Some aspects of the optimization over the copositive and the completely positive cone

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Zusammenfassung

Optimierungsprobleme tauchen in vielen praktischen Anwendungsbereichen auf. Zu den einfachsten Problemen gehören lineare Optimierungsprobleme. Oft reichen lineare Probleme allerdings zur Modellierung praktischer Anwendungen nicht aus, sondern es muss die Ganzzahligkeit von Variablen gefordert werden oder es tauchen nichtlineare Nebenbedingungen oder eine nichtlineare Zielfunktion auf. Eine wichtige Problemklasse stellen hierbei quadratische Probleme dar, welche im Allgemeinen aber schwer zu lösen sind. Ein Ansatz, der sich in den letzten Jahren entwickelt und verbreitet hat, besteht in der Umformulierung quadratischer Probleme in sogenannte kopositive Programme. Kopositive Programme sind lineare Optimierungsprobleme über dem Kegel der kopositiven Matrizen

$$\mathcal{C}_n = \{A \in \mathbb{R}^{n\times n} : A = A^T,\ x^T A x \geq 0 \text{ für alle } x \in \mathbb{R}^n,\ x \geq 0\},$$

oder dem Dualkegel, dem Kegel der vollständig positiven Matrizen

$$\mathcal{C}_n^* = \Big\{ \sum_{i=1}^{m} x_i x_i^T : x_i \in \mathbb{R}^n,\ x_i \geq 0 \text{ für alle } i = 1, \ldots, m \Big\}.$$

Die Schwierigkeit dieser Probleme liegt in der Kegelbedingung. Aber nicht nur das Optimieren über diesen Kegeln ist schwierig. Wie von Murty und Kabadi (1987) und Dickinson und Gijben (2013) gezeigt ist es NP-schwer zu testen, ob eine gegebene Matrix kopositiv oder vollständig positiv ist. Ein besseres Verständnis dieser Kegel trägt daher zum besseren Verständnis und zum Finden neuer Lösungsmethoden für quadratische Probleme bei.

Eine verbreitete Vorgehensweise bei der Betrachtung kopositiver Programme besteht darin, den kopositiven beziehungsweise den vollständig positiven Kegel durch Approximationskegel zu ersetzen. Wenn die daraus resultierenden Probleme numerisch gelöst werden können, erlaubt dies die Berechnung von Schranken für den gesuchten Optimalwert. In den letzten Jahren wurden verschiedene Approximationen vorgestellt (Parrilo, 2000; Bomze and de Klerk, 2002; de Klerk and Pasechnik, 2002; Peña et al., 2007; Bundfuss and Dür,

2009). Bei allen Ansätzen führt das Optimieren über den Approximationskegeln zu linearen oder semidefiniten Programmen.

Die zweite grundsätzliche Vorgehensweise besteht in der Verwendung von Schnittebenen. Ersetzt man den vollständig positiven Kegel in der Kegelbedingung beispielsweise durch den positiv semidefiniten Kegel, führt dies zu einer Relaxierung des Problems, die eine Schranke für den gesuchten Optimalwert liefert. Im Allgemeinen ist eine Optimallösung dieser Relaxierung jedoch nicht vollständig positiv und das Hinzufügen einer Schnittebene, die diese Optimallösung vom vollständig positiven Kegel separiert, führt zu einer schärferen Relaxierung und einer besseren Schranke.

In der vorliegenden Dissertation beschäftigen wir uns mit verschiedenen Aspekten der kopositiven Optimierung. Wir führen zunächst die relevanten Begriffe und Ergebnisse zum kopositiven und vollständig positiven Kegel sowie der kopositiven Optimierung ein. Dann zeigen wir, wie die Projektion einer Matrix auf diese Kegel berechnet werden kann. Diese Projektionen werden im Anschluss verwendet, um Faktorisierungen vollständig positiver Matrizen zu berechnen. Eine zweite Anwendung besteht in der Berechnung von Schnittebenen für Optimierungsprobleme über dem vollständig positiven Kegel. Der vorgestellte Ansatz ist der erste, mit dem eine beliebige nicht vollständig positive Matrix vom vollständig positiven Kegel separiert werden kann. Für Matrizen, deren Graph dreiecksfrei ist, beschreiben wir eine alternative Methode zur Berechnung von Schnittebenen, die diese besondere Struktur ausnutzt. Schließlich betrachten wir kopositive und vollständig positive Programme, die sich als Umformulierungen quadratischer Optimierungsprobleme ergeben. Dabei beschäftigen wir uns zunächst mit dem Standard-quadratischen Optimierungsproblem. Wir untersuchen verschiedene Klassen von Zielfunktionen, für die der Optimalwert des Problems durch das Lösen eines linearen oder semidefiniten Programms bestimmt werden kann. Dies führt zu zwei Algorithmen zum Lösen Standard-quadratischer Optimierungsprobleme. Die Algorithmen werden anhand numerischer Beispiele illustriert und diskutiert. Die vorgestellten Methoden lassen sich nicht ohne Weiteres auf kopositive Formulierungen von allgemeineren quadratischen Optimierungsproblemen übertragen. Dies verdeutlichen wir anhand von Beispielen.

Contents

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Introduction

Copositive programming is concerned with the problem of optimizing a linear function over the copositive cone

$$\mathcal{C}_n = \{A \in \mathbb{R}^{n\times n} : A = A^T,\ x^T Ax \geq 0 \text{ for all } x \in \mathbb{R}^n,\ x \geq 0\},$$

or its dual, the completely positive cone

$$\mathcal{C}_n^* = \Big\{ \sum_{i=1}^{m} x_i x_i^T : x_i \in \mathbb{R}^n,\ x_i \geq 0 \text{ for all } i = 1, \dots, m \Big\}.$$

It is an active field of research and has received a growing amount of attention in recent years. This is because many combinatorial as well as quadratic problems can be formulated as copositive optimization problems.

The concept of copositivity seems to go back to Motzkin (1952) who gave a criterion for a quadratic form to be nonnegative over the nonnegative orthant. Since then, many copositivity criteria have been developed. However, copositive programming is a relatively young field in mathematical optimization. Quist et al. (1998) were the first to formulate optimization problems over the copositive and completely positive cones in order to strengthen the positive semidefinite relaxation of quadratic programs. The first exact completely positive representation of a quadratic program is due to Bomze et al. (2000) who considered the standard quadratic optimization problem. Their result has been generalized by Burer (2009) who showed that every nonconvex quadratic optimization problem with continuous and binary variables can be written as a linear problem over the completely positive cone. This includes many NP-hard combinatorial problems such as the maximum clique problem, the quadratic assignment problem and graph partitioning. The complexity of these problems is then moved entirely to the cone constraint, showing that general copositive programs are hard to solve. In fact, even checking whether a given matrix is copositive or completely positive is an NP-hard problem (Murty and Kabadi, 1987; Dickinson and Gijben, 2013). A better understanding of the copositive and the completely positive cone can therefore help in solving (certain classes of) quadratic problems.

There are basically two approaches for solving copositive and completely positive optimization problems. The first one uses (inner or outer) approximating cones. Replacing the copositive or the completely positive cone by a tractable cone allows to compute a bound on the optimal value. An obvious choice is to replace the copositive by the positive semidefinite cone. Better bounds can be obtained by using a converging approximation hierarchy. The first inner approximation hierarchy of the copositive cone has been introduced by Parrilo (2000) and is based on sum-of-squares decompositions of polynomials. Based on Parrilo's results, Bomze and de Klerk (2002), de Klerk and Pasechnik (2002) and Peña, Vera and Zuluaga (2007) developed similar hierarchies. All have in common that optimizing over the approximating cones amounts to solving linear or semidefinite programs. Bundfuss and Dür (2009) introduced copositivity criteria which are based on simplicial partitions of the standard simplex leading to an inner and outer approximation hierarchy of the copositive as well as of the completely positive cone. As all cones in this hierarchy are polyhedral, this leads to linear optimization problems.

The second approach is to use cutting planes in order to improve relaxations of completely positive optimization problems. Replacing the completely positive cone by a tractable cone as the positive semidefinite cone leads to a relaxation of the problem providing a bound on the optimal value. In general, an optimal solution of this relaxation is not completely positive and adding a cut, i.e., a linear constraint that separates the obtained solution from the completely positive cone, results in a tighter relaxation yielding a better bound. Since Bomze, Locatelli and Tardella (2008) introduced the idea of using copositive cuts, several methods to compute such cutting planes have been developed.

We will consider several aspects of copositive programming. We start by studying the problem of computing the projection of a given matrix onto the copositive and the completely positive cone. We will see how these projections can be used to compute factorizations of completely positive matrices. As a second application, we use them to construct cutting planes to separate a matrix from the completely positive cone. Besides the cuts based on copositive projections, we will study another approach to separate a triangle-free doubly nonnegative matrix from the completely positive cone. A special focus is on copositive and completely positive programs that arise as reformulations of quadratic optimization problems. Among those we start by studying the standard quadratic optimization problem. We will show that for several classes of objective functions, the relaxation resulting from replacing the copositive or the completely positive cone in the conic reformulation by a tractable cone is exact. Based on these results, we develop two algorithms for solving standard quadratic optimization problems. The methods presented cannot immediately be adapted to general quadratic optimization problems. This is illustrated with examples.

The thesis is organized as follows. We start in Chapter 1 by introducing basic terminology from linear algebra and graph theory. In Chapter 2, the copositive and the completely positive cone are defined, and criteria for copositivity and complete positivity, and approximations of both cones are presented. Basic terminology and results from conic optimization are introduced in Chapter 3. After that, we concentrate on the special case of completely positive programs and explain the relation of copositive and quadratic programming. Chapter 4 deals with the problem of projecting a matrix onto the copositive respectively completely positive cone. Moreover, we show how these projections can be used to compute factorizations of completely positive matrices. In Chapter 5, we study the conic reformulation of the standard quadratic optimization problem in more detail. We show that for special classes of objective functions, the optimal value can be obtained by solving a linear or semidefinite program. Based on these results, we present two algorithms to solve standard quadratic optimization problems and discuss numerical results. A focus is on the 5-dimensional standard quadratic optimization problem. The chapter concludes with a discussion of more general quadratic programs, in particular, of sufficient conditions for relaxations of these to be exact. Chapter 6 deals with the computation of copositive cuts. We first survey the literature about cutting planes. Then we present two new approaches. The first one is based on the copositive projections introduced in Chapter 4. The second one applies to matrices that have a triangle-free graph. For both approaches numerical results are discussed. We conclude with a short summary and state some open questions arising from the results presented in the thesis.

Contributions

In the following, we state the main contributions of the thesis.

- Based on the inner and outer approximations of the copositive cone introduced by Bundfuss and Dür (2009), we show how the projection of a matrix onto the copositive cone can be computed. Using a decomposition theorem of Moreau, we also show how to project a matrix onto the completely positive cone. These projections can be used to compute factorizations of completely positive matrices. The presented method is the first to compute factorizations of arbitrary matrices lying in the interior of the completely positive cone. The results are presented in Chapter 4 and were published in Sponsel and Dür (2012).

- Using the copositive projections from Chapter 4, we develop a method to compute cutting planes to cut off an arbitrary matrix $A \notin \mathcal{C}_n^*$ from the completely positive cone. This method is explained in Section 6.3. Moreover, we illustrate the approach by computing cutting planes for the semidefinite relaxation of some stable set problems. These results were also published in Sponsel and Dür (2012).

- In Section 6.4, we present an approach to separate triangle-free doubly nonnegative matrices from the completely positive cone. We compare the resulting cuts to the ones introduced in Bomze et al. (2010a) since the basic structure is quite similar. Moreover, we discuss numerical results for some stable set problems. The results presented in this section are prepared for publication in Berman et al. (2013).

- Extending the result of Anstreicher and Burer (2005) that every standard quadratic optimization problem with a positive semidefinite matrix in the objective function can be stated as a semidefinite program, we study more classes for which the problem has an exact linear or positive semidefinite representation. This leads to two algorithms to solve standard quadratic optimization problems. We also study more general quadratic problems. The results are presented in Chapter 5.

1. Notation and preliminaries

In this chapter, we introduce some basic terminology from linear algebra and graph theory that we will need later on.

1.1. Vectors and matrices

We denote scalars and vectors by lowercase letters and matrices by uppercase letters. For $x \in \mathbb{R}^n$, the relation $x \geq 0$ is understood entrywise and we denote the set of all nonnegative n-vectors by $\mathbb{R}^n_+$. The set of all n-vectors having only positive entries is denoted $\mathbb{R}^n_{++}$. The i-th entry of a vector $x \in \mathbb{R}^n$ is referred to as x_i, and similarly, the entries of a matrix $A \in \mathbb{R}^{m \times n}$ are referred to as A_{ij}. For $D \in \mathbb{R}^{n \times n}$ and $d \in \mathbb{R}^n$, let $\operatorname{diag}(D)$ denote the diagonal of D and denote by $\operatorname{Diag}(d)$ the square diagonal matrix whose diagonal is d. Throughout the thesis, let I denote the identity matrix, e the all-ones vector and $E = ee^T$ the all-ones matrix. Furthermore, we denote by e_i the i-th unit vector, i.e., e_i is the vector whose i-th entry is one and all other entries are zero. For $A \in \mathbb{R}^{n \times n}$, let $\operatorname{rank}(A)$ be the rank of the matrix A and $\operatorname{trace}(A)$ its trace.

The *inner product* of two matrices $A, B \in \mathbb{R}^{m \times n}$ is defined as

$$\langle A, B \rangle = \operatorname{trace}(B^T A) = \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} B_{ij}.$$

Note that for $A \in \mathbb{R}^{n \times n}$ and $x \in \mathbb{R}^n$, we have

$$x^T A x = \langle A, xx^T \rangle. \tag{1.1}$$

The *Hadamard product* of two matrices $A, B \in \mathbb{R}^{m \times n}$ is the matrix $A \circ B$ with entries $(A \circ B)_{ij} = A_{ij} B_{ij}$. Observe that for symmetric matrices $A, B, C \in \mathbb{R}^{n \times n}$, we have

$$\langle A \circ B, C \rangle = \langle A, B \circ C \rangle = \langle A \circ C, B \rangle. \tag{1.2}$$

Let $\mathcal{S}_n$ denote the set of all symmetric $n \times n$ matrices, i.e.,

$$\mathcal{S}_n = \left\{ A \in \mathbb{R}^{n \times n} : A = A^T \right\}.$$

We define the set of (entrywise) nonnegative matrices as

$$\mathcal{N}_n = \{A \in \mathcal{S}_n : A_{ij} \geq 0 \text{ for all } i, j = 1, \ldots, n\}$$

and write $A \geq 0$ if A is nonnegative.

The set of positive semidefinite matrices is defined as

$$\begin{aligned}\mathcal{S}_n^+ &= \left\{A \in \mathcal{S}_n : x^T A x \geq 0 \text{ for all } x \in \mathbb{R}^n\right\} \\ &= \left\{\sum_{i=1}^k a_i a_i^T : a_i \in \mathbb{R}^n,\ i = 1, \ldots, k\right\},\end{aligned}$$

and the set of positive definite matrices is

$$\mathcal{S}_n^{++} = \left\{A \in \mathcal{S}_n : x^T A x > 0 \text{ for all } x \neq 0\right\}.$$

We write $A \succ 0$ ($A \succeq 0$) if A is positive (semi-)definite.

A matrix $A \in \mathcal{S}_n$ is *reducible* if there is a permutation matrix P such that

$$PAP^T = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$$

with symmetric matrices A_1, A_2. A matrix that is not reducible is said to be *irreducible*. The *spectral radius* of a matrix $A \in \mathbb{R}^{n\times n}$ is defined as

$$\rho(A) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } A\}.$$

We will need the following result on the spectral radius of nonnegative (irreducible) matrices, see Horn and Johnson (1985, Theorems 8.3.1 and 8.4.4).

Theorem 1.1.1 (Perron–Frobenius Theorem) *If $A \in \mathcal{N}_n$, then the spectral radius $\rho(A)$ is an eigenvalue of A, and A has a nonnegative eigenvector u corresponding to $\rho(A)$. If, in addition, A is irreducible, then there is a positive vector u such that $Au = \rho(A)u$.*

The eigenvalue $\rho(A)$ of an irreducible nonnegative matrix A is called the *Perron root* of A, and a positive eigenvector corresponding to the eigenvalue $\rho(A)$ is called a *Perron vector* of A.

Finally, we introduce some notation related to subsets of $\mathbb{R}^n$. Let $M \subseteq \mathbb{R}^n$. We denote by

$$\operatorname{span}(M) = \left\{\sum_{i=1}^k \lambda_i x_i : x_i \in M,\ \lambda_i \in \mathbb{R},\ i = 1, \ldots, k\right\}$$

the linear hull of M, by

$$\operatorname{aff}(M) = \left\{ \sum_{i=1}^{k} \lambda_i x_i : x_i \in M,\ \lambda_i \in \mathbb{R},\ i = 1, \dots, k,\ \sum_{i=1}^{k} \lambda_i = 1 \right\}$$

the affine hull of M, and by

$$\operatorname{conv}(M) = \left\{ \sum_{i=1}^{k} \lambda_i x_i : x_i \in M,\ \lambda_i \geq 0,\ i = 1, \dots, k,\ \sum_{i=1}^{k} \lambda_i = 1 \right\}$$

the convex hull of M. Let $\operatorname{int}(M)$ denote the interior of M, $\operatorname{relint}(M)$ its relative interior and $\operatorname{cl}(M)$ its closure. If M is convex, then $x \in M$ is an *extreme point* of M if

$$x = \lambda y + (1 - \lambda) z,\ y, z \in M,\ 0 < \lambda < 1 \quad \Rightarrow \quad y = x = z.$$

A *face* of a closed convex set M is a subset $F \subseteq M$ such that every closed line segment $\operatorname{conv}(\{x, y\})$ in M with a relative interior point in F has both endpoints u, v in F. Consequently, $x \in M$ is an extreme point of M if it is a zero-dimensional face of M.

1.2. Graphs

Let $\binom{V}{2}$ denote the set of all 2-element subsets of a set V. In this thesis, we only consider simple graphs G, i.e., $G = (V, E)$ where $V \neq \emptyset$ is a finite set and $E \subseteq \binom{V}{2}$. The elements of V are called *vertices* and the elements of E are called *edges* of the graph. We write $V(G)$ to denote the vertex set of G and $E(G)$ to denote its edge set. Two vertices $i, j \in V$ are called *adjacent* if there is an edge $\{i, j\} \in E$. A graph G can be represented by its *adjacency matrix* A_G which is defined as

$$(A_G)_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in E(G) \\ 0, & \text{else} \end{cases}.$$

Clearly, the adjacency matrix is symmetric and its diagonal is zero. Conversely, given a matrix $X \in \mathcal{S}_n$, we define the graph $G(X)$ of X as the graph on the vertices $1, \dots, n$ with i, j being adjacent if and only if $i \neq j$ and $X_{ij} \neq 0$.

Two graphs $G = (V, E)$ and $G' = (V', E')$ are *isomorphic* if there is a bijection $\varphi : V \to V'$ such that i and j are adjacent in G if and only if $\varphi(i)$ and $\varphi(j)$ are adjacent in G'.

The *complementary graph* of $G = (V, E)$, denoted $\bar{G}$, is the graph $(V, \bar{E})$ with $\bar{E} = \binom{V}{2} \setminus E$.

A *subgraph* of $G = (V, E)$ is a graph $H = (V', E')$ with $V' \subseteq V$ and $E' \subseteq \binom{V'}{2} \cap E$. If $E' = \binom{V'}{2} \cap E$, we say that H is an *induced subgraph* of G or that H is the subgraph of G induced by V'.

A graph is *bipartite* if there is a partition of the vertex set $V = V_1 \cup V_2$ with $V_1 \cap V_2 = \emptyset$ such that no two vertices in V_1 and no two vertices in V_2 are adjacent.

A graph is said to be *complete* if all of its vertices are pairwise adjacent. The complete graph on n vertices is denoted by K_n. K_3 is a *triangle*. A graph that has no subgraph isomorphic to K_3 is called *triangle-free*.

A *cycle* (of length n) or *n-cycle*, denoted C_n, is a graph (V, E) of the form

$$V = \{1, 2, \ldots, n\} \quad \text{and} \quad E = \{\{1, 2\}, \{2, 3\}, \ldots, \{n-1, n\}, \{n, 1\}\}.$$

We also write $C_n = (1, 2, \ldots, n, 1)$. A cycle of odd (even) length is called *odd (even) cycle*. If a graph G has an induced subgraph which is isomorphic to C_k for some $k \geq 4$, then we refer to this subgraph as *hole* of G. Similarly, an *antihole* is an induced subgraph isomorphic to $\bar{C}_k$ for some $k \geq 4$.

A *path* (of length n) is a graph (V, E) whose vertices can be ordered such that

$$V = \{1, \ldots, n\} \quad \text{and} \quad E = \{\{1, 2\}, \{2, 3\}, \ldots, \{n-1, n\}\}.$$

We also write $P = (1, 2, \ldots, n)$ to denote a path from 1 to n. We define the *distance* $d_G(i, j)$ of two vertices i, j in G as the length of a shortest path from i to j. If no such path exists, we set $d_G(i, j) = \infty$. The *diameter* of G is defined as the greatest distance between any two vertices in G.

A graph $G = (V, E)$ is said to be *connected* if for any two vertices $i, j \in V$ there is a path from i to j. A maximal connected subgraph of G is called *component* of G. A graph that is not connected has thus more than one component. If a component consists of only one vertex, then this vertex is an *isolated vertex*.

A *clique* in G is a subset $V' \subseteq V$ such that the subgraph induced by V' is complete. The maximum size of a clique in G is called the *clique number* of G and denoted by $\omega(G)$. The problem to compute the clique number of a graph is called the *maximum clique problem*. Karp (1972) has shown that this problem is NP-complete, so, unless $P = NP$, there is no algorithm that returns a solution in a time that is polynomially bounded by the number of vertices.

A *stable set* in G is a subset $V' \subseteq V$ such that the vertices in V' are pairwise nonadjacent. The size of a maximum stable set in G is called *stability number* of G and denoted by $\alpha(G)$. The problem of determining the stability number of a graph is referred to as the stable set problem. Obviously, we have $\omega(G) = \alpha(\bar{G})$. The maximum clique problem is thus equivalent to computing the stability number of the complementary graph.

A *vertex coloring* is a map $c : V \to C$ such that for any two adjacent vertices $i, j \in V$ we have $c(i) \neq c(j)$. The smallest number $k \in \mathbb{N}$ such that there is a vertex coloring $c : V \to C$ with $|C| = k$, where $|C|$ denotes the number of elements in C, is called *chromatic number*. We denote the chromatic number of a graph G by $\chi(G)$. As for the maximum clique problem, computing the chromatic number of a graph is NP-complete (Karp, 1972).

Since in a coloring all vertices in a clique have to be colored differently, the chromatic number of a graph is bounded by its clique number, i.e., we have $\omega(G) \leq \chi(G)$. A graph G is *perfect* if $\omega(H) = \chi(H)$ for any induced subgraph H of G. Chudnovsky, Robertson, Seymour and Thomas (2006) have shown that a graph is perfect if and only if it does neither have an odd hole nor an odd antihole. This characterization of perfect graphs is known as the strong perfect graph theorem.

For more details and a thorough introduction to graph theory, we refer to Diestel (2005). More information on the maximum clique problem and perfect graphs can be found in Schrijver (2003).

2. The copositive and the completely positive cone

In this chapter, we introduce the copositive cone and its dual, the completely positive cone. We start by giving some basic definitions and results on cones in Section 2.1, before we consider the copositive cone in Section 2.2 and the completely positive cone in Section 2.3. Finally, in Section 2.4, we introduce approximations of these cones. More information on both cones can be found in the survey papers (Ikramov and Savel'eva, 2000; Dür, 2010; Bomze, 2012; Bomze et al., 2012) and references therein.

2.1. Cones

We will introduce some basic definitions and properties related to cones.

Definition 2.1.1 A set $\mathcal{K} \subseteq \mathbb{R}^n$ is a *cone* if for every $x \in \mathcal{K}$ and $\alpha \geq 0$ we have $\alpha x \in \mathcal{K}$.

The following result follows immediately from the definition.

Lemma 2.1.2 *$\mathcal{K}$ is a convex cone if and only if for every $x, y \in \mathcal{K}$ and $\alpha, \beta \geq 0$, $\alpha x + \beta y \in \mathcal{K}$.*

Obviously, the closure of a convex cone is also a convex cone. Moreover, the intersection as well as the sum of two convex cones are again convex cones.

Definition 2.1.3 A convex cone $\mathcal{K}$ is *pointed* if $\mathcal{K} \cap (-\mathcal{K}) = \{0\}$, and *solid* if it has a nonempty interior. A closed convex cone that is pointed and solid is called a *proper cone*.

For $M \subseteq \mathbb{R}^n$, we denote by

$$\text{cone}(M) = \left\{ \sum_{i=1}^{k} \lambda_i x_i : x_i \in M,\ \lambda_i \geq 0,\ i = 1, \ldots, k \right\}$$

the conic hull of M. It is the intersection of all convex cones containing M.

Definition 2.1.4 A convex cone $\mathcal{K}$ is a *polyhedral cone* if it is finitely generated, i.e., $\mathcal{K} = \text{cone}(M)$ for some finite set M.

Definition 2.1.5 Let $x \in \mathbb{R}^n$. The *ray generated by* x is the set $\{\alpha x : \alpha \geq 0\}$. If $\mathcal{K} \subseteq \mathbb{R}^n$ is a convex cone and $x \in \mathcal{K}$, then the ray generated by x is contained in $\mathcal{K}$.

Definition 2.1.6 Let $\mathcal{K}$ be a closed convex cone and $x \in \mathcal{K}$. The ray generated by x is an *extreme ray* of $\mathcal{K}$ if

$$x = y + z,\ y, z \in \mathcal{K} \quad \Rightarrow \quad y, z \in \{\alpha x : \alpha \geq 0\}.$$

We denote the set of vectors generating extreme rays of $\mathcal{K}$ by $\text{Ext}(\mathcal{K})$.

The following theorem is a version of Carathéodory's theorem for convex cones.

Theorem 2.1.7 *Let $\mathcal{K} = \text{cone}(M)$ be a convex cone in $\mathbb{R}^n$. Then every $x \in \mathcal{K}$ can be represented as a nonnegative combination of at most n elements of M.*

This is a well-known result. See for example Berman and Shaked-Monderer (2003, Theorem 1.34). For the sake of completeness, we state the proof here.

Proof Let $x \in \mathcal{K}$. Then $x = \sum_{i=1}^m \lambda_i x_i$ for some $x_1, \ldots, x_m \in M$ and $\lambda_1, \ldots, \lambda_m > 0$. If $m > n$, then $x_1, \ldots, x_m$ are linearly dependent. Hence there exist coefficients $\mu_1, \ldots, \mu_m \in \mathbb{R}$, not all zero, such that $\sum_{i=1}^m \mu_i x_i = 0$. We may assume that at least one μ_i is positive. Define $a = \min\{\frac{\lambda_i}{\mu_i} : \mu_i > 0\}$ and $\alpha_i = \lambda_i - a\mu_i$, $i = 1, \ldots, m$. Note that by definition all coefficients α_i are nonnegative. Then

$$x = \sum_{i=1}^m \lambda_i x_i - 0 = \sum_{i=1}^m \lambda_i x_i - a \sum_{i=1}^m \mu_i x_i = \sum_{i=1}^m (\lambda_i - a\mu_i) x_i = \sum_{i=1}^m \alpha_i x_i.$$

Since at least one coefficient α_i is zero, this shows that x can be represented as a nonnegative combination of less than m elements of M. □

We now define the dual of a set.

Definition 2.1.8 Let $\mathcal{K} \subseteq \mathbb{R}^n$. The set

$$\mathcal{K}^* = \{y \in \mathbb{R}^n : \langle x, y \rangle \geq 0 \text{ for all } x \in \mathcal{K}\}$$

is called the *dual* of $\mathcal{K}$. If $\mathcal{K}$ is a cone with $\mathcal{K}^* = \mathcal{K}$, then $\mathcal{K}$ is said to be *self-dual*.

The following theorem states some basic duality properties. For a proof see (Ben-Israel, 1969, Theorem 1.3, Theorem 1.5 and Corollary 1.7).

Theorem 2.1.9 *Let $\mathcal{K}$, $\mathcal{K}_1$ and $\mathcal{K}_2$ be nonempty subsets of $\mathbb{R}^n$. Then*

(i) *$\mathcal{K}^*$ is a closed convex cone.*

(ii) *If $\mathcal{K}_1 \subseteq \mathcal{K}_2$, then $\mathcal{K}_2^* \subseteq \mathcal{K}_1^*$.*

(iii) *$\mathcal{K} \subseteq \mathcal{K}^{**}$, and if $\mathcal{K}$ is a convex cone, then $\operatorname{cl}\mathcal{K} = \mathcal{K}^{**}$.*

(iv) *$\mathcal{K}_1^* \cap \mathcal{K}_2^* \subseteq (\mathcal{K}_1 + \mathcal{K}_2)^*$, and if $0 \in \mathcal{K}_1 + \mathcal{K}_2$, then $(\mathcal{K}_1 + \mathcal{K}_2)^* \subseteq \mathcal{K}_1^* \cap \mathcal{K}_2^*$.*

(v) *If $\mathcal{K}_1$ and $\mathcal{K}_2$ are closed convex cones, then $\operatorname{cl}(\mathcal{K}_1^* + \mathcal{K}_2^*) = (\mathcal{K}_1 \cap \mathcal{K}_2)^*$.*

The interior of $\mathcal{K}^*$ can be characterized as follows (cf. Berman (1973)).

Lemma 2.1.10 *If $\mathcal{K} \subseteq \mathbb{R}^n$ is a closed convex pointed cone, then*

$$\operatorname{int}(\mathcal{K}^*) = \{y \in \mathcal{K}^* : \langle x, y\rangle > 0 \textit{ for all } x \in \mathcal{K} \setminus \{0\}\}.$$

Closely related to the dual is the concept of the polar cone.

Definition 2.1.11 The *polar cone* of a set $\mathcal{K} \subseteq \mathbb{R}^n$ is the closed convex cone

$$\mathcal{K}^\circ = \{y \in \mathbb{R}^n : \langle y, x\rangle \leq 0 \text{ for all } x \in \mathcal{K}\}.$$

From the definition, it is immediately clear that $\mathcal{K}^\circ = -\mathcal{K}^*$.

2.2. The copositive cone

In this section, we consider the copositive cone. We start by defining $\mathcal{K}$-semidefiniteness which is a generalization of positive semidefiniteness and copositivity.

Definition 2.2.1 Let $\mathcal{K} \subseteq \mathbb{R}^n$ be a nonempty set. A matrix $A \in \mathcal{S}_n$ is called *$\mathcal{K}$-semidefinite* if

$$x^T A x \geq 0 \quad \text{for all } x \in \mathcal{K}.$$

If

$$x^T A x > 0 \quad \text{for all } x \in \mathcal{K},\ x \neq 0,$$

then A is called *$\mathcal{K}$-definite*.

The set of all $\mathcal{K}$-semidefinite matrices forms a cone that we denote by $\mathcal{C}_{\mathcal{K}}$. The dual of $\mathcal{C}_{\mathcal{K}}$ is given in the following lemma (cf. Eichfelder and Povh (2013, Lemma 2 and Lemma 4)).

Lemma 2.2.2 *Let $\mathcal{K} \subseteq \mathbb{R}^n$ be nonempty. Then*

$$\mathcal{C}_{\mathcal{K}}^* = \operatorname{cl}\operatorname{cone}\{xx^T : x \in \mathcal{K}\} = \operatorname{conv}\{xx^T : x \in \operatorname{cl}\operatorname{cone}\mathcal{K}\}.$$

For $\mathcal{K} = \mathbb{R}^n$, the cone $\mathcal{C}_{\mathcal{K}}$ is simply the cone of all positive semidefinite matrices or the positive semidefinite cone, for short. We will be interested in the case $\mathcal{K} = \mathbb{R}^n_+$.

Definition 2.2.3 A matrix $A \in \mathcal{S}_n$ is *copositive* if

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

and *strictly copositive* if

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

The *copositive cone*, denoted $\mathcal{C}_n$, is the set of all copositive $n \times n$ matrices, i.e.,

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

By Lemma 2.2.2, the dual of $\mathcal{C}_n$ is given by

$$\mathcal{C}_n^* = \operatorname{conv}\{xx^T : x \in \mathbb{R}^n_+\}$$

which is called the *completely positive cone*. In Section 2.3, we will study this cone in more detail.

The following theorem states some basic properties of the copositive cone.

