.2.2, and so $(XB^T e)(XB^T e)^T \in \mathcal{C}$. Further, $Z \in \mathcal{C}_{bd} \subseteq \mathcal{C}$. Because X satisfies (4.4) with $\lambda \geq 0$, we see $X \in \mathcal{C}$. □

As a representation result, (4.4) is quite interesting since it demonstrates that the structure of $\mathcal{C}$ depends heavily on the structure of $\mathcal{C}_{\text{bd}}$. Algorithmically, however, the nonlinearity seems to preclude explicit computation except when X is fixed, which is the case within Algorithm 1. In the next subsection, we explore a similar, but different, representation of $\mathcal{C}$ that is amenable to computation. Still, the following proposition shows that, under a certain simple condition, the nonlinear representation reduces to a linear one:

Proposition 4.3.2. *Let $X \in \mathcal{C}$, and suppose BXB^T has a zero entry. Define $x := XB^T e \in P$ in accordance with Lemma 4.2.2. It holds that:*

(i) if $x \in \text{bd}(P)$, then $\lambda = 0$ in some representation (4.4) of X;

(ii) if $x \in \text{relint}_{>}(P)$, then $\lambda = 0$ in all representations (4.4) of X.

Proof. Write (4.4) as $X = \lambda x x^T + Z$. For (i), since $x \in \text{bd}(P)$, we have $xx^T \in \mathcal{C}_{\text{bd}}$. Hence, $\lambda x x^T$ can be subsumed into Z, yielding a new representation of X with $\lambda = 0$. For (ii), pre- and post-multiply $X = \lambda x x^T + Z$ by B and B^T, respectively, to yield

$$BXB^T = \lambda(Bx)(Bx)^T + BZB^T.$$

Because $Bx > 0$ and $BZB^T \geq 0$, the zero entry of BXB^T ensures $\lambda = 0$. □

Another interpretation of Proposition 4.3.2 is that $\mathcal{C}_{\text{bd}}$, which is an inner approximation of $\mathcal{C}$, is actually exact on certain faces of $\mathcal{C}$.

4.3.3 A class of convex relaxations

Motivated by the nonlinear representation (4.4) of $\mathcal{C}$ in the previous subsection, we now explore a new class of relaxations for $\mathcal{C}$, each of which is at least as strong as $\mathcal{D}$. The derivation of the relaxations are different than the derivation of (4.4), but they share similar structural elements.

Let a "step direction" $d \in P$ be fixed, and define

$$\mathcal{C}(d) := \mathcal{C}(P; d) := \left\{ X = \zeta dd^T + dz^T + zd^T + Z \ : \ \begin{array}{c} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P, \ Z \in \mathcal{C}_{\text{bd}} \end{array} \right\}.$$

Proposition 4.3.3. *$\mathcal{C} \subseteq \mathcal{C}(d) \subseteq \mathcal{D}$ for all nonzero $d \in P$.*

Proof. Let $X \in \mathcal{C}(d)$. It is easy to verify that the equation

$$X = \begin{pmatrix} d & I \end{pmatrix} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \begin{pmatrix} d^T \\ I \end{pmatrix}$$

holds and implies $X \succeq 0$. Also $AX = 0$ and $BXB^T \geq 0$ hold because $d, z \in P$ and $Z \in \mathcal{C}_{\text{bd}} \subseteq \mathcal{C}$. So $\mathcal{C}(d) \subseteq \mathcal{D}$.

Next, we show that every extreme ray of $\mathcal{C}$ is in $\mathcal{C}(d)$, which will prove $\mathcal{C} \subseteq \mathcal{C}(d)$. Note every extreme ray of $\mathcal{C}$ has form $X := xx^T$ with $x \in P$ [72, Lemma 1]. Let $\alpha \geq 0$ be the smallest step-size such that $x - \alpha d \in \text{bd}(P)$. Note that α is well-defined because $-d \notin P$ due to Assumption 4.2.2. Then define

$$\zeta := \alpha^2$$

$$z := \alpha(x - \alpha d) \in P$$

$$Z := (x - \alpha d)(x - \alpha d)^T \in \mathcal{C}_{\text{bd}}$$

so that

$$\begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} = \begin{pmatrix} \alpha \\ x - \alpha d \end{pmatrix} \begin{pmatrix} \alpha \\ x - \alpha d \end{pmatrix}^T \succeq 0.$$

So $xx^T = \zeta dd^T + dz^T + zd^T + Z \in \mathcal{C}(d)$. □

The next proposition, which is analogous to Proposition 4.3.2, shows that if $d \in \text{relint}_>(P)$, then a zero entry in BXB^T forces $\zeta = 0$ and $z = 0$ in $\mathcal{C}(d)$.

Proposition 4.3.4. *Let $d \in \text{relint}_>(P)$, and let $X \in \mathcal{C}(d)$ be given with associated (ζ, z, Z). Suppose BXB^T has a zero entry. Then $\zeta = 0$ and $z = 0$.*

Proof. Pre- and post-multiplying $X = \zeta dd^T + dz^T + zd^T + Z$ by B and B^T, respectively, yields

$$BXB^T = \zeta(Bd)(Bd)^T + (Bd)(Bz)^T + (Bz)(Bd)^T + BZB^T,$$

Since $Bd > 0$, $Bz \geq 0$ and $BZB^T \geq 0$, the zero entry of BXB^T ensures $\zeta = 0$, which in turn forces $z = 0$ by positive semidefiniteness of $(\zeta, z^T; z, Z)$. □

We next show that, if we allow d to vary, the intersection of all $\mathcal{C}(d)$ captures $\mathcal{C}$ exactly.

Proposition 4.3.5. $\mathcal{C} = \cap_{d \in P} \mathcal{C}(d)$.

Proof. Since $\mathcal{C} \subseteq \mathcal{C}(d) \subseteq \mathcal{D}$, it suffices to show that, for any $X \in \mathcal{D} \setminus \mathcal{C}$, there exists $d \in P$ such that $X \notin \mathcal{C}(d)$. To do so, let $Q \in \mathcal{C}^*$ separate X with $\langle Q, X \rangle < 0$, and let d be a global minimizer of $\langle x, Qx \rangle$ over the nonempty, bounded slice $P \cap \{x : \langle e, Bx \rangle = 1\}$. We know $\delta := \langle d, Qd \rangle \geq 0$ since $Q \in \mathcal{C}^*$. In fact, we may assume without loss of generality that $\delta = 0$; otherwise, we may replace Q by the shifted $Q - \delta B^T ee^T B$. This shift ensures that the new Q remains in $\mathcal{C}^*$ because, for all $x \in P \cap \{x : \langle e, Bx \rangle = 1\}$,

$$\langle Q - \delta B^T ee^T B, xx^T \rangle = \langle Q, xx^T \rangle - \delta \geq 0.$$

Also, the new Q still satisfies $\langle Q, X\rangle < 0$ because $X \in \mathcal{D}$ implies

$$\langle Q - \delta B^T ee^T B, X\rangle \leq \langle Q, X\rangle < 0.$$

We claim $X \notin \mathcal{C}(d)$. Assuming otherwise, let (ζ, z, Z) be associated with X in $\mathcal{C}(d)$. Since $Z \in \mathcal{C}_{\text{bd}} \subseteq \mathcal{C}$, it holds that $\langle Q, Z\rangle \geq 0$. Hence,

$$0 > \langle Q, X\rangle = \langle Q, \zeta dd^T + dz^T + zd^T + Z\rangle = \zeta\delta + 2\langle Q, dz^T\rangle + \langle Q, Z\rangle \geq 2\langle Q, dz^T\rangle.$$

On the other hand, $d + \rho z \in P$ for all $\rho \geq 0$, and so

$$0 \leq \langle Q, (d + \rho z)(d + \rho z)^T\rangle = 2\rho\langle Q, dz^T\rangle + \rho^2\langle Q, zz^T\rangle.$$

In particular, for $\rho > 0$, $\langle Q, dz^T\rangle \geq -\rho\langle Q, zz^T\rangle$. Taking $\rho \to 0$, we see $\langle Q, dz^T\rangle \geq 0$, a contradiction. □

Notice that $\mathcal{C}(d) = \mathcal{C}(\kappa d)$ for all $\kappa > 0$, and so, without loss of generality we may assume $\langle e, Bd\rangle = 1$. Also, in the context of the preceding proof, a similar argument as in Theorem 4.3.1 shows Q is not positive semidefinite on the linear subspace $\{x : Ax = 0, \langle e, Bx\rangle = 0\}$. This implies that Proposition 4.3.5 still holds even if d is taken only over $\text{bd}(P)$.

We now heuristically compare the equation $X = \zeta dd^T + dz^T + zd^T + Z$ for $X \in \mathcal{C}(d)$ with the nonlinear representation $X = \lambda(XB^Te)(XB^Te)^T + Z$ for $X \in \mathcal{C}_n$ as depicted in (4.4) of the previous subsection. The two representations share $Z \in \mathcal{C}_{\text{bd}}$, and for given $d \in P$, the rank-3, linear term $\zeta dd^T + dz^T + zd^T$ functions as an approximation of the rank-1, nonlinear term $\lambda(XB^Te)(XB^Te)^T$. By allowing d to vary over P, Proposition 4.3.5 shows that, in some sense, the rank-3, linear term is enough to enforce the rank-1, nonlinear term.

The two representations share an additional characteristic. Recall Proposition 4.3.2 showed that the nonlinear representation of $X \in \mathcal{C}$ simplifies to a linear one when BXB^T is known to have a zero component. In particular, the rank-1, nonlinear term $\lambda(XB^Te)(XB^Te)^T$ vanishes. For $\mathcal{C}(d)$ with $d \in \text{relint}_>(P)$, as shown in

Proposition 4.3.4, the rank-3, linear term vanishes under the same condition.

A disadvantage of $\mathcal{C}(d)$ is that is generally intractable due to its dependence on $\mathcal{C}_{\text{bd}}$. However, using the equation $\mathcal{C}_{\text{bd}} = \sum_i \mathcal{C}_i$, we can relax $\mathcal{C}_i$ to $\mathcal{D}_i := \mathcal{D}(P_i)$ in $\mathcal{C}(d)$—where $\mathcal{D}(P_i)$ is defined in analogy with (4.1), respecting the fixed equality $\langle b_i, x \rangle = 0$—to obtain the following tractable relaxation:

$$\mathcal{D}(d) := \mathcal{D}(P; d) := \left\{ X = \zeta dd^T + dz^T + zd^T + Z \ : \ \begin{array}{c} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P, \ Z \in \sum_i \mathcal{D}_i \end{array} \right\}.$$

Proposition 4.3.4 extends to $\mathcal{D}(d)$ by the same proof:

Proposition 4.3.6. *Let $d \in \text{relint}_>(P)$, and let $X \in \mathcal{D}(d)$ be given with associated (ζ, z, Z). Suppose BXB^T has a zero entry. Then $\zeta = 0$ and $z = 0$.*

In addition, $\mathcal{D}(d)$ is at least as strong as $\mathcal{D}$.

Theorem 4.3.2. *$\mathcal{D}(d) \subseteq \mathcal{D}$ for all nonzero $d \in P$.*

Proof. Let $X = \zeta dd^T + dz^T + zd^T + Z \in \mathcal{D}(d)$. We need to show that X satisfies all constraints of $\mathcal{D}$.

We first claim $X \succeq 0$. If $\zeta = 0$, then $z = 0$ and $X = Z \succeq 0$. If $\zeta > 0$, we have

$$\begin{aligned} X &= \zeta dd^T + dz^T + zd^T + \zeta^{-1} zz^T + Z - \zeta^{-1} zz^T \\ &= (\sqrt{\zeta} d + \sqrt{\zeta^{-1}} z)(\sqrt{\zeta} d + \sqrt{\zeta^{-1}} z)^T + Z - \zeta^{-1} zz^T, \end{aligned}$$

which expresses X as the sum of two semidefinite matrices, which implies $X \succeq 0$.

It remains to show that X satisfies all the linear constraints of $\mathcal{D}$. Since $P_i \subseteq P$ for all i, $\mathcal{D}_i \subseteq \mathcal{D}$ for all i. This implies Z satisfies all constraints. Since $d, z \in P$, we also see that dd^T and $dz^T + zd^T$ satisfy all constraints, which proves the result. □

Combining Proposition 4.3.3 and Theorem 4.3.2, we have the inclusions $\mathcal{C} \subseteq \mathcal{C}(d) \subseteq \mathcal{D}(d) \subseteq \mathcal{D}$. We were unable to prove or disprove whether $\cap_{d \in P} \mathcal{D}(d)$ equals $\mathcal{C}$.

4.3.4 A recursive hierarchy of convex relaxations

The ideas of the previous subsection can be extended to obtain a recursive hierarchy of convex relaxations for $\mathcal{C}$. In contrast to other hierarchies such as the one proposed by Parrilo [62] for completely positive matrices (see the discussion in Section 1.3), the number of relaxations in our hierarchy is finite. However, the hierarchy depends on a specific choice of vectors in P. In particular, a different choice of vectors yields a different finite hierarchy. In this sense, we actually propose an infinite family of finite hierarchies.

As it will turn out, $\mathcal{C}(d) := \mathcal{C}(P; d)$ and $\mathcal{D}(d) := \mathcal{D}(P; d)$ of the previous subsection will constitute the first level of the hierarchy for a specific choice $d \in P$. In order to define the higher levels of the hierarchy, we first need to introduce some definitions and notation.

Let m denote the number of inequalities in $Bx \geq 0$. For any $I \subseteq \{1, \ldots, m\}$, define

$$P_I := P \cap \{x : b_i^T x = 0 \ \forall \ i \in I\}$$

to be the face of P having all inequalities $\langle b_i, x \rangle \geq 0$, $i \in I$, set to equality. For example, $P_\emptyset = P$. Defining $J := \{1, \ldots, m\} \setminus I$, we write

$$P_I = \{x : A_I x = 0, B_J x \geq 0\},$$

where: A_I consists of the rows of A combined with the rows b_i^T of B for $i \in I$; and B_J consists of the remaining rows of B, i.e., b_j^T such that $j \in J$.

As mentioned above, the hierarchy will be defined in terms of a specific choice of vectors in P. Specifically, for all $I \subseteq \{1, \ldots, m\}$ with $|I| < m$, choose $v_I \in P_I$, and let $\mathcal{V}$ denote the collection of all v_I. If $P_I = \emptyset$, we consider the corresponding v_I to be non-existent in $\mathcal{V}$. The collection $\mathcal{V}$ will then serve as the basis for the hierarchy.