Theorem 2.2.4 (i) *$\mathcal{C}_n$ is a proper cone.*

(ii) *$\mathcal{C}_n$ is nonpolyhedral (unless $n = 1$).*

(iii) $\operatorname{int}(\mathcal{C}_n) = \left\{A \in \mathcal{S}_n : x^T Ax > 0 \textit{ for all } x \in \mathbb{R}^n_+ \setminus \{0\}\right\}$.

For a proof of (i) see for example Berman and Shaked-Monderer (2003, Proposition 1.24). A proof of (ii) and (iii) can be found in Bundfuss (2009, Lemma 2.3). However, for a better understanding of the copositive cone, we give proofs of the three properties.

Proof (i): Let $(A_i)_{i\in\mathbb{N}}$ be a sequence of copositive matrices with $\lim_{i\to\infty} A_i = A$. For any $x \in \mathbb{R}^n_+$, we have

$$x^T A x = x^T \lim_{i\to\infty} A_i x = \lim_{i\to\infty} x^T A_i x \geq 0$$

by continuity of the quadratic form, hence $A \in \mathcal{C}_n$ showing that the copositive cone is closed.

To show convexity, let $A_1, A_2 \in \mathcal{C}_n$ and $0 \leq \lambda \leq 1$. For $x \in \mathbb{R}^n_+$, we have

$$x^T(\lambda A_1 + (1-\lambda)A_2)x = \lambda x^T A_1 x + (1-\lambda)x^T A_2 x \geq 0.$$

Next, assume $A \in \mathcal{C}_n \cap (-\mathcal{C}_n)$. Then for all $x \in \mathbb{R}^n_+$, we have $x^T A x \geq 0$ and $-x^T A x \geq 0$ implying $x^T A x = 0$. Taking $x = e_i$ shows that $A_{ii} = 0$ for all $i = 1, \ldots, n$. Furthermore, for $x = e_i + e_j$, $i \neq j$, we get $(e_i + e_j)^T A (e_i + e_j) = A_{ii} + A_{ij} + A_{ji} + A_{jj} = 2A_{ij} = 0$ and thus $A_{ij} = 0$.

Finally, to show that $\mathcal{C}_n$ has a nonempty interior, let $B \in \mathcal{C}_n^* \setminus \{0\}$. Then $B \geq 0$ and $B \neq 0$. We thus have $\langle E, B\rangle = \sum_{i,j=1}^n B_{ij} > 0$. By Lemma 2.1.10, $E \in \operatorname{int}(\mathcal{C}_n^{**})$, and by Theorem 2.1.9 (iii), $\mathcal{C}_n^{**} = \mathcal{C}_n$ showing that the copositive matrix E lies in the interior of $\mathcal{C}_n$.

(ii): We first show that $\mathcal{C}_2 = \mathcal{S}_2^+ \cup \mathcal{N}_2$. Obviously, we have $\mathcal{S}_2^+ \cup \mathcal{N}_2 \subseteq \mathcal{C}_2$. To show the other inclusion, let $A \in \mathcal{C}_2$. If $A \notin \mathcal{N}_2$, then $A_{12} = A_{21} < 0$ and

$$x^T A x = A_{11}x_1^2 + A_{22}x_2^2 + 2A_{12}x_1x_2 \geq A_{11}x_1^2 + A_{22}x_2^2 + 2A_{12}|x_1||x_2| \geq 0$$

for all $x \in \mathbb{R}^2$ by copositivity of A. Thus, A is positive semidefinite.

As $\mathcal{S}_2^+ \cup \mathcal{N}_2$ is nonpolyhedral, which can be seen by illustrating this cone (cf. Bundfuss (2009, Figure 2.1)), we have that $\mathcal{C}_2$ is nonpolyhedral. Now assume that $\mathcal{C}_n$ is polyhedral for some n. Then

$$\mathcal{C}_n \cap \{A \in \mathcal{S}_n : A_{ij} = 0 \text{ for all } 2 < i, j \leq n\}$$

is polyhedral as well. But since this intersection is the cone $\mathcal{C}_2$ embedded in a higher-dimensional space, it is nonpolyhedral contradicting the assumption that $\mathcal{C}_n$ is polyhedral.

(iii): Let $A \in \operatorname{int}(\mathcal{C}_n)$. For $x \in \mathbb{R}^n_+$, $x \neq 0$, we have $xx^T \in \mathcal{C}_n^* \setminus \{0\}$. By Lemma 2.1.10, we have $x^T A x = \langle A, xx^T\rangle > 0$, showing that A is strictly copositive.

Now let A be strictly copositive, and $B \in \mathcal{C}_n^* \setminus \{0\}$. Then B can be written as $B = \sum_{i=1}^m b_i b_i^T$ with $b_i \in \mathbb{R}_+^n \setminus \{0\}$. We thus have

$$\langle A, B \rangle = \left\langle A, \sum_{i=1}^m b_i b_i^T \right\rangle = \sum_{i=1}^m \langle A, b_i b_i^T \rangle = \sum_{i=1}^m b_i^T A b_i > 0,$$

and by Lemma 2.1.10, $A \in \operatorname{int}(\mathcal{C}_n)$. □

Furthermore, the copositive cone is invariant under permutation and scaling with positive diagonal matrices.

Lemma 2.2.5 (i) *Let P be a permutation matrix. Then $A \in \mathcal{S}_n$ is (strictly) copositive if and only if PAP^T is (strictly) copositive.*

(ii) *Let $D = \operatorname{Diag}(d)$ with $d \in \mathbb{R}_{++}^n$. Then $A \in \mathcal{S}_n$ is (strictly) copositive if and only if DAD is (strictly) copositive.*

Proof The statements follow immediately from the fact that $\mathbb{R}_+^n$ and $\mathbb{R}_{++}^n$ are invariant under permutation and scaling, and from the definition of copositivity. □

It is easy to see that every nonnegative matrix is copositive. The same holds for positive semidefinite matrices. We thus have

$$\mathcal{N}_n + \mathcal{S}_n^+ \subseteq \mathcal{C}_n.$$

As we have seen in the proof of Theorem 2.2.4 (ii), $\mathcal{C}_2 = \mathcal{N}_2 \cup \mathcal{S}_2^+$. For $n = 3, 4$, we have $\mathcal{C}_n = \mathcal{N}_n + \mathcal{S}_n^+$ (Diananda, 1962). For $n \geq 5$, however, there are copositive matrices that cannot be represented as the sum of a nonnegative and a positive semidefinite matrix. An example is the well known Horn matrix

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}. \tag{2.1}$$

The corresponding quadratic form can be written as

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

Let $x \in \mathbb{R}^5_+$. By the first expression $x^T H x \geq 0$ if $x_5 \geq x_4$, and the second expression shows that $x^T H x \geq 0$ if $x_4 \geq x_5$. Consequently, H is copositive. As shown for example in Hall Jr. and Newman (1963), the Horn matrix cannot be written as the sum of a nonnegative and a positive semidefinite matrix.

A matrix is said to be *extreme copositive* if it generates an extreme ray of the copositive cone. The set of extreme copositive matrices is invariant under permutation and scaling (see for example Dickinson (2013a, Theorem 8.20 iv)).

Theorem 2.2.6 *Let P be a permutation matrix and $D = \mathrm{Diag}(d)$ with $d \in \mathbb{R}^n_{++}$. Then $A \in \mathrm{Ext}(C_n)$ if and only if $PDADP^T \in \mathrm{Ext}(\mathcal{C}_n)$.*

For $n \leq 4$, the extreme rays of $\mathcal{C}_n$ are the extreme rays of $\mathcal{N}_n + \mathcal{S}_n^+$ which are characterized in the following theorem.

Theorem 2.2.7 (Hall Jr. and Newman (1963)) *The extreme rays of $\mathcal{C}_n$ which belong to $\mathcal{N}_n + \mathcal{S}_n^+$ are generated by $e_i e_j^T$, $i, j = 1, \ldots, n$, and by aa^T with $a \in \mathbb{R}^n$ having both positive and negative entries.*

For the characterization of the extreme rays of $\mathcal{C}_5$ we have to introduce the *Hildebrand matrices* (Hildebrand, 2012)

$$T(\varphi) = \begin{pmatrix} 1 & \sin\varphi_4 & -\cos(\varphi_4+\varphi_5) & -\cos(\varphi_2+\varphi_3) & \sin\varphi_3 \\ \sin\varphi_4 & 1 & \sin\varphi_5 & -\cos(\varphi_5+\varphi_1) & -\cos(\varphi_3+\varphi_4) \\ -\cos(\varphi_4+\varphi_5) & \sin\varphi_5 & 1 & \sin\varphi_1 & -\cos(\varphi_1+\varphi_2) \\ -\cos(\varphi_2+\varphi_3) & -\cos(\varphi_5+\varphi_1) & \sin\varphi_1 & 1 & \sin\varphi_2 \\ \sin\varphi_3 & -\cos(\varphi_3+\varphi_4) & -\cos(\varphi_1+\varphi_2) & \sin\varphi_2 & 1 \end{pmatrix}$$

with $\varphi_i > -\frac{\pi}{2}$, $i = 1, \ldots, 5$, and $\sum_{i=1}^5 \varphi_i < -\frac{3\pi}{2}$.

Theorem 2.2.8 (Hildebrand (2012, Theorem 3.1)) *The extreme rays of $\mathcal{C}_5$ that do not belong to $\mathcal{N}_5 + \mathcal{S}_5^+$ are generated by matrices of the form $PDHDP^T$, where H denotes the Horn matrix, P is a permutation matrix and $D = \mathrm{Diag}(d)$ with $d \in \mathbb{R}^5_{++}$, and by matrices of the form $PDT(\varphi)DP^T$, where $T(\varphi)$ is a Hildebrand matrix.*

For $n > 5$, the set of extreme rays $\mathrm{Ext}(\mathcal{C}_n)$ is not fully known. A characterization of the extreme rays whose entries are all 0, 1 or -1 and whose diagonal entries are all 1 has been given in Hoffman and Pereira (1973) (see also Theorem A.1). For an overview of results on extreme copositive matrices we refer to Dickinson (2013a, Theorem 8.20).

A matrix $A \in \mathcal{S}_n$ that is not copositive can be copositive of order k for some $k < n$, which is defined as follows.

Definition 2.2.9 A matrix A is called *copositive of order k*, if every principal submatrix of A of order k is copositive. A is called *copositive of exact order k* if it is copositive of order k but not of order $k+1$.

We will need the following result about matrices that are copositive of exact order $n-1$.

Theorem 2.2.10 (Väliaho (1986, Theorem 3.8)) *Let $A \in \mathcal{S}_n$. If A is copositive of exact order $n-1$, then $A^{-1} \leq 0$.*

2.2.1. Copositivity criteria

Although in some cases it is easy to see whether a matrix is copositive, for example if the matrix is nonnegative or positive semidefinite, in general testing copositivity is a co-NP-complete problem, i.e., the problem to test whether a given matrix is not copositive is NP-complete (Murty and Kabadi, 1987). However, there are many criteria for copositivity, but because testing copositivity is a hard problem, these can in general not be checked in polynomial time. We will now present some copositivity criteria that we will need in the following chapters.

Many criteria are based on principal submatrices. We start with the following result which follows immediately from the definition of copositivity.

Proposition 2.2.11 *Every principal submatrix of a (strictly) copositive matrix is (strictly) copositive. In particular, all diagonal entries of a (strictly) copositive matrix are nonnegative (positive).*

The next theorem gives a necessary and sufficient condition for copositivity in terms of the eigenvalues and eigenvectors of the principal submatrices.

Theorem 2.2.12 (Kaplan (2000, Theorem 2)) *Let $A \in \mathcal{S}_n$. Then A is copositive if and only if every principal submatrix of A has no positive eigenvector associated with a negative eigenvalue.*

We now consider a criterion which is similar to the Schur complement condition for positive (semi-)definiteness, see Li and Feng (1993, Theorem 2).

Theorem 2.2.13 *We consider the following partition of a matrix $A \in \mathcal{S}_n$*

$$A = \begin{pmatrix} a & b^T \\ b & C \end{pmatrix},$$

where $a \in \mathbb{R}, b \in \mathbb{R}^{n-1}, C \in \mathcal{S}_{n-1}$. The matrix A is copositive if and only if each of the following holds:

(i) *$a \geq 0$,*

(ii) *C is copositive,*

(iii) *Any $x \geq 0$ with $x \neq 0$ and $b^T x \leq 0$ satisfies*

$$x^T(aC - bb^T)x \geq 0.$$

For $b \leq 0$, the criterion can be reduced to the following.

Corollary 2.2.14 *Under the assumptions of Theorem 2.2.13, let $b \leq 0$. The matrix A is copositive if and only if $a \geq 0$ and $aC - bb^T$ is copositive.*

The statement follows directly from Theorem 2.2.13. A proof can also be found in Andersson et al. (1995, Theorem 2.1).

As stated in the following proposition, for matrices with a special structure, testing copositivity can be reduced to testing semidefiniteness (see for example Ikramov and Savel'eva (2000, Theorem 4.21)).

Proposition 2.2.15 *A matrix $A \in \mathcal{S}_n$ having only nonpositive off-diagonal entries is copositive if and only if it is positive semidefinite.*

Proof If $A \in \mathcal{S}_n$ is positive semidefinite, it clearly is copositive. To show the converse, assume that $A \in \mathcal{C}_n$ has only nonpositive off-diagonal entries, and let $x \in \mathbb{R}^n$. Then

$$x^T A x = \sum_{i=1}^n A_{ii} x_i^2 + \sum_{i \neq j} A_{ij} x_i x_j \geq \sum_{i=1}^n A_{ii} x_i^2 + \sum_{i \neq j} A_{ij} |x_i||x_j| \geq 0$$

by copositivity of A, showing that A is positive semidefinite. □

Finally, we present two results on copositivity regarding the Hadamard product with rank one matrices (cf. Berman et al. (2013)). For the proofs, the following notation will be useful. We denote by $x^{\dashv}$ the vector such that

$$(x^{\dashv})_i = \begin{cases} x_i^{-1} & \text{if } x_i \neq 0 \\ 0 & \text{if } x_i = 0, \end{cases} \tag{2.2}$$

and if $x \geq 0$, then $\sqrt{x}$ denotes the vector with $(\sqrt{x})_i = \sqrt{x_i}$.

Moreover, note that for $u \in \mathbb{R}^n$, combining (1.1) and (1.2) yields

$$x^T(A \circ uu^T)x = \langle A \circ uu^T, xx^T \rangle = \langle A, (u \circ x)(u \circ x)^T \rangle = (u \circ x)^T A (u \circ x). \tag{2.3}$$

The following theorem gives a characterization of copositivity of a matrix A.

Theorem 2.2.16 *Let $A \in \mathcal{S}_n$. Then the following are equivalent:*

(i) $A \in \mathcal{C}_n$,

(ii) $A \circ uu^T \in \mathcal{C}_n$ *for every nonnegative* $u \in \mathbb{R}^n$,

(iii) $A \circ uu^T \in \mathcal{C}_n$ *for every positive* $u \in \mathbb{R}^n$,

(iv) *There exists a positive* $u \in \mathbb{R}^n$ *such that* $A \circ uu^T \in \mathcal{C}_n$.

Proof Clearly, we only have to prove (i)⇒(ii) and (iv)⇒(i).
(i)⇒(ii): If $A \in \mathcal{C}_n$ and u is a nonnegative vector, then (2.3) implies that

$$x^T(A \circ uu^T)x = (u \circ x)^T A(u \circ x) \geq 0,$$

for every nonnegative $x \in \mathbb{R}^n$. That is, $A \circ uu^T \in \mathcal{C}_n$.
(iv)⇒(i): If $A \circ uu^T \in \mathcal{C}_n$ for a positive $u \in \mathbb{R}^n$, then

$$A = (A \circ uu^T) \circ (u^{\dashv})(u^{\dashv})^T \in \mathcal{C}_n,$$

since (i) implies (ii). □

The next theorem gives a similar characterization for extreme copositive matrices.

Theorem 2.2.17 *Let $A \in \mathcal{S}_n$. Then the following are equivalent:*

(i) *A is an extreme copositive matrix,*

(ii) *$A \circ uu^T$ is an extreme copositive matrix for every positive $u \in \mathbb{R}^n$,*

(iii) *There exists a positive $u \in \mathbb{R}^n$ such that $A \circ uu^T$ is an extreme copositive matrix.*

Proof If $u \in \mathbb{R}^n_{++}$ and $D = \text{Diag}(u)$, then $A \circ uu^T = DAD$. So the equivalence of (i), (ii) and (iii) is the known fact about preservation of extremality under scaling by a positive diagonal matrix as stated in Theorem 2.2.6. □

Remark 2.2.18 Note that if $u \geq 0$ and A is an extreme copositive matrix, then $A \circ uu^T$ may not be extreme. To see this, we consider the Horn matrix H which is an extreme 5×5 matrix and has 2×2 principal submatrices of all ones, which are not extreme in $\mathcal{C}_2$. For example, take the principal submatrix on rows and columns 1 and 3. So if the entries 1 and 3 of u are equal to one, and all other entries of u are zeros, then $H \circ uu^T$ is not extreme.

More copositivity criteria can be found in the survey paper on conditionally definite matrices by Ikramov and Savel'eva (2000) and the references therein. Bundfuss and Dür (2008) have introduced criteria that are based on simplicial partitions of the standard simplex. These lead to inner and outer approximations of the copositive cone which we will present in Section 2.4.1. Parrilo (2000) introduced sufficient copositivity conditions which are based on sum-of-squares decompositions of polynomials, and which yield an approximation hierarchy that we present in Section 2.4.2. Bomze and Eichfelder (2013) introduced copositivity criteria based on difference-of-convex decompositions.

2.3. The completely positive cone

We now study the dual of $\mathcal{C}_n$, the completely positive cone, in more detail.

Definition 2.3.1 A matrix $B \in \mathcal{S}_n$ is *completely positive* if it can be written as

$$B = \sum_{i=1}^{m} a_i a_i^T \quad \text{with } a_i \in \mathbb{R}^n_+. \tag{2.4}$$

This representation is called *rank one representation*.

By defining A as the matrix whose i-th column is a_i, we get the following representation of B, which is equivalent to (2.4),

$$B = AA^T \quad \text{with } A \in \mathbb{R}^{n \times m},\ A \geq 0.$$

The set of all completely positive $n \times n$ matrices is denoted $\mathcal{C}_n^*$. This notation will be justified in Theorem 2.3.5.

Like the copositive cone, the completely positive cone is invariant under permutation and scaling.

Lemma 2.3.2 (i) *Let P be a permutation matrix. Then $A \in \mathcal{S}_n$ is completely positive if and only if PAP^T is completely positive.*

(ii) *Let $D = \mathrm{Diag}(d)$ with $d \in \mathbb{R}^n_{++}$. Then $A \in \mathcal{S}_n$ is completely positive if and only if DAD is completely positive.*

Proof As in the copositive case, the statement follows from the fact that $\mathbb{R}^n_+$ is invariant under permutation and scaling. □

The interior of the completely positive cone has first been characterized by Dür and Still (2008). A less restrictive characterization has been found by Dickinson.

Theorem 2.3.3 (Dickinson (2010, Theorem 3.5)) *We have*

$$\operatorname{int}(\mathcal{C}_n^*) = \left\{ \sum_{i=1}^{m} a_i a_i^T : a_1 \in \mathbb{R}^n_{++},\ a_i \in \mathbb{R}^n_+ \ \forall i,\ \operatorname{span}\{a_1, \dots, a_m\} = \mathbb{R}^n \right\}$$
$$= \{AA^T : \operatorname{rank}(A) = n,\ A = [a|B],\ a \in \mathbb{R}^n_{++},\ B \geq 0\}.$$

In contrast to the set of extreme rays of the copositive cone, which is not completely known, the set of extreme rays of the completely positive cone has a simple description.

Theorem 2.3.4 (Hall Jr. and Newman (1963, Theorem 3.1 (iii))) *The extreme rays of $\mathcal{C}_n^*$ are the rank one matrices aa^T with $a \in \mathbb{R}^n_+ \setminus \{0\}$.*

The following theorem states some basic properties of $\mathcal{C}_n^*$.

Theorem 2.3.5 (i) *$\mathcal{C}_n^*$ is a proper cone.*

(ii) *$\mathcal{C}_n^*$ is nonpolyhedral (unless $n = 1$).*

(iii) *$\mathcal{C}_n$ and $\mathcal{C}_n^*$ are the duals of each other.*

A proof of (i) can be found in Dickinson (2013a, Theorem 5.5). For proofs of (ii) and (iii) see Berman and Shaked-Monderer (2003). However, for a better understanding of the completely positive cone, we will give proofs here.

Proof (i): Convexity of $\mathcal{C}_n^*$ is obvious from the definition. For a proof of closedness we refer to Berman and Shaked-Monderer (2003, Theorem 2.2). We have $\mathcal{C}_n^* \subseteq \mathcal{C}_n$. As the copositive cone is pointed (cf. Theorem 2.2.4 (i)), the same holds for the completely positive cone. By Theorem 2.3.3, $I + E$ lies in the interior of the completely positive cone showing that $\mathcal{C}_n^*$ is solid.

(ii): Statement (ii) follows from the fact that $\mathcal{C}_n^*$ has infinitely many extreme rays (cf. Theorem 2.3.4).

(iii): To avoid confusion during the proof, we denote the cone of all completely positive $n \times n$ matrices by $\mathcal{CP}_n$ for the moment. We want to show that the copositive and the completely positive cone are the duals of each other, i.e., $\mathcal{CP}_n^* = \mathcal{C}_n$ and $\mathcal{C}_n^* = \mathcal{CP}_n$.

By definition, $A \in \mathcal{C}_n$ if and only if $\langle A, bb^T \rangle = b^T A b \geq 0$ for all $b \in \mathbb{R}^n_+$. Since this is equivalent to $\langle A, B \rangle \geq 0$ for all $B \in \mathcal{CP}_n$, we have $\mathcal{CP}_n^* = \mathcal{C}_n$.

By Theorem 2.1.9 (iii), we then have $\mathcal{CP}_n = \mathrm{cl}(\mathcal{CP}_n) = (\mathcal{CP}_n^*)^* = \mathcal{C}_n^*$. This result also justifies the notation of the completely positive cone as $\mathcal{C}_n^*$. □

By Definition 2.3.1, it is immediately clear that every completely positive matrix is nonnegative as well as positive semidefinite, i.e., we have

$$\mathcal{C}_n^* \subseteq \mathcal{S}_n^+ \cap \mathcal{N}_n.$$

A matrix that is both nonnegative and positive semidefinite is called *doubly nonnegative*. We will denote the set of all doubly nonnegative $n \times n$ matrices by $\mathcal{D}_n$. Since $\mathcal{S}_n^+$ and $\mathcal{N}_n$ are proper, self-dual cones (cf. Berman and Shaked-Monderer (2003, Proposition 1.20 and 1.21)), we have by Theorem 2.1.9 (iv) and (v) that $\mathcal{D}_n$ and $\mathcal{S}_n^+ + \mathcal{N}_n$ are duals of each other. Consequently, for $n \leq 4$, we have

$$\mathcal{C}_n^* = \mathcal{S}_n^+ \cap \mathcal{N}_n,$$

whereas for $n \geq 5$ strict inclusion holds.

Definition 2.3.6 The minimal number m for which $B \in \mathcal{C}_n^*$ has a rank one representation

$$B = \sum_{i=1}^{m} a_i a_i^T \quad \text{with } a_i \in \mathbb{R}_+^n$$

is called the *cp-rank* of B.

By a simple observation, $\text{cp-rank}(B) \geq \text{rank}(B)$. Whereas for matrices $B \in \mathcal{C}_n^*$ with $\text{rank}(B) \leq 2$ or $n \leq 3$, equality holds (cf. Berman and Shaked-Monderer (2003, Theorem 3.1 and 3.2)), for matrices of higher rank or higher order, the cp-rank can be greater than its rank. By Theorem 2.1.7, the cp-rank of a matrix $B \in \mathcal{C}_n^*$ can be bounded by $\text{cp-rank}(B) \leq \frac{1}{2}n(n+1)$. In Drew et al. (1994), it is conjectured that an upper bound for the cp-rank is $\lfloor n^2/4 \rfloor$. For more details on the cp-rank we refer to Berman and Shaked-Monderer (2003) and Berman and Rothblum (2006).

2.3.1. Complete positivity criteria

Checking whether a given matrix is completely positive is an NP-hard problem (Dickinson and Gijben, 2013). For special cases, however, this can be done in linear time (see Dickinson and Dür (2012) and the references therein). Most criteria for complete positivity are based on properties of the graph associated to the matrix (cf. Section 1.2) or on the structure of the matrix.

Similar to Proposition 2.2.11, we have the following result on principal submatrices of completely positive matrices, see Berman and Shaked-Monderer (2003, Proposition 2.4).

Proposition 2.3.7 *Every principal submatrix of a completely positive matrix is completely positive.*

Another well-known property yielding a necessary condition for a matrix with zeros on the diagonal to be completely positive is the following.

Proposition 2.3.8 *Let* $B \in \mathcal{C}_n^*$. *If* $B_{ii} = 0$ *for some* $i \in \{1, \dots, n\}$, *then* $B_{ij} = 0$ *for all* j.

Proof Let $B \in \mathcal{C}_n^*$. Then B can be represented as $B = \sum_{k=1}^m a_k a_k^T$ with $a_k \in \mathbb{R}_+^n$ for all $k = 1, \dots, m$. If $B_{ii} = 0$, then $(a_k)_i = 0$ for all k, and thus $B_{ij} = \sum_{k=1}^m (a_k)_i (a_k)_j = 0$. □

The next result gives a necessary and sufficient condition for a matrix whose associated graph is triangle-free to be completely positive. To state it, we have to define the comparison matrix $M(B)$ of a square matrix B. It is defined by

$$(M(B))_{ij} = \begin{cases} |B_{ij}| & \text{if } i = j \\ -|B_{ij}| & \text{if } i \neq j. \end{cases}$$

Theorem 2.3.9 (Drew et al. (1994, Theorem 5)) *If* $B \in \mathcal{S}_n$ *is nonnegative and* $G(B)$ *is triangle-free, then* B *is completely positive if and only if its comparison matrix can be represented as* $M(B) = \alpha I - P$ *with* $P \geq 0$ *and* $\alpha \geq \rho(P)$.

The following special case will be needed in Chapter 6.

Corollary 2.3.10 *If* $B \in \mathcal{N}_n$ *with* $\operatorname{diag}(B) = e$ *has a triangle-free graph, then* B *is completely positive if and only if* $\rho(B - I) \leq 1$.

Proof Since $G(B)$ is triangle-free, Theorem 2.3.9 gives us that $B \in \mathcal{C}_n^*$ if and only if its comparison matrix $M(B)$ can be written as $M(B) = \alpha I - P$ with $P \in \mathcal{N}_n$ and $\alpha \geq \rho(P)$. In our case, we have

$$M(B) = I - (B - I),$$

which immediately gives the result. □

We now characterize complete positivity of a matrix B in terms of copositivity of the Hadamard product of B with copositive matrices.

Theorem 2.3.11 *Let $B \in \mathcal{S}_n$. The following are equivalent:*

(i) $B \in \mathcal{C}_n^*$,

(ii) $A \circ B \in \mathcal{C}_n$ *for every* $A \in \mathcal{C}_n$,

(iii) $A \circ B \in \mathcal{C}_n$ *for every extreme copositive matrix* $A \in \mathcal{C}_n$,

(iv) $A \circ B \in \mathcal{C}_n$ *for every extreme copositive matrix* $A \in \mathcal{C}_n$ *each of whose diagonal entries is either zero or one.*

Proof It is sufficient to prove (i)⇒(ii) and (iv)⇒(i).

(i)⇒(ii): If $B \in \mathcal{C}_n^*$, then $B = \sum_{i=1}^m u_i u_i^T$, where $u_i \in \mathbb{R}^n$ is nonnegative for all i. Then, for every $A \in \mathcal{C}_n$, the matrix $A \circ B = \sum_{i=1}^m A \circ u_i u_i^T$ is copositive as a sum of copositive matrices by Theorem 2.2.16.

(iv)⇒(i): Let A be an arbitrary extreme copositive matrix. Define $d = \operatorname{diag}(A)$ and $u = \sqrt{d^{\dashv}}$, where $d^{\dashv}$ is defined as in (2.2). Then $A \circ uu^T \in \mathcal{C}_n$ and all its diagonal entries are either zero or one. Since by assumption $(A \circ uu^T) \circ B \in \mathcal{C}_n$, we get from Theorem 2.2.16 that $A \circ B = (A \circ uu^T) \circ B \circ \sqrt{d}\sqrt{d}^T \in \mathcal{C}_n$. Consequently, $0 \leq e^T(A \circ B)e = \langle B, A \rangle$. Since A was an arbitrary extreme copositive matrix, this means that B is in the dual cone of $\mathcal{C}_n$, that is, $B \in \mathcal{C}_n^*$. □

Corollary 2.3.12 *If $B \in \mathcal{D}_n$, then $B \in \mathcal{C}_n^*$ if and only if $A \circ B \in \mathcal{C}_n$ for every (extreme) $A \in \mathcal{C}_n \setminus (\mathcal{S}_n^+ + \mathcal{N}_n)$.*

Proof If $A \in (\mathcal{S}_n^+ + \mathcal{N}_n)$, then clearly $A \circ B \in (\mathcal{S}_n^+ + \mathcal{N}_n)$. Hence $B \in \mathcal{C}_n^*$ if and only if $A \circ B \in \mathcal{C}_n$ for every (extreme) copositive matrix which is not in $(\mathcal{S}_n^+ + \mathcal{N}_n)$. □

2.4. Approximations

As we have seen, the copositive and the completely positive cone are computationally not tractable. Therefore, one approach to solve optimization problems over these cones consists in replacing the copositive respectively completely positive cone by a sequence of tractable approximations which allows to approximate the optimal value. We will introduce two different approximation schemes yielding inner and outer approximation hierarchies of the copositive and the completely positive cone.

2.4.1. Approximations based on simplicial partitions

In this section, we present polyhedral inner and outer approximations of the copositive and the completely positive cone which have been introduced in Bundfuss and Dür (2009). We will use these approximations to approximate the solution of optimization problems over $\mathcal{C}_n$, in particular the projection of an arbitrary matrix onto the copositive cone as explained in Section 4.2.

2.4.1.1. Simplicial partitions

Since the approximations to be described here are based on simplicial partitions of the standard simplex, we start with the definition of this concept.

Definition 2.4.1 Let $k \le n$. A *k-simplex* is the convex hull of $k+1$ affinely independent points in $\mathbb{R}^n$.

The *standard simplex*

$$\Delta^S = \{x \in \mathbb{R}^n_+ : \|x\|_1 = 1\}$$

is the convex hull of the n unit vectors $e_1, \dots, e_n \in \mathbb{R}^n$.

Definition 2.4.2 Let Δ be a simplex in $\mathbb{R}^n$. A family $\mathcal{P} = \{\Delta^1, \dots, \Delta^m\}$ of simplices satisfying

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

is called a *simplicial partition* of Δ. We denote by $V_{\mathcal{P}}$ the set of all vertices of simplices in $\mathcal{P}$, and by $E_{\mathcal{P}}$ the set of all edges of simplices in $\mathcal{P}$.

We will now show how a simplicial partition can be generated. Let $\Delta = \operatorname{conv}\{v_1, \dots, v_n\}$ and $w \in \Delta \setminus \{v_1, \dots, v_n\}$. Then

$$w = \sum_{i=1}^{n} \lambda_i v_i \quad \text{with} \quad \lambda_i \ge 0,\ 1 \le i \le n, \quad \text{and} \quad \sum_{i=1}^{n} \lambda_i = 1.$$

For every $i \in \{1, \dots, n\}$ with $\lambda_i > 0$, we obtain a subsimplex of Δ by replacing v_i by w, i.e.,

$$\Delta^i = \operatorname{conv}\{v_1, \dots, v_{i-1}, w, v_{i+1}, \dots, v_n\}.$$

The subsimplices Δ^i form a simplicial partition of Δ (see Horst (1976, Lemma 1)). A special case of this method is the *bisection* where w is chosen as the midpoint of an edge of Δ.