We next define a convex cone recursively in terms of P_I, $\mathcal{V}$, and any integer t satisfying $0 \le t \le |J|$. For notational convenience, let $P_{Ij} := P_{I \cup \{j\}}$. The convex cone is

$$\mathcal{C}^{(t)}(P_I;\mathcal{V}) := \left\{ X = \zeta v_I v_I^T + v_I z^T + z v_I^T + Z \;:\; \begin{array}{c} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P_I,\; Z \in \sum_{j \in J} \mathcal{C}^{(t-1)}(P_{Ij};\mathcal{V}) \end{array} \right\},$$

where the base-case of the recursion is defined as follows:

$$\mathcal{C}^{(0)}(P_\bullet;\mathcal{V}) := \mathcal{C}(P_\bullet),$$

i.e., the "zero-th" cone is simply the cone of completely positive matrices over the given argument. For example, consider $P_\emptyset = P$ with chosen $\mathcal{V}$, and define $P_j := P_{\{j\}}$. Then $t = 0$ yields $\mathcal{C}^{(0)}(P,\mathcal{V}) = \mathcal{C}(P)$, and $t = 1$ gives

$$\mathcal{C}^{(1)}(P;\mathcal{V}) := \left\{ X = \zeta v_\emptyset v_\emptyset^T + v_\emptyset z^T + z v_\emptyset^T + Z \;:\; \begin{array}{c} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P,\; Z \in \sum_{j=1}^m \mathcal{C}(P_j) \end{array} \right\},$$

which is precisely $\mathcal{C}(P;d)$ of the previous subsection with $d = v_\emptyset$.

An important property of $\mathcal{C}^{(t)}(P_I;\mathcal{V})$ is the following inclusion relationship.

Lemma 4.3.3. *Given P_I, $\mathcal{V}$, and $0 \le t < |J|$, it holds that $\mathcal{C}^{(t)}(P_I;\mathcal{V}) \subseteq \mathcal{C}^{(t+1)}(P_I;\mathcal{V})$.*

Proof. Using a proof similar to that of Proposition 4.3.3, we can show $\mathcal{C}^{(0)}(P_\bullet;\mathcal{V}) \subseteq \mathcal{C}^{(1)}(P_\bullet;\mathcal{V})$ for any argument. So assuming $\mathcal{C}^{(t-1)}(P_\bullet;\mathcal{V}) \subseteq \mathcal{C}^{(t)}(P_\bullet;\mathcal{V})$, we proceed by induction. The only difference between the definitions of $\mathcal{C}^{(t)}(P_I;\mathcal{V})$ and $\mathcal{C}^{(t+1)}(P_I;\mathcal{V})$ is the respective constraints

$$Z \in \sum_{j \in J} \mathcal{C}^{(t-1)}(P_{Ij};\mathcal{V}) \qquad \text{and} \qquad Z \in \sum_{j \in J} \mathcal{C}^{(t)}(P_{Ij};\mathcal{V}).$$

By induction, $\mathcal{C}^{(t-1)}(P_{Ij};\mathcal{V}) \subseteq \mathcal{C}^{(t)}(P_{Ij};\mathcal{V})$, and so the second constraint is looser, which implies $\mathcal{C}^{(t)}(P_I;\mathcal{V}) \subseteq \mathcal{C}^{(t+1)}(P_I;\mathcal{V})$, as desired. □

This result establishes the following hierarchy of relaxations for $\mathcal{C}(P)$:

$$\mathcal{C}(P) = \mathcal{C}^{(0)}(P;\mathcal{V}) \subseteq \mathcal{C}^{(1)}(P;\mathcal{V}) \subseteq \cdots \subseteq \mathcal{C}^{(m)}(P;\mathcal{V}).$$

Via recursion, the relaxation $\mathcal{C}^{(t)}(P;\mathcal{V})$ is ultimately based on a number of convex cones of the generic form $\mathcal{C}(P_\bullet) = \mathcal{C}^{(0)}(P_\bullet;\mathcal{V})$. For this reason, in practice, one cannot expect to optimize efficiently over $\mathcal{C}^{(t)}(P;\mathcal{V})$ since $\mathcal{C}(P_\bullet)$ is generally intractable. However, if one further relaxes $\mathcal{C}(P_\bullet)$ to $\mathcal{D}(P_\bullet)$, then the resulting relaxation will be in fact tractable. Formally, in analogy with $\mathcal{C}^{(t)}(P;\mathcal{V})$, we define

$$\mathcal{D}^{(t)}(P_I;\mathcal{V}) := \left\{ X = \zeta v_I v_I^T + v_I z^T + z v_I^T + Z \ : \ \begin{matrix} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P_I,\ Z \in \sum_{j\in J} \mathcal{D}^{(t-1)}(P_{Ij};\mathcal{V}) \end{matrix} \right\}$$

and

$$\mathcal{D}^{(0)}(P_\bullet;\mathcal{V}) := \mathcal{D}(P_\bullet),$$

For example, letting $v_j := v_{\{j\}}$ and $P_{jk} := P_{\{j,k\}}$ for notational convenience, we have

$$\mathcal{D}^{(2)}(P;\mathcal{V}) = \left\{ X = \zeta v_\emptyset v_\emptyset^T + v_\emptyset z^T + z v_\emptyset^T + Z \ : \ \begin{matrix} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P,\ Z \in \sum_{j=1}^m \mathcal{D}^{(1)}(P_j;\mathcal{V}) \end{matrix} \right\},$$

where

$$\mathcal{D}^{(1)}(P_j;\mathcal{V}) = \left\{ X = \zeta v_j v_j^T + v_j z^T + z v_j^T + Z \ : \ \begin{matrix} \begin{pmatrix} \zeta & z^T \\ z & Z \end{pmatrix} \succeq 0 \\ z \in P_j,\ Z \in \sum_{k\neq j} \mathcal{D}(P_{jk}) \end{matrix} \right\}.$$

Just as Lemma 4.3.3 established an important inclusion property of $\mathcal{C}^{(t)}(P_I;\mathcal{V})$, a related—but different—inclusion holds for $\mathcal{D}^{(t)}(P_I;\mathcal{V})$.

Lemma 4.3.4. *Given P_I, $\mathcal{V}$, and $0 \le t < |J|$, it holds that $\mathcal{D}^{(t)}(P_I;\mathcal{V}) \supseteq \mathcal{D}^{(t+1)}(P_I;\mathcal{V})$.*

Proof. Using a proof similar to that of Theorem 4.3.2, we can show $\mathcal{D}^{(0)}(P_\bullet;\mathcal{V}) \supseteq \mathcal{D}^{(1)}(P_\bullet;\mathcal{V})$ for any $P_\bullet$. The proof now follows the proof of Lemma 4.3.3, except that all inclusions are reversed. □

This result establishes the following hierarchy of restrictions of $\mathcal{D}(P)$:

$$\mathcal{D}(P) = \mathcal{D}^{(0)}(P;\mathcal{V}) \supseteq \mathcal{D}^{(1)}(P;\mathcal{V}) \supseteq \cdots \supseteq \mathcal{D}^{(m)}(P;\mathcal{V}).$$

The next proposition brings together the above hierarchies for $\mathcal{C}(P)$ and $\mathcal{D}(P)$.

Proposition 4.3.7. *Given $\mathcal{V}$, it holds that*

$$\mathcal{C}(P) \subseteq \mathcal{C}^{(1)}(P;\mathcal{V}) \subseteq \cdots \subseteq \mathcal{C}^{(m)}(P;\mathcal{V}) \subseteq \mathcal{D}^{(m)}(P;\mathcal{V}) \subseteq \cdots \subseteq \mathcal{D}^{(1)}(P;\mathcal{V}) \subseteq \mathcal{D}(P).$$

Proof. We need only establish that $\mathcal{C}^{(m)}(P;\mathcal{V}) \subseteq \mathcal{D}^{(m)}(P;\mathcal{V})$ because the remaining inclusions follow from Lemmas 4.3.3 and 4.3.4.

In fact, we prove more generally that $\mathcal{C}^{(t)}(P_\bullet;\mathcal{V}) \subseteq \mathcal{D}^{(t)}(P_\bullet;\mathcal{V})$. This follows because the only true difference in the definitions of $\mathcal{C}^{(t)}(P_\bullet;\mathcal{V})$ and $\mathcal{D}^{(t)}(P_\bullet;\mathcal{V})$ occurs at the lowest level of recursion, where $\mathcal{C}(P_*)$ is relaxed to $\mathcal{D}(P_*)$. □

In the preceding proposition, the hierarchy is expressed fully via m levels, where m is the number of linear inequalities defining P. In some cases, one can prove strict inclusion for some levels. For example, for the completely positive case in Section 2.2, one can show that $\mathcal{C}^{(1)}(P,\mathcal{V})$ is a proper subset of $\mathcal{C}^{(2)}(P,\mathcal{V})$, if each $v_I \in \text{relint}_>(P_I)$ and $n \geq 5$. However, generally it may happen that some of the levels of the hierarchy may be identical, e.g., $\mathcal{C}^{(m-1)}(P;\mathcal{V}) = \mathcal{C}^{(m)}(P;\mathcal{V}) = \mathcal{D}^{(m)}(P;\mathcal{V}) = \mathcal{D}^{(m-1)}(P;\mathcal{V})$, making the full hierarchy unnecessary. For example, in Section 2.2, results therein imply that the levels of the hierarchy are identical for $t \geq m-4$.

Finally, we claim that $D^{(t)}(P;\mathcal{V})$ is tractable when t is constant with respect to the size of P. Let p be the total number of linear constraints defining P (i.e., the number of linear equalities plus the number m of linear inequalities). We already know that $\mathcal{D}(P) = \mathcal{D}^{(0)}(P;\mathcal{V})$ requires a single positive-semidefinite variable of size $n \times n$, which is constrained by $O(p^2)$ linear constraints. In fact $\mathcal{D}(P_\bullet) = \mathcal{D}^{(0)}(P_\bullet;\mathcal{V})$

for any argument $P_\bullet$ has the same size since $P_\bullet$ also lives in $\Re^n$ and is defined by p linear constraints. Additionally, one can see from the recursion that $\mathcal{D}^{(t)}(P;\mathcal{V})$ is ultimately based on $O(m^t)$ cones of the form $\mathcal{D}(P_\bullet)$. So the description of $\mathcal{D}^{(t)}(P;\mathcal{V})$ requires roughly $O(m^t)$ semidefinite variables of size $n \times n$ and $O(m^t p^2)$ linear constraints. This shows that, if t is constant with respect to n and p, the level-t relaxation $\mathcal{D}^{(t)}(P;\mathcal{V})$ is tractable.

4.4 Application: Completely Positive Matrices

In this section, we apply the results of Section 4.3 to the case when P equals the nonnegative orthant $\Re^+_n$. $I + \frac{1}{n^2}E$ is an interior point [28]; this is also implied by Proposition 4.2.1. To emphasize the dimension n, in this section we employ the notation $P^n := \Re^+_n$, $\mathcal{C}^n := \mathcal{C}(\Re^+_n)$ and $\mathcal{D}^n := \mathcal{D}(\Re^+_n)$.

As mentioned in the Introduction, A empty and $B = I$ give rise to $P = \Re^+_n$. Assumptions 4.2.1–4.2.3 are straightforward to verify, so that all results in Section 4.3 apply.

To apply the separation algorithm, Algorithm 1, to $\mathcal{C}^n$, we note that

$$P_1^n := \left\{ \begin{pmatrix} 0 \\ \tilde{x} \end{pmatrix} : \tilde{x} \in P^{n-1} \right\}.$$

In other words, P_1^n is just a copy of P^{n-1} embedded in $\Re_n$. The same holds for P_i^n except the embedding sets the i-th coordinate to zero. Similarly,

$$C_1^n := \mathcal{C}(P_1^n) = \left\{ \begin{pmatrix} 0 & 0^T \\ 0 & \tilde{X} \end{pmatrix} : \tilde{X} \in \mathcal{C}^{n-1} \right\}$$

and C_i^n more generally are simply embeddings of $\mathcal{C}^{n-1}$. So Algorithm 1 amounts to the optimization problem (4.2) over n copies of the cone $(\mathcal{C}^{n-1})^*$. To complete the specification of Algorithm 1, we need a matrix $X^0 \in \text{relint}(\sum_i \mathcal{C}_i^n)$. One such choice, which we use in the examples below, is to define X_i^0 to be the appropriate embedding of $\tilde{I} + \frac{1}{(n-1)^2}\tilde{e}\tilde{e}^T \in \text{int}(\mathcal{C}^{n-1})$ into $\mathcal{C}_i^n$ and then set $X^0 := \sum_i \frac{1}{n} X_i^0$.

Since $\mathcal{C}^{n-1} = \mathcal{D}^{n-1}$ is tractable for $n \leq 5$, we have the following corollary of Theorem 4.3.1:

Corollary 4.4.1. *Algorithm 1 correctly solves the separation problem for $\mathcal{C}(\Re_5^+)$.*

This is the first separation algorithm for $\mathcal{C}^5$ and successfully answers the open question as to whether or not $\mathcal{C}^5$ is tractable.

Example 4.4.1. The paper [21] studies the set $\mathcal{D}^n \backslash \mathcal{C}^n$ of so-called *bad* matrices. In particular, the authors give a characterization of the extreme rays of $\mathcal{D}^5$, which are not in $\mathcal{C}^5$; they call these *extremely bad* matrices. The authors show how to separate 5×5 extremely bad matrices but are unable to separate nearby bad matrices.

Consider the following 5×5 extremely bad matrix Z, permutation matrix P, and doubly nonnegative matrix $X := 0.93Z + 0.07PZP^T$, which is close to Z:

$$Z = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 6 & 2 & 0 & 0 \\ 0 & 2 & 1 & 1 & 0 \\ 0 & 0 & 1 & 5 & 2 \\ 1 & 0 & 0 & 2 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad X = \begin{pmatrix} 1.00 & 0.93 & 0.07 & 0.07 & 0.93 \\ 0.93 & 5.65 & 1.86 & 0.14 & 0.07 \\ 0.07 & 1.86 & 1.07 & 0.93 & 0.14 \\ 0.07 & 0.14 & 0.93 & 5.07 & 1.86 \\ 0.93 & 0.07 & 0.14 & 1.86 & 2.21 \end{pmatrix}.$$

As detailed in [21], the copositive matrix

$$K = \begin{pmatrix} 9.00 & -4.50 & 10.50 & 4.50 & -7.50 \\ -4.50 & 2.25 & -5.25 & 2.25 & 3.75 \\ 10.50 & -5.25 & 12.25 & -5.25 & 8.75 \\ 4.50 & 2.25 & -5.25 & 2.25 & -3.75 \\ -7.50 & 3.75 & 8.75 & -3.75 & 6.25 \end{pmatrix}$$

separates Z, but one can check that it does not separate X. By using Algorithm 1 in a Matlab implementation using SeDuMi [71], we are able to verify that $X \notin \mathcal{C}^5$

via separation with the copositive matrix

$$Q \approx \begin{pmatrix} 0.380 & -0.190 & 0.409 & 0.161 & -0.263 \\ -0.190 & 0.095 & -0.205 & 0.080 & 0.131 \\ 0.409 & -0.205 & 0.441 & -0.173 & 0.283 \\ 0.161 & 0.080 & -0.173 & 0.068 & -0.111 \\ -0.263 & 0.131 & 0.283 & -0.111 & 0.182 \end{pmatrix}.$$

The SeDuMi solution time is approximately 0.1 seconds on a 2.40 GHz Linux machine.