Figure 2.1 illustrates the partitioning method on a small example. We consider the simplex $\Delta = \text{conv}\{v_1, v_2, v_3\}$ and choose

$$w_1 = \tfrac{1}{3}v_1 + \tfrac{1}{3}v_2 + \tfrac{1}{3}v_3 \quad \text{and} \quad w_2 = \tfrac{1}{2}v_1 + \tfrac{1}{2}v_2.$$

For w_1, one obtains the simplicial partition $\mathcal{P} = \{\Delta^1, \Delta^2, \Delta^3\}$ with

$$\begin{aligned} \Delta^1 &= \text{conv}\{w_1, v_2, v_3\}, \\ \Delta^2 &= \text{conv}\{v_1, w_1, v_3\}, \\ \Delta^3 &= \text{conv}\{v_1, v_2, w_1\}. \end{aligned}$$

For the bisection point w_2, the simplicial partition consists of the subsimplices

$$\Delta^1 = \text{conv}\{w_2, v_2, v_3\} \quad \text{and} \quad \Delta^2 = \text{conv}\{v_1, w_2, v_3\}.$$

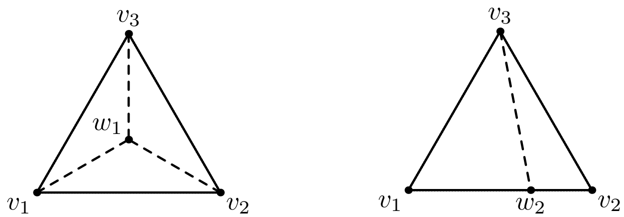

Figure 2.1.: Simplicial partition

By the *diameter* $\delta(\mathcal{P})$ of a simplicial partition $\mathcal{P}$, we mean the length of a longest edge in $E_{\mathcal{P}}$, i.e.,

$$\delta(\mathcal{P}) = \max_{\{u,v\} \in E_{\mathcal{P}}} \|u - v\|_2.$$

If we repeatedly subdivide subsimplices Δ^i of Δ such that the bisection point is an almost arbitrary point on a longest edge, then we get a sequence $(\mathcal{P}_l)_l$ of simplicial partitions of Δ with $\delta(\mathcal{P}_l) \to 0$. For details see Horst (1997) or the recent paper Dickinson (2013b).

2.4.1.2. Approximations of the copositive cone

We now define inner and outer approximations of the copositive cone.

Theorem 2.4.3 *Let $\mathcal{P}$ be a simplicial partition of Δ^S. The set*

$$\mathcal{I}_{\mathcal{P}} = \{X \in \mathcal{S}_n : v^T X v \geq 0 \text{ for all } v \in V_{\mathcal{P}},\\ u^T X v \geq 0 \text{ for all } \{u, v\} \in E_{\mathcal{P}}\}$$

is an inner approximation of $\mathcal{C}_n$, and the set

$$\mathcal{O}_{\mathcal{P}} = \{X \in \mathcal{S}_n : v^T X v \geq 0 \text{ for all } v \in V_{\mathcal{P}}\}$$

is an outer approximation of $\mathcal{C}_n$.

For a proof see Bundfuss and Dür (2009, Lemma 3.1 and Lemma 3.4).

It is easy to see that $\mathcal{I}_{\mathcal{P}}$ and $\mathcal{O}_{\mathcal{P}}$ are closed convex polyhedral cones. If partitions $\mathcal{P}_l$ are constructed by successive bisection of subsimplices of Δ^S, then the approximations are nested, that is, we have $\mathcal{I}_{\mathcal{P}_l} \subseteq \mathcal{I}_{\mathcal{P}_{l+1}}$ and $\mathcal{O}_{\mathcal{P}_l} \supseteq \mathcal{O}_{\mathcal{P}_{l+1}}$ for all $l \in \mathbb{N}$. Nested or not, the approximations converge towards $\mathcal{C}_n$ in the following sense:

Theorem 2.4.4 *Let $(\mathcal{P}_l)_l$ be a sequence of simplicial partitions of Δ^S with $\delta(\mathcal{P}_l) \to 0$ as $l \to \infty$. Then we have*

$$\mathcal{C}_n = \operatorname{cl}\Big(\bigcup_{l \in \mathbb{N}} \mathcal{I}_{\mathcal{P}_l}\Big) \quad \text{and} \quad \mathcal{C}_n = \bigcap_{l \in \mathbb{N}} \mathcal{O}_{\mathcal{P}_l}.$$

For a proof see Bundfuss and Dür (2009, Theorems 3.3 and 3.6).

2.4.1.3. Approximations of the completely positive cone

By Theorem 2.1.9, taking the dual of an inner approximation of the copositive cone yields an outer approximation of the completely positive cone. Likewise, the dual of an outer approximation of $\mathcal{C}_n$ is an inner approximation of $\mathcal{C}_n^*$. As observed in Bundfuss and Dür (2009, Section 3.3), the dual cones of the inner and outer approximations $\mathcal{I}_{\mathcal{P}}$ and $\mathcal{O}_{\mathcal{P}}$ of $\mathcal{C}_n$ can be described as

$$\mathcal{I}_{\mathcal{P}}^* = \left\{ \sum_{\{u,v\} \in E_{\mathcal{P}}} \lambda_{uv}(uv^T + vu^T) + \sum_{v \in V_{\mathcal{P}}} \lambda_v vv^T : \lambda_{uv}, \lambda_v \in \mathbb{R}_+ \right\}$$

which is an outer approximation of $\mathcal{C}_n^*$, and as

$$\mathcal{O}_{\mathcal{P}}^* = \left\{ \sum_{v \in V_{\mathcal{P}}} \lambda_v v v^T : \lambda_v \in \mathbb{R}_+ \right\}$$

which is an inner approximation of $\mathcal{C}_n^*$.

Let $(\mathcal{P}_l)_l$ again be a sequence of simplicial partitions of Δ^S with $\delta(\mathcal{P}_l) \to 0$. From Theorem 2.4.4 we get

$$\mathcal{C}_n^* = \bigcap_{l \in \mathbb{N}} \mathcal{I}_{\mathcal{P}_l}^* \quad \text{and} \quad \mathcal{C}_n^* = \mathrm{cl}\left(\bigcup_{l \in \mathbb{N}} \mathcal{O}_{\mathcal{P}_l}^* \right).$$

2.4.1.4. Generalization of the approach

As described in Bundfuss (2009) and Sponsel et al. (2012), the approach can be generalized to get better approximations of the copositive cone. We will briefly present the underlying idea.

As a simplex Δ is determined by its vertices, it can be represented by a matrix V_Δ whose columns are these vertices. V_Δ is nonsingular and unique up to a permutation of its columns. We refer to the set of all matrices corresponding to simplices in a partition $\mathcal{P}$ as

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

Let $\mathcal{M} \subset \mathcal{C}_n$. Then we can define the following approximation hierarchy of the copositive cone

$$\mathcal{K}_{\mathcal{M},\mathcal{P}} = \{A \in \mathcal{S}_n : V^T A V \in \mathcal{M} \text{ for all } V \in M(\mathcal{P})\}.$$

Note that for $\mathcal{M} = \mathcal{N}_n$, these approximations equal the inner approximations $\mathcal{I}_{\mathcal{P}}$ introduced in Section 2.4.1.2.

In Sponsel et al. (2012, Theorem 2.1) it has been shown that $\mathcal{K}_{\mathcal{M},\mathcal{P}} \subset \mathcal{C}_n$ for any $\mathcal{M} \subset \mathcal{C}_n$ and all partitions $\mathcal{P}$ of the standard simplex. Moreover, assuming $\mathcal{N}_n \subseteq \mathcal{M}$, we have

$$\mathrm{int}(\mathcal{C}_n) \subset \bigcup_{\varepsilon > 0} \bigcup_{\delta(\mathcal{P}) < \varepsilon} \mathcal{K}_{\mathcal{M},\mathcal{P}}$$

(see Sponsel et al. (2012, Theorem 2.2)).

An important issue that affects the quality of the approximations is the choice of the set $\mathcal{M}$. To get a good approximation $\mathcal{K}_{\mathcal{M},\mathcal{P}}$, the set $\mathcal{M}$ should be a good approximation of $\mathcal{C}_n$. On the other hand, to keep $\mathcal{K}_{\mathcal{M},\mathcal{P}}$ tractable, it should be computationally cheap to check membership of $\mathcal{M}$. Possible choices of $\mathcal{M}$ as well as numerical results for testing copositivity using this approximation hierarchy are discussed in Sponsel et al. (2012).

2.4.2. Approximations based on polynomials

In this section, we introduce three inner approximation hierarchies of the copositive cone which are based on polynomials. Optimizing over the cones of these hierarchies can be done by solving linear or semidefinite programs.

For $A \in \mathcal{S}_n$ and $x \in \mathbb{R}^n$, we define

$$P_A(x) = (x \circ x)^T A (x \circ x) = \sum_{i,j=1}^{n} A_{ij} x_i^2 x_j^2.$$

Since any nonnegative n-vector can be written as $(x \circ x)^T = (x_1^2, x_2^2, \ldots, x_n^2)^T$ with $x \in \mathbb{R}^n$, the matrix A is copositive if and only if $P_A(x) \geq 0$ for all $x \in \mathbb{R}^n$. A sufficient condition for the polynomial $P_A(x)$ to be nonnegative is that it can be written as a sum of squares, i.e., $P_A(x) = \sum_{i=1}^{t} p_i(x)^2$ where p_i, $i = 1, \ldots, t$, are polynomial functions. Parrilo (2000) showed that $P_A(x)$ has a sum of squares representation if and only if $A \in \mathcal{S}_n^+ + \mathcal{N}_n$, which is a sufficient copositivity condition that we have already seen in Section 2.2.

Stronger sufficient copositivity conditions can be obtained by considering the polynomials

$$P_A^r(x) = P_A(x) \left(\sum_{i=1}^{n} x_i^2 \right)^r = \left(\sum_{i,j=1}^{n} A_{ij} x_i^2 x_j^2 \right) \left(\sum_{i=1}^{n} x_i^2 \right)^r$$

for $r \geq 0$ integer. Parrilo (2000) showed that if $P_A^r(x)$ has a sum of squares decomposition, then $P_A^{r+1}(x)$ is also a sum of squares, and if $P_A^r(x)$ is nonnegative for some r, then the same holds for $P_A(x)$. We thus get an inner approximation hierarchy for the copositive cone by defining

$$\mathcal{K}_n^r = \left\{ A \in \mathcal{S}_n : \left(\sum_{i,j=1}^{n} A_{ij} x_i^2 x_j^2 \right) \left(\sum_{i=1}^{n} x_i^2 \right)^r \text{ is a sum-of-squares} \right\}.$$

As shown by Parrilo (2000), we have

$$\mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{K}_n^0 \subseteq \mathcal{K}_n^1 \subseteq \mathcal{K}_n^2 \subseteq \ldots \subseteq \mathcal{C}_n \quad \text{and} \quad \mathrm{cl}\left(\bigcup_{r \in \mathbb{N}} \mathcal{K}_n^r \right) = \mathcal{C}_n.$$

The condition that a matrix lies in $\mathcal{K}_n^r$ can be checked by solving a system of linear matrix inequalities (cf. Parrilo (2000)), and therefore, optimizing over $\mathcal{K}_n^r$ amounts to solving a semidefinite program. But as the size of the matrix variable grows quickly with r, current SDP-solvers can only handle problems over $\mathcal{K}_n^r$ for small values of r.

We now consider the case $r = 1$ in more detail. By Parrilo (2000, Theorem 5.2) and Bomze and de Klerk (2002, Theorem 2.3), a matrix A is in $\mathcal{K}_n^1$ if and only if there are matrices $M^1, \ldots, M^n \in \mathcal{S}_n$ such that the following system of linear matrix inequalities is fulfilled

$$A - M^i \succeq 0\,,\ i = 1, \ldots, n \tag{2.5}$$

$$M^i_{ii} = 0\,,\ i = 1, \ldots, n \tag{2.6}$$

$$M^i_{jj} + 2M^j_{ij} = 0\,,\ \forall\, i \neq j \tag{2.7}$$

$$M^i_{jk} + M^j_{ik} + M^k_{ij} \geq 0\,,\ \forall\, i < j < k\,. \tag{2.8}$$

For $n = 5$, Dickinson, Dür, Gijben and Hildebrand (2013) have shown that every copositive matrix can be scaled such that the scaled matrix lies in $\mathcal{K}_5^1$, i.e., we have the following.

Theorem 2.4.5 (Dickinson et al. (2013, Theorem 3.4)) *Let $A \in \mathcal{S}_5$ and let $D \in \mathcal{S}_5$ be a diagonal matrix with strictly positive diagonal entries such that $(DAD)_{ii} \in \{0, 1\}$ for all $1 \leq i \leq 5$. Then $A \in \mathcal{C}_5$ if and only if $DAD \in \mathcal{K}_5^1$.*

Clearly, the same holds for scalings with $(DAD)_{ii} \in \{0, k\}$ for any $k > 0$. This means that for any 5×5 matrix, copositivity can be checked by scaling and testing if the scaled matrix lies in $\mathcal{K}_5^1$.

Based on Parrilo's results, Bomze and de Klerk (2002) and de Klerk and Pasechnik (2002) introduced the following approximation hierarchy

$$\mathcal{C}_n^r = \left\{ A \in \mathcal{S}_n : \left(\sum_{i,j=1}^n A_{ij} x_i^2 x_j^2 \right) \left(\sum_{i=1}^n x_i^2 \right)^r \text{ has nonnegative coefficients} \right\},$$

and showed that

$$\mathcal{N}_n = \mathcal{C}_n^0 \subseteq \mathcal{C}_n^1 \subseteq \mathcal{C}_n^2 \subseteq \ldots \subseteq \mathcal{C}_n \quad \text{and} \quad \text{cl}\Big(\bigcup_{r \in \mathbb{N}} \mathcal{C}_n^r \Big) = \mathcal{C}_n.$$

Obviously, these approximations are weaker, i.e., $\mathcal{C}_n^r \subseteq \mathcal{K}_n^r$ for all r, but since optimizing over $\mathcal{C}_n^r$ amounts to solving a linear program, these problems can be solved more easily.

A third hierarchy has been introduced by Peña, Vera and Zuluaga (2007). They define the following set of polynomials

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

where for $\beta \in \mathbb{N}^n$ the notations $|\beta| = \beta_1 + \ldots, \beta_n$ and $x^\beta = x_1^{\beta_1} \ldots x_n^{\beta_n}$ are used. They show that the cones

$$\mathcal{Q}_n^r = \left\{ A \in \mathcal{S}_n : x^T A x \left(\sum_{i=1}^n x_i^2 \right)^r \in \mathcal{E}_n^r \right\}$$

form an inner approximation hierarchy of the copositive cone, i.e.,

$$\mathcal{Q}_n^0 \subseteq \mathcal{Q}_n^1 \subseteq \mathcal{Q}_n^2 \subseteq \ldots \subseteq \mathcal{C}_n \quad \text{and} \quad \mathrm{cl}\left(\bigcup_{r \in \mathbb{N}} \mathcal{Q}_n^r \right) = \mathcal{C}_n.$$

Moreover, they show that $\mathcal{C}_n^r \subseteq \mathcal{Q}_n^r \subseteq \mathcal{K}_n^r$ for all r, and $\mathcal{Q}_n^r = \mathcal{K}_n^r$ for $r \in \{0, 1\}$. As for $\mathcal{K}_n^r$, the condition that a matrix lies in $\mathcal{Q}_n^r$ can be checked by solving a system of linear matrix inequalities which means that optimizing over $\mathcal{Q}_n^r$ can be done by solving a semidefinite program.

By Theorem 2.1.9, taking the dual of an inner approximation of the copositive cone yields an outer approximation of the completely positive cone. In Dong (2013) two outer approximation hierarchies of the completely positive cone are constructed. The first one is a sequence of polyhedral cones, and the second one is a sequence of cones represented by semidefinite constraints. Furthermore, Dong showed that the cones of the first hierarchy are the duals of $\mathcal{C}_n^r$ and the cones of the second hierarchy are the duals of Q_n^r. For details we refer to Dong (2013).

3. Conic optimization

In this chapter we consider conic optimization problems, i.e., optimization problems with a linear objective function, linear constraints and an additional constraint that the variable lies in a cone $\mathcal{K}$. In Section 3.1, we introduce the basic terminology and state two duality results, before we consider the special case of copositive programming in Section 3.2.

3.1. Conic optimization and duality

Let $\mathcal{K} \subseteq \mathbb{R}^n$ be a closed convex cone. Let $c \in \mathbb{R}^n$, $a_i \in \mathbb{R}^n$, $i = 1, \dots, m$, and $b_i \in \mathbb{R}$, $i = 1, \dots, m$. We consider the following pair of conic optimization problems

$$\begin{array}{ll} \inf & \langle c, x \rangle \\ \text{s. t.} & \langle a_i, x \rangle = b_i, \; i = 1, \dots, m \\ & x \in \mathcal{K}, \end{array} \tag{P}$$

$$\begin{array}{ll} \sup & \langle b, y \rangle \\ \text{s. t.} & c - \sum_{i=1}^m y_i a_i \in \mathcal{K}^* \\ & y \in \mathbb{R}^m. \end{array} \tag{D}$$

Problem (P) is referred to as the *primal problem* and (D) as the *dual problem*. Special cases are linear programming when $\mathcal{K} = \mathcal{K}^* = \mathbb{R}^n_+$, and semidefinite programming when $\mathcal{K} = \mathcal{K}^* = \mathcal{S}_n^+ \subseteq \mathbb{R}^{n \times n}$, which we can identify with $\mathbb{R}^{n^2}$.

The *feasible set* of (P), denoted Feas(P), is the set of all feasible solutions of (P), i.e., the set of all $x \in \mathcal{K}$ that fulfill the equality constraints, and similarly, the feasible set of (D) is the set of all $y \in \mathbb{R}^m$ with $c - \sum_{i=1}^m y_i a_i \in \mathcal{K}^*$. Let $\bar{p}$ and $\bar{d}$ denote the *optimal values* of (P) respectively (D), i.e.,

$$\bar{p} = \inf\{\langle c, x \rangle : \langle a_i, x \rangle = b_i, \; i = 1, \dots, m, \text{ and } x \in \mathcal{K}\}$$

and

$$\bar{d} = \sup\{\langle b, y \rangle : c - \sum_{i=1}^m y_i a_i \in \mathcal{K}^*\}.$$

An *optimal solution* of (P) is a feasible solution $\bar{x}$ with $\langle c, \bar{x}\rangle = \bar{p}$, and similarly, an optimal solution of (D) is a feasible solution $\bar{y}$ with $\langle b, \bar{y}\rangle = \bar{d}$. If the feasible set of (P) is empty, we say that the problem is *infeasible* and set $\bar{p} = \infty$. Likewise, if the constraints of (D) are infeasible, we set $\bar{d} = -\infty$. If there are feasible points x_k of (P) with $\langle c, x_k\rangle \to -\infty$ as $k \to \infty$ then $\bar{p} = -\infty$ and we say that the problem is *unbounded*. Similarly, problem (D) is unbounded if there are feasible points y_k with $\langle b, y_k\rangle \to \infty$ as $k \to \infty$.

The following theorem states the well-known result that weak duality holds.

Theorem 3.1.1 (Weak Conic Duality Theorem) *Let x be feasible for (P) and y be feasible for (D). Then*

$$\langle c, x\rangle \geq \langle b, y\rangle.$$

Proof If x and y are feasible solutions of (P) respectively (D), then by duality

$$\langle c, x\rangle - \langle b, y\rangle = \langle c, x\rangle - \sum_{i=1}^{m} b_i y_i = \langle c, x\rangle - \sum_{i=1}^{m} \langle a_i, x\rangle y_i = \left\langle c - \sum_{i=1}^{m} y_i a_i, x \right\rangle \geq 0.$$

□

Under additional assumptions, this result can be strengthened. We say that x is a *strictly feasible solution* of (P) if x is feasible and lies in the interior of $\mathcal{K}$. Similarly, y is a *strictly feasible solution* of (D) if $c - \sum_{i=1}^{m} y_i a_i \in \operatorname{int}(\mathcal{K}^*)$.

Theorem 3.1.2 (Strong Conic Duality Theorem) *If there exists a strictly feasible solution of (P), and a feasible solution of (D), then $\bar{p} = \bar{d}$ and the supremum in (D) is attained. Similarly, if there exists a strictly feasible solution of (D) and a feasible solution of (P), then $\bar{p} = \bar{d}$ and the infimum in (P) is attained.*

For a proof we refer to Renegar (2001, Section 3.2).

3.2. Copositive programming

We now consider completely positive programs which are conic optimization problems over the completely positive cone. These problems are closely related to quadratic optimization problems. The first completely positive representation of a quadratic optimization problem is due to Bomze et al. (2000) who studied the standard quadratic optimization problem

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & e^T x = 1 \\ & x \geq 0 \end{array} \qquad \text{(StQP)}$$

with $Q \in \mathcal{S}_n$. By nonnegativity of x, the linear constraint $e^T x = 1$ can equivalently be stated as $(e^T x)^2 = x^T e e^T x = 1$. The problem can thus be written as

$$\begin{array}{ll} \min & \langle Q, xx^T \rangle \\ \text{s.t.} & \langle E, xx^T \rangle = 1 \\ & x \geq 0. \end{array}$$

Introducing the matrix variable $X = xx^T$, we get

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s.t.} & \langle E, X \rangle = 1 \\ & X = xx^T \\ & x \geq 0. \end{array}$$

Relaxing the rank one constraint yields the following completely positive program

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s.t.} & \langle E, X \rangle = 1 \\ & X \in \mathcal{C}_n^*. \end{array} \qquad (\mathrm{P}_{\mathcal{C}^*})$$

To show that this problem is not only a relaxation but an exact reformulation of (StQP), we need the following characterization of the extreme points of the feasible set of $(\mathrm{P}_{\mathcal{C}^*})$.

Lemma 3.2.1 *The extreme points of the feasible set of $(P_{\mathcal{C}^*})$ are exactly the rank one matrices $X = xx^T$ with $x \in \Delta^S$.*

This result has been shown in Bomze et al. (2000, Lemma 5). For the sake of completeness, we state the proof here.

Proof Let $X = xx^T$ with $x \in \Delta^S$. Obviously, $X \in \mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$. Assume by contradiction, that X is not extreme, i.e., $X = \lambda Y + (1 - \lambda) Z$ with $Y, Z \in \mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$, $Y, Z \neq X$, and $0 < \lambda < 1$. Choose an orthogonal basis $\{x_1, \ldots, x_n\}$

of $\mathbb{R}^n$ with $x_n = x$. Then

$$\begin{aligned} 0 &= (x_i^T x)^2 = x_i^T (xx^T) x_i \\ &= x_i^T (\lambda Y + (1-\lambda) Z) x_i \\ &= \lambda x_i^T Y x_i + (1-\lambda) x_i^T Z x_i \end{aligned} \tag{3.1}$$

for all $i < n$. Since Y, Z are feasible for $(\mathrm{P}_{\mathcal{C}^*})$ and thus positive semidefinite, equation (3.1) implies that $x_i^T Y x_i = x_i^T Z x_i = 0$ for all $i < n$. Therefore, Y and Z have rank one, whence $Y = yy^T$ and $Z = zz^T$ for some $y, z \in \mathbb{R}^n_+$. We then obtain that $x_i^T y = x_i^T z = 0$ for all $i < n$ which implies that Y and Z must be multiples of $X = xx^T$. By $\langle E, Y \rangle = \langle E, Z \rangle = 1$, we then get $Y = Z = X$ and consequently, X is an extreme point of $\mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$.

To show the converse, assume that X is an extreme point of $\mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$. By complete positivity, we have $X = \sum_{i=1}^m \lambda_i x_i x_i^T$ with $x_i \in \mathbb{R}^n \setminus \{0\}$ and $\lambda_i \geq 0$ for all $i = 1, \ldots, m$, and $\sum_{i=1}^m \lambda_i = 1$. By the linear constraint, we get

$$1 = \langle E, X \rangle = \sum_{i=1}^m \lambda_i (e^T x_i)^2. \tag{3.2}$$

Since $x_i \in \mathbb{R}^n_+ \setminus \{0\}$ for $i = 1, \ldots, m$, we have $e^T x_i > 0$ for all i. We define $y_i = \frac{1}{e^T x_i} x_i$. Then $y_i \in \Delta^S$ and $Y_i = y_i y_i^T \in \mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$. Consequently,

$$X = \sum_{i=1}^m \lambda_i x_i x_i^T = \sum_{i=1}^m \lambda_i (e^T x_i)^2 y_i y_i^T = \sum_{i=1}^m \lambda_i (e^T x_i)^2 Y_i$$

is a convex combination of matrices $Y_i \in \mathrm{Feas}(\mathrm{P}_{\mathcal{C}^*})$. Note that by (3.2), the sum of the coefficients is one. By assumption, X is an extreme point, whence $X = Y_1 = \ldots = Y_m$ and $X = y_1 y_1^T$ with $y_1 \in \Delta^S$. □

By linearity of the objective function in $(\mathrm{P}_{\mathcal{C}^*})$, an optimal solution $\bar{X}$ of this problem is attained at an extreme point of the feasible set, and by Lemma 3.2.1, this solution is a rank one matrix, i.e., $\bar{X} = \bar{x}\bar{x}^T$ with $\bar{x} \in \Delta^S$. Since $\langle Q, \bar{X} \rangle = \bar{x}^T Q \bar{x}$ and $\bar{x}$ is feasible for the standard quadratic optimization problem, this shows that the relaxation $(\mathrm{P}_{\mathcal{C}^*})$ is an exact reformulation of (StQP).

Burer (2009) generalized this result and showed that every optimization problem with quadratic objective, linear constraints and continuous and binary variables can equivalently be written as a linear problem over $\mathcal{C}_n^*$. He considered the problem

$$\begin{array}{ll} \min & x^T Q x + 2c^T x \\ \text{s.t.} & a_i^T x = b_i, \ i = 1, \ldots, m \\ & x \geq 0 \\ & x_j \in \{0, 1\} \quad \forall j \in B, \end{array} \tag{QP}$$

where $x \in \mathbb{R}^n$ and $B \subseteq \{1, \dots, n\}$. We assume Feas$(QP) \neq \emptyset$. This setting includes many NP-hard combinatorial problems.

We assume that for all $x \geq 0$ with $a_i^T x = b_i$, $i = 1, \dots, m$, we have $0 \leq x_j \leq 1$ for all $j \in B$. Then the following equivalence result can be shown.

Theorem 3.2.2 (Burer (2009, Theorem 2.6)) *The completely positive program*

$$\begin{array}{ll} \min & \langle Q, X \rangle + 2c^T x \\ \text{s.t.} & a_i^T x = b_i, \ i = 1, \dots, m \\ & a_i^T X a_i = b_i^2, \ i = 1, \dots, m \\ & x_j = X_{jj} \quad \forall j \in B \\ & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}_{n+1}^* \end{array} \qquad (\text{QP}_{\mathcal{C}^*})$$

is equivalent to (QP), i.e., it has the same optimal value, and if $(\bar{x}, \bar{X})$ is optimal for (QP$_{\mathcal{C}^*}$) then $\bar{x}$ is in the convex hull of optimal solutions of (QP).

Moreover, Burer showed that if

$$\text{there is a } y \in \mathbb{R}^m \text{ such that } \sum_{i=1}^m y_i a_i \geq 0, \ \sum_{i=1}^m y_i b_i = 1, \qquad (3.3)$$

then x can be eliminated in (QP$_{\mathcal{C}^*}$).

Theorem 3.2.3 (Burer (2009, Theorem 3.1)) *Suppose that (3.3) holds, and define $\alpha = \sum_{i=1}^m y_i a_i$. Then*

$$\begin{array}{ll} \min & \langle Q, X \rangle + 2c^T X\alpha \\ \text{s.t.} & a_i^T X\alpha = b_i, \ i = 1, \dots, m \\ & a_i^T X a_i = b_i^2, \ i = 1, \dots, m \\ & (X\alpha)_j = X_{jj} \quad \forall j \in B \\ & \alpha^T X \alpha = 1 \\ & X \in \mathcal{C}_n^* \end{array} \qquad (\text{QP}_{\mathcal{C}^*}\text{'})$$

is equivalent to (QP), i.e., it has the same optimal value, and if $\bar{X}$ is optimal for (QP$_{\mathcal{C}^*}$), then $\bar{X}\alpha$ is in the convex hull of optimal solutions of (QP).

Note that by reformulating (QP) as a linear optimization problem over the completely positive cone, the complexity of the problem is shifted entirely to the cone constraint. Therefore, a better understanding of the completely positive cone helps in solving nonconvex quadratic problems.

The result generalizes earlier results on the completely positive reformulation of the standard quadratic optimization problem (Bomze et al., 2000) presented above, the maximum stable set problem (de Klerk and Pasechnik, 2002), the quadratic assignment problem (Povh, 2006; Povh and Rendl, 2009), and the graph 3-partitioning problem (Povh, 2006; Povh and Rendl, 2007).

We briefly return to the standard quadratic optimization problem. In the setting of (QP), we have $c = 0$, $a = e$, $b = 1$ and $B = \emptyset$. For $y = 1$, property (3.3) holds, and we have $\alpha = e$. The completely positive reformulation we get by applying Theorem 3.2.3, is equivalent to ($\mathrm{P}_{\mathcal{C}^*}$).

Burer's result has been extended to problems where the nonnegativity constraint on x is replaced by a constraint $x \in \mathcal{K}$ where $\mathcal{K} \subseteq \mathbb{R}^n$ is a nonempty closed (convex) set respectively a closed convex cone. The conic reformulation is then a linear problem over the cone $\mathcal{C}^*_{\mathcal{K}}$. For details we refer to Dickinson et al. (2012) and Burer (2012). Another extension due to Burer and Dong (2012) concerns nonconvex quadratically constrained programs.

4. Copositive projection

We investigate the problem of projecting a matrix $A \in \mathcal{S}_n$ onto the copositive cone $\mathcal{C}_n$ and the completely positive cone $\mathcal{C}_n^*$.

We start by explaining the algorithm to project onto $\mathcal{C}_n$. Since an exact projection is hard to compute, we project the matrix onto the inner and outer approximations of $\mathcal{C}_n$ introduced in Section 2.4.1. As these approximations converge to $\mathcal{C}_n$, we can approximate the projection of A onto $\mathcal{C}_n$ with arbitrary precision. We will deduce this statement from a more general result presented in Section 4.1.

After that, we proceed to study projections onto $\mathcal{C}_n^*$ which can be derived through projections onto $\mathcal{C}_n$ via a decomposition theorem by Moreau.

Finally, in Section 4.4, we show how these projections can be used to compute factorizations of completely positive matrices.

The results of this chapter were published in Sponsel and Dür (2012).

4.1. Optimization by approximation

In this section, we show how we can use approximations to solve optimization problems over the intractable cones $\mathcal{C}_n$ and $\mathcal{C}_n^*$. The results in this section are similar to those in Bundfuss and Dür (2009) where this was done for linear problems. Here, we provide more general convergence results for nonlinear problems. We will use these results in Section 4.2 and Section 4.3 for the projection onto $\mathcal{C}_n$ and $\mathcal{C}_n^*$.

Let $\mathcal{K}$ be a closed convex cone in $\mathbb{R}^n$ with nonempty interior. We consider the problem

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & g_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_j(x) = 0, \quad j = 1, \dots p \\ & x \in \mathcal{K} \end{array} \tag{$\mathrm{P}_{\mathcal{F}\cap\mathcal{K}}$}$$

with $f, g_i, h_j : \mathbb{R}^n \to \mathbb{R}$ continuous. To facilitate notation, denote by $\mathcal{F}$ the set of points in $\mathbb{R}^n$ that fulfill the equality and inequality constraints in $(\mathrm{P}_{\mathcal{F}\cap\mathcal{K}})$.

We assume that both the objective function f and the set $\mathcal{F}$ are convex. Moreover, we assume that $(\mathrm{P}_{\mathcal{F}\cap\mathcal{K}})$ is bounded from below, i.e.,

$$f_{\min} := \inf\{f(x) : x \in \mathcal{F} \cap \mathcal{K}\} > -\infty.$$

Let $(\mathcal{I}_l)_l$ and $(\mathcal{O}_l)_l$ be nested sequences of inner respectively outer approximations of $\mathcal{K}$ such that for $l \to \infty$ we have $\mathcal{I}_l \to \mathcal{K}$ (in the sense that for all $x \in \operatorname{int}(\mathcal{K})$ there is an $L \in \mathbb{N}$ such that $x \in \mathcal{I}_l$ for all $l \geq L$) and $\mathcal{O}_l \to \mathcal{K}$ (i.e., $\bigcap_{l\in\mathbb{N}} \mathcal{O}_l = \mathcal{K}$).

The following theorem shows that we can approximate the optimal value of $(\mathrm{P}_{\mathcal{F}\cap\mathcal{K}})$ with arbitrary precision by minimizing f over a sequence of inner approximations of $\mathcal{K}$.