We now turn our attention to the relaxations $\mathcal{C}(d)$ and $\mathcal{D}(d)$, for given $d \in \Re^+_n$, introduced in Section 4.3.3. Recall the inclusions $\mathcal{C} \subseteq \mathcal{C}(d) \subseteq \mathcal{D}(d) \subseteq \mathcal{D}$. Here, we do not include a superscript for the dimension n.

Example 4.4.2. Let $n = 5$, in which case $\mathcal{C}(d) = \mathcal{D}(d)$ since $\mathcal{C}_{\text{bd}}$ is based on five copies of $\mathcal{C}(\Re^+_4)$. To illustrate the strength of $\mathcal{D}(d)$ for various d, we consider the optimization problem $\mu(d) := \min\{\langle H, X\rangle : X \in \mathcal{D}(d), \langle I, X\rangle \le 1\}$, where $H \in \mathcal{C}^* \setminus \mathcal{D}^*$ is the well-known Horn matrix:

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

It is known that

$$0 = \min\{\langle H, X\rangle : X \in \mathcal{C}, \langle I, X\rangle \le 1\},$$

$$-0.2361 \approx 2 - \sqrt{5} = \min\{\langle H, X\rangle : X \in \mathcal{D}, \langle I, X\rangle \le 1\}.$$

Hence, for any $d \ge 0$, it must hold that $-0.2361 \le \mu(d) \le 0$, and the closeness to 0 gives an indirect indication of the strength of $\mathcal{D}(d)$. Table 4.1 summarizes our computational experiment.

Table 4.1: Strength of $\mathcal{D}_5(d)$ for various d

d	$\mu(d)$
$(1,0,0,0,0)^T$	-0.2361
$(1,1,0,0,0)^T$	0
$(1,0,1,0,0)^T$	-0.1249
$(1,1,1,0,0)^T$	-0.0787
$(1,1,1,1,0)^T$	0
$(1,1,1,1,1)^T$	0

In our opinion, the preceding example and Proposition 4.3.6 suggest that $d = e$ is a reasonable default choice for $\mathcal{D}(d)$.

Example 4.4.3. Again let $n = 5$, and let Z be an extremely bad matrix in $\mathcal{D}\backslash\mathcal{C}$ [21], which necessarily has a zero entry. We claim $Z \notin \mathcal{D}(e)$. Suppose for contradiction that Z is in $\mathcal{D}(e)$. Then Proposition 4.3.6 implies $Z \in \sum_{i=1}^{5} D_i$, where $\mathcal{D}_i$ is precisely all 5×5 completely positive matrices with row i and column i equal to 0. In other words, $\mathcal{D}_i$ is isomorphic to the 4×4 doubly nonnegative matrices, which are precisely the 4×4 completely positive matrices by Theorem 1.1.1. So Z is the sum of completely positive matrices and hence completely positive, which contradicts the assumption that $Z \in \mathcal{D} \setminus \mathcal{C}$.

To further gauge the strength of $\mathcal{D}(e)$ relative to $\mathcal{C}$, we calculate the distance of Z to $\mathcal{D}(e)$ and compare it to the distance of Z to $\mathcal{C}$. The distances are calculated by solving the following optimization problems:

$$\operatorname{dist}(Z, \mathcal{D}(e)) := \min\{\|X - Z\|_F : X \in \mathcal{D}(e)\},$$

$$\operatorname{dist}(Z, \mathcal{C}) := \min\{\|X - Z\|_F : X \in \mathcal{C}\},$$

where $\|\cdot\|_F$ is the Frobenius norm induced by the inner product $\langle\cdot,\cdot\rangle$. In practice, $\text{dist}(Z, \mathcal{C})$ is calculated by first solving over $\mathcal{D}$ and then repeatedly adding copositive cuts produced by Algorithm 1. We then calculate the percentage

$$\frac{\text{dist}(Z, \mathcal{D}(e))}{\text{dist}(Z, \mathcal{C})} \times 100\%.$$

By definition, this percentage is between 0% and 100%, and the closer it is to 100%, the better $\mathcal{D}(e)$ approximates $\mathcal{C}$ near Z.

For 1000 randomly generated extremely bad Z with $\langle ee^T, Z\rangle = 1$, we calculated the above percentage. The average of the 1000 percentages was 99.935%, and the standard deviation was 0.241%. This means that, on average, $\mathcal{D}(e)$ cuts away about 99.9% of the distance between the extremely bad matrix Z and $\mathcal{C}$. In addition the minimum percentage over all 1000 Z was 97.958%. We feel this is convincing evidence that $\mathcal{D}(e)$ approximates $\mathcal{C}$ well and is certainly much stronger than $\mathcal{D}$.

In the next example, we numerically examine the recursive hierarchy of tractable convex relaxations $\mathcal{D}^{(t)} \subseteq \cdots \subseteq \mathcal{D}^{(1)} \subseteq \mathcal{D}$ introduced in Section 4.3.4. The result shows that indeed $\mathcal{D}^{(t)}$ gets much stronger with increased depth t.

Example 4.4.4. Let $n = 7$, and consider the following 7×7 exceptional and extremal copositive matrix (the so-called *Hoffman-Pereira matrix*) [47]:

$$Q := \begin{pmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{pmatrix}$$

Also consider the optimization $\min\{\langle Q, X\rangle : \langle I, X\rangle \le 1, X \in \mathcal{C}\}$, whose optimal value is 0 by definition. To compute lower bounds for this problem, we replace $\mathcal{C}$ by its level-1, level-2, and level-3 relaxations $\mathcal{D}^{(1)}(\Re^7_+;\mathcal{V})$, $\mathcal{D}^{(2)}(\Re^7_+;\mathcal{V})$, and $\mathcal{D}^{(3)}(\Re^7_+;\mathcal{V})$, respectively, where $\mathcal{V}$ consists of vectors v_I defined as follows: $[v_I]_i = 0$ for all $i \in I$, and $[v_I]_j = 1$ for all $j \in J := \{1,\ldots,n\} \setminus I$. Note that, when $n = 7$, $\mathcal{D}^{(3)}(\Re^7_+;\mathcal{V})$ is the deepest relaxation one needs to consider since it is based on $\mathcal{D}(\Re^+_4) = \mathcal{C}(\Re^+_4)$. We calculated the following four relaxation values:

$$\begin{aligned}
-0.1099 &\approx \min\{\langle Q,X\rangle : \langle I,X\rangle \le 1, X \in \mathcal{D}\} \\
-0.0824 &\approx \min\left\{\langle Q,X\rangle : \langle I,X\rangle \le 1, X \in \mathcal{D}^{(1)}(\Re^7_+;\mathcal{V})\right\} \\
-0.0824 &\approx \min\left\{\langle Q,X\rangle : \langle I,X\rangle \le 1, X \in \mathcal{D}^{(2)}(\Re^7_+;\mathcal{V})\right\} \\
0.0000 &\approx \min\left\{\langle Q,X\rangle : \langle I,X\rangle \le 1, X \in \mathcal{D}^{(3)}(\Re^7_+;\mathcal{V})\right\}.
\end{aligned}$$

This experiment shows the potential power of the recursive relaxations. However, it should be noted that the relaxations grow exponentially in size with the recursive depth. For example, in our Yalmip/SeDuMi implementation, the first relaxation required 1.3 seconds, while the last one required 3.8.

4.4.1 The simplex

As mentioned in the Introduction, $\mathcal{C}(\Re^+_n)$ is closely related to $\mathcal{C}(\hom(\Delta_{n-1}))$. In the first case, A is empty and $B = I$, while in the second, $A = (-1, \tilde{e}^T)$ and $B = (0, \tilde{I})$. This case certainly satisfies Assumptions 4.2.1–4.2.3.