Theorem 4.1.1 *Let $(\mathcal{I}_l)_l$ be a nested sequence of inner approximations of $\mathcal{K}$ as described above. Assume that $(P_{\mathcal{F}\cap\mathcal{K}})$ has a strictly feasible point, i.e., a point $\hat{x} \in \mathcal{F} \cap \operatorname{int}(\mathcal{K})$. Let $f_l := \inf\{f(x) : x \in \mathcal{F} \cap \mathcal{I}_l\}$. Then*

$$\lim_{l\to\infty} f_l = f_{\min}.$$

If the optimal values f_l are attained in the points x_l, then any accumulation point $\bar{x}$ of the sequence $(x_l)_l$ is a minimizer of $(P_{\mathcal{F}\cap\mathcal{K}})$, so $f_{\min} = f(\bar{x})$ is also attained and $\bar{x}$ is a global solution to $(P_{\mathcal{F}\cap\mathcal{K}})$.

Proof The inner approximation property implies $f_l \geq f_{\min}$ for all $l \in \mathbb{N}$. The sequence $(f_l)_l$ is monotone and bounded whence the limit exists. Consequently, $\lim_{l\to\infty} f_l \geq f_{\min}$.

To see the converse, take an $\varepsilon \in (0,1)$ and a point $y_\varepsilon \in \mathcal{F} \cap \mathcal{K}$ with $f(y_\varepsilon) \leq f_{\min} + \varepsilon$. Define

$$z_\varepsilon = (1-\varepsilon)y_\varepsilon + \varepsilon\hat{x}.$$

By construction, $z_\varepsilon \in \operatorname{int}(\mathcal{K}) \cap \mathcal{F}$. By the assumptions of the theorem, for each ε there exists an $l_\varepsilon \in \mathbb{N}$ such that $z_\varepsilon \in \mathcal{I}_l$ for all $l \geq l_\varepsilon$. It follows that

$$\lim_{l\to\infty} f_l \leq f(z_\varepsilon) \leq (1-\varepsilon)[f_{\min} + \varepsilon] + \varepsilon f(\hat{x}).$$

Letting $\varepsilon \to 0$, we arrive at $\lim\limits_{l\to\infty} f_l \leq f_{\min}$, as desired.

Now assume that the optimal values f_l are attained in $x_l \in \mathcal{F} \cap \mathcal{I}_l$, and take an accumulation point $\bar{x}$ along with a subsequence $(x_k)_k$ converging to it. Then we get from continuity of f that

$$f(\bar{x}) = \lim_{k\to\infty} f(x_k) = f_{\min},$$

so $f_{\min} = f(\bar{x})$ is attained and $\bar{x}$ is a minimizer of $(\mathrm{P}_{\mathcal{F}\cap\mathcal{K}})$. □

We get the same result for sequences of outer approximations.

Theorem 4.1.2 *Let $(\mathcal{O}_l)_l$ be a nested sequence of outer approximations of $\mathcal{K}$ as described above. Let $f_l := \inf\{f(x) : x \in \mathcal{F} \cap \mathcal{O}_l\}$. Then*

$$\lim_{l\to\infty} f_l = f_{\min}.$$

If the optimal values f_l are attained in the points x_l, then any accumulation point $\bar{x}$ of the sequence $(x_l)_l$ is a minimizer of ($P_{\mathcal{F}\cap\mathcal{K}}$), so $f_{\min} = f(\bar{x})$ is also attained and $\bar{x}$ is a global solution to ($P_{\mathcal{F}\cap\mathcal{K}}$).

Proof As before, we immediately get from the outer approximation property that $f_l \leq f_{\min}$ for all $l \in \mathbb{N}$. The sequence is monotone and bounded, so the limit exists and we have

$$\lim_{l\to\infty} f_l \leq f_{\min}. \tag{4.1}$$

There exists a sequence of points $o_l \in \mathcal{F} \cap \mathcal{O}_l$ with

$$\lim_{l\to\infty} f(o_l) = \lim_{l\to\infty} f_l.$$

Because of $\bigcap_{l\in\mathbb{N}} \mathcal{O}_l = \mathcal{K}$, we have

$$\operatorname{dist}(o_l, \mathcal{F} \cap \mathcal{K}) := \inf_{x\in\mathcal{F}\cap\mathcal{K}} \|o_l - x\| \to 0.$$

So there exists a sequence $x_l \in \mathcal{F} \cap \mathcal{K}$ with $\lim_{l\to\infty} \|x_l - o_l\| = 0$, and, by continuity of f, we have $\lim_{l\to\infty}[f(x_l) - f(o_l)] = 0$. Clearly, all of these x_l fulfill $f_{\min} \leq f(x_l)$, so we get

$$0 = \lim_{l\to\infty} [f(x_l) - f(o_l)] \geq \lim_{l\to\infty} [f_{\min} - f(o_l)] = f_{\min} - \lim_{l\to\infty} f_l.$$

Combined with (4.1), this gives $f_{\min} = \lim_{l\to\infty} f_l$, as desired. Note that this also shows that $\lim_{l\to\infty} f_l > -\infty$, even if some of the $f_l = -\infty$.

If the optimal values f_l are attained, similar reasoning as in the proof of Theorem 4.1.1 ensures the result. □

Remark 4.1.3 Observe that the infimum in ($\mathrm{P}_{\mathcal{F}\cap\mathcal{K}}$) and the auxiliary problems is not necessarily attained. For a thorough discussion of this see Bomze et al. (2012). Even if the minima are attained, the sequences $(x_l)_l$ with $x_l \in \operatorname{Argmin}_{x\in\mathcal{F}\cap\mathcal{I}_l} f(x)$ respectively $x_l \in \operatorname{Argmin}_{x\in\mathcal{F}\cap\mathcal{O}_l} f(x)$ do not necessarily have an accumulation point. Stronger assumptions can be imposed which guarantee existence of the accumulation points and convergence of the solutions.

We will use the results of this section for the projection onto the cones of copositive and completely positive matrices. But note that Theorem 4.1.1 and Theorem 4.1.2 do not only hold for cones but for any closed convex set $\mathcal{K}$ having a point $\hat{x} \in \operatorname{int}(\mathcal{K})$.

4.2. Projection onto the copositive cone

The problem of projecting a matrix $A \in \mathcal{S}_n$ onto the copositive cone can be formulated as

$$\begin{aligned} \min \quad & \|X - A\| \\ \text{s. t.} \quad & X \in \mathcal{C}_n. \end{aligned} \tag{P$_\mathcal{C}$}$$

Obviously, this is a special case of (P$_{\mathcal{F}\cap\mathcal{K}}$). We use the Frobenius norm, i.e., $\|A\| = \sqrt{\sum_{i,j=1}^n |A_{ij}|^2}$, although our results can be generalized to arbitrary strictly convex norms. So the problem has a unique solution which we denote by $\operatorname{pr}(\mathcal{C}_n, A)$.

4.2.1. The algorithm

As in Section 2.4.1.2, let $(\mathcal{P}_l)_l$ be a sequence of simplicial partitions of Δ^S and let

$$\begin{aligned} \mathcal{I}_{\mathcal{P}_l} = \{X \in \mathcal{S}_n : \; & v^T X v \geq 0 \text{ for all } v \in V_{\mathcal{P}_l}, \\ & u^T X v \geq 0 \text{ for all } \{u, v\} \in E_{\mathcal{P}_l}\} \end{aligned}$$

and

$$\mathcal{O}_{\mathcal{P}_l} = \{X \in \mathcal{S}_n : v^T X v \geq 0 \text{ for all } v \in V_{\mathcal{P}_l}\}$$

be the corresponding inner respectively outer approximations of $\mathcal{C}_n$. Furthermore, for a partition $\mathcal{P}$, let $\operatorname{pr}(\mathcal{I}_\mathcal{P}, A)$ and $\operatorname{pr}(\mathcal{O}_\mathcal{P}, A)$ denote the projection of A onto $\mathcal{I}_\mathcal{P}$ respectively $\mathcal{O}_\mathcal{P}$. For a given $\varepsilon > 0$, we want to compute an ε-optimal solution of (P$_\mathcal{C}$), i.e., a feasible solution $\operatorname{pr}(\mathcal{I}_\mathcal{P}, A)$ which satisfies a certain ε-optimality condition, like

$$\|\operatorname{pr}(\mathcal{I}_\mathcal{P}, A) - A\| - \|\operatorname{pr}(\mathcal{O}_\mathcal{P}, A) - A\| < \varepsilon$$

for absolute, or

$$\frac{\|\operatorname{pr}(\mathcal{I}_\mathcal{P}, A) - A\|}{\|\operatorname{pr}(\mathcal{O}_\mathcal{P}, A) - A\|} < 1 + \varepsilon$$

for relative ε-optimality.

We start with $\mathcal{P} = \{\Delta^S\}$ and project A onto the corresponding inner approximation of $\mathcal{C}_n$. If $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A) = A$, then $\mathrm{pr}(\mathcal{C}_n, A) = A$, so we can stop. Otherwise, we project A onto the corresponding outer approximation. If $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ and $\mathrm{pr}(\mathcal{O}_\mathcal{P}, A)$ satisfy the ε-optimality condition, then $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ is an ε-optimal solution of $(\mathrm{P}_\mathcal{C})$ and we can stop. Otherwise, we refine our partition through bisection and iterate. The procedure is stated in Algorithm 4.2.1.

Algorithm 4.2.1: Projection of a symmetric matrix A onto the copositive cone.

Input: $A \in \mathcal{S}_n$, $\varepsilon > 0$

$\mathcal{P} \leftarrow \{\Delta^S\}$

solve

$$\begin{array}{ll} \min & \|X - A\| \\ \text{s.t.} & X \in \mathcal{I}_\mathcal{P} \end{array} \qquad (\mathrm{P}_{\mathcal{I}_\mathcal{P}})$$

let $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ denote the solution of this problem

if $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A) = A$ **then**

  STOP: $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A) = \mathrm{pr}(\mathcal{C}_n, A)$

end

solve

$$\begin{array}{ll} \min & \|X - A\| \\ \text{s.t.} & X \in \mathcal{O}_\mathcal{P} \end{array} \qquad (\mathrm{P}_{\mathcal{O}_\mathcal{P}})$$

let $\mathrm{pr}(\mathcal{O}_\mathcal{P}, A)$ denote the solution of this problem

if $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ *and* $\mathrm{pr}(\mathcal{O}_\mathcal{P}, A)$ *fulfill the stopping criterion* **then**

  STOP: $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ is an ε-optimal solution of $(\mathrm{P}_\mathcal{C})$

end

choose $\Delta \in \mathcal{P}$

bisect $\Delta = \Delta^1 \cup \Delta^2$

$\mathcal{P} \leftarrow \mathcal{P} \setminus \{\Delta\} \cup \{\Delta^1, \Delta^2\}$

go to 2

Output: ε-optimal solution $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$

In the described procedure, we repeatedly have to solve problems of the form $(\mathrm{P}_{\mathcal{I}_\mathcal{P}})$ and $(\mathrm{P}_{\mathcal{O}_\mathcal{P}})$. This can be done by reformulating these problems as second order cone problems and using suitable interior point solvers. An alternative option is to use active set methods (see for example Lawson and Hanson (1974) and Arioli et al. (1984)). The advantage of active set algorithms is that they are well suited for warm starts which is advantageous in our setting, since in successive iterations the corresponding problems $(\mathrm{P}_{\mathcal{I}_\mathcal{P}})$ and $(\mathrm{P}_{\mathcal{O}_\mathcal{P}})$ differ in a small number of constraints only. Furthermore, we have $\mathcal{I}_{\mathcal{P}_l} \subseteq \mathcal{I}_{\mathcal{P}_{l+1}}$ for all $l \in \mathbb{N}$ which means that in each iteration $\mathrm{pr}(\mathcal{I}_\mathcal{P}, A)$ can be used as a feasible starting point for problem $(\mathrm{P}_{\mathcal{I}_\mathcal{P}})$ in the next iteration.

For the outer approximations, $\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A)$ in iteration l is feasible in the next iteration if and only if it fulfills $\omega_l^T \mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A)\omega_l \geq 0$ where ω_l denotes the bisection point of iteration l. In that case, $\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A)$ is also optimal for the next subproblem $(\mathrm{P}_{\mathcal{O}_{\mathcal{P}_{l+1}}})$. Otherwise, we can easily compute a new feasible starting point. Let

$$X_\lambda = \lambda \, \mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) + (1-\lambda) \, \mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A)$$

with $0 \leq \lambda \leq 1$. Then, the matrix X_{λ^*} with $\lambda^* = \min\{\lambda : \omega_l^T X_\lambda \omega_l \geq 0\}$ is feasible for problem $(\mathrm{P}_{\mathcal{O}_{\mathcal{P}_{l+1}}})$, which means that we can take it as starting point.

There is some freedom in the algorithm concerning how an edge is selected and bisected. This question as well as the problem of redundancies appearing in the subproblems are discussed in Bundfuss and Dür (2009, Section 5). Similar techniques can be used here.

4.2.1.1. Convergence of the algorithm

We can use Theorems 4.1.1 and 4.1.2 to prove convergence of the algorithm. Note that the problems $(\mathrm{P}_{\mathcal{I}_\mathcal{P}})$ and $(\mathrm{P}_{\mathcal{O}_\mathcal{P}})$ are projections onto closed convex sets with a strictly convex norm. Therefore, each problem has a unique optimal solution.

Theorem 4.2.1 *Let $(\mathcal{P}_l)_l$ be a sequence of simplicial partitions of Δ^S with $\delta(\mathcal{P}_l) \to 0$ as $l \to \infty$. Then $\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) \to \mathrm{pr}(\mathcal{C}_n, A)$ and $\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A) \to \mathrm{pr}(\mathcal{C}_n, A)$.*

Proof We first show that the sequences $(\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A))_l$ and $(\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A))_l$ possess accumulation points, and then we apply Theorems 4.1.1 and 4.1.2.

We have $0 \in \mathcal{I}_{\mathcal{P}_l}$ and $0 \in \mathcal{O}_{\mathcal{P}_l}$ for all $l \in \mathbb{N}$, so 0 is a feasible solution of all $(\mathrm{P}_{\mathcal{I}_{\mathcal{P}_l}})$ and $(\mathrm{P}_{\mathcal{O}_{\mathcal{P}_l}})$. It follows that for all $l \in \mathbb{N}$

$$\|\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) - A\| \leq \|0 - A\| = \|A\|$$

and

$$\|\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A) - A\| \leq \|0 - A\| = \|A\|.$$

Hence, we have for all $l \in \mathbb{N}$ that

$$\|\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A)\| = \|\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) - A + A\| \leq \underbrace{\|\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) - A\|}_{\leq \|A\|} + \|A\| \leq 2\|A\|$$

and similarly

$$\|\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A)\| \leq 2\|A\|.$$

Since $\mathcal{I}_{\mathcal{P}_l} \subseteq \mathcal{C}_n$, the sequence $(\mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A))_l$ lies in the compact set

$$\{X \in \mathcal{C}_n : \|X\| \leq 2\|A\|\}\,.$$

Likewise, since $\mathcal{O}_{\mathcal{P}_{l+1}} \subseteq \mathcal{O}_{\mathcal{P}_l}$ for all l, the sequence $(\mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A))_l$ lies in the compact set

$$\{X \in \mathcal{O}_{\mathcal{P}_0} : \|X\| \leq 2\|A\|\}\,.$$

Consequently, both sequences have accumulation points which we denote by $X_{\mathcal{I}}$ and $X_{\mathcal{O}}$, respectively. Theorems 4.1.1 and 4.1.2 imply that $X_{\mathcal{I}}$ and $X_{\mathcal{O}}$ are global minimizers of ($\mathrm{P}_{\mathcal{C}}$), and since this problem has a unique solution, it follows that $X_{\mathcal{I}} = \mathrm{pr}(\mathcal{C}_n, A) = X_{\mathcal{O}}$. We therefore have $\lim_{l\to\infty} \mathrm{pr}(\mathcal{I}_{\mathcal{P}_l}, A) = \mathrm{pr}(\mathcal{C}_n, A)$ and $\lim_{l\to\infty} \mathrm{pr}(\mathcal{O}_{\mathcal{P}_l}, A) = \mathrm{pr}(\mathcal{C}_n, A)$, as desired. □

4.2.1.2. Example

To illustrate the algorithm, we consider the following example

$$\begin{aligned} \min \quad & \|X - A\| \\ \text{s. t.} \quad & \left\langle \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}, X \right\rangle = 2 \\ & X \in \mathcal{C}_2 \end{aligned} \tag{P}$$

with $A = \begin{pmatrix} 0.6 & -1.2 \\ -1.2 & 1.6 \end{pmatrix}$. The feasible set, which is the same as in Bundfuss and Dür (2009, Example 4.1), is displayed in Figure 4.1. Since we consider

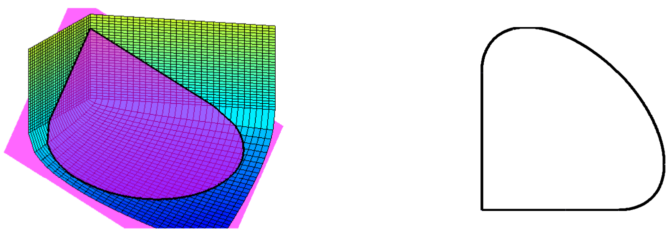

Figure 4.1.: Feasible set of (P)

symmetric matrices, $\mathcal{C}_2$ is a cone in $\mathbb{R}^3$, i.e., we identify $X \in \mathcal{C}_2$ with the vector $(X_{11}, X_{22}, X_{12})^T$. The copositive cone consists of all points above the multicolored surface. The feasible set, which is the set of all points that lie in the intersection of the copositive cone with the hyperplane that comes from the linear constraint, is thus two dimensional.

We now want to approximate the projection of A onto the feasible set of (P) by applying Algorithm 4.2.1. Figure 4.2 shows the first iterations.

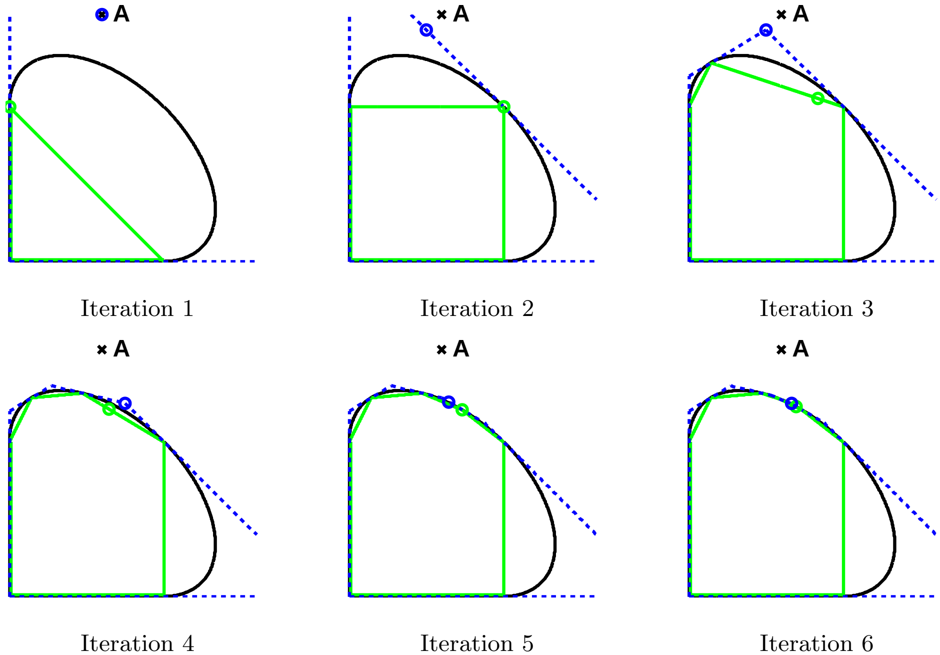

Figure 4.2.: Iterations of the projection algorithm

As before, the feasible set is the set of all points bounded by the black curved line. The inner approximations are represented by the green solid line and the outer approximations by the blue dashed line. The projections onto the inner and outer approximations are marked by small green and blue circles. Note that in the first iteration, A lies in the outer approximation whence the projection onto the outer approximation equals A.

In Figure 4.2, the projection of A does not look like the orthogonal projection. This comes from the fact that for drawing the 2-dimensional picture we mapped every matrix X of the feasible set onto the vector $(X_{11}, X_{22})^T$. The off-diagonal entries of the matrices are not displayed but implicitly given by the linear constraint. However, the restriction of the mapping

$$\begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \mapsto \begin{pmatrix} X_{11} \\ X_{22} \end{pmatrix}$$

to the plane given by the linear constraint is not isometric. Therefore, we computed an orthogonal basis of the plane given by the linear constraint in order to determine an isometric mapping of this plane to $\mathbb{R}^2$. This basis is given by the matrices

$$\frac{1}{\sqrt{5}} \begin{pmatrix} \phi & -1 \\ -1 & 1-\phi \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{5}} \begin{pmatrix} \phi & -1 \\ -1 & 1-\phi \end{pmatrix}$$

(where $\phi = (1+\sqrt{5})/2$ is the golden ratio) and these were used to produce the metrically faithful pictures in Figure 4.3.

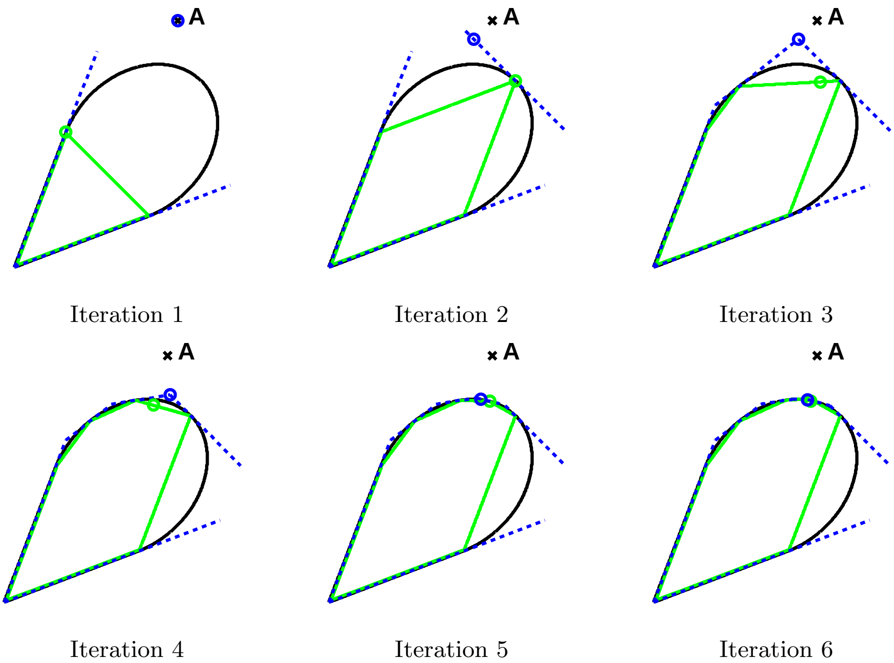

Figure 4.3.: Iterations of the projection algorithm, metrically faithful

4.3. Projection onto the completely positive cone

Next, we study the problem of projecting a matrix $A \in \mathcal{S}_n$ onto the completely positive cone $\mathcal{C}_n^*$. As in the copositive case, we can approximate this projection by projecting A onto a sequence of inner and outer approximations of $\mathcal{C}_n^*$. Again, let $(\mathcal{P}_l)_l$ be a sequence of simplicial partitions of Δ^S and let $\mathcal{O}_{\mathcal{P}_l}^*$ and $\mathcal{I}_{\mathcal{P}_l}^*$ be the corresponding inner and outer approximations of $\mathcal{C}_n^*$ as introduced in Section 2.4.1.3. Recall that they were defined as

$$\mathcal{I}_{\mathcal{P}_l}^* = \left\{ \sum_{\{u,v\} \in E_{\mathcal{P}_l}} \lambda_{uv}(uv^T + vu^T) + \sum_{v \in V_{\mathcal{P}_l}} \lambda_v vv^T : \lambda_{uv}, \lambda_v \in \mathbb{R}_+ \right\}$$

and

$$\mathcal{O}_{\mathcal{P}_l}^* = \left\{ \sum_{v \in V_{\mathcal{P}_l}} \lambda_v vv^T : \lambda_v \in \mathbb{R}_+ \right\}.$$

As in the previous section, for a partition $\mathcal{P}$, we denote by $\operatorname{pr}(\mathcal{O}_{\mathcal{P}}^*, A)$ and $\operatorname{pr}(\mathcal{I}_{\mathcal{P}}^*, A)$ the projection of A onto $\mathcal{O}_{\mathcal{P}}^*$ respectively $\mathcal{I}_{\mathcal{P}}^*$.

Although both $\mathcal{I}_{\mathcal{P}}^*$ and $\mathcal{O}_{\mathcal{P}}^*$ are polyhedral cones, neither of them is given by a set of defining inequalities but rather through an "inner" description – in contrast to the approximations $\mathcal{I}_{\mathcal{P}}$ and $\mathcal{O}_{\mathcal{P}}$ of the copositive cone. Therefore, solving even a linear problem over $\mathcal{I}_{\mathcal{P}}^*$ or $\mathcal{O}_{\mathcal{P}}^*$ is not straightforward. However, we can use a dual approach, and instead of projecting the matrix A directly onto $\mathcal{I}_{\mathcal{P}}^*$ respectively $\mathcal{O}_{\mathcal{P}}^*$, we can work with $\mathcal{I}_{\mathcal{P}}$ respectively $\mathcal{O}_{\mathcal{P}}$. This approach uses a decomposition theorem by Moreau (1962) for which we need the concept of the polar cone $\mathcal{K}^\circ$ introduced in Section 2.1.

Theorem 4.3.1 (Moreau) *Let $\mathcal{K}$ be a closed convex cone in $\mathbb{R}^n$. For $x, x_1, x_2 \in \mathbb{R}^n$, the following are equivalent:*

(i) $x = x_1 + x_2$ *with* $x_1 \in \mathcal{K}$, $x_2 \in \mathcal{K}^\circ$ *and* $\langle x_1, x_2 \rangle = 0$,

(ii) $x_1 = \operatorname{pr}(\mathcal{K}, x)$ *and* $x_2 = \operatorname{pr}(\mathcal{K}^\circ, x)$.

The decomposition described in the theorem is illustrated in Figure 4.4.

For any closed convex cone $\mathcal{K}$ we have

$$\operatorname{pr}(\mathcal{K}, -x) = -\operatorname{pr}(-\mathcal{K}, x).$$

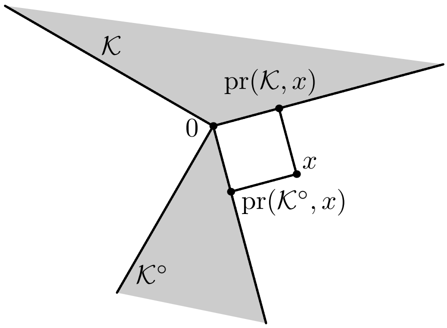

Figure 4.4.: Illustration of Moreau's decomposition theorem

(cf. Hiriart-Urruty and Lemaréchal (1993, Section III.3.2)). Combined with $\mathcal{C}_n^\circ = -\mathcal{C}_n^*$, this gives

$$\operatorname{pr}(\mathcal{C}_n^*, A) = \operatorname{pr}(\mathcal{C}_n, -A) + A.$$

The same holds for the approximating cones, i.e.,

$$\operatorname{pr}(\mathcal{I}_{\mathcal{P}}^*, A) = \operatorname{pr}(\mathcal{I}_{\mathcal{P}}, -A) + A \tag{4.2}$$

and

$$\operatorname{pr}(\mathcal{O}_{\mathcal{P}}^*, A) = \operatorname{pr}(\mathcal{O}_{\mathcal{P}}, -A) + A. \tag{4.3}$$

If $(\mathcal{P}_l)_l$ is a sequence of simplicial partitions of Δ^S with $\delta(\mathcal{P}_l) \to 0$ as $l \to \infty$, then according to Theorem 4.2.1 we have $\operatorname{pr}(\mathcal{I}_{\mathcal{P}_l}, A) \to \operatorname{pr}(\mathcal{C}_n, A)$ and $\operatorname{pr}(\mathcal{O}_{\mathcal{P}_l}, A) \to \operatorname{pr}(\mathcal{C}_n, A)$. This implies

$$\lim_{l\to\infty} \operatorname{pr}(\mathcal{I}_{\mathcal{P}_l}^*, A) = \lim_{l\to\infty} \operatorname{pr}(\mathcal{I}_{\mathcal{P}_l}, -A) + A = \operatorname{pr}(\mathcal{C}_n, -A) + A = \operatorname{pr}(\mathcal{C}_n^*, A)$$

and

$$\lim_{l\to\infty} \operatorname{pr}(\mathcal{O}_{\mathcal{P}_l}^*, A) = \lim_{l\to\infty} \operatorname{pr}(\mathcal{O}_{\mathcal{P}_l}, -A) + A = \operatorname{pr}(\mathcal{C}_n, -A) + A = \operatorname{pr}(\mathcal{C}_n^*, A).$$

So instead of projecting A onto $\mathcal{I}_{\mathcal{P}}^*$ respectively $\mathcal{O}_{\mathcal{P}}^*$ we can project $-A$ onto $\mathcal{I}_{\mathcal{P}}$ respectively $\mathcal{O}_{\mathcal{P}}$, which are again second order cone problems over cones given by a set of defining inequalities.

4.4. Factorization of a completely positive matrix

To the best of our knowledge, no algorithm is known for the problem of finding a factorization of a general completely positive matrix $A = XX^T$. Jarre and

Schmallowsky (2009) present a heuristic algorithm which for a given matrix $A \in \mathcal{S}_n$ determines a matrix $X \in \mathcal{N}_n$ such that either $XX^T = A$ proving that $A \in \mathcal{C}_n^*$, or such that XX^T is in some sense close to A. Bomze (2009) deals with the question of how to extend the factorization of an $n \times n$ matrix A to a factorization of an $(n+1)\times(n+1)$ matrix containing A as a principal submatrix. Dickinson and Dür (2012) study special cases where complete positivity of a matrix can be checked in linear time, and show how to compute a minimal rank one representation if such a matrix is found to be completely positive. While the first approach may stagnate, the second requires knowledge about the factorization of a principal submatrix, and the third one requires a special structure of the matrix, we will show how to use projections to compute a factorization for any matrix A lying in the interior of $\mathcal{C}_n^*$. The basic idea is to find an inner approximation $\mathcal{O}_{\mathcal{P}}^*$ of $\mathcal{C}_n^*$ such that $A \in \mathcal{O}_{\mathcal{P}}^*$, and then use the definition of this $\mathcal{O}_{\mathcal{P}}^*$ to extract a factorization of A.

So consider an $n \times n$ completely positive matrix A. If $\operatorname{pr}(\mathcal{O}_{\mathcal{P}}^*, A) = A$ for some partition $\mathcal{P}$ of the standard simplex, then we have $A \in \mathcal{O}_{\mathcal{P}}^*$ and hence

$$A = \sum_{v \in V_{\mathcal{P}}} \lambda_v v v^T \quad \text{with } \lambda_v \in \mathbb{R}_+. \tag{4.4}$$

Therefore, we can find a nonnegative factorization of A by computing a feasible solution λ_v of (4.4). This can be done by solving a linear optimization problem with an arbitrary (linear) objective function and (4.4) as constraints. Obviously, we are interested in sparse solutions, i.e., we want as few nonzero λ_v's in (4.4) as possible. Now if the linear feasibility problem is solved with the simplex algorithm, then the optimal solution $\bar{\lambda}$ is a vertex of the feasible region and at most $\frac{1}{2}n(n+1)$ of its entries are nonzero. It was shown in Li et al. (2004) that in this case the number of nonzero coefficients can be reduced to $\frac{1}{2}n(n+1) - 1$. But even then, the factorization obtained by this procedure is not necessarily minimal.

Assuming the approximations to be nested, if $A \in \operatorname{int}(\mathcal{C}_n^*)$ and $(\mathcal{P}_l)_l$ is a sequence of simplicial partitions of Δ^S with $\delta(\mathcal{P}_l) \to 0$, then there is an $L \in \mathbb{N}$ such that $A \in \mathcal{O}_{\mathcal{P}_l}^*$ for all $l \geq L$. So for matrices $A \in \operatorname{int}(\mathcal{C}_n^*)$, the procedure described above is finite. For matrices on the boundary of $\mathcal{C}_n^*$, we may not find an inner approximation $\mathcal{O}_{\mathcal{P}}^*$ with $A \in \mathcal{O}_{\mathcal{P}}^*$, even after a large number of iterations. Nevertheless our approach is a substantial progress, since it allows (at least in theory) to find factorizations of arbitrary matrices in $\operatorname{int}(\mathcal{C}_n^*)$.

4.4.1. An illustrative example

We now illustrate our method with a small example. The interior of the completely positive cone has been characterized in Dür and Still (2008) and Dickinson (2010), so we know how to construct a matrix $A \in \operatorname{int}(\mathcal{C}_n^*)$. Consider

$$A = \begin{pmatrix} 2 & 1 & 1 & 1 & 2 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & 2 & 6 & 5 & 1 \\ 1 & 1 & 5 & 6 & 2 \\ 2 & 1 & 1 & 2 & 3 \end{pmatrix}.$$

Since A can be written as

$$A = \begin{pmatrix}1\\1\\1\\1\\1\end{pmatrix}\begin{pmatrix}1\\1\\1\\1\\1\end{pmatrix}^T + \begin{pmatrix}0\\1\\1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\1\\0\\0\end{pmatrix}^T + \begin{pmatrix}0\\0\\2\\2\\0\end{pmatrix}\begin{pmatrix}0\\0\\2\\2\\0\end{pmatrix}^T + \begin{pmatrix}0\\0\\0\\1\\1\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\\1\end{pmatrix}^T + \begin{pmatrix}1\\0\\0\\0\\1\end{pmatrix}\begin{pmatrix}1\\0\\0\\0\\1\end{pmatrix}^T, \tag{4.5}$$

we have $A \in \operatorname{int}(\mathcal{C}_5^*)$ according to Theorem 2.3.3. Furthermore, the factorization (4.5) is minimal. This also follows from Theorem 2.3.3.

We now construct a simplicial partition $\mathcal{P}$ of Δ^S such that $A \in \mathcal{O}_\mathcal{P}^*$, and then we compute a factorization of A with respect to the vertices of this partition. We do this by projecting the matrix onto a sequence of inner approximations of $\mathcal{C}_5^*$ and we attempt to guide the partitioning through the results of the projections.

We start by explaining the partitioning strategy. Observe the following: Since $A \in \mathcal{C}_5^* \subseteq \mathcal{I}_\mathcal{P}^*$, we have $\operatorname{pr}(\mathcal{I}_\mathcal{P}^*, A) = A$. As long as $A \notin \mathcal{O}_\mathcal{P}^*$, we have that $\operatorname{pr}(\mathcal{O}_\mathcal{P}^*, A) \neq A = \operatorname{pr}(\mathcal{I}_\mathcal{P}^*, A)$. According to (4.2) and (4.3), this is equivalent to

$$\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) \neq \operatorname{pr}(\mathcal{I}_\mathcal{P}, -A). \tag{4.6}$$

We claim that then $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) \notin \mathcal{I}_\mathcal{P}$. To see this, observe that $\mathcal{I}_\mathcal{P} \subset \mathcal{O}_\mathcal{P}$ implies

$$\|-A - \operatorname{pr}(\mathcal{O}_\mathcal{P}, -A)\| \leq \|-A - \operatorname{pr}(\mathcal{I}_\mathcal{P}, -A)\|. \tag{4.7}$$

Now assume by contradiction that $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) \in \mathcal{I}_\mathcal{P}$. Then by optimality of $\operatorname{pr}(\mathcal{I}_\mathcal{P}, -A)$ we have

$$\|-A - \operatorname{pr}(\mathcal{O}_\mathcal{P}, -A)\| \geq \|-A - \operatorname{pr}(\mathcal{I}_\mathcal{P}, -A)\|. \tag{4.8}$$

From (4.7) and (4.8) and uniqueness of the projection we get $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) = \operatorname{pr}(\mathcal{I}_\mathcal{P}, -A)$ which is a contradiction to (4.6). Therefore, we have $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) \notin \mathcal{I}_\mathcal{P}$.

By the definition of $\mathcal{I}_\mathcal{P}$ and $\mathcal{O}_\mathcal{P}$, this means that there exists a *violating* edge, i.e., an edge $\{u, v\} \in E_\mathcal{P}$ with

$$u^T \operatorname{pr}(\mathcal{O}_\mathcal{P}, -A)v < 0.$$

This suggests the following strategy to generate partitions: Starting with $\mathcal{P} = \{\Delta^S\}$, after each projection of $-A$ onto $\mathcal{O}_\mathcal{P}$ we refine the current partition by bisecting a longest violating edge. We do this until we have found a partition $\mathcal{P}$ with $u^T \operatorname{pr}(\mathcal{O}_\mathcal{P}, -A)v \geq 0$ for all $\{u, v\} \in E_\mathcal{P}$, which is equivalent to $A \in \mathcal{O}^*_\mathcal{P}$. To see this, first observe that $u^T \operatorname{pr}(\mathcal{O}_\mathcal{P}, -A)v \geq 0$ for all $\{u, v\} \in E_\mathcal{P}$ is equivalent to $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) \in \mathcal{I}_\mathcal{P}$. By (4.7) and (4.8), the latter is equivalent to $\operatorname{pr}(\mathcal{O}_\mathcal{P}, -A) = \operatorname{pr}(\mathcal{I}_\mathcal{P}, -A)$. Applying (4.2) and (4.3), this can be written as $\operatorname{pr}(\mathcal{O}^*_\mathcal{P}, A) = \operatorname{pr}(\mathcal{I}^*_\mathcal{P}, A) = A$ whence $A \in \mathcal{O}^*_\mathcal{P}$.

Strictly speaking, this partitioning strategy does not guarantee $\delta(\mathcal{P}_l) \to 0$, however it seems to work well in numerical tests.

We implemented our approach in Matlab and computed the projections with SeDuMi (Sturm, 1999). For the feasibility problem (4.4) we used the Matlab solver `linprog`. For our example, we obtained a partition with 102 vertices. In the optimal solution of the feasibility problem (4.4), 15 of the coefficients λ_v are nonzero. These nonzero coefficients and the corresponding vertices are

$$\begin{aligned}
v_1 &= \begin{pmatrix}0.0000 & 0.0000 & 0.5000 & 0.5000 & 0.0000\end{pmatrix}, & \lambda_{v_1} &= 13.2572,\\
v_2 &= \begin{pmatrix}0.5000 & 0.0000 & 0.0000 & 0.0000 & 0.5000\end{pmatrix}, & \lambda_{v_2} &= 0.9799,\\
v_3 &= \begin{pmatrix}0.2500 & 0.2500 & 0.2500 & 0.0000 & 0.2500\end{pmatrix}, & \lambda_{v_3} &= 3.6273,\\
v_4 &= \begin{pmatrix}0.1250 & 0.1250 & 0.2500 & 0.2500 & 0.2500\end{pmatrix}, & \lambda_{v_4} &= 2.3089,\\
v_5 &= \begin{pmatrix}0.0000 & 0.2500 & 0.5000 & 0.2500 & 0.0000\end{pmatrix}, & \lambda_{v_5} &= 3.6723,\\
v_6 &= \begin{pmatrix}0.0000 & 0.0000 & 0.2500 & 0.5000 & 0.2500\end{pmatrix}, & \lambda_{v_6} &= 0.9664,\\
v_7 &= \begin{pmatrix}0.5000 & 0.1250 & 0.1250 & 0.0000 & 0.2500\end{pmatrix}, & \lambda_{v_7} &= 3.2720,\\
v_8 &= \begin{pmatrix}0.2500 & 0.3750 & 0.1250 & 0.0000 & 0.2500\end{pmatrix}, & \lambda_{v_8} &= 1.6844,\\
v_9 &= \begin{pmatrix}0.0000 & 0.4375 & 0.3125 & 0.1250 & 0.1250\end{pmatrix}, & \lambda_{v_9} &= 1.9127,\\
v_{10} &= \begin{pmatrix}0.0625 & 0.1875 & 0.3750 & 0.3750 & 0.0000\end{pmatrix}, & \lambda_{v_{10}} &= 2.9066,\\
v_{11} &= \begin{pmatrix}0.1875 & 0.0000 & 0.0625 & 0.3750 & 0.3750\end{pmatrix}, & \lambda_{v_{11}} &= 9.3450,\\
v_{12} &= \begin{pmatrix}0.0000 & 0.1875 & 0.0625 & 0.3750 & 0.3750\end{pmatrix}, & \lambda_{v_{12}} &= 0.8167,
\end{aligned}$$

$$\begin{aligned}
v_{13} &= \begin{pmatrix}0.3750 & 0.1250 & 0.3750 & 0.0000 & 0.1250\end{pmatrix}, & \lambda_{v_{13}} &= 0.1880, \\
v_{14} &= \begin{pmatrix}0.1250 & 0.3750 & 0.3750 & 0.1250 & 0.0000\end{pmatrix}, & \lambda_{v_{14}} &= 4.1370, \\
v_{15} &= \begin{pmatrix}0.1875 & 0.1875 & 0.0625 & 0.1875 & 0.3750\end{pmatrix}, & \lambda_{v_{15}} &= 3.9257.
\end{aligned}$$

The obtained factorization $A = \sum_{i=1}^{15} \lambda_{v_i} v_i v_i^T$ is very different from (4.5). Not only does it need 15 factors instead of 5, it also uses different points $v \in \Delta^S$. Only (scaled versions of) v_1 and v_2 can be found in the original factorization (4.5).

It is possible to reconstruct the original factorization with the above procedure, but this needs prior knowledge of the desired result. The following partitioning shows how this can be achieved: Start with the standard simplex $\Delta^S = \text{conv}(\{e_1, \dots, e_5\})$ and successively construct the bisection points

$$\begin{aligned}
w_1 &= \tfrac{1}{2}(e_2 + e_3) &&= \begin{pmatrix}0.00 & 0.50 & 0.50 & 0.00 & 0.00\end{pmatrix}, \\
w_2 &= \tfrac{1}{2}(e_3 + e_4) &&= \begin{pmatrix}0.00 & 0.00 & 0.50 & 0.50 & 0.00\end{pmatrix}, \\
w_3 &= \tfrac{1}{2}(e_4 + e_5) &&= \begin{pmatrix}0.00 & 0.00 & 0.00 & 0.50 & 0.50\end{pmatrix}, \\
w_4 &= \tfrac{1}{2}(e_1 + e_5) &&= \begin{pmatrix}0.50 & 0.00 & 0.00 & 0.00 & 0.50\end{pmatrix}, \\
w_5 &= \tfrac{1}{2}(w_1 + w_3) &&= \begin{pmatrix}0.00 & 0.25 & 0.25 & 0.25 & 0.25\end{pmatrix}, \\
w_6 &= \tfrac{1}{5}e_1 + \tfrac{4}{5}w_5 &&= \begin{pmatrix}0.20 & 0.20 & 0.20 & 0.20 & 0.20\end{pmatrix}.
\end{aligned}$$

For the resulting partition $\mathcal{P}$ with 11 vertices it turns out that $A \in \mathcal{O}_{\mathcal{P}}^*$, and we get a factorization with only 5 nonzero coefficients:

$$A = 4w_1w_1^T + 16w_2w_2^T + 4w_3w_3^T + 4w_4w_4^T + 25w_6w_6^T.$$

This factorization corresponds to the factorization of A in (4.5). Adapting the partitioning strategy in this way was possible since we know how A was constructed. Guiding the partitioning in an efficient way would be desirable since the subdivision strategy has a crucial influence on the number of iterations. For general matrices, however, finding a suitable partitioning strategy seems a difficult problem.

5. Standard quadratic optimization problems

In this chapter, we study the standard quadratic optimization problem, which will be introduced in Section 5.1. As we have seen in Section 3.2, the problem can be reformulated as a completely positive respectively copositive program. In Section 5.2, we show that for special classes of objective functions, the relaxation resulting from replacing the completely positive respectively copositive cone in the conic reformulation by a tractable one is exact. Based on these results, in Section 5.3, we construct two algorithms to solve standard quadratic optimization problems.

Since for $n \leq 4$, every copositive and completely positive program can be reformulated as a positive semidefinite program, the smallest dimension where hard instances appear is $n = 5$. In Section 5.4, we will consider this case in more detail and try two different approaches to handle the problem. Finally, in Section 5.5, we study more general quadratic programs.

5.1. The standard quadratic optimization problem

Recall that the standard quadratic optimization problem (StQP) consists of minimizing a quadratic function over the standard simplex, i.e.,

$$\begin{array}{ll} \min & x^T Q x \\ \text{s. t.} & e^T x = 1 \\ & x \geq 0, \end{array} \qquad \text{(StQP)}$$

where Q is a symmetric $n \times n$ matrix. In the following, we denote an optimal solution of (StQP) by $\bar{x}$ and the corresponding objective value by $\bar{y}$. Solving general standard quadratic optimization problems is an NP-hard problem. This follows from the fact that the maximum clique problem can be written as a standard quadratic optimization problem (cf. Bomze (1998)).

As stated for example in Bomze (1998), the standard quadratic optimization problem is shift-invariant, i.e., we have the following.

Lemma 5.1.1 *The minimizers of (StQP) remain the same if Q is replaced by $Q + cE$, $c \in \mathbb{R}$.*

Proof Let $x \in \Delta^S$ and $c \in \mathbb{R}$. Then

$$x^T(Q + cE)x = x^TQx + cx^Tee^Tx = x^TQx + c. \qquad \square$$

We have seen in Section 3.2 that the standard quadratic optimization problem has an exact reformulation as a completely positive optimization problem. This reformulation is of the form

$$\begin{array}{ll} \min & \langle Q, X\rangle \\ \text{s.t.} & \langle E, X\rangle = 1 \\ & X \in \mathcal{C}_n^*. \end{array} \tag{$\mathrm{P}_{\mathcal{C}^*}$}$$

The dual of problem ($\mathrm{P}_{\mathcal{C}^*}$) is

$$\begin{array}{ll} \max & y \\ \text{s.t.} & Q - yE \in \mathcal{C}_n. \end{array} \tag{$\mathrm{P}_{\mathcal{C}}$}$$

Note that for $y < \min\{Q_{ij} : i, j = 1, \ldots, n\}$ the matrix $Q - yE$ is positive and lies thus in the interior of $\mathcal{C}_n$. Furthermore, the matrix $B = \frac{1}{n^2+n}(E + I)$ is feasible for ($\mathrm{P}_{\mathcal{C}^*}$), and by Theorem 2.3.3 we have $B \in \operatorname{int}(\mathcal{C}_n^*)$. By the strong conic duality theorem (cf. Theorem 3.1.2), we thus know that the optimal values of ($\mathrm{P}_{\mathcal{C}^*}$) and ($\mathrm{P}_{\mathcal{C}}$) are attained and equal (cf. Bomze et al. (2012)).

5.1.1. Optimal solutions

It is easy to see that any convex combination of matrices xx^T, where x is an optimal solution of (StQP), is optimal for ($\mathrm{P}_{\mathcal{C}^*}$). We now assume that we have an optimal solution $\bar{X}$ of ($\mathrm{P}_{\mathcal{C}^*}$) and want to derive an optimal solution of (StQP).

Proposition 5.1.2 *Let $\bar{X}$ be an optimal solution of problem ($\mathrm{P}_{\mathcal{C}^*}$). Then for any factorization $\bar{X} = \sum_{i=1}^m x_i x_i^T$ with $x_i \geq 0$, $x_i \neq 0$ for all $i = 1, \ldots, m$, the vector $\frac{1}{e^T x_i} x_i$ is an optimal solution of (StQP).*

Proof Let $\bar{X}$ be optimal for ($\mathrm{P}_{\mathcal{C}^*}$). Then $\bar{X}$ is completely positive which means that it can be written as

$$\bar{X} = \sum_{i=1}^m x_i x_i^T \tag{5.1}$$

with $x_i \geq 0$, $x_i \neq 0$ for all $i = 1, \dots, m$. Furthermore, from the linear constraint we get

$$\langle E, \bar{X} \rangle = \sum_{i=1}^{m} (e^T x_i)^2 = 1. \tag{5.2}$$

Defining $z_i = \frac{1}{e^T x_i} x_i$ and $\mu_i = (e^T x_i)^2$, $i = 1, \dots, m$, we have

$$\bar{X} = \sum_{i=1}^{m} (e^T x_i)^2 \big(\frac{1}{e^T x_i} x_i\big)\big(\frac{1}{e^T x_i} x_i\big)^T = \sum_{i=1}^{m} \mu_i z_i z_i^T. \tag{5.3}$$

The coefficients μ_i are all positive and by (5.2) we have $\sum_{i=1}^m \mu_i = 1$. Consequently, $\bar{X}$ is a convex combination of the matrices $z_i z_i^T$, and by definition all vectors z_i are feasible for (StQP). This means that $z_i^T Q z_i \geq \bar{y}$ for all $i = 1, \dots, m$, where $\bar{y}$ denotes the optimal value of (StQP).

We now want to show that the vectors z_i are also all optimal. We assume by contradiction that z_j is not optimal for some $j \in \{1, \dots, m\}$, i.e., $z_j^T Q z_j > \bar{y}$. Then

$$\langle Q, \bar{X} \rangle = \sum_{i \neq j} \mu_i \underbrace{z_i^T Q z_i}_{\geq \bar{y}} + \mu_j \underbrace{z_j^T Q z_j}_{> \bar{y}} > (1 - \mu_j)\bar{y} + \mu_j \bar{y} = \bar{y}$$

which contradicts optimality of $\bar{X}$. Consequently, for any factorization $\bar{X} = \sum_{i=1}^m x_i x_i^T$ with $x_i \geq 0$, $x_i \neq 0$, $i = 1, \dots, m$, we have that the vectors $\frac{1}{e^T x_i} x_i$ are optimal for (StQP). □

Note that, unless Q is a multiple of E, an optimal solution $\bar{X}$ of (P$_{\mathcal{C}^*}$) necessarily lies on the boundary of $\mathcal{C}_n^*$. Therefore, the procedure of Section 4.4 does not necessarily produce a factorization of $\bar{X}$. Hence, it is not clear how to compute the vectors x_i respectively $z_i = \frac{1}{e^T x_i} x_i$.

In the special case of $\bar{X}$ being of rank one, we have $\bar{X} = xx^T$ with $x \geq 0$ and $(e^T x)^2 = 1$ implying $e^T x = 1$. This means that the vector x lies in the feasible set of (StQP), and since problem (P$_{\mathcal{C}^*}$) and (StQP) have the same optimal value, it follows that x is also optimal for (StQP). We can compute x by multiplying $\bar{X}$ with the all-ones vector, i.e., we have $\bar{X} = xx^T$ with $x \in \Delta^S$ implying $\bar{X}e = xx^T e = x$. We have thus shown the following.

Proposition 5.1.3 *If an optimal solution $\bar{X}$ of (P$_{\mathcal{C}^*}$) is of rank one, then $\bar{X}e$ is an optimal solution of (StQP).*

Note that problem (P$_{\mathcal{C}^*}$) has at least one optimal solution of rank one: By linearity of the objective function in (P$_{\mathcal{C}^*}$), an optimal solution $\bar{X}$ of this problem is attained at an extreme point of the feasible set, and by Lemma 3.2.1, this solution is a rank one matrix.

If, on the other hand, $\bar{X}$ has rank $r > 1$, then for any factorization of the form (5.1) we have $m \geq 2$. We now want to analyze whether in that case $\bar{X}e$ is still optimal for (StQP). As we have seen above, we can rewrite any factorization of $\bar{X}$ of the form (5.1) as convex combination of rank one matrices $z_i z_i^T$ with $z_i \in \Delta^S$ as in (5.3). Therefore, we have

$$\bar{X}e = \sum_{i=1}^{m} \mu_i z_i z_i^T e = \sum_{i=1}^{m} \mu_i z_i.$$

This shows that $\bar{X}e$ can be written as convex combination of vectors $z_i \in \Delta^S$, $i = 1, \ldots, m$, and that $\bar{X}e$ is thus feasible for (StQP). Consequently, we have

$$(\bar{X}e)^T Q(\bar{X}e) \geq \bar{y}.$$

If the objective function of (StQP) is convex, we also have

$$(\bar{X}e)^T Q(\bar{X}e) = \big(\sum_{i=1}^{r} \mu_i z_i\big)^T Q\big(\sum_{i=1}^{r} \mu_i z_i\big) \leq \sum_{i=1}^{r} \mu_i z_i^T Q z_i = \langle Q, \bar{X}\rangle = \bar{y}$$

and thus optimality of $\bar{X}e$. This result is stated in the following proposition.

Proposition 5.1.4 *If (StQP) has a convex objective function and $\bar{X}$ is an optimal solution of ($P_{\mathcal{C}^*}$), then $\bar{X}e$ is an optimal solution of (StQP).*

If, however, the quadratic form is not convex, then in general $\bar{X}e$ is not optimal for (StQP). To see this, we consider the 2×2 matrix $Q = -I$. Then $\bar{X} = \frac{1}{2}I$ is an optimal solution of ($P_{\mathcal{C}^*}$) with $\bar{y} = -1$ but $(\bar{X}e)^T Q(\bar{X}e) = -\frac{1}{2} > \bar{y}$ which shows that $\bar{X}e$ is not optimal for (StQP).

5.2. Relaxations

Since standard quadratic optimization problems are hard to solve in general, we study relaxations of the completely positive reformulation ($P_{\mathcal{C}^*}$) and the copositive reformulation ($P_{\mathcal{C}}$) resulting from replacing $\mathcal{C}_n^*$ respectively $\mathcal{C}_n$ by a tractable cone. In Section 5.2.1 we consider special problem classes for which such a relaxation can be shown to be exact and in Section 5.2.2, we show under which conditions we can derive an optimal solution $\bar{x}$ of (StQP) from an optimal solution $\bar{X}$ of an exact relaxation of ($P_{\mathcal{C}^*}$).

5.2.1. Special classes of objective functions

Replacing $\mathcal{C}_n$ in problem ($\mathrm{P}_{\mathcal{C}}$) by a tractable cone like $\mathcal{N}_n$, $\mathcal{S}_n^+$ or $\mathcal{S}_n^+ + \mathcal{N}_n$ results in a linear respectively semidefinite program providing a lower bound for the original problem. Depending on properties of the matrix Q in the objective function, we will exhibit cases when the solutions of these problems provide not only bounds but give the exact optimal value of ($\mathrm{P}_{\mathcal{C}}$) and thus of (StQP). On the dual side, this corresponds to replacing the completely positive cone in ($\mathrm{P}_{\mathcal{C}^*}$) by $\mathcal{N}_n$, $\mathcal{S}_n^+$ respectively $\mathcal{S}_n^+ \cap \mathcal{N}_n$ yielding a relaxation of the completely positive program. By the conic duality theorem, if replacing the copositive cone in ($\mathrm{P}_{\mathcal{C}}$) by $\mathcal{N}_n$, $\mathcal{S}_n^+$ respectively $\mathcal{S}_n^+ + \mathcal{N}_n$ results in an equivalent problem then the corresponding dual problem is an exact relaxation of ($\mathrm{P}_{\mathcal{C}^*}$).

5.2.1.1. Diagonal matrices

We assume that Q is a diagonal matrix with $Q_{11} \geq Q_{22} \geq \ldots \geq Q_{nn}$. First we consider the case $Q_{nn} \leq 0$.

Proposition 5.2.1 *If $Q_{nn} \leq 0$, then $Q - \bar{y}E \in \mathcal{N}_n$.*

Proof We will show that $\bar{y} = Q_{nn}$. Clearly, $\bar{y} \leq Q_{nn}$ since otherwise $(Q - \bar{y}E)_{nn} < 0$ which contradicts copositivity of this matrix. On the other hand, we have $Q_{ij} \geq Q_{nn}$ for all $1 \leq i, j \leq n$ which implies $Q - Q_{nn}E \in \mathcal{N}_n \subseteq \mathcal{C}_n$. Therefore, we have $\bar{y} = Q_{nn}$. □

Remark 5.2.2 If $Q_{nn} = 0$, we have $Q - \bar{y}E = Q$ which implies that the matrix is positive semidefinite as well as nonnegative.

We now consider the case $Q_{nn} > 0$. Note that in that case Q is positive semidefinite which means that (StQP) is a convex optimization problem. The following result is a special case of a result of Anstreicher and Burer (2005) (cf. Proposition 5.2.7).

Proposition 5.2.3 *If $Q_{nn} > 0$, then $Q - \bar{y}E \in \mathcal{S}_n^+$.*

Proof Note that Q being a diagonal matrix with $Q_{11} \geq Q_{22} \geq \ldots \geq Q_{nn} > 0$ implies that Q is nonnegative and thus copositive. Consequently, we have $\bar{y} \geq 0$ implying that the copositive matrix $Q - \bar{y}E$ has only nonpositive off-diagonal entries. By Proposition 2.2.15, we can conclude that the matrix is positive semidefinite. □

We now want to determine the optimal value $\bar{y}$. To this end, we will apply the copositivity criterion of Theorem 2.2.13 to a sequence of principal submatrices of $Q - yE$. Note that under the assumption of Q being a diagonal matrix with $Q_{11} \geq Q_{22} \geq \ldots \geq Q_{nn} > 0$, we have $\bar{y} \geq 0$ and thus $b = -\bar{y}e^T \leq 0$. We can therefore apply the reduced criterion of Corollary 2.2.14 to show the following.

Proposition 5.2.4 *If Q is a diagonal matrix with diagonal entries $Q_{11} \geq Q_{22} \geq \ldots, Q_{nn} > 0$, then the optimal value $\bar{y}$ of (StQP) can be computed recursively, i.e., we have $\bar{y} = \bar{y}_1$, where $\bar{y}_n = Q_{nn}$ and $\bar{y}_i = (\bar{y}_{i+1}Q_{ii})/(\bar{y}_{i+1} + Q_{ii})$ for $i = n-1, \ldots, 1$.*

Proof For $1 \leq i \leq n$, we denote by $(Q - yE)^{(i)}$ the submatrix of $Q - yE$ consisting of the rows and columns $i, \ldots, n$ and consider these matrices for $i = n, n-1, \ldots, 1$. Furthermore, we denote by $\bar{y}_i$ the maximum value of y for which $(Q - yE)^{(i)}$ is copositive. Starting with $(Q - yE)^{(n)} = (Q_{nn} - y)$, we immediately get $\bar{y}_n = Q_{nn}$. Applying Corollary 2.2.14 to the following partitions of $(Q - yE)^{(i)}$, $i = n-1, \ldots, 1$,

$$(Q - yE)^{(i)} = \begin{pmatrix} Q_{ii} - y & -ye^T \\ -ye & (Q - yE)^{(i+1)} \end{pmatrix},$$

we have that $\bar{y}_i = \min\{Q_{ii}, \hat{y}_i\}$, where $\hat{y}_i$ is the maximum value of y such that

$$(Q_{ii} - y)(Q - yE)^{(i+1)} - y^2 E$$

is copositive. Note that for $y = Q_{ii}$ we have

$$(Q_{ii} - y)(Q - yE)^{(i+1)} - y^2 E = -y^2 E = -Q_{ii}^2 E$$

which is not copositive since by assumption $Q_{ii} > 0$. This shows that $\hat{y}_i < Q_{ii}$ and thus $\bar{y}_i = \hat{y}_i$. Moreover, for $y < Q_{ii}$ we have $\frac{1}{Q_{ii} - y} > 0$ which means that copositivity of

$$(Q_{ii} - y)(Q - yE)^{(i+1)} - y^2 E$$

is equivalent to copositivity of

$$(Q - yE)^{(i+1)} - \frac{y^2}{Q_{ii} - y} E = \left(Q - \frac{y(Q_{ii} - y) + y^2}{Q_{ii} - y} E\right)^{(i+1)}.$$

This matrix is copositive if

$$\frac{y(Q_{ii} - y) + y^2}{Q_{ii} - y} \leq \bar{y}_{i+1}$$

which is equivalent to

$$y \leq \frac{\bar{y}_{i+1} Q_{ii}}{\bar{y}_{i+1} + Q_{ii}} .$$

Since $\hat{y}_i$ denotes the maximum value of y such that $(Q_{ii} - y)(Q - yE)^{(i+1)} - y^2 E$ is copositive, we can conclude that

$$\hat{y}_i = \frac{\bar{y}_{i+1} Q_{ii}}{\bar{y}_{i+1} + Q_{ii}} .$$

Therefore, we have

$$\bar{y}_i = \min\{Q_{ii}, \frac{\bar{y}_{i+1} Q_{ii}}{\bar{y}_{i+1} + Q_{ii}}\} = \frac{\bar{y}_{i+1} Q_{ii}}{\bar{y}_{i+1} + Q_{ii}} .$$

Recursively, we get $\bar{y} = \bar{y}_1$, where $\bar{y}_n = Q_{nn}$ and $\bar{y}_i = (\bar{y}_{i+1} Q_{ii})/(\bar{y}_{i+1} + Q_{ii})$ for $i = n-1, \ldots, 1$. □

Remark 5.2.5 The same result can be obtained by applying the preprocessing described in Bomze and Locatelli (2012, Section 3.1) which applies to standard quadratic optimization problems with a separable objective function $Q = D + \frac{1}{2}(ce^T + ec^T)$ where D is a diagonal matrix with $0 < D_{ii} \leq D_{jj}$ for some $i \neq j$, $c \in \mathbb{R}^n$ and $c_i = c_j$. In that case, the problem can be reduced to a standard quadratic optimization problem with a separable objective function in $\mathbb{R}^{n-1}$, i.e., the problem can be rewritten as

$$\begin{array}{ll} \min & x^T \tilde{Q} x \\ \text{s. t.} & e^T x = 1 \\ & x \geq 0, \end{array}$$

with $\tilde{Q} = \tilde{D} + \frac{1}{2}(\tilde{c}e^T + e\tilde{c}^T)$ where $\tilde{c} = (c_i, c_{[i,j]}^T)^T$ and

$$\tilde{D} = \begin{pmatrix} \frac{D_{ii} D_{jj}}{D_{ii} + D_{jj}} & 0 \\ 0 & D_{[i,j]} \end{pmatrix},$$

with $c_{[i,j]}$ resulting from c by deleting the i-th and j-th entry and $D_{[i,j]}$ denoting the principal submatrix of D resulting from deleting the i-th and j-th row and column.

Since we have $c_i = 0$ for all $i \in \{1, \ldots, n\}$, the procedure can be applied $n - 1$ times until we have a problem of dimension one and can immediately deduce the optimal value.

5.2.1.2. Positive semidefinite matrices

As stated in Anstreicher and Burer (2005), for positive semidefinite matrices we have the following result.

Proposition 5.2.6 *For $Q \in \mathcal{S}_n^+$ problem (StQP) is equivalent to the Shor relaxation*

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s. t.} \quad & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{S}_{n+1}^+ \\ & x \in \Delta^S. \end{aligned} \tag{Shor}$$

Proof Let $\bar{y}$ and $\bar{y}_{\mathrm{S}}$ denote the optimal solution values of (StQP) and (Shor) respectively. An optimal solution $\bar{x}$ of (StQP) gives a feasible solution (x, X) of (Shor) by setting $x = \bar{x}$ and $X = \bar{x}\bar{x}^T$. Since the corresponding solution value equals $\bar{y}$, we obviously have $\bar{y}_{\mathrm{S}} \leq \bar{y}$.

We now want to show that $\bar{y} \leq \bar{y}_{\mathrm{S}}$. To this let $(\bar{x}_{\mathrm{S}}, \bar{X}_{\mathrm{S}})$ denote an optimal solution of (Shor). We assume by contradiction $\bar{y}_{\mathrm{S}} < \bar{y}$ which can equivalently be written as $\langle Q, \bar{X}_{\mathrm{S}} - \bar{x}\bar{x}^T \rangle < 0$, thus $\langle Q, \bar{X}_{\mathrm{S}} - xx^T \rangle < 0$ for all $x \in \Delta^S$. Since by assumption Q is positive semidefinite, this implies $\bar{X}_{\mathrm{S}} - xx^T \notin \mathcal{S}_n^+$ for all $x \in \Delta^S$ which contradicts feasibility of $(\bar{x}_{\mathrm{S}}, \bar{X}_{\mathrm{S}})$. Therefore we have $\bar{y} \leq \bar{y}_{\mathrm{S}}$ and thus equivalence of (StQP) and the Shor relaxation. □

We now want to consider the reformulation $(\mathrm{P}_{\mathcal{C}})$ of the standard quadratic optimization problem and the question if for $Q \in \mathcal{S}_n^+$ we can replace $\mathcal{C}_n$ by a computationally tractable cone. Anstreicher and Burer (2005) have shown that for positive semidefinite Q, the relaxation resulting from replacing the completely positive cone in $(\mathrm{P}_{\mathcal{C}^*})$ by $\mathcal{S}_n^+ \cap \mathcal{N}_n$ is equivalent to $(\mathrm{P}_{\mathcal{C}^*})$. Let $A = Q - yE$ for some $y < \min\{Q_{ij} : i, j = 1, \ldots, n\}$ and let $B = \frac{1}{n^2+n}(E + I)$. By Lemma 2.1.10, A is strictly feasible for the relaxation of $(\mathrm{P}_{\mathcal{C}})$ resulting from replacing $\mathcal{C}_n$ by $\mathcal{S}_n^+ + \mathcal{N}_n$, and B is strictly feasible for the doubly nonnegative relaxation of $(\mathrm{P}_{\mathcal{C}^*})$. We can thus apply the strong conic duality theorem to conclude the following.