Anstreicher and Burer [5] showed that $\mathcal{C}(\hom(\Delta_{n-1})) = \mathcal{D}(\hom(\Delta_{n-1}))$ if and only if $n \le 5$. Note that this result does not follow directly from Theorem 1.1.1 since $\mathcal{C}(\hom(\Delta_4))$ is a subset of $\mathcal{C}(\Re^+_5)$, the completely positive matrices of size 5×5. Using Algorithm 1, we have for the first time a separation algorithm for $\mathcal{C}(\hom(\Delta_5))$, which is a subset of the 6×6 completely positive matrices:

Corollary 4.4.2. *Algorithm 1 correctly solves the separation problem for* $\mathcal{C}(\hom(\Delta_5))$.

To implement the separation algorithm, we note that, for $P = \hom(\Delta_{n-1})$, P_i is simply an embedding of $\hom(\Delta_{n-2})$. Also, a point X^0 can be generated using arguments found in the proof of Proposition 4.2.1.

4.5 Application: The Box

In this section, we apply the results of Section 4.3 to the case when P equals the homogenization of the box $\square_{n-1}$.

4.5.1 Literature review

For $P = \hom(\square_{n-1})$, $\mathcal{C}$ has been formally studied in the papers [5, 24]. In the latter paper, the slice

$$\{X \in \mathcal{C} : X_{11} = 1\} = \text{conv} \left\{ \begin{pmatrix} 1 \\ \tilde{x} \end{pmatrix} \begin{pmatrix} 1 \\ \tilde{x} \end{pmatrix}^T : \tilde{x} \in \square_{n-1} \right\}$$

is denoted QPB_{n-1}. $\mathcal{C}$ is full-dimensional, e.g., [24] showed that

$$\lambda \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T + \sum_{j=1}^{n-1} \begin{pmatrix} 1 \\ \tilde{e}_j \end{pmatrix} \begin{pmatrix} 1 \\ \tilde{e}_j \end{pmatrix}^T + \sum_{j=1}^{n-1} \begin{pmatrix} 1 \\ \frac{1}{2}\tilde{e}_j \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2}\tilde{e}_j \end{pmatrix}^T + \sum_{1 \le j < k \le n-1} \begin{pmatrix} 1 \\ \tilde{e}_j + \tilde{e}_k \end{pmatrix} \begin{pmatrix} 1 \\ \tilde{e}_j + \tilde{e}_k \end{pmatrix}^T \right]$$

lies in the relative interior of QPB_{n-1}, where $\lambda := [n(n+1)/2]^{-1}$ and $\tilde{e}_j$ is the standard coordinate vector in $\Re_{n-1}$. Since QPB_{n-1} is a slice of $\mathcal{C}$, the above point is an interior point of $\mathcal{C}$. The semidefinite relaxation $\mathcal{D}$ has also been studied in several papers, and the slice $\{X \in \mathcal{D} : X_{11} = 1\}$ is often written PSD$\cap$RLT since $\mathcal{D}$ combines both positive semidefiniteness and the linear inequalities arising from the reformulation-linearization technique of Sherali and Adams [70].

To emphasize the dimension, we use the notation $P^n := \hom(\square_{n-1})$, $\mathcal{C}^n := \mathcal{C}(\hom(\square_{n-1}))$ and $\mathcal{D}^n := \mathcal{D}(\hom(\square_{n-1}))$. Anstreicher and Burer [5] proved $QPB_{n-1} =$ PSD$\cap$RLT if and only if $n \le 3$. In terms of the cones presented here, the result is as follows:

Theorem 4.5.1. *$\mathcal{C}^n = \mathcal{D}^n$ if and only if $n \le 3$.*

For $n > 3$, Burer and Letchford [24] showed that additional valid inequalities for $\mathcal{C}^n$ can be derived from valid inequalities of the *boolean quadric polytope* [61]

$$BQP_{n-1} := \text{conv}\left\{ \begin{pmatrix} 1 \\ \tilde{x} \end{pmatrix} \begin{pmatrix} 1 \\ \tilde{x} \end{pmatrix}^T : \tilde{x} \in \{0,1\}^{n-1} \right\}.$$

Proposition 4.5.1. *Let $Q \in (BQP_{n-1})^*$ with $Q_{22} = \cdots = Q_{nn} = 0$. Then $Q \in (QPB_{n-1})^* = (\mathcal{C}^n)^*$.*

Such valid inequalities include for example the well-known triangle inequalities, which along with the RLT constraints, capture BQP_3 exactly. However, in [24], it is shown by example that the relaxation PSD ∩ RLT ∩ TRI which incorporates the triangle inequalities to tighten the slice $\{X \in \mathcal{D} : X_{11} = 1\}$ still does not characterize QPB_3 exactly. In terms of cones, $\mathcal{C}^4 \subsetneq \mathcal{D}^4 \cap \text{TRI}$.

Using a different approach, [5] provides an exact, disjunctive formulation of $\mathcal{C}^4$. Otherwise, little is known about the structure of $\mathcal{C}^n$. In particular, it has not been known whether there is a separation procedure for $\mathcal{C}^4$ that is closely related to the cone $\mathcal{D}^4$ and whether separation over $\mathcal{C}^5$ is tractable.

4.5.2 More when $n = 4$

As mentioned in the previous subsection, the cone $\mathcal{C}^4 := \mathcal{C}(\text{hom}(\square_3))$ is properly contained in the cone $\mathcal{D}^4 \cap \text{TRI}$. Specifically, the set TRI incorporates the following four triangle inequalities:

$$X_{23} + X_{24} \leq X_{12} + X_{34}$$

$$X_{23} + X_{34} \leq X_{13} + X_{24}$$

$$X_{24} + X_{34} \leq X_{14} + X_{23}$$

$$X_{12} + X_{13} + X_{14} \leq X_{23} + X_{24} + X_{34} + 1.$$

The following proposition provides a nonempty class of points that is guaranteed to be in this difference.

Proposition 4.5.2. *Suppose* $X \in \mathcal{D}^4 \cap \text{TRI}$ *satisfies the following conditions:* $\text{rank}(X) = 3$, $X_{22} > 0$, $X_{32} = X_{42} = 0$, $0 < X_{43} < \min\{X_{33}, X_{44}\}$, $X_{33} = X_{31}$, *and* $X_{44} = X_{41}$. *Then* $X \notin \mathcal{C}^4$.

Proof. We suppose $X \in \mathcal{C}^4$ and derive a contradiction. Write a minimal representation $X = \sum_{k=1}^{K} x^k (x^k)^T$, where $K \geq 3$ and $0 \neq x^k \in P^4$. In particular, by the characterization of P and that of all extreme rays of $\mathcal{C}$, $0 \neq x^k$ implies $x_1^k > 0$ for all k. Since $X_{22} > 0$, we may assume without loss of generality that $x_2^1 > 0$, which implies $x_3^1 = x_4^1 = 0$ since $X_{32} = X_{42} = 0$. Hence

$$X = \begin{pmatrix} x_1^1 \\ x_2^1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} x_1^1 \\ x_2^1 \\ 0 \\ 0 \end{pmatrix}^T + \sum_{k=2}^{K} x^k (x^k)^T.$$

Next, the conditions $X_{33} = X_{31}$ and $X_{44} = X_{41}$ imply $x_j^k \in \{0, x_1^k\}$ for all k and all $j \in \{3, 4\}$. Then, since $X_{43} > 0$, we may assume $x_3^2 = x_4^2 = x_1^2$, which in turn implies $x_2^2 = 0$ since $X_{32} = 0$. So

$$X = \begin{pmatrix} x_1^1 \\ x_2^1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} x_1^1 \\ x_2^1 \\ 0 \\ 0 \end{pmatrix}^T + \begin{pmatrix} x_1^2 \\ 0 \\ x_1^2 \\ x_1^2 \end{pmatrix} \begin{pmatrix} x_1^2 \\ 0 \\ x_1^2 \\ x_1^2 \end{pmatrix}^T + \sum_{k=3}^{K} x^k (x^k)^T.$$