Proposition 5.2.7 *If Q is positive semidefinite, then $Q - \bar{y}E \in \mathcal{S}_n^+ + \mathcal{N}_n$.*

We cannot reduce $\mathcal{S}_n^+ + \mathcal{N}_n$ to one of the two cones $\mathcal{S}_n^+$ or $\mathcal{N}_n$, since in general $Q \in \mathcal{S}_n^+$ does neither imply $Q - \bar{y}E \in \mathcal{S}_n^+$ nor $Q - \bar{y}E \in \mathcal{N}_n$ as the following two examples show.

Example 5.2.8 We consider the standard quadratic optimization problem whose objective function is given by the matrix

$$Q = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix} \in \mathcal{S}_2^{++}.$$

The optimal solution of (StQP) is $\bar{x} = (0,1)^T$ with objective function value $\bar{y} = 1$. However, the matrix

$$Q - \bar{y}E = \begin{pmatrix} 4 & 1 \\ 1 & 0 \end{pmatrix}$$

is not positive semidefinite.

Example 5.2.9 Consider the following positive definite matrix

$$Q = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \in \mathcal{S}_2^{++}.$$

The optimal solution of the corresponding (StQP) is $\bar{x} = (0.5, 0.5)^T$ with objective function value $\bar{y} = 0.5$. The matrix

$$Q - \bar{y}E = \begin{pmatrix} 1.5 & -1.5 \\ -1.5 & 1.5 \end{pmatrix}$$

does not lie in the nonnegative cone.

Note that any completely positive matrix is positive semidefinite. Therefore, the results of this section also apply to standard quadratic optimization problems with $Q \in \mathcal{C}_n^*$.

5.2.1.3. Negative semidefinite matrices

If Q is negative semidefinite, then the associated quadratic form is a concave function and by the following lemma, the optimal value of (StQP) is the lowest entry of Q along the diagonal.

Lemma 5.2.10 *The minimum of a concave function over a compact convex set $\mathcal{K}$ is attained at an extreme point of $\mathcal{K}$.*

For a proof, see Rockafellar (1970, Corollary 32.3.1).

Since the extreme points of the standard simplex are the vertices e_i, $i = 1, \dots, n$, this means that

$$\bar{y} = \min\{Q_{ii} : i = 1, \dots, n\},$$

and if j is such that $Q_{jj} = \bar{y}$, then e_j is an optimal solution. We deduce the following result.

Proposition 5.2.11 *If Q is negative semidefinite, then $Q - \bar{y}E \in \mathcal{N}_n$.*

Proof Let Q_{ii} denote the lowest entry of Q along the diagonal implying $\bar{y} = Q_{ii}$ according to Lemma 5.2.10. Then $Q_{kl} \geq Q_{ii}$ for all $1 \leq k, l \leq n$, since otherwise the quadratic form takes a positive value for $x = e_k - e_l$ which contradicts the assumption that Q is negative semidefinite. Consequently, we have $Q - \bar{y}E = Q - Q_{ii}E \in \mathcal{N}_n$. □

5.2.1.4. Interior matrices

A matrix $Q \in \mathcal{S}_n$ is said to be *interior* if the corresponding (StQP) has an optimal solution $\bar{x}$ which lies in the interior of the standard simplex, i.e., $\bar{x}$ has no zero entries. The problem can have other optimal solutions having zero entries. As in Johnson and Reams (2008), consider for example the matrix

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

Then the standard quadratic optimization problem with Q in the objective function has $(\frac{1}{4}, \frac{1}{2}, \frac{1}{4})^T$ as optimal solution which implies that the matrix is interior, although the point $(\frac{1}{2}, \frac{1}{2}, 0)^T$ is also optimal.

We will use the following result about copositive interior matrices.

Lemma 5.2.12 (Johnson and Reams (2008, Corollary 2)) *If a matrix is copositive and interior, then it is positive semidefinite.*

With this result we can prove the following.

Proposition 5.2.13 *If Q is interior, then $Q - \bar{y}E \in \mathcal{S}_n^+$.*

Proof Let Q be interior. Then, by Lemma 5.1.1, the copositive matrix $Q - \bar{y}E$ is also interior since it has the same minimizers as Q. Thus it is positive semidefinite according to Lemma 5.2.12. □

Note that every diagonal matrix with $Q_{nn} > 0$ is interior. Therefore, the result is a generalization of Proposition 5.2.3.

5.2.1.5. Rank one matrices

We consider the case that Q is a rank one matrix, i.e., $Q = qq^T$ for some $q \in \mathbb{R}^n$. Our treatment of this case differs from the other special cases described before in the sense that we do not use reformulation ($\mathrm{P}_{\mathcal{C}}$) but show how problem (StQP) can be transformed into a linear program. To this end, we take a look at the objective function. We want to minimize

$$x^TQx = x^Tqq^Tx = (q^Tx)^2.$$

The value of $(q^Tx)^2$ is minimal if and only if $|q^Tx|$ is minimal. To minimize $|q^Tx|$, we introduce a variable $z \in \mathbb{R}$ and solve the following linear program

$$\begin{array}{ll} \min & z \\ \text{s.t.} & z \geq q^Tx \\ & z \geq -q^Tx \\ & x \in \Delta^S. \end{array} \tag{5.4}$$

If $(\bar{x}, \bar{z})$ is an optimal solution of (5.4), then $\bar{x}$ is a minimizer of (StQP) and the optimal value of (StQP) is $\bar{z}^2 = (q^T\bar{x})^2 = \bar{x}^TQ\bar{x}$.

5.2.1.6. Some other classes of objective functions

We want to consider some more special classes of objective functions. Since standard quadratic optimization problems are shift invariant, we can perturb every matrix Q such that it is nonnegative, i.e. we consider $Q + cE$ with $c \geq \max\{-Q_{ij} : i, j = 1, \dots, n\}$. This shows that assuming Q to be nonnegative is no restriction.

For any cone $\mathcal{K} \subsetneq \mathcal{C}_n$ there is a copositive matrix $Q \notin \mathcal{K}$, and we have $Q + cE \in \mathcal{N}_n$. This shows that for $Q \in \mathcal{N}_n$ replacing the copositive cone in ($\mathrm{P}_{\mathcal{C}}$) by a cone $\mathcal{K} \subsetneq \mathcal{C}_n$ does not yield an exact reformulation of the problem. Therefore, for $Q \in \mathcal{N}_n$ there is in general no exact reformulation of ($\mathrm{P}_{\mathcal{C}^*}$) resulting from replacing the completely positive cone by some tractable cone $\mathcal{K} \supsetneq \mathcal{C}_n^*$. Consequently, the same is true for a general matrix $Q \in \mathcal{S}_n^+ + \mathcal{N}_n$. Since any nonnegative matrix is copositive, the same holds for $Q \in \mathcal{C}_n$, i.e., for $Q \in \mathcal{C}_n$, there is in general no tractable exact reformulation of ($\mathrm{P}_{\mathcal{C}^*}$).

We now consider the cones $\mathcal{K}_n^r$ of Parrilo's approximation hierarchy (cf. Section 2.4.2). By similar reasoning, we can show that if $Q \in \mathcal{K}_n^r$, $r \in \mathbb{N}$, replacing the copositive cone in ($\mathrm{P}_{\mathcal{C}}$) by $\mathcal{K}_n^r$ does not yield an exact reformulation of the problem. For any $r \in \mathbb{N}$, there is a copositive matrix Q which does not lie in $\mathcal{K}_n^r$. The perturbed matrix $Q + cE$ with $c = \max\{-Q_{ij} : i, j = 1, \dots, n\}$ is nonnegative and is thus an element of $\mathcal{K}_n^r$ for all $r \in \mathbb{N}$ by

$$Q + cE \in \mathcal{N}_n \subseteq \mathcal{S}_n^+ + \mathcal{N}_n = \mathcal{K}_n^0 \subseteq \mathcal{K}_n^r \quad \text{for all } r \in \mathbb{N}.$$

This shows that we cannot replace the copositive cone in problem $(\mathrm{P}_{\mathcal{C}})$ by $\mathcal{K}_n^r$ since $Q \notin \mathcal{K}_n^r$.

5.2.2. Deriving an optimal solution for the standard quadratic optimization problem

We have seen in Section 5.1.1 that if $\bar{X}$ is an optimal solution of $(\mathrm{P}_{\mathcal{C}^*})$ and the quadratic form $x^T Q x$ is convex on Δ^S, then $\bar{X}e$ is optimal for (StQP). The same holds for general instances if $\bar{X}$ is of rank one. If replacing the completely positive cone by a tractable cone yields an exact relaxation of $(\mathrm{P}_{\mathcal{C}^*})$, this means that solving this relaxation gives us the optimal value of (StQP). But the corresponding optimal solution $\bar{X}$ is not necessarily completely positive. Therefore, the question arises if $\bar{X}e$ is feasible for (StQP), and under which conditions it is also optimal.

In the following, we assume that $\bar{X}$ is an optimal solution of

$$\begin{array}{ll} \min & \langle Q, X\rangle \\ \text{s.t.} & \langle E, X\rangle = 1 \\ & X \in \mathcal{S}_n^+ \cap \mathcal{N}_n \end{array} \qquad (\mathrm{P}_{\mathcal{S}^+\cap\mathcal{N}})$$

and that $(\mathrm{P}_{\mathcal{S}^+\cap\mathcal{N}})$ is an exact relaxation of $(\mathrm{P}_{\mathcal{C}^*})$. As we have seen in Section 5.2.1, this holds for example if Q is a diagonal matrix, an interior matrix, or if it is positive or negative semidefinite.

First note that $\langle E, \bar{X}\rangle = 1$ is equivalent to $e^T(\bar{X}e) = 1$. Since $\bar{X}$ is nonnegative we have $\bar{X}e \geq 0$, and consequently, $\bar{X}e$ is feasible for (StQP).

We first consider the case that $\bar{X}$ is a rank one matrix. Since $\bar{X}$ is positive semidefinite, we have $\bar{X} = xx^T$ for some $x \in \mathbb{R}^n$. By nonnegativity of $\bar{X}$, the vector x is either nonnegative or nonpositive. Since the matrix xx^T is the same in both cases, we can assume x to be nonnegative. Consequently, $\bar{X}$ is optimal for $(\mathrm{P}_{\mathcal{C}^*})$ and, as shown in Section 5.1.1, $\bar{X}e = x$ is optimal for (StQP). This result is stated in the following proposition.

Proposition 5.2.14 *Assume that $(P_{\mathcal{S}^+\cap\mathcal{N}})$ is an exact relaxation of $(P_{\mathcal{C}^*})$. If an optimal solution $\bar{X}$ of $(P_{\mathcal{S}^+\cap\mathcal{N}})$ is of rank one, then $\bar{X}e$ is an optimal solution of (StQP).*

We now assume that $\bar{X}$ has rank $r \geq 2$. To analyze optimality of $\bar{X}e$ we will use the following lemma (Tian, 2012, Theorem 50).

Lemma 5.2.15 *Let $A \in \mathcal{S}_n^{++}$, $b \in \mathbb{R}^n$ and $B = bb^T$. If a nonzero matrix $X \in \mathcal{S}_n$ with* $\operatorname{rank}(X) = r$ *satisfies*

$$\begin{aligned} \langle A, X \rangle &\leq 1 \\ \langle B, X \rangle &= 1 \\ X &\in \mathcal{S}_n^+, \end{aligned}$$

then there exists a decomposition $X = \sum_{i=1}^r \mu_i x_i x_i^T$ with $\sum_{i=1}^r \mu_i = 1$ and $\mu_i > 0$, $x_i^T A x_i \leq 1$, $b^T x_i = 1$ for all $i = 1, \ldots, r$.

To apply the lemma we set $b = e$ and $B = ee^T$. Furthermore, we have to find a matrix $A \in \mathcal{S}_n^{++}$ such that adding $\langle A, X \rangle \leq 1$ to the constraints of $(\mathrm{P}_{\mathcal{S}^+ \cap \mathcal{N}})$ does not change the feasible set. Note that $\langle E, X \rangle = 1$ and $X \in \mathcal{N}_n$ implies $\langle I, X \rangle \leq 1$. We can thus set $A = I$. Then by Lemma 5.2.15, there exists a decomposition $\bar{X} = \sum_{i=1}^r \mu_i x_i x_i^T$ with $\sum_{i=1}^r \mu_i = 1$ and $\mu_i > 0$, $x_i^T I x_i \leq 1$, $e^T x_i = 1$ for all $i = 1, \ldots, r$, where r is the rank of $\bar{X}$. Consequently, we have

$$\bar{X}e = \sum_{i=1}^r \mu_i x_i x_i^T e = \sum_{i=1}^r \mu_i x_i.$$

Since $\bar{X}e$ is feasible for (StQP), we have

$$(\bar{X}e)^T Q (\bar{X}e) \geq \bar{y}.$$

As in Section 5.1.1, if the objective function of (StQP) is convex, we also have

$$(\bar{X}e)^T Q (\bar{X}e) = \big(\sum_{i=1}^r \mu_i x_i\big)^T Q \big(\sum_{i=1}^r \mu_i x_i\big) \leq \sum_{i=1}^r \mu_i x_i^T Q x_i = \langle Q, \bar{X} \rangle = \bar{y}$$

and thus optimality of $\bar{X}e$. This result is stated in the following proposition.

Proposition 5.2.16 *Assume that $(\mathrm{P}_{\mathcal{S}^+ \cap \mathcal{N}})$ is an exact relaxation of $(\mathrm{P}_{\mathcal{C}^*})$. If (StQP) has a convex objective function and $\bar{X}$ is an optimal solution of $(\mathrm{P}_{\mathcal{S}^+ \cap \mathcal{N}})$, then $\bar{X}e$ is an optimal solution of (StQP).*

If Q is positive semidefinite, then the corresponding quadratic form clearly is convex. Note that this includes the special case of diagonal matrices having no negative diagonal entry. We now want to show that we can also assume convexity for Q being interior. As stated in Proposition 5.2.13, if Q is interior then $Q - \bar{y}E \in \mathcal{S}_n^+$ and the quadratic form $x^T(Q - \bar{y}E)x$ is thus convex. Since for $x \in \Delta^S$ we have $x^T(Q - \bar{y}E)x = x^TQx - \bar{y}$, it follows that the quadratic form x^TQx is convex on Δ^S.

If the quadratic form is not convex, in particular if Q is a diagonal matrix having a negative entry or if Q is negative semidefinite, then in general $\bar{X}e$ is not optimal for (StQP) even if the relaxation ($\mathrm{P}_{\mathcal{S}^+\cap\mathcal{N}}$) is exact. This follows from the fact that even for $\bar{X}$ being completely positive, $\bar{X}e$ is in general not optimal for (StQP) (cf. Section 5.1.1).

5.3. Algorithms

In this section, we present two algorithms to solve standard quadratic optimization problems. Both are based on the idea to split the problem into subproblems of smaller dimension. This process is iterated until the resulting problems have a structure that allows to solve them. We will first explain the algorithms in Section 5.3.1 and 5.3.2 and then apply them to some test instances and compare the results in Section 5.3.4.

5.3.1. Algorithm 1

We present an algorithm to solve standard quadratic optimization problems by subdividing the problem into subproblems with decreasing dimension. As we have seen in Section 5.2.1.2 and 5.2.1.3, if the matrix Q is either positive or negative semidefinite we can compute the optimal value of (StQP) by solving a semidefinite respectively linear program. If, in contrast, the matrix is indefinite, we will first reformulate the problem. To this end, note that for any feasible solution x we have $x_n = 1 - \sum_{i=1}^{n-1} x_i$. Using this property, we reformulate the problem as follows

$$\begin{array}{ll} \min & \tilde{x}^T\tilde{Q}\tilde{x} + \tilde{c}^T\tilde{x} + \tilde{d} \\ \text{s.t.} & e^T\tilde{x} \leq 1 \\ & \tilde{x} \geq 0\ , \end{array} \tag{StQP'}$$

where $\tilde{Q}$ is an $(n-1)\times(n-1)$ matrix, $\tilde{c}$ is a vector of dimension $n-1$, $\tilde{d}$ is a constant, and $\tilde{x}$ is a vector in $\mathbb{R}^{n-1}$. We want to determine $\tilde{Q}$, $\tilde{c}$ and $\tilde{d}$ such that (StQP') and (StQP) are equivalent in the sense that they have the same optimal value and such that $\tilde{x}$ is an optimal solution of (StQP') if and only if $(\tilde{x}_1, ..., \tilde{x}_{n-1}, 1 - \sum_{i=1}^{n-1} \tilde{x}_i)^T$ is an optimal solution of (StQP). To do so, we consider problem (StQP) and set $x_n = 1 - \sum_{i=1}^{n-1} x_i$. We have

$$x^T Q x = \sum_{i,j=1}^{n-1} x_i x_j Q_{ij} + \sum_{j=1}^{n-1} x_n x_j Q_{nj} + \sum_{i=1}^{n-1} x_n x_i Q_{in} + x_n^2 Q_{nn} \,. \tag{5.5}$$

Replacing x_n by $1 - \sum_{i=1}^{n-1} x_i$, we get

$$\sum_{j=1}^{n-1} x_n x_j Q_{nj} = \sum_{j=1}^{n-1} \Big(1 - \sum_{i=1}^{n-1} x_i\Big) x_j Q_{nj} = \sum_{j=1}^{n-1} x_j Q_{nj} - \sum_{i,j=1}^{n-1} x_i x_j Q_{nj} \,,$$

$$\sum_{i=1}^{n-1} x_n x_i Q_{in} = \sum_{i=1}^{n-1} \Big(1 - \sum_{j=1}^{n-1} x_j\Big) x_i Q_{in} = \sum_{i=1}^{n-1} x_i Q_{in} - \sum_{i,j=1}^{n-1} x_i x_j Q_{in}$$

and

$$\begin{aligned} x_n^2 Q_{nn} &= \Big(1 - \sum_{i=1}^{n-1} x_i\Big)^2 Q_{nn} = \Big(1 - 2\sum_{i=1}^{n-1} x_i + \Big(\sum_{i=1}^{n-1} x_i\Big)^2\Big) Q_{nn} \\ &= Q_{nn} - 2\sum_{i=1}^{n-1} x_i Q_{nn} + \sum_{i,j=1}^{n-1} x_i x_j Q_{nn} \end{aligned}$$

Consequently, equation (5.5) can equivalently be written as

$$\begin{aligned} x^T Q x = \sum_{i=1,j}^{n-1} x_i x_j Q_{ij} + \sum_{j=1}^{n-1} x_j Q_{nj} - \sum_{i,j=1}^{n-1} x_i x_j Q_{nj} + \sum_{i=1}^{n-1} x_i Q_{in} - \sum_{i,j=1}^{n-1} x_i x_j Q_{in} \\ + Q_{nn} - 2\sum_{i=1}^{n-1} x_i Q_{nn} + \sum_{i,j=1}^{n-1} x_i x_j Q_{nn} \,. \end{aligned}$$

For $x \in$ Feas(StQP) and $\tilde{x} \in$ Feas(StQP'), we thus have

$$x^T Q x = \tilde{x}^T \tilde{Q} \tilde{x} + \tilde{c}^T \tilde{x} + \tilde{d}$$

with

$$\tilde{Q}_{ij} = Q_{ij} - Q_{in} - Q_{nj} + Q_{nn} \quad \text{for } i, j = 1, \ldots, n-1, \tag{5.6}$$

$$\tilde{c}_i = 2(Q_{ni} - Q_{nn}) \quad \text{for } i = 1, \ldots, n-1, \tag{5.7}$$

$$\tilde{d} = Q_{nn} \,. \tag{5.8}$$

We consider problem (StQP'). If $\tilde{Q}$ is positive semidefinite, the problem is convex and can be solved in polynomial time, for example by interior-point methods (for details see Nesterov and Nemirovskii (1987)). If $\tilde{Q}$ is negative semidefinite, then by Lemma 5.2.10, the minimum is achieved at an extreme point of the feasible set and

$$\bar{y} = \min\{\tilde{Q}_{ii} + \tilde{c}_i + \tilde{d} : i = 1, \ldots, n-1\}.$$

Otherwise, if $\tilde{Q}$ is indefinite, we will use the following property to decrease the dimension of the problem.

Proposition 5.3.1 (Tuy (1998, Proposition 3.18)) *The minimum (or maximum) of an indefinite quadratic function on a compact set is attained at a boundary point.*

This means that at least one of the constraints in (StQP') is active at the optimal solution. By setting one of the constraints active at a time, we get n subproblems of (StQP'): If the linear constraint is active we get

$$\begin{array}{ll} \min & \tilde{x}^T \tilde{Q} \tilde{x} + \tilde{c}^T \tilde{x} + \tilde{d} \\ \text{s.t.} & e^T \tilde{x} = 1 \\ & \tilde{x} \geq 0\,. \end{array} \tag{5.9}$$

For the nonnegativity constraint, we get for each $i = 1, \ldots, n-1$ a subproblem of the following form

$$\begin{array}{ll} \min & \tilde{x}^T \tilde{Q} \tilde{x} + \tilde{c}^T \tilde{x} + \tilde{d} \\ \text{s.t.} & e^T \tilde{x} \leq 1 \\ & \tilde{x} \geq 0 \\ & \tilde{x}_i = 0\,. \end{array}$$

The latter is equivalent to

$$\begin{array}{ll} \min & x^T \tilde{Q}_{[i,i]} x + \tilde{c}_{[i]}^T x + \tilde{d} \\ \text{s.t.} & e^T x \leq 1 \\ & x \geq 0\,, \end{array} \tag{5.10}$$

where $\tilde{Q}_{[i,i]}$ denotes the principal submatrix of $\tilde{Q}$ resulting from deleting the i-th row and column, $\tilde{c}_{[i]}$ is the vector c without the i-th entry and x is a vector in $\mathbb{R}^{n-2}$. We then get the optimal value $\bar{y}$ of (StQP') respectively (StQP) by taking the minimum over the optimal values of (5.9) and (5.10).

We now consider these subproblems in more detail. Since the feasible set of problem (5.9) is the standard simplex in $\mathbb{R}^{n-1}$, we can reformulate the problem as

$$\begin{array}{ll} \min & \tilde{x}^T M \tilde{x} \\ \text{s. t.} & e^T \tilde{x} = 1 \\ & \tilde{x} \geq 0 \end{array}$$

with $M = \tilde{Q} + \frac{1}{2}(\tilde{c}e^T + e\tilde{c}^T) + \tilde{d}E$. This is a standard quadratic optimization problem in $\mathbb{R}^{n-1}$ which means that we can again apply the described method to solve it iteratively. Problem (5.10) is of the form (StQP') and we can either solve it directly if the matrix in the objective function is positive or negative semidefinite, or we subdivide the problem into subproblems of smaller dimension and iterate.

The described procedure is stated in Algorithm 5.3.1.

5.3.2. Algorithm 2

We present a similar algorithm to solve standard quadratic optimization problems which is also based on subdividing the problem into subproblems with decreasing dimension. Again, if the matrix Q is either positive or negative semidefinite, we can compute the optimal value of (StQP) by solving a semidefinite respectively linear program. If, on the other hand, the matrix is indefinite then we will use the concept of interior matrices. Depending whether the matrix is interior or not we either get the optimal value by solving a semidefinite program or we can subdivide the problem into subproblems of smaller dimension. To check whether Q is interior, we will use the following characterization due to Johnson and Reams (2008, Theorem 1).

Theorem 5.3.2 *A matrix $A \in \mathcal{S}_n$ is interior if and only if (i) and (ii) hold.*

(i) *There exists $u > 0$, $\|u\|_1 = 1$, and $\mu \in \mathbb{R}$ such that $Au = \mu e$.*

(ii) *$y^T A y \geq 0$ for all $y \in \mathbb{R}^n$ such that $e^T y = 0$.*

Note that (i) is numerically difficult to check because of the strict inequality $u > 0$. We will show that we can reformulate property (i) in Theorem 5.3.2 such that it can be checked by solving a linear feasibility problem.

Lemma 5.3.3 *The following are equivalent*

(i) *there exists $u > 0$, $\|u\|_1 = 1$, and $\mu \in \mathbb{R}$ such that $Au = \mu e$;*

(i') *there exists* $v \in \mathbb{R}^n$, $v_i \geq 1$ *for all* $i = 1, \ldots, n$, *and* $\eta \in \mathbb{R}$ *such that* $Av = \eta e$.

Algorithm 5.3.1: Computing the optimal value $\bar{y}$ of (StQP).

Input: $Q \in \mathcal{S}_n$

$\mathcal{J}_1 \leftarrow \{Q\}$

$\mathcal{J}_2 \leftarrow \emptyset$

$\bar{y} \leftarrow \infty$

while $\mathcal{J}_1 \neq \emptyset$ *or* $\mathcal{J}_2 \neq \emptyset$ **do**

if $\mathcal{J}_1 \neq \emptyset$ **then**

choose $A \in \mathcal{J}_1$, let k denote the number of rows of A

if A *is positive semidefinite* **then**

$\hat{y} = \max\{y : A - yE \in \mathcal{S}_k^+ + \mathcal{N}_k\}$

$\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$

$\mathcal{J}_1 \leftarrow \mathcal{J}_1 \setminus \{A\}$

else if A *is negative semidefinite* **then**

$\hat{y} = \max\{y : A - yE \in \mathcal{N}_k\}$

$\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$

$\mathcal{J}_1 \leftarrow \mathcal{J}_1 \setminus \{A\}$

else

$\mathcal{J}_2 \leftarrow \mathcal{J}_2 \cup \{(\tilde{A}, \tilde{c}, \tilde{d})\}$ with $\tilde{Q}$, $\tilde{c}$ and $\tilde{d}$ derived from A as in (5.6)-(5.8)

end

else

choose $(A, c, d) \in \mathcal{J}_2$, let k denote the number of rows of A

if A *is positive semidefinite* **then**

solve

$$\begin{array}{ll} \min & x^T Ax + c^T x + d \\ \text{s. t.} & e^T x \leq 1 \\ & x \geq 0 \end{array}$$

denote the solution value by $\hat{y}$

$\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$

$\mathcal{J}_2 \leftarrow \mathcal{J}_2 \setminus \{(A, c, d)\}$

else if A *is negative semidefinite* **then**

$\hat{y} = \min\{A_{ii} + c_i + d_i : i = 1, \ldots, k\}$

$\bar{y} = \min\{\hat{y}, \bar{y}\}$

$\mathcal{J}_2 \leftarrow \mathcal{J}_2 \setminus \{(A, c, d)\}$

else

$\mathcal{J}_1 \leftarrow \mathcal{J}_1 \cup \{A + \frac{1}{2}(ce^T + ec^T) + dE\}$

$\mathcal{J}_2 \leftarrow \mathcal{J}_2 \cup \{(A_{[1,1]}, c_{[1]}, d), (A_{[2,2]}, c_{[2]}, d), \ldots, (A_{[k,k]}, c_{[k]}, d)\}$

end

end

end

Output: optimal solution value $\bar{y}$ of (StQP)

Proof Assume that property (i) holds, i.e., there exists $u > 0$, $\|u\|_1 = 1$, and $\mu \in \mathbb{R}$ such that $Au = \mu e$. Let $u_{\min} = \min\{u_i : i = 1, \dots, n\}$ and set $v = \frac{1}{u_{\min}} u$. Then $v_i \geq 1$ for all $i = 1, \dots, n$, and $Av = \frac{1}{u_{\min}} Au = \frac{1}{u_{\min}} \mu e$. Setting $\eta = \frac{1}{u_{\min}} \mu$, we get $Av = \eta e$ showing that (i') holds.

Next we show that (i') implies (i). To this assume that there exists $v \in \mathbb{R}^n$, $v_i \geq 1$ for all $i = 1, \dots, n$, and $\eta \in \mathbb{R}$ such that $Av = \eta e$. Let $u = \frac{1}{\|v\|_1} v$. Then $u > 0$ and $\|u\|_1 = 1$. Furthermore, for $\mu = \frac{1}{\|v\|_1} \eta$ we get $Au = \frac{1}{\|v\|_1} Av = \frac{1}{\|v\|_1} \eta e = \mu e$ showing that (i) holds. □

If Q is indefinite, we first check if property (i') of Lemma 5.3.3 holds. If there is a $v \in \mathbb{R}^n$ and an $\eta \in \mathbb{R}$ fulfilling the conditions in (i'), we still have to check property (ii) to know if Q is interior. Instead of doing this directly, we solve the following semidefinite program which is a relaxation of ($\mathrm{P}_{\mathcal{C}^*}$)

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s. t.} & \langle E, X \rangle = 1 \\ & X \in \mathcal{S}_n^+ . \end{array} \tag{$\mathrm{P}_{\mathcal{S}^+}$}$$

By Proposition 5.2.13, if Q is interior then ($\mathrm{P}_{\mathcal{S}^+}$) is an exact relaxation of (StQP) and, in particular, it is bounded. Therefore, we can conclude that Q is not interior if ($\mathrm{P}_{\mathcal{S}^+}$) is unbounded. Assuming that (i') holds, this means that (ii) has to be violated.

We now consider the case that ($\mathrm{P}_{\mathcal{S}^+}$) is bounded and want to show that in that case the relaxation is exact, i.e., we get the optimal value $\bar{y}$ of ($\mathrm{P}_{\mathcal{C}^*}$) respectively (StQP). To this we need the following lemma.

Lemma 5.3.4 *If there exists $y \in \mathbb{R}^n$, $e^T y = 0$ such that $y^T Q y < 0$, then the problem ($P_{\mathcal{S}^+}$) in unbounded.*

Proof Assume that there exists $y \in \mathbb{R}^n$, $e^T y = 0$ such that $y^T Q y < 0$. Let X be feasible for ($\mathrm{P}_{\mathcal{S}^+}$). Then $X + \lambda y y^T$ is feasible for ($\mathrm{P}_{\mathcal{S}^+}$) for all $\lambda \geq 0$ and $\langle Q, X + \lambda y y^T \rangle \to -\infty$ as $\lambda \to \infty$ which shows that the problem is unbounded. □

Therefore, if the problem is bounded, we know by the result of Lemma 5.3.4 that property (ii) holds. Under the assumption that (i') holds, this means that the matrix Q is interior and, by Proposition 5.2.13, we get the optimal solution value $\bar{y}$ of (StQP) by solving problem ($\mathrm{P}_{\mathcal{S}^+}$).

If (i') or (ii) is violated, we can conclude that the matrix is not interior which means that the optimal solution $\bar{x}$ of (StQP) has at least one zero entry. For each $i = 1, \dots, n$, we consider the subproblem

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & e^T x = 1 \\ & x \geq 0 \\ & x_i = 0 \end{array}$$

which is equivalent to the following standard quadratic optimization problem in $\mathbb{R}^{n-1}$

$$\begin{array}{ll} \min & x^T Q_{[i,i]} x \\ \text{s.t.} & e^T x = 1 \\ & x \geq 0\,, \end{array}$$

where again $Q_{[i,i]}$ denotes the principal submatrix of Q resulting from deleting the i-th row and column. Denoting the optimal value of each of these subproblems by $\bar{y}_i$, we get the optimal value $\bar{y}$ of (StQP) by taking the minimum over these values. As before, if the matrix $Q_{[i,i]}$ is either positive or negative semidefinite we can compute $\bar{y}_i$ by solving a semidefinite respectively linear program. Otherwise the matrix is indefinite and we again check if it is interior. If it is, we solve the SDP-relaxation ($\mathrm{P}_{\mathcal{S}^+}$) to get the optimal solution value. Otherwise, we subdivide the problem into subproblems of smaller dimension and iterate. The described procedure is stated in Algorithm 5.3.2.

5.3.2.1. An extension

In every iteration of Algorithm 5.3.2, if the matrix A in question is indefinite, we first have to solve a linear feasibility problem and possibly a semidefinite program to check if A is interior. To make the algorithm more efficient, we want to reduce the number of semidefinite programs that have to be solved. To this end, we consider perturbations of A of the form $A + cE$, $c \in \mathbb{R}$, and start with the following observation.

Lemma 5.3.5 *Let $A \in \mathcal{S}_n$ and $c \in \mathbb{R}$. Then A is interior if and only if $A + cE$ is interior.*

Proof The statement follows immediately from the fact that for every $c \in \mathbb{R}$ the matrix $A + cE$ has the same minimizers as A. □

We now set $c = -\min\{Q_{ij} : i, j = 1, \dots, n\}$. As every matrix $A \in \mathcal{J}$ in the algorithm is a principal submatrix of Q or equals Q, it follows that $A + cE$ is nonnegative and thus copositive. By Lemma 5.2.12, every copositive interior

Algorithm 5.3.2: Computing the optimal value $\bar{y}$ of (StQP).

Input: $Q \in \mathcal{S}_n$
1 $\mathcal{J} \leftarrow \{Q\}$
2 $\bar{y} \leftarrow \infty$
3 **while** $\mathcal{J} \neq \emptyset$ **do**
4 choose $A \in \mathcal{J}$, let k denote the number of rows of A
5 **if** *A is positive semidefinite* **then**
6 $\hat{y} = \max\{y : A - yE \in \mathcal{S}_k^+ + \mathcal{N}_k\}$
7 $\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$
8 $\mathcal{J} \leftarrow \mathcal{J} \setminus \{A\}$
9 **else if** *A is negative semidefinite* **then**
10 $\hat{y} = \max\{y : A - yE \in \mathcal{N}_k\}$
11 $\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$
12 $\mathcal{J} \leftarrow \mathcal{J} \setminus \{A\}$
13 **else**
14 **if** *$\exists v \in \mathbb{R}^k$, $v_i \geq 1$ $\forall i = 1, \ldots, k$, and $\eta \in \mathbb{R}$ such that $Av = \eta e$* **then**
15 solve

$$\begin{array}{ll} \min & \langle A, X \rangle \\ \text{s.t.} & \langle E, X \rangle = 1 \\ & X \in \mathcal{S}_k^+. \end{array}$$

16 **if** *the problem is unbounded* **then**
17 $\mathcal{J} \leftarrow \mathcal{J} \setminus \{A\} \cup \{A_{[1,1]}, A_{[2,2]}, \ldots, A_{[k,k]}\}$
18 go to 4
19 **else**
20 denote the solution value by $\hat{y}$
21 $\bar{y} \leftarrow \min\{\hat{y}, \bar{y}\}$
22 $\mathcal{J} \leftarrow \mathcal{J} \setminus \{A\}$
23 **end**
24 **end**
25 **end**
26 **end**
Output: optimal solution value $\bar{y}$ of (StQP)

matrix is positive semidefinite. We can therefore conclude that if $A + cE$ has negative eigenvalues, then the matrix is not interior. By Lemma 5.3.5, this implies that A is not interior either.

By applying the following lemma, we can even say more.

Lemma 5.3.6 *Let A be a symmetric $n \times n$ matrix with eigenvalues $\lambda_1(A) \geq \lambda_2(A) \geq \ldots \geq \lambda_n(A)$, and let A_0 be a $k \times k$ principal submatrix of A. Then*

$$\lambda_{\min}(A_0) \leq \lambda_k(A) \tag{5.11}$$

with $\lambda_{\min}(A_0)$ *denoting the minimum eigenvalue of* A_0.

A proof can be found in Bernstein (2009, Corollary 8.4.6).

If the matrix $A + cE$ has p negative eigenvalues $\lambda_{n-p+1}, \ldots, \lambda_n$, then by Lemma 5.3.6 every principal submatrix of $A + cE$ of order $k \geq n - p + 1$ has at least one negative eigenvalue implying that the corresponding principal submatrix of A is not interior by the same reasoning as above.

Instead of checking for every indefinite matrix $A \in \mathcal{J}$ in the algorithm if it is interior by solving the linear feasibility problem in line 14 and the semidefinite program in line 15, we thus compute the eigenvalues of $A + cE$. Let p denote the number of negative eigenvalues. If $p \geq 1$, then in line 17, we remove A from the set $\mathcal{J}$ and add all principal submatrices of order $n - p$. If $p = 0$, we cannot decide if A is interior or not as the following example shows. Let

$$Q_1 = \begin{pmatrix} 4.25 & 1.25 \\ 1.25 & 0.25 \end{pmatrix} \quad \text{and} \quad Q_2 = \begin{pmatrix} 0 & -2 \\ -2 & 0 \end{pmatrix}.$$

The matrices are both indefinite and the matrices $Q_k + c_k E$ with

$$c_k = -\min\{(Q_k)_{ij} : i, j = 1, 2\},$$

$k = 1, 2$, have no negative eigenvalue, i.e., $p_k = 0$ for $k = 1, 2$. The first matrix Q_1 is not interior whereas the second matrix Q_2 is interior showing that both cases can occur. Consequently, if $p = 0$, we have to check property (i) and (ii) by solving the linear feasibility problem and the semidefinite program in line 14 respectively line 15 of Algorithm 5.3.2 to decide if A is interior.

Nevertheless, if $p \geq 1$, it is not necessary to check property (i) and (ii), and if $p > 1$, when subdividing the problem into subproblems, the dimension can even be decreased by more than one.

5.3.3. Computing an optimal solution of (StQP)

By slightly modifying Algorithm 5.3.1 and Algorithm 5.3.2, it is possible not only to compute the optimal value of a standard quadratic optimization problem but also an optimal solution $\bar{x}$.

We first consider the case where A is positive semidefinite or interior. If we determine the optimal value $\hat{y}$ of the subproblem by solving the doubly nonnegative relaxation of $(\mathrm{P}_{\mathcal{C}^*})$, which is exact for these cases, then according to the results of Section 5.2.2, the vector $\hat{X}e$, with $\hat{X}$ denoting the optimal solution of the doubly nonnegative program, is optimal for (StQP).

If A is negative semidefinite, by Lemma 5.2.10, we have $\hat{y} = \min\{A_{ii} : i = 1, \ldots, n\}$ and e_j with j chosen such that $A_{jj} = \hat{y}$, is an optimal solution of the standard quadratic optimization problem with the matrix A in the objective function.

For the subproblems with $(A, c, d) \in \mathcal{J}_2$ in Algorithm 5.3.1 positive or negative semidefinite, we also get an optimal solution $\hat{x}$ for each subproblem.

This means that for every subproblem that is considered in the algorithms we can compute an optimal solution $\hat{x}$ and in the updating steps for the optimal value $\bar{y}$, we can also update $\bar{x}$ and thus compute an optimal solution of (StQP).

5.3.4. Numerical results

To illustrate the behavior of the algorithms presented in Section 5.3.1 and 5.3.2, we apply them to some instances of the standard quadratic optimization problem taken from Bomze and de Klerk (2002).

The matrix in the objective function of the first test instance is

$$Q_1 = \begin{pmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{pmatrix}$$

and the corresponding (StQP) has optimal value $\bar{y} = 0.5$.

The second instance is a standard quadratic optimization problem with

$$Q_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

in the objective function and optimal value $\bar{y} = \frac{1}{3}$.

The objective of the third example is to maximize the quadratic form $x^T Q_3 x$ over the standard simplex with

$$Q_3 = \begin{pmatrix} 14 & 15 & 16 & 0 & 0 \\ 15 & 14 & 12.5 & 22.5 & 15 \\ 16 & 12.5 & 10 & 26.5 & 16 \\ 0 & 22.5 & 26.5 & 0 & 0 \\ 0 & 15 & 16 & 0 & 14 \end{pmatrix}.$$

The optimal value of this instance is $\bar{y} = 16\frac{1}{3}$. We will transform this problem to a minimization problem before solving it.

The last problem that we consider is a standard quadratic optimization problem with

$$Q_4 = \tilde{Q} - 0.1\, rr^T + 0.4012\, E$$

where

$$\tilde{Q} = \begin{pmatrix} 0.82 & -0.23 & 0.155 & -0.013 & -0.314 \\ -0.23 & 0.484 & 0.346 & 0.197 & 0.592 \\ 0.155 & 0.346 & 0.298 & 0.143 & 0.419 \\ -0.013 & 0.197 & 0.143 & 0.172 & 0.362 \\ -0.314 & 0.592 & 0.419 & 0.362 & 0.916 \end{pmatrix} \quad \text{and} \quad r = \begin{pmatrix} 1.78 \\ 0.37 \\ 0.237 \\ 0.315 \\ 0.49 \end{pmatrix}.$$

The optimal value of this problem is $\bar{y} = 0.4839$.

We want to solve these instances with Algorithm 5.3.1 from Section 5.3.1 and with both the basic and the extended version of Algorithm 5.3.2 described in Section 5.3.2. To this end, we implemented the approaches in Matlab and used Yalmip (Löfberg, 2004) and SeDuMi (Sturm, 1999) to solve the semidefinite programs.

To decrease the number of quadratic programs that have to be solved, before adding an instance $(A_{[i,i]}, c_{[i]}, d)$ to the set $\mathcal{J}_2$ in line 16 or line 31 of Algorithm 5.3.1, we first check if this matrix is already in $\mathcal{J}_2$ or has been in the set in some previous iteration, and only add it if this is not the case. Moreover, we only add a matrix to $\mathcal{J}_1$ in line 30 of the algorithm, if it has not been added to the set before. In Algorithm 5.3.2, we do the same check before adding a principal submatrix to the set $\mathcal{J}$ in line 17.

The results can be found in Tables 5.1 to 5.3. Table 5.1 shows for every instance the number of iterations and the number of times that a matrix $A \in \mathcal{J}_1$ respectively $A \in \mathcal{J}_2$ is positive or negative semidefinite. The number of times that a matrix A is found to be positive or negative semidefinite is relatively small compared to the number of iterations. This means that in most iterations, the considered matrix is indefinite and the problem is thus subdivided into subproblems with smaller dimension.

		$A \in \mathcal{J}_1$		$A \in \mathcal{J}_2$	
Inst.	# it.	# A psd	# A nsd	# A psd	# A nsd
Q_1	20	3	0	5	0
Q_2	3485	11	0	10	0
Q_3	43	0	0	12	4
Q_4	25	3	0	13	0

Table 5.1.: Results for Algorithm 5.3.1

Table 5.2 and Table 5.3 show for every instance the number of iterations, the number of positive semidefinite matrices A, the number of negative semidefinite matrices A and the number of times that the linear feasibility problem and the semidefinite program had to be solved to check if A is interior.

Inst.	# it.	# A psd	# A nsd	# LP	# SDP
Q_1	13	5	0	8	1
Q_2	2307	12	0	2295	243
Q_3	27	0	6	21	14
Q_4	20	14	0	6	0

Table 5.2.: Results for Algorithm 5.3.2

As in Table 5.1, for both versions of Algorithm 5.3.2, the number of iterations is considerably higher than the number of times that the considered matrix is positive or negative semidefinite which means that it is indefinite most of the time.

Comparing the results of Table 5.1 and Table 5.2, we see that using the concept of interior matrices allows to reduce the number of iterations. Another substantial decrease of iterations as well as of the number of linear feasibility problems and semidefinite programs is obtained by applying the extended version of Algorithm 5.3.2. In Table 5.3, the number of linear and semidefinite programs to check if the considered matrix A is interior is small compared to

Inst.	# it.	# A psd	# A nsd	# LP	# SDP
Q_1	9	5	0	0	0
Q_2	1586	12	0	1	1
Q_3	22	0	6	6	6
Q_4	20	14	0	0	0

Table 5.3.: Results for the extended version of Algorithm 5.3.2

the number of iterations. This comes from the fact that every time that A is indefinite and p, the number of negative eigenvalues of $A + cE$, is at least one, no linear or semidefinite program has to be solved. In these cases, the matrix is removed from the set $\mathcal{J}$ and replaced by the principal submatrices of order $n - p$. Moreover, these submatrices are only added to $\mathcal{J}$ if they have not been added to the set before. It can thus happen that in some iterations a matrix is removed from J without adding any of its principal submatrices.

As the results show, the number of iterations of both types of algorithms quickly increases with growing dimension of the problem. On the other hand, for the test instances, the number of convex quadratic, linear or semidefinite programs that have to be solved is relatively small which seems promising. Comparing Algorithm 5.3.2 with the extended version, the strategy of the extended version already allows to notably decrease the number of iterations. This comes from the fact that in that approach, when subdividing the problem into subproblems, the dimension can often be reduced by more than one. But to make the algorithm applicable to larger problems it is necessary to find strategies to reduce the number of iterations even more.

5.4. Standard quadratic optimization problems in $\mathbb{R}^5$

For $n \leq 4$, we have $\mathcal{C}_n = \mathcal{S}_n^+ + \mathcal{N}_n$ which means that we can compute the optimal value of (StQP) by replacing the copositive cone in the reformulation ($\mathrm{P}_{\mathcal{C}}$) by $\mathcal{S}_n^+ + \mathcal{N}_n$ or the completely positive cone in ($\mathrm{P}_{\mathcal{C}^*}$) by $\mathcal{S}_n^+ \cap \mathcal{N}_n$ and solve the resulting semidefinite program. For $n \geq 5$, this does not hold anymore and we now want to study different approaches to solve standard quadratic optimization problems in $\mathbb{R}^5$ since this is the smallest dimension where hard instances appear. Unfortunately, the approaches do not lead to a method for solving standard quadratic optimization problems, reinforcing how hard it is to solve these problems even in small dimensions.

5.4.1. Reducing the dimension

Since copositive and completely positive programs in $\mathbb{R}^4$ can be reformulated as semidefinite programs and then be solved, an obvious approach to solve standard quadratic optimization problems in $\mathbb{R}^5$ is to consider the conic reformulation ($\mathrm{P}_{\mathcal{C}}$) or ($\mathrm{P}_{\mathcal{C}^*}$) and to try to reduce the dimension of the problem. In Section 5.3, we have already seen two algorithms that are based on the idea to subdivide the problem into subproblems of smaller dimension. We now want to describe another approach to reduce the dimension of the problem.

Considering the copositivity criterion of Theorem 2.2.13 for a matrix $A \in \mathcal{S}_n$, we see that the dimension of the matrices considered in the three conditions is at most $n-1$. Therefore, we consider reformulation ($\mathrm{P}_{\mathcal{C}}$) of the standard quadratic optimization problem and try to reduce the dimension of the problem by applying this criterion. To solve ($\mathrm{P}_{\mathcal{C}}$) we have to maximize y such that the matrix $Q-yE$ is copositive. Applying Theorem 2.2.13 to the following partition of $Q-yE$

$$Q - yE = \begin{pmatrix} a-y & (b-ye)^T \\ b-ye & C-yE \end{pmatrix}$$

with $a \in \mathbb{R}$, $b \in \mathbb{R}^4$ and $C \in \mathcal{S}_4$, we get that $Q-yE$ is copositive if and only if each of the following is fulfilled:

(i) $a - y \geq 0$,

(ii) $C - yE$ is copositive,

(iii) Each $x \geq 0$ with $x \neq 0$ and $(b-ye)^T x \leq 0$ satisfies

$$x^T\big((a-y)(C-yE) - (b-ye)(b-ye)^T\big)x \geq 0. \tag{5.12}$$

Let $\bar{y}_{(i)}$, $\bar{y}_{(ii)}$ respectively $\bar{y}_{(iii)}$ denote the maximum value of y such that property (i), (ii) respectively (iii) is fulfilled. Then the optimal solution value of ($\mathrm{P}_{\mathcal{C}}$) is

$$\bar{y} = \min\{\bar{y}_{(i)}, \bar{y}_{(ii)}, \bar{y}_{(iii)}\}.$$

Obviously, the optimal value of the first property is $\bar{y}_{(i)} = a$. The maximum value of y such that property (ii) holds can be determined by solving a semidefinite program, since $C - yE$ is a 4×4 matrix and thus copositive if and only if it has a representation as the sum of a positive semidefinite and a nonnegative matrix.

We now consider the third property in more detail. First note that the inequality in (5.12) is always fulfilled for $x = 0$. We can therefore rewrite (iii) as

(iii') Each $x \geq 0$ with $(b - ye)^T x \leq 0$ satisfies

$$x^T\big((a-y)(C-yE) - (b-ye)(b-ye)^T\big)x \geq 0.$$

This means that we want to maximize y such that the matrix

$$\begin{aligned} M(y) &= (a-y)(C-yE) - (b-ye)(b-ye)^T \\ &= aC - yaE - yC + y^2E - bb^T + ybe^T + yeb^T - y^2E \\ &= (aC - bb^T) - y(C + aE - be^T - eb^T) \end{aligned}$$

is $\mathcal{K}(y)$-semidefinite with

$$\mathcal{K}(y) = \{x \in \mathbb{R}^4 : x \geq 0,\ (b-ye)^T x \leq 0\}.$$

Note that this cone depends on y. By the following result, $\mathcal{K}$-semidefiniteness can be reduced to copositivity.

Lemma 5.4.1 (Eichfelder and Jahn (2008, Corollary 2.21)) *Let $\mathcal{K} \subseteq \mathbb{R}^n$ be a polyhedral cone and let $A \in \mathcal{S}_n$. Then there is a matrix $\bar{K} \in \mathbb{R}^{n \times s}$ with*

$$\mathcal{K} = \{x \in \mathbb{R}^n : x = \bar{K}u, u \in \mathbb{R}^s_+\},$$

and A is $\mathcal{K}$-semidefinite if and only if $\bar{K}^T A \bar{K}$ is copositive.

For the sake of readability, in the following we will not distinguish between an extreme ray and a vector generating this extreme ray.

Applying Lemma 5.4.1, we want to maximize y such that the matrix $\bar{K}_y^T M(y) \bar{K}_y$ is copositive. To do so, we first have to determine the matrix $\bar{K}_y$ which has the extreme rays of $\mathcal{K}(y) = \{x \in \mathbb{R}^4 : x \geq 0,\ (b-ye)^T x \leq 0\}$ as columns.

To determine the extreme rays of $\mathcal{K}(y)$, we need the concept of adjacent extreme rays. Two extreme rays $u \neq v$ of a pointed polyhedral cone P are called *adjacent* if the minimal face of P containing u and v contains no other extreme rays. This can be characterized as follows, see Fukuda and Prodon (1996, Proposition 7).

Proposition 5.4.2 *Let $P = \{x \in \mathbb{R}^n : Ax \leq 0\}$, where A is an $m \times n$ matrix with rows $a_1^T, \ldots, a_m^T$ and* $\operatorname{rank}(A) = n$. *Two extreme rays u and v in P are adjacent if and only if* $\operatorname{rank}(A_J) = n - 2$, *where $J = I(u) \cap I(v)$ with $I(u) = \{i : a_i^T u = 0\}$, $I(v) = \{i : a_i^T v = 0\}$, and A_J denotes the matrix with rows a_j^T, $j \in J$.*

We write $\mathcal{K}(y)$ as

$$\mathcal{K}(y) = \mathbb{R}^4_+ \cap \{x \in \mathbb{R}^4 : (b - ye)^T x \leq 0\}$$

and first determine which of the extreme rays of $P = \mathbb{R}^4_+ = \{x \in \mathbb{R}^4 : Ax \leq 0\}$ with $A = -I$ are adjacent. The set of extreme rays of $\mathbb{R}^4_+$ is $V = \{e_1, \ldots, e_4\}$ and for each extreme ray e_i we have $I(e_i) = \{1, \ldots, 4\} \setminus \{i\}$. Consequently, we have $I(e_i) \cap I(e_j) = \{1, \ldots, 4\} \setminus \{i, j\}$ and $|I(e_i) \cap I(e_j)| = n - 2$ for all $i \neq j$ implying that $\operatorname{rank}(A_{I(e_i) \cap I(e_j)}) = n - 2$ for all $i \neq j$. By Proposition 5.4.2, all extreme rays in V are adjacent.

Next, we use the following lemma to determine the extreme rays of $\mathcal{K}(y)$.

Lemma 5.4.3 *Let $P = \{x \in \mathbb{R}^n : Ax \leq 0\}$ with $A \in \mathbb{R}^{m \times n}$ and* $\operatorname{rank}(A) = n$. *Let V be the set of extreme rays of P, and $a \in \mathbb{R}^n$. Then*

$$\begin{aligned} W = \{&v \in V : a^T v \leq 0\} \\ &\cup \{(a^T u)v - (a^T v)u : u, v \text{ adjacent in } V,\ a^T u > 0,\ a^T v < 0\} \end{aligned}$$

is the set of extreme rays of $P \cap \{x \in \mathbb{R}^n : a^T x \leq 0\}$.

A proof can be found in Fukuda and Prodon (1996, Lemma 8).

Applying Lemma 5.4.3, the set of extreme rays of

$$\mathcal{K}(y) = \mathbb{R}^4_+ \cap \{x \in \mathbb{R}^4 : (b - ye)^T x \leq 0\}$$

is

$$\begin{aligned} W(y) &= \{e_i : (b - ye)^T e_i \leq 0\} \\ &\quad \cup \{((b - ye)^T e_i)e_j - ((b - ye)^T e_j)e_i : i \neq j,\ (b - ye)^T e_i > 0, \\ &\qquad\qquad (b - ye)^T e_j < 0\} \\ &= \{e_i : b_i \leq y\} \cup \{(b_i - y)e_j - (b_j - y)e_i : i \neq j,\ b_i > y,\ b_j < y\}. \end{aligned}$$

Clearly, the extreme rays of $\mathcal{K}(y)$ also depend on y. The number of extreme rays depends on the signs of the entries of $b - ye$. If the vector $b - ye$ has three positive and one negative entry, or if it has two positive, one zero and one negative entry, or if it has one positive, two zero and one negative entry, then $\mathcal{K}(y)$ has four extreme rays. If $b - ye$ has one positive, one zero and two negative entries, then $\mathcal{K}(y)$ has five extreme rays. And if $b-ye$ has one positive and three negative entries, or if it has two positive and two negative entries, then $\mathcal{K}(y)$ has six extreme rays. Consequently, the matrix $M(y)$ is of order $s = 4$, $s = 5$ or $s = 6$.

For $s = 4$, the matrix $\bar{K}_y^T M(y) \bar{K}_y$ is copositive if and only if it can be written as the sum of a positive semidefinite and a nonnegative matrix. For $s = 5$ and $s = 6$, copositivity is difficult to check. We will therefore reduce the dimension of the matrices under consideration by applying Theorem 2.1.7.

Recall that our goal is to maximize y such that $\bar{K}_y^T M(y) \bar{K}_y$ is copositive or, equivalently, such that $M(y)$ is $\mathcal{K}(y)$-semidefinite. By definition, the matrix $M(y)$ is $\mathcal{K}(y)$-semidefinite if $x^T M(y) x \geq 0$ for all $x \in \mathcal{K}(y)$, which is equivalent to $x^T M(y) x \geq 0$ for all $x \in \mathcal{K}_1 \cup \ldots \cup \mathcal{K}_m$, where $\{\mathcal{K}_1, \ldots, \mathcal{K}_m\}$ is any partition of $\mathcal{K}(y)$ such that $\mathcal{K}_j \subseteq \mathcal{K}(y)$ for all $j = 1, \ldots, m$, and $\bigcup_{j=1}^m \mathcal{K}_j = \mathcal{K}(y)$. The latter means that $M(y)$ is $\mathcal{K}_j$-semidefinite for all $j = 1, \ldots, m$.

By Theorem 2.1.7, every $x \in \mathcal{K}(y)$ can be represented as a nonnegative combination of at most four extreme rays of $\mathcal{K}(y)$. Therefore, every $x \in \mathcal{K}(y)$ lies in some set $\mathcal{K}_j$ if we partition $\mathcal{K}(y)$ as follows: Let $\mathcal{K}_j = \operatorname{cone}(W_j)$ where W_j, $j = 1, \ldots, \binom{s}{4}$, are the four-element subsets of the set of extreme rays of $\mathcal{K}(y)$. Then the matrix $M(y)$ is $\mathcal{K}(y)$-semidefinite if and only if it is $\mathcal{K}_j$-semidefinite for all $j = 1, \ldots, \binom{s}{4}$. Denoting by $\bar{K}_j$ the matrix having the extreme rays of $\mathcal{K}_j$ as columns, this means that we want to determine the maximum value of y such that $\bar{K}_j^T M(y) \bar{K}_j$ is copositive for all $j = 1, \ldots, \binom{s}{4}$. As these are matrices of order 4, copositivity of the matrices is equivalent to $\bar{K}_j^T M(y) \bar{K}_j$ having a representation as the sum of a positive semidefinite and a nonnegative matrix. But note that not only $M(y)$ but also the extreme rays of $\mathcal{K}(y)$ and thus the matrices $\bar{K}_j$ depend on y.

We have thus reduced the standard quadratic programming problem in $\mathbb{R}^5$ to the problem of maximizing y such that one or several 4×4 matrices are copositive. The problem in this approach is that the dependence of the considered 4×4 matrices $\bar{K}_j^T M(y) \bar{K}_j$ on y is not linear and hence, it is hard to solve these programs. Moreover, also the number of matrices $\bar{K}_j^T M(y) \bar{K}_j$ depends on y.

For a fixed value of y, however, we can test copositivity of the matrices $\bar{K}_j^T M(y) \bar{K}_j$, $j =, \ldots, \binom{s}{4}$, by solving a semidefinite program. This allows us to compute bounds on $\bar{y}$.

Danninger (1990) presents a generalized version of this approach to check copositivity of symmetric $n \times n$ matrices. The reduction of dimension and partitioning of cones is then iterated until small dimensions are reached such that copositivity can be checked by applying known copositivity criteria.

5.4.2. Optimizing over $\mathcal{K}_5^1$

By Theorem 2.4.5, every copositive 5×5 matrix can be scaled into $\mathcal{K}_5^1$. This means that for any 5×5 matrix, copositivity can be checked by scaling and testing if the scaled matrix lies in $\mathcal{K}_5^1$. Therefore, we will try to reformulate the copositive reformulation of the standard quadratic optimization problem in $\mathbb{R}^5$ as a problem over the cone $\mathcal{K}_5^1$.

We want to maximize y such that the matrix $Q - yE$ is copositive which is, by Theorem 2.4.5, equivalent to the following problem

$$\begin{array}{ll} \max & y \\ \text{s.t.} & D(Q - yE)D \in \mathcal{K}_5^1 \\ & D \in \mathcal{D}\,, \end{array} \qquad (\mathrm{P}_{\mathcal{K}_5^1})$$

where $\mathcal{D}$ denotes the set of diagonal matrices with strictly positive diagonal entries, i.e.,

$$\mathcal{D} = \{\mathrm{Diag}(d) : d \in \mathbb{R}^n_{++}\}\,.$$

As we have seen in Section 2.4.2, testing if a matrix is in $\mathcal{K}_n^1$ can be done by solving the system of linear matrix inequalities (2.5)–(2.8). Consequently, the matrix $D(Q - yE)D$ is in $\mathcal{K}_5^1$ if and only if there are matrices $M^1, \ldots, M^5 \in \mathcal{S}_5$ such that

$$D(Q - yE)D - M^i \succeq 0\,,\ i = 1, \ldots, 5 \qquad (5.13)$$

$$M^i_{ii} = 0\,,\ i = 1, \ldots, 5 \qquad (5.14)$$

$$M^i_{jj} + 2M^j_{ij} = 0\,,\ \forall\, i \neq j \qquad (5.15)$$

$$M^i_{jk} + M^j_{ik} + M^k_{ij} \geq 0\,,\ \forall\, i < j < k\,. \qquad (5.16)$$

We want to reformulate this system by using the well known fact that the positive semidefinite cone is invariant under scaling:

Lemma 5.4.4 *Let $D \in \mathcal{D}$. Then $A \in \mathcal{S}_n^+$ if and only if $DAD \in \mathcal{S}_n^+$.*

Proof Let $D \in \mathcal{D}$, $x \in \mathbb{R}^n$ and $y = D^{-1}x$. Note that the mapping $x \mapsto D^{-1}x$ is a bijection on $\mathbb{R}^n$. Then

$$x^T A x = (DD^{-1}x)^T A (DD^{-1}x) = (Dy)^T A (Dy) = y^T DADy$$

showing the result. □

For $D \in \mathcal{D}$ we also have $D^{-1} \in \mathcal{D}$. Consequently, inequality (5.13) holds if and only if

$$Q - yE - D^{-1}M^iD^{-1} \succeq 0 \quad \text{for } i = 1, \dots, 5\,. \tag{5.17}$$

Setting $Z^i = D^{-1}M^iD^{-1}$, $i = 1, \dots, 5$, inequality (5.17) can be written as

$$Q - yE - Z^i \succeq 0 \quad \text{for } i = 1, \dots, 5\,,$$

and since $d_i > 0$, this is equivalent to

$$\tfrac{1}{d_i}Q - y\tfrac{1}{d_i}E - \tfrac{1}{d_i}Z^i \succeq 0 \quad \text{for } i = 1, \dots, 5\,.$$

Considering (5.14), we have

$$M^i_{ii} = 0 \quad \Leftrightarrow \quad \tfrac{1}{d_i^2}M^i_{ii} = (D^{-1}M^iD^{-1})_{ii} = Z^i_{ii} = 0 \quad \Leftrightarrow \quad \tfrac{1}{d_i}Z^i_{ii} = 0\,.$$

For (5.15), we have

$$\begin{aligned} & M^i_{jj} + 2M^j_{ij} = d_j^2 Z^i_{jj} + 2d_id_jZ^j_{ij} = 0 \\ \Leftrightarrow \quad & \tfrac{1}{d_i}Z^i_{jj} + 2\tfrac{1}{d_j}Z^j_{ij} = 0\,. \end{aligned}$$

Considering (5.16), we have

$$\begin{aligned} & M^i_{jk} + M^j_{ik} + M^k_{ij} = d_jd_kZ^i_{jk} + d_id_kZ^i_{ik} + d_id_jZ^k_{ij} \geq 0 \\ \Leftrightarrow \quad & \tfrac{1}{d_i}Z^i_{jk} + \tfrac{1}{d_j}Z^j_{ik} + \tfrac{1}{d_k}Z^k_{ij} \geq 0\,. \end{aligned}$$

Setting $W^i = \frac{1}{d_i}Z^i$ and $p_i = \frac{1}{d_i}$, we can thus conclude that there are matrices $M^1, \dots, M^5 \in \mathcal{S}_5$ such that the system (5.13)-(5.16) holds if and only if there are matrices $W^1, \dots, W^5 \in \mathcal{S}_5$ such that

$$p_iQ - p_iyE - W^i \succeq 0\,,\ i = 1, \dots, 5 \tag{5.18}$$

$$W^i_{ii} = 0\,,\ i = 1, \dots, 5 \tag{5.19}$$

$$W^i_{jj} + 2W^j_{ij} = 0\,,\ \forall\, i \neq j \tag{5.20}$$

$$W^i_{jk} + W^j_{ik} + W^k_{ij} \geq 0\,,\ \forall\, i < j < k\,. \tag{5.21}$$

Consequently, the matrix $Q - yE$ is copositive if and only if there are scalars $p_1, \dots, p_5 > 0$ such that the system (5.18)-(5.21) has a solution. The difficulty appearing here lies in the fact that, for y considered as a variable that we want to maximize, inequality (5.18) is not linear but bilinear. We thus get a bilinear semidefinite optimization problem which is NP-hard (Toker and Özbay, 1995). However, there exists software to solve nonlinear semidefinite programs, for example PENNON (Kočvara and Stingl, 2008). But since this thesis is concerned with linear conic problems only, we do not pursue this approach any further.

5.5. Quadratic programs

In this section, we study more general quadratic programs. We start with quadratic programs with linear constraints and then consider single quadratic constraint programs. In both cases, we first reformulate the problem as a completely positive program. Then, in analogy to the results of Section 5.2, we analyze if there are special cases where replacing the completely positive cone by a tractable cone leads to an exact relaxation of the problem.

5.5.1. Quadratic program with linear constraints

The problem that we consider first is of the form

$$\begin{aligned} \min \quad & x^T Q x \\ \text{s.t.} \quad & Ax = b \\ & x \geq 0\,, \end{aligned} \tag{QP}$$

with $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. We assume that A is nonzero since for $A = 0$ and $b \neq 0$ the problem is infeasible, whereas for $A = 0$ and $b = 0$ the problem is equivalent to testing copositivity of Q. In that case, if the matrix Q is copositive, the optimal value of (QP) is zero, and if Q is not copositive the problem is unbounded.

Clearly this setting includes the standard quadratic optimization problem as a special case. Moreover, it can easily be verified that quadratic problems over polyhedral cones can be written in this form.

5.5.1.1. Reformulation as a standard quadratic optimization problem

We want to show that under the assumption that the feasible set of (QP) is bounded we can reformulate the problem as a standard quadratic optimization problem.