Next, note that, for all $k \geq 3$, we have $x_3^k \neq x_1^k$ or $x_4^k \neq x_1^k$; otherwise, $x_2^k = 0$ and the representation for X is not minimal. So, for all $k \geq 3$, we have

$$x^k = \begin{pmatrix} x_1^k \\ 0 \\ x_1^k \\ 0 \end{pmatrix}, \quad x^k = \begin{pmatrix} x_1^k \\ 0 \\ 0 \\ x_1^k \end{pmatrix}, \quad \text{or} \quad x^k = \begin{pmatrix} x_1^k \\ x_2^k \\ 0 \\ 0 \end{pmatrix}.$$

Because $\text{rank}(X) = 3$, at most one of the first two possibilities may occur in the representation, and by minimality, if one possibility does occur, it occurs at most once. Suppose the first one occurs once; then $X_{43} = X_{44} = (x_1^2)^2$. If the second occurs once, then $X_{43} = X_{33} = (x_1^2)^2$. If neither occurs, then $X_{43} = X_{33} = X_{44} = (x_1^2)$. Whatever the case, this contradicts the condition $X_{43} < \min\{X_{33}, X_{44}\}$. □

One can solve a semidefinite program (e.g., with constraints such as $X_{22} \geq \varepsilon$ for fixed small $\varepsilon > 0$) to see that there exist $X \in \mathcal{D}^4 \cap \mathrm{TRI}$ satisfying the conditions of the proposition. One concrete example is the following:

$$\begin{pmatrix} 1 & 1/3 & 1/3 & 1/3 \\ 1/3 & 1/4 & 0 & 0 \\ 1/3 & 0 & 1/3 & 1/15 \\ 1/3 & 0 & 1/15 & 1/3 \end{pmatrix}.$$

4.5.3 Application and examples

As mentioned in Section 4.1, A empty and

$$B = \begin{pmatrix} 0 & \tilde{I} \\ \tilde{e} & -\tilde{I} \end{pmatrix}$$

give rise to $P = \hom(\square_{n-1})$. Assumptions 4.2.1–4.2.3 are straightforward to verify, so that all results in Section 4.3 apply.

To apply the separation algorithm, Algorithm 1, to $\mathcal{C}^n$, we note that

$$P^n_{n-1} := \left\{ \begin{pmatrix} \tilde{x} \\ 0 \end{pmatrix} : \tilde{x} \in P^{n-1} \right\},$$

$$P^n_{2(n-1)} := \left\{ \begin{pmatrix} \tilde{x} \\ \tilde{x}_1 \end{pmatrix} : \tilde{x} \in P^{n-1} \right\}.$$

In other words, P^n_{n-1} and $P^n_{2(n-1)}$ are just copies of P^{n-1} embedded in $\Re_n$. The same holds for P^n_i and P^n_{i+n-1} for $i = 1, \ldots, n-1$ generally except the embedding sets the i-th coordinate to zero and $\tilde{x}_1$, respectively. Similarly,

$$C^n_{n-1} := \mathcal{C}(P^n_{n-1}) = \left\{ \begin{pmatrix} \tilde{X} & 0 \\ 0^T & 0 \end{pmatrix} : \tilde{X} \in \mathcal{C}^{n-1} \right\},$$

$$C^n_{2(n-1)} := \mathcal{C}(P^n_{2(n-1)}) = \left\{ \begin{pmatrix} \tilde{X} & \tilde{X}_{\cdot 1} \\ \tilde{X}^T_{\cdot 1} & \tilde{X}_{11} \end{pmatrix} : \tilde{X} \in \mathcal{C}^{n-1} \right\},$$

and $\mathcal{C}^n_i$ and $\mathcal{C}^n_{n-1+i}$ are simply embeddings of $\mathcal{C}^{n-1}$. So Algorithm 1 amounts to the optimization problem (4.2) over $2(n-1)$ copies of the cone $(\mathcal{C}^{n-1})^*$. To complete the specification of Algorithm 1, we need a matrix $X^0 \in \mathrm{int}(\sum_{i=1}^{2(n-1)} \mathcal{C}^n_i)$. One such choice, which we use in the examples below, is to define X^0_i to be the appropriate embedding of the $\square_{n-2}$ version of the interior point given in Section 4.5.1 and then set $X^0 := \sum_{i=1}^{2(n-1)} \frac{1}{2(n-1)} X^0_i$.

Since $\mathcal{C}^{n-1} = \mathcal{D}^{n-1}$ is tractable for $n \leq 3$, we have the following corollary of Theorem 4.3.1:

Corollary 4.5.1. *Algorithm 1 correctly solves the separation problem for* $\mathcal{C}^4 = \mathcal{C}(\mathrm{hom}(\square_3))$.

This is the first separation algorithm for $\mathcal{C}^4$ that is closely related to the cone $\mathcal{D}^4$. Using the disjunctive formulation of $\mathcal{C}^4$ given in [5], we also obtain a separation procedure for $\mathcal{C}^5$.

Corollary 4.5.2. *Algorithm 1 correctly solves the separation problem for* $\mathcal{C}^5 = \mathcal{C}(\mathrm{hom}(\square_4))$.

This answers the open question as to whether or not $\mathcal{C}^4$ and $\mathcal{C}^5$ are tractable.

Example 4.5.1. Burer and Letchford [24] considered the following optimization:

$\min\{\langle \tilde{x}, \tilde{Q}\tilde{x}\rangle + 2\langle \tilde{c}, \tilde{x}\rangle : \tilde{x} \in \square_3\}$, where

$$\tilde{Q} = \begin{pmatrix} 2.25 & 3 & 3 \\ 3 & 0 & 0.5 \\ 3 & 0.5 & -1 \end{pmatrix}, \quad \tilde{c} = \begin{pmatrix} -1.5 \\ -0.5 \\ 0 \end{pmatrix}.$$

From basic principles, one can verify that the optimal value is -1. However, after conversion to the form $\{\langle Q, X\rangle : X \in \mathcal{C}^4, X_{11} = 1\}$ and relaxation via $\mathcal{D}^4 \cap \mathrm{TRI}$, the relaxation value is approximately -1.0929 for a gap of 9.29%.

In [31], Dong and Anstreicher reconsidered the same problem but from the point of view of its completely-positive formulation [18], which lies in the cone $\mathcal{C}(\Re^+_7)$. By iteratively generating copositive cuts based on the zero structure of the solution to the relaxation over $\mathcal{D}(\Re^+_7)$, the gap to the optimal value can be closed to 0%. In a similar spirit, one could also separate 5×5 completely positive submatrices of the completely-positive formulation using Algorithm 1 in Section 2.2.

Here, we focus on the box structure and generate cuts in $(\mathcal{C}^4)^*$ using Algorithm 1. Similar to [31], the gap is reduced to 0% after the addition of 20 cuts. In contrast to [31], however, our separation requires no special structure in the solution of the relaxation.

In Example 4.5.1, the relaxation over $\mathcal{D}^4 \cap \mathrm{TRI}$ yields a gap of 9.29%, and so the optimal solution $\bar{X}$ of the relaxation is in the difference $\mathcal{D}^4 \cap \mathrm{TRI} \setminus \mathcal{C}^4$. In fact, we found that the optimal $\bar{X}$ numerically satisfies the assumptions of Proposition 4.5.2, which is necessarily cut off by $\mathcal{D}^4(d)$ by the following corollary of Proposition 4.3.6.