If the feasible set is bounded, it can be represented as the convex hull of its vertices, i.e.,

$$\begin{aligned} \operatorname{Feas}(\mathrm{QP}) &= \{x \in \mathbb{R}^n : Ax = b, x \geq 0\} \\ &= \operatorname{conv}\{v^1, \dots, v^k\} \end{aligned}$$

with $v^1, \dots, v^k$ denoting the vertices of Feas(QP). Every point $x \in$ Feas(QP) can then be written as a convex combination of the vertices, i.e.,

$$x = \sum_{i=1}^{k} \lambda_i v^i \text{ with } \lambda_i \geq 0,\ \sum_{i=1}^{k} \lambda_i = 1.$$

Denoting by V the matrix with columns $v^1, \dots, v^k$, we can thus rewrite (QP) as a standard quadratic program

$$\begin{aligned} \min \quad & \lambda^T (V^T Q V) \lambda \\ \text{s.t.} \quad & e^T \lambda = 1 \\ & \lambda \geq 0 \,. \end{aligned}$$

It is thus clear that all results of Section 5.2 can be applied here by considering properties of the matrix $V^T Q V$. If the matrix Q is positive respectively negative semidefinite, then it can easily be shown that the same holds for $V^T Q V$. In this case, the standard quadratic program can be solved in polynomial time by replacing the copositive cone in the conic programming formulation by a tractable cone as shown in Section 5.2.1. But in general the representation of (QP) as standard quadratic optimization problem has higher dimension than the original problem, and moreover, the vertices of Feas(QP) have to be known. Therefore, it might be advantageous to consider other conic reformulations of problem (QP).

5.5.1.2. Reformulation as a completely positive program and relaxations

We now want to consider a different conic reformulation of (QP) which is due to Burer (2009). By Theorem 3.2.2, problem (QP) can be written in the following form

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & Ax = b \\ & a_i^T X a_i = b_i^2 \ , \ i = 1, \dots, m \\ & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{C}^*_{n+1}, \end{aligned} \tag{QP$_{\mathcal{C}^*}$}$$

where a_i^T denotes the i-th row of A. Replacing the completely positive cone by the positive semidefinite cone, adding the constraint that x has to be nonnegative and deleting the linear constraints on X leads to a generalized version of the Shor relaxation from Section 5.2.1.2

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{S}^+_{n+1} \\ & Ax = b \\ & x \geq 0. \end{aligned} \tag{QP$_{\text{Shor}}$}$$

For $Q \in \mathcal{S}^+_n$ this relaxation is exact which can be proven in the same way as for the standard quadratic optimization problem in Section 5.2.1.2. Moreover, if $Q \in \mathcal{S}_n^+$ and $(\bar{x}, \bar{X})$ is an optimal solution of $(\mathrm{QP}_{\mathrm{Shor}})$ or $(\mathrm{QP}_{\mathcal{C}^*})$, then $\bar{x}$ is an optimal solution of (QP): First note that

$$\begin{pmatrix} 1 & \bar{x}^T \\ \bar{x} & \bar{X} \end{pmatrix} \in \mathcal{S}_{n+1}^+$$

which implies that $\bar{X} - \bar{x}\bar{x}^T$ is positive semidefinite. Together with $Q \in \mathcal{S}_n^+$ we get $\langle Q, \bar{X} - \bar{x}\bar{x}^T \rangle \geq 0$ which is equivalent to $\bar{x}^T Q \bar{x} \leq \langle Q, \bar{X} \rangle$. On the other hand, $(\bar{x}, \bar{x}\bar{x}^T)$ is feasible for $(\mathrm{QP}_{\mathrm{Shor}})$ respectively $(\mathrm{QP}_{\mathcal{C}^*})$, whence $\bar{x}^T Q \bar{x} \geq \langle Q, \bar{X} \rangle$. Therefore, we have $\bar{x}^T Q \bar{x} = \langle Q, \bar{X} \rangle$. Since the relaxation is exact for $Q \in \mathcal{S}_n^+$, this implies that $\bar{x}$ is an optimal solution of (QP).

If $Q \notin \mathcal{S}_n^+$, then the generalized Shor relaxation $(\mathrm{QP}_{\mathrm{Shor}})$ is unbounded: If $Q \notin \mathcal{S}_n^+$, then there exists a matrix $U \in \mathcal{S}_n^+$ with $\langle Q, U \rangle < 0$. Let $x \in \mathrm{Feas}(\mathrm{QP})$. Then $(x, xx^T + \mu U) \in \mathrm{Feas}(\mathrm{QP}_{\mathrm{Shor}})$ for all $\mu \geq 0$ and

$$\langle Q, xx^T + \mu U \rangle = \langle Q, xx^T \rangle + \mu \langle Q, U \rangle \to -\infty \quad \text{for } \mu \to \infty.$$

The problem is that there is too much freedom for the matrix X. To avoid unboundedness of the problem, one has to add constraints to bound X, but in general it is difficult to find such constraints that are valid for all (x, xx^T) with $x \in \mathrm{Feas}(\mathrm{QP})$ in order to guarantee that the new problem is still a relaxation of (QP).

Since $(\mathrm{QP}_{\mathcal{C}^*})$ is an exact reformulation of (QP), it is clear that we can add a nonnegativity constraint on X respectively replace the positive semidefinite cone in $(\mathrm{QP}_{\mathrm{Shor}})$ by the doubly nonnegative cone. But this only guarantees boundedness of the problem if Q is copositive. Otherwise, there is a nonnegative vector u with $u^T Q u < 0$. Let x be feasible for (QP). Then for all $\mu \geq 0$, the point $(x, xx^T + \mu uu^T)$ is feasible for the doubly nonnegative version of $(\mathrm{QP}_{\mathrm{Shor}})$ resulting from replacing the positive semidefinite cone in $(\mathrm{QP}_{\mathrm{Shor}})$ by the doubly nonnegative cone. But as $\langle Q, xx^T + \mu uu^T \rangle \to -\infty$ for $\mu \to \infty$, this shows that the doubly nonnegative relaxation is unbounded if Q is not copositive.

Considering reformulation $(\mathrm{QP}_{\mathcal{C}^*})$, we see that other constraints that could be added are $a_i^T X a_i = b_i^2$, $i = 1, \ldots, m$, where a_i^T denotes the i-th row of A.

5.5.2. Single quadratic constraint program

The single quadratic constraint problem is of the following form

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & x^T A x = b \\ & x \geq 0\,, \end{array} \tag{SQC}$$

i.e., we want to minimize a quadratic function over the set of all nonnegative vectors that satisfy a single quadratic constraint. The matrix A is assumed to be strictly copositive and the vector b must be strictly positive. Preisig studied this problem and showed that it can be reformulated as a copositive program, see Preisig (1996, Theorem 3.5).

Theorem 5.5.1 *Let $\bar{y}$ denote the optimal value of (SQC) with A being strictly copositive and $b = 1$. Then*

$$\bar{y} = \max\{y : Q - yA \in \mathcal{C}_n\}.$$

The assumption that $b = 1$ can easily be generalized to any strictly positive value. If we consider problem (SQC) and assume $b > 0$, then we can rewrite the problem as follows

$$\begin{array}{ll} \min & x^T Q x \\ \text{s. t.} & x^T(\frac{1}{b}A)x = 1 \\ & x \geq 0 \ . \end{array}$$

According to Theorem 5.5.1, this problem is equivalent to

$$\max\{\lambda : Q - \lambda \tfrac{1}{b} B \in \mathcal{C}_n\}.$$

Setting $y = \frac{\lambda}{b}$, we get the following copositive reformulation of (SQC)

$$\begin{array}{ll} \max & by \\ \text{s. t.} & Q - yA \in \mathcal{C}_n \end{array} \qquad (\text{SQC}_{\mathcal{C}})$$

with the corresponding dual problem

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s. t.} & \langle A, X \rangle = b \\ & X \in \mathcal{C}_n^* \ . \end{array} \qquad (\text{SQC}_{\mathcal{C}^*})$$

We now want to show equivalence of the copositive and the completely positive reformulation of (SQC). By assumption, the matrix A is strictly copositive. Consequently, for $y < \bar{y}$ if $b = 1$, respectively for $y < b\bar{y}$ in the general case, we have that $Q - yA$ is strictly copositive. On the other hand, the matrix $X = \frac{b}{n} D$, where D is the diagonal matrix with diagonal entries $D_{ii} = \frac{1}{A_{ii}}$ for all $i = 1, \ldots, n$, is feasible for ($\text{SQC}_{\mathcal{C}^*}$). Moreover, X lies in the interior of the completely positive cone which can easily be seen by applying Theorem 2.3.3. By the conic duality theorem (cf. Theorem 3.1.2), this implies that the problems ($\text{SQC}_{\mathcal{C}}$) and ($\text{SQC}_{\mathcal{C}^*}$) are equivalent in the sense that they have the same optimal value. A more detailed proof to show equivalence of the single quadratic constraint problem and its copositive and completely positive reformulation can be found in Bundfuss (2009, Lemma 4.1).

As stated in Preisig (1996), Theorem 5.5.1 implies that the single quadratic constraint problem is NP-complete. One algorithm that Preisig proposes to determine $\bar{y}$ is a bisection algorithm where a number of copositivity tests has to be done. First, a lower bound y_l and an upper bound y_u are chosen such that $Q - y_l A$ is strictly copositive and $Q - y_u A$ is not strictly copositive. Let $y = (y_l + y_u)/2$. If $Q - yA$ is strictly copositive, set $y_l = y$, otherwise set $y_u = y$. If $Q - y_u A$ is copositive, or if $y_u - y_l$ is below a chosen tolerance, then let $y_{\text{opt}} = y_u$ and stop. Otherwise iterate the procedure. The computed y_{opt} is greater or equal than the optimal value $\bar{y}$.

5.5.2.1. Relaxations

We have seen that the single quadratic constraint problem can be reformulated as a completely positive program which is equivalent to the dual copositive program, i.e., problem (SQC) is equivalent to the problems ($\text{SQC}_{\mathcal{C}^*}$) and ($\text{SQC}_{\mathcal{C}}$). We now want to study if for special classes of matrices Q in the objective function, replacing the copositive respectively the completely positive cone in the conic reformulations of (SQC) by a tractable cone leads to equivalent problems.

To do so, we first consider the following instance of a single quadratic constraint problem in $\mathbb{R}^5$ where $Q = 6I$, $A = -H + 6I$ with H denoting the Horn matrix, and $b = 1$. Note that A is strictly diagonally dominant which implies that it is positive definite and thus strictly copositive. We now want to maximize y such that the matrix $Q - yA$ is copositive. For $y = 1$ we have $Q - yA = H \in \mathcal{C}_5$. We can conclude that $\bar{y} \geq 1$. On the other hand, for $y = 1 + k$ with $k > 0$, we have $Q - yA = H - kA$ which is not copositive. This can be seen by computing the value of $x^T(H - kA)x$ for $x = (1, 1, 0, 0, 0)^T$ which is negative. Consequently, we have $\bar{y} = 1$. Since $Q - \bar{y}A = H$ does not lie in $\mathcal{S}_5^+ + \mathcal{N}_5$, replacing the copositive cone in ($\text{SQC}_{\mathcal{C}}$) by the positive semidefinite cone, the nonnegative cone or $\mathcal{S}_5^+ + \mathcal{N}_5$ does not yield an equivalent problem. Since Q is a diagonal matrix with positive diagonal entries, thus positive semidefinite as well as interior, this implies that for those classes of matrices, replacing the completely positive cone in ($\text{SQC}_{\mathcal{C}^*}$) by the positive semidefinite, the nonnegative or the doubly nonnegative cone does result in a relaxation of the problem which is in general not exact.

We now consider an example with $Q \in \mathcal{S}_5$ being a diagonal matrix with negative entries on the diagonal and thus being negative semidefinite. Let

$Q = -I$, $A = H + I$ which is strictly copositive, and $b = 1$. For $y = -1$ we have $Q - yA = H$ which is copositive. Since for $y > -1$ the quadratic form $x^T(Q - yA)x$ takes a negative value for $x = (1, 1, 0, 0, 0)^T$ showing that the matrix is not copositive, we have $\bar{y} = -1$. As in the first example, we have $Q - \bar{y}A = H$. Consequently, for negative semidefinite matrices, replacing the copositive cone in (SQC$_{\mathcal{C}}$) by the nonnegative cone, the semidefinite cone or $\mathcal{S}_n^+ + \mathcal{N}_n$ respectively replacing the completely positive cone in (SQC$_{\mathcal{C}^*}$) by the nonnegative, the positive semidefinite or the doubly nonnegative cone does not result in an exact reformulation of the problem.

We conclude that in contrast to the standard quadratic optimization problem which can be seen as a special case of the single quadratic constraint problem (since for $x \geq 0$ we have that $e^T x = 1$ if and only if $(e^T x)^2 = x^T E x = 1$), for the general single quadratic constraint problem we could not find exact relaxations of the completely positive reformulation (SQC$_{\mathcal{C}^*}$) for special classes of matrices Q. The problem is that there is too much freedom for the matrix A in the quadratic constraint.

6. Cutting planes

In this chapter, we study the problem of separating a doubly nonnegative matrix which is not completely positive from the completely positive cone. In other words, given $X \in \mathcal{D}_n \setminus \mathcal{C}_n^*$, we want to find a copositive matrix K such that $\langle K, X\rangle < 0$.

In Section 6.1, we start by motivating the problem and we give a short overview of existing separation procedures from the literature. We then survey the separation of 5×5 matrices in more detail in Section 6.2. In Section 6.3, we present the first algorithm to separate an arbitrary matrix $X \notin \mathcal{C}_n^*$ from the completely positive cone. This approach is based on (approximate) projections onto the copositive cone as described in Chapter 4 and has been published in Sponsel and Dür (2012). Finally, in Section 6.4, we show how to separate doubly nonnegative matrices that have a triangle-free graph from the completely positive cone. The results of that section are contained in the preprint Berman et al. (2013).

6.1. Cutting planes for completely positive programs

As we have seen in Section 3.2, every optimization problem with quadratic objective, linear constraints, and binary variables can equivalently be written as a linear problem over $\mathcal{C}_n^*$. The completely positive cone in the resulting optimization problem is often relaxed to a weaker but tractable cone like the cone of doubly nonnegative matrices. Consider the completely positive problem

$$\begin{aligned} \min \quad & \langle C, X\rangle \\ \text{s.t.} \quad & \langle A_i, X\rangle = b_i, \quad i = 1,\dots,m \\ & X \in \mathcal{C}_n^* \end{aligned} \qquad (\mathrm{P}_{\mathcal{C}^*})$$

and its doubly nonnegative relaxation

$$\begin{aligned} \min \quad & \langle C, X\rangle \\ \text{s.t.} \quad & \langle A_i, X\rangle = b_i, \quad i = 1,\dots,m \\ & X \in \mathcal{D}_n. \end{aligned} \qquad (\mathrm{P}_{\mathcal{D}})$$

Solving this relaxation gives a lower bound on the optimal value of ($\mathrm{P}_{\mathcal{C}^*}$). Let $\bar{X}$ denote the solution obtained by solving ($\mathrm{P}_{\mathcal{D}}$). In general, $\bar{X}$ is not completely positive. Therefore, it is desirable to construct a cut that separates this solution from the cone $\mathcal{C}_n^*$. We thus want to find a copositive matrix K such that $\langle K, X \rangle < 0$. Adding the linear constraint

$$\langle K, X \rangle \geq 0 \tag{6.1}$$

to ($\mathrm{P}_{\mathcal{D}}$) yields a tighter relaxation of ($\mathrm{P}_{\mathcal{C}^*}$) and a potentially improved bound on its optimal value. Note that by duality, (6.1) holds for all $X \in \mathcal{C}_n^*$ which means that all feasible solutions of the original problem ($\mathrm{P}_{\mathcal{C}^*}$) are still feasible after adding the cut to ($\mathrm{P}_{\mathcal{D}}$).

The idea of using copositive cuts was first introduced by Bomze, Locatelli and Tardella (2008) and further applied to the maximum clique problem by Bomze, Frommlet and Locatelli (2010a). We will describe the cuts from Bomze et al. (2010a) in more detail when comparing them in Section 6.4.2.1 to the cuts that we will introduce in Section 6.4.1.

Burer, Anstreicher and Dür (2009) characterize 5×5 extreme doubly nonnegative matrices which are not completely positive and show how to separate such a matrix from the completely positive cone. Dong and Anstreicher (2013) generalize this procedure to matrices $X \in \mathcal{D}_5 \setminus \mathcal{C}_5^*$ that have at least one off-diagonal zero, and to larger matrices having block structure. Extending the results of Burer et al. (2009) and Dong and Anstreicher (2013), Burer and Dong (2013) establish the first full separation algorithm for 5×5 completely positive matrices. We will present these approaches in more detail in Section 6.2 where we consider the separation of 5×5 matrices from the completely positive cone.

In contrast to the approaches that either apply only to one specific problem or need a special structure of the considered matrix, we will show in Section 6.3 how an arbitrary matrix $X \notin \mathcal{C}_n^*$ can be separated from the cone of completely positive matrices.

6.2. Separating 5×5 matrices from the completely positive cone

We first consider 5×5 matrices, since this is the smallest dimension where $\mathcal{D}_n \setminus \mathcal{C}_n^*$ is nonempty. We start by giving an overview of separation procedures from the literature, and then present a new approach from Berman et al. (2013).

Burer, Anstreicher and Dür (2009) show that 5×5 extreme doubly nonnegative matrices which are not completely positive can be characterized as follows.

Theorem 6.2.1 (Burer et al. (2009, Corollary 1)) *Let $X \in \mathcal{D}_5$. Then $X \in \mathrm{Ext}(\mathcal{D}_5) \setminus \mathcal{C}_5^*$ if and only if $\mathrm{rank}(X) = 3$ and X is cyclic, i.e., $G(X)$ is a 5-cycle.*

Another characterization is based on the fact that these matrices can be represented as $P^T X P = DRR^T D$ with P, D and R defined as in the following theorem.

Theorem 6.2.2 (Burer et al. (2009, Theorem 3)) *A matrix $X \in \mathcal{S}_5$ is extreme doubly nonnegative but not completely positive if and only if there exists a permutation matrix P, a diagonal matrix D with strictly positive diagonal entries, and a 5×3 matrix*

$$R = \begin{pmatrix} 1 & 0 & 0 \\ r_{21} & r_{22} & 1 \\ 0 & 1 & 0 \\ 0 & 1 & -r_{22} \\ 1 & 0 & -r_{21} \end{pmatrix} \qquad (r_{21}, r_{22} > 0)$$

such that $P^T X P = DRR^T D$.

Based on these results, Burer, Anstreicher and Dür (2009) show how to separate such a matrix from the completely positive cone. To construct a cut, the Horn matrix H as defined in (2.1) is used.

Theorem 6.2.3 (Burer et al. (2009, Lemma 4 and Theorem 8)) *Let $X \in \mathrm{Ext}(\mathcal{D}_5)$ be a cyclic matrix with $\mathrm{rank}(X) = 3$, and let $P^T X P = DRR^T D$ be its representation provided by Theorem 6.2.2. Define $u = -(P^T X P \circ H)^{-1} e$ and $K = P(H \circ uu^T)P^T$. Then $u > 0$ and the copositive matrix K is a cut that separates X from the completely positive cone.*

Dong and Anstreicher (2013) generalize this separation procedure to matrices $X \in \mathcal{D}_5 \setminus \mathcal{C}_5^*$ having at least one off-diagonal zero. In the following, we assume that X has the form

$$X = \begin{pmatrix} X_{11} & \alpha_1 & \alpha_2 \\ \alpha_1^T & 1 & 0 \\ \alpha_2^T & 0 & 1 \end{pmatrix} \qquad (X_{11} \in \mathcal{D}_3)$$

which can always be achieved by applying an appropriate permutation and scaling. Then we have the following.

Theorem 6.2.4 (Dong and Anstreicher (2013, Theorem 6)) *If $X \in \mathcal{D}_5$, then $X \in \mathcal{D}_5 \setminus \mathcal{C}_5^*$ if and only if there is a matrix*

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

and $\langle K, X \rangle < 0$.

In general, the matrix K is not copositive. But by slightly modifying K, we get a copositive matrix that cuts off X.

Theorem 6.2.5 (Dong and Anstreicher (2013, Theorem 7)) *Let $X \in \mathcal{D}_5 \setminus \mathcal{C}_5^*$ and let K satisfy the conditions of Theorem 6.2.4. Define*

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

Then $\langle K(s), X \rangle < 0$ for any s, and $K(s) \in \mathcal{C}_5$ for $s \geq \sqrt{\gamma_1 \gamma_2}$.

As shown in Dong and Anstreicher (2013), the matrix K can be obtained by numerically minimizing $\langle K, X \rangle$ such that K satisfies the conditions in Theorem 6.2.4 and is normalized via $\langle I, K \rangle = 1$ or a similar constraint. This approach can be extended to larger matrices having block structure. For details see Dong and Anstreicher (2013).

Extending the results of Burer et al. (2009) and Dong and Anstreicher (2013), Burer and Dong (2013) establish the first full separation algorithm for 5×5 completely positive matrices. Let

$$(\mathcal{C}_5^*)^{(1)} = \left\{ \begin{pmatrix} 0 & 0 \\ 0 & X \end{pmatrix} : X \in \mathcal{C}_4^* \right\}$$

and, for $i = 2, \ldots, 5$, let $(\mathcal{C}_5^*)^{(i)}$ be the respective embedding of $\mathcal{C}_4^*$ in $\mathcal{S}_5$. That is, $(\mathcal{C}_5^*)^{(i)}$ is the set of completely positive 5×5 matrices whose i-th row and column are zero. Furthermore, for $i = 1, \ldots, 5$, denote by X_i^0 an appropriate embedding of $I + \frac{1}{16}E \in \mathcal{S}_4$ into $(\mathcal{C}_5^*)^{(i)}$, i.e., X_i^0 is the 5×5 matrix whose i-th row and column are zero and such that the principal submatrix resulting from deleting the i-th row and column is $I + \frac{1}{16}E$. Define $X^0 = \sum_{i=1}^5 \frac{1}{5} X_i^0$. Then, the following theorem gives a separation algorithm for $\mathcal{C}_5^*$, see Burer and Dong (2013, Theorem 2 and Corollary 1).

Theorem 6.2.6 *Suppose $X \in \mathcal{D}_5$. Let $\bar{y}$ denote the optimal value of*

$$\min\left\{\langle X, K\rangle : K \in \mathcal{S}_5,\ K_{[i,i]} \in \mathcal{D}_4^* \ \forall i = 1, \ldots, 5, \\ \langle X^0, K\rangle \leq 1,\ \langle XKX, E\rangle \geq 0\right\}, \tag{6.2}$$

where $K_{[i,i]}$ is the principal submatrix of K resulting from deleting the i-th row and column. If $\bar{y} \geq 0$, then $X \in \mathcal{C}_5^*$. If, on the contrary, $\bar{y} < 0$, then $X \notin \mathcal{C}_5^*$ and any optimal solution K of (6.2) is copositive and separates X from the completely positive cone.

We now describe another approach (Berman et al., 2013). Suppose that $X \in \mathcal{D}_5$. Let H stand for either the Horn matrix or a Hildebrand matrix, or a suitable permutation of one of these matrices, and define $B = X \circ H$. Assume that $B \notin \mathcal{C}_n$. Then according to Theorem 2.3.11, $X \notin \mathcal{C}_n^*$. We next demonstrate how to construct a cut in this case.

Since $X \in \mathcal{D}_5$, all principal 4×4 submatrices of X are completely positive, and hence all principal 4×4 submatrices of B are copositive. This means that B is copositive of order 4. We thus have

$$B \text{ is not copositive} \quad \Leftrightarrow \quad B \text{ is copositive of exact order 4.}$$

From Theorem 2.2.10 we get that in this case $B^{-1} \leq 0$ or equivalently $-B^{-1} \geq 0$. By Theorem 1.1.1, the spectral radius ρ of $-B^{-1}$ is an eigenvalue of $-B^{-1}$, and the matrix has a nonnegative eigenvector u corresponding to ρ. Then u is also an eigenvector of B corresponding to the negative eigenvalue $\lambda = -\frac{1}{\rho}$ of B. Define the matrix $K := H \circ uu^T$ which is copositive according to Theorem 2.2.16. Then

$$\langle K, X\rangle = \langle H \circ uu^T, X\rangle = \langle uu^T, X \circ H\rangle = u^T(X \circ H)u = u^T B u = \lambda u^T u < 0,$$

which shows that K provides a cut as desired.

Although the approach is different, the basic structure of this cut is the same as for the cuts in Theorem 6.2.3. As we have seen above, these cuts are also of the form $H \circ uu$ with H denoting the Horn matrix. However, the vector u is different from the one we use here. Also note that the construction in Theorem 6.2.3 works for extreme doubly nonnegative matrices only, whereas the procedure outlined above works for arbitrary 5×5 doubly nonnegative matrices.

6.3. Cutting planes based on copositive projection

Let $(\mathrm{P}_{\mathcal{C}^*})$ be the completely positive program from Section 6.1 and let $(\mathrm{P}_{\mathcal{D}})$ be its doubly nonnegative relaxation. We will show in Section 6.3.1 that if the optimal solution $\bar{X}$ of $(\mathrm{P}_{\mathcal{D}})$ is not completely positive, we can find a cutting plane that separates $\bar{X}$ from the set of feasible solutions of $(\mathrm{P}_{\mathcal{C}^*})$ by projecting $\bar{X}$ onto an outer approximation of $\mathcal{C}_n^*$. Adding the cut to $(\mathrm{P}_{\mathcal{D}})$ results in a tighter relaxation of the original problem and an improved lower bound on its optimal value. In Section 6.3.2, we will apply the separation procedure to some stable set problems and discuss the numerical results.

6.3.1. Constructing a cut

In the following, we assume that $\bar{X} \in \mathcal{D}_n \setminus \mathcal{C}_n^*$. As we have seen in Section 4.3, we can project $\bar{X}$ onto an outer approximation $\mathcal{I}_{\mathcal{P}}^*$ of $\mathcal{C}_n^*$ by projecting $-\bar{X}$ on the corresponding inner approximation $\mathcal{I}_{\mathcal{P}}$ of $\mathcal{C}_n$, i.e.,

$$\mathrm{pr}(\mathcal{I}_{\mathcal{P}}^*, \bar{X}) = \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}) + \bar{X}. \tag{6.3}$$

If $\bar{X} \notin \mathcal{C}_n^*$, we can find an outer approximation $\mathcal{I}_{\mathcal{P}}^*$ of $\mathcal{C}_n^*$ such that $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$. We will show that in this case the inequality

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), X \right\rangle \geq 0$$

cuts off $\bar{X}$. To this end, we need the following proposition (Hiriart-Urruty and Lemaréchal, 1993, Proposition III.3.1.3).

Proposition 6.3.1 *Let $\mathcal{K}$ be a nonempty closed convex set in $\mathbb{R}^n$. For all $x_1, x_2 \in \mathbb{R}^n$, we have*

$$\|\mathrm{pr}(\mathcal{K}, x_1) - \mathrm{pr}(\mathcal{K}, x_2)\|^2 \leq \langle \mathrm{pr}(\mathcal{K}, x_1) - \mathrm{pr}(\mathcal{K}, x_2), x_1 - x_2 \rangle .$$

If $0 \in \mathcal{K}$, this proposition implies

$$\|\mathrm{pr}(\mathcal{K}, x)\|^2 \leq \langle \mathrm{pr}(\mathcal{K}, x), x \rangle \quad \text{for all } x \in \mathbb{R}^n.$$

Consequently, we have $\left\| \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}) \right\|^2 \leq \left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), -\bar{X} \right\rangle$ or equivalently

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), \bar{X} \right\rangle \leq - \left\| \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}) \right\|^2 . \tag{6.4}$$

From (6.3) we get

$$\bar{X} \in \mathcal{I}_{\mathcal{P}}^* \quad \Leftrightarrow \quad \mathrm{pr}(\mathcal{I}_{\mathcal{P}}^*, \bar{X}) = \bar{X} \quad \Leftrightarrow \quad \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}) = 0$$

and thus

$$\bar{X} \in \mathcal{I}_{\mathcal{P}}^* \quad \Leftrightarrow \quad \|\mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X})\|^2 = 0. \tag{6.5}$$

Combining (6.4) and (6.5), we get

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), \bar{X} \right\rangle < 0 \quad \text{for all } \bar{X} \notin \mathcal{I}_{\mathcal{P}}^*.$$

On the other hand, the matrix $\mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X})$ is copositive by construction, which means that we have

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), X \right\rangle \geq 0 \quad \text{for all } X \in \mathcal{C}_n^*.$$

Therefore, we have shown the following result:

Theorem 6.3.2 *Let $\bar{X} \notin \mathcal{C}_n^*$ and let $\mathcal{I}_{\mathcal{P}}^*$ be an outer approximation of $\mathcal{C}_n^*$ such that $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$. Then the inequality*

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), X \right\rangle \geq 0$$

is a cut which separates $\bar{X}$ from the completely positive cone.

Consequently, if $\bar{X}$ is the solution of the relaxation $(\mathrm{P}_{\mathcal{D}})$ and $\mathcal{I}_{\mathcal{P}}^*$ is such that $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$, then the inequality

$$\left\langle \mathrm{pr}(\mathcal{I}_{\mathcal{P}}, -\bar{X}), X \right\rangle \geq 0$$

is a cut that separates $\bar{X}$ from the feasible set of $(\mathrm{P}_{\mathcal{C}^*})$.

6.3.2. Numerical results for some stable set problems

We will illustrate the separation procedure by discussing computational results for some stable set problems. Let G be a graph and A_G its adjacency matrix. As shown in de Klerk and Pasechnik (2002), the problem of computing the stability number α of G can be stated as a completely positive optimization problem:

$$\frac{1}{\alpha} = \min\{\langle I + A_G, X\rangle : \langle E, X\rangle = 1, X \in \mathcal{C}_n^*\}. \tag{6.6}$$

Replacing $\mathcal{C}_n^*$ by $\mathcal{D}_n$ results in a relaxation of the problem providing an upper bound on α. This bound ϑ' is called Lovász–Schrijver bound:

$$\frac{1}{\vartheta'} = \min\{\langle I + A_G, X\rangle : \langle E, X\rangle = 1, X \in \mathcal{D}_n\}. \tag{6.7}$$

We consider the 5-cycle C_5 and the graphs G_8, G_{11}, G_{14} and G_{17} from Peña et al. (2007) for which $\vartheta' \neq \alpha$ implying that the solution matrix $\bar{X}$ of (6.7) is not completely positive. For each of the optimization problems associated to these graphs, we want to find an outer approximation $\mathcal{I}_{\mathcal{P}}^*$ of $\mathcal{C}_n^*$ such that $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$. According to Theorem 6.3.2, we can then compute a cut that separates $\bar{X}$ from the feasible set of (6.6).

As long as $\bar{X} \in \mathcal{I}_{\mathcal{P}}^*$, the matrix can be written as

$$\bar{X} = \sum_{\{u,v\}\in E_{\mathcal{P}}} \lambda_{uv}(uv^T + vu^T) + \sum_{v\in V_{\mathcal{P}}} \lambda_v vv^T \quad \text{with } \lambda_{uv}, \lambda_v \in \mathbb{R}_+. \tag{6.8}$$

This leads to the following partitioning strategy: We start with the standard simplex and compute a factorization of $\bar{X}$ according to (6.8). If the problem is feasible, we reorder all edges $\{u, v\}$ such that the corresponding coefficients λ_{uv} are in decreasing order, and bisect those edges with $\lambda_{uv} \geq p\cdot \max_{\{u_i,v_i\}\in E_{\mathcal{P}}} \lambda_{u_i v_i}$ for some $0 \leq p \leq 1$. We iterate the process of computing a factorization and refining the partition until the factorization problem becomes infeasible which means that $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$. Then we project $-\bar{X}$ onto $\mathcal{I}_{\mathcal{P}}$, add the resulting cut to (6.7) and compute a new bound on α. If the solution matrix of this new problem is not completely positive we can repeat the procedure and compute a cut that separates it from the feasible set of (6.6).

We implemented this approach in Matlab and used Yalmip (Löfberg, 2004) and SeDuMi (Sturm, 1999) to solve the relaxations. To compute a feasible solution of the factorization, we maximized the function $\sum_{\{u,v\}\in E_{\mathcal{P}}} \langle I + A_G, uv^T + vu^T\rangle \lambda_{uv}$ and set the constant p to 0.95. The factorization as well as the projections were computed with SeDuMi. The resulting bounds on the stability number after adding one and ten cuts computed by this method can be found in Table 6.1. The numbers in parentheses indicate the total number of bisections. Furthermore, for each graph, the stability number α, the Lovász–Schrijver bound ϑ' and the bounds ϑ^{BFL} from Bomze et al. (2010a), $\vartheta^{\text{DA}^*}_{\text{mean}}$ from Dong and Anstreicher (2011) and $\vartheta^{\text{DA}}_{\text{mean}}$ from