Corollary 4.5.3. *Let $X \in \mathcal{D}^4 \cap \mathrm{TRI}$ satisfy the assumptions of Proposition 4.5.2 so that $X \notin \mathcal{C}^4$, and let $d \in \mathrm{relint}_>(P^4)$. Then $X \notin \mathcal{D}^4(d) := \mathcal{D}(P^4; d)$.*

Proof. We prove the contrapositive. Suppose $X \in \mathcal{D}^4(d)$. The condition $X_{42} = 0$

implies (via Proposition 4.3.6) that any X in $\mathcal{D}^4(d)$ can be written as the sum of six matrices (essentially) in $\mathcal{D}^3 = \mathcal{C}^3$ (by Theorem 4.5.1). This in turn implies $X \in \mathcal{C}^4$. □

Example 4.5.2. We consider the same problem as in Example 4.5.1, where instead we solve over the relaxation $\mathcal{D}^4(d)$, where $d = (1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})^T$. The above corollary guarantees that the gap of 9.29% must be improved. In fact, our Yalmip-CSDP [54, 15] implementation achieves a gap of 0%, i.e., it solves the quadratic problem over $\square_3$ exactly.

Random numerical experiments suggest that encountering an X in the difference $\mathcal{D}^4 \cap \text{TRI} \setminus \mathcal{C}^4$ does not happen often. In other words, notwithstanding the preceding examples, $\mathcal{D}^4 \cap \text{TRI}$ seems to be a good approximation of $\mathcal{C}^4$. The following example provides some evidence for this viewpoint.

Example 4.5.3. We created a simple procedure to generate randomly a $Z \in \mathcal{D}^4 \cap \text{TRI} \setminus \mathcal{C}^4$ with $Z_{11} = 1$ in accordance with Proposition 4.5.2. For 1000 such Z, we calculated the normalized distance

$$\text{normdist}(X, \mathcal{C}^4) := \frac{\min\{\|X - Z\|_F : X \in \mathcal{C}^4, X_{11} = 1\}}{\|Z\|_F}.$$

by first relaxing to $\mathcal{D}^4$ and then repeatedly adding $(\mathcal{C}^4)^*$ cuts produced by Algorithm 1. The average normalized distance was 0.0022 with standard deviation 0.0026. The maximum normalized distance was 0.0135.

4.6 Two Remarks

There are many avenues to extend the research of this chapter. It would be interesting to determine the relationship, if any, between our hierarchy for $\mathcal{C}(\Re^+_n)$ and Parrilo's hierarchy. The relationship between $\cap_{d \in P} \mathcal{D}(d)$ and $\mathcal{C}$ could also be explored. In particular, are these two sets equal? Given $X \in \mathcal{D}$, it would also be nice to compute $d \in P$ such that $X \notin \mathcal{D}(d)$ if such a d exists. This would allow one to generate d intelligently instead of using an *a priori* choice of d.

Another important direction for this research is to investigate the hierarchy of relaxations computationally for large n. This will undoubtedly be a challenge due to their large size. On the other hand, the relaxations are well structured, which may lead to opportunities for computational improvements. The results of this paper could also be applied to large n by focusing on small groups of nonnegative or bounded variables. For example, given n bounded variables in a quadratic program, one could focus separately on triples of variables and separate valid inequalities for $\mathcal{C}(\text{hom}(\square_3))$.

CHAPTER 5
OPEN QUESTIONS AND FUTURE WORK

There are many interesting open questions in the field of copositive programming. We conclude this thesis by mentioning a few of them. First, since copositive programming is a special case of linear conic programming, and classical interior point framework for solving LCPs requires a smooth barrier function, it is natural to ask whether the CP cone, $\mathcal{C}$, or its dual $\mathcal{C}^*$, admits any kind of barrier function, that allows to design an (most likely computationally intensive) interior point algorithm for copositive programs. Another related question is whether there exists efficiently computable barrier functions for cones $\mathcal{T}_n^r$ and $\mathcal{TD}_n^r$. In other words, what is the most effective way to exploit the tensor structures algorithmically? Can one give an explicit characterization of all facets of $\mathcal{T}_n^r$? Research on these directions could lead to more practical algorithms for solving relaxations of copositive programs.

In Chapter 3 and Chapter 4, we studied the separation problem via two approaches. One natural direction of research is to study the possibility of employing these linear cutting planes effectively in practice. Although current SDP solvers cannot handle large semidefinite programs efficiently, small SDPs are typically solved very fast and stably. Therefore, it is especially interesting to examine the effectiveness of adding low dimensional (say 5×5) copositive cuts in some global solution framework for mixed integer quadratic programs.

Another long known open question is whether the CP cone, $\mathcal{C}$, is SDP - representable. In other words, for any fixed n, can $\mathcal{C}_n$ be represented as a projection of a high dimensional semidefinite cone intersected with some affine space? Our boundary cone approach sheds some light on this problem. For example, by using the results in Section 4.4, we are able to reduce the separation problem for $\mathcal{C}_{n+1}$ to an optimization problem over direct products of multiple copies of $\mathcal{C}_n$. Since $\mathcal{C}_4$ is SDP-representable ($\mathcal{C}_4 = \mathcal{D}_4$), and one can optimize using merely separation oracles (ellipsoid method), in principle one can solve any copositive program for fixed n by recursively employing ellipsoid method and our reduction in Section 4.4. One question is, does this approach somehow implicitly provide a computable characterization for $\mathcal{C}_n$, where $n \geq 4$? For now we are unable to answer this question.

One final remark is in order. Most current approximation hierarchies for the CP cone $\mathcal{C}$ and its dual cone $\mathcal{C}^*$, including $\{\mathcal{L}^r\}$, $\{\mathcal{K}^r\}$ and $\{\mathcal{Q}^r\}$ as explained in Section 1.3, as well as the tensor hierarchies $\{\mathcal{T}^r\}$ and $\{\mathcal{TD}^r\}$ in Chapter 2, seem to suffer one same problem: they are not "diagonally rescaling invariant". However, $\mathcal{C}$ and $\mathcal{C}^*$ are. In particular, let D be an $n \times n$ diagonal matrix with $D_{ii} > 0, \forall i$, then a matrix $X \in \mathcal{C}_n$ if and only if $DXD \in \mathcal{C}_n$. Similarly $M \in \mathcal{C}_n^*$ if and only if $DMD \in \mathcal{C}_n^*$. However, such a relation does not seem to hold for all the aforementioned approximation sets. For such an outer approximation set $\mathcal{R} \supseteq \mathcal{C}_n$, it is natural to define its diagonally strengthened version:

$$\tilde{\mathcal{R}} := \{X \mid DXD \in \mathcal{R}, \forall D \textit{ diagonal }, D_{ii} > 0\}.$$

It is straightforward to verify that $\mathcal{R} \supseteq \tilde{\mathcal{R}} \supseteq \mathcal{C}_n$. Similarly for an inner approximation $\mathcal{P} \subseteq \mathcal{C}_n^*$, define

$$\tilde{\mathcal{P}} := \mathbf{cl}\,\mathrm{conv}\{M \mid \exists D \textit{ diagonal }, D_{ii} > 0, \textit{ s.t. } DMD \in \mathcal{P}\}.$$

Then $\mathcal{P} \subseteq \tilde{\mathcal{P}} \subseteq \mathcal{C}_n^*$. It is an interesting question if the original approximation set $\mathcal{R}$ and $\mathcal{P}$ are tractable, under what condition are these "improved" versions also tractable.

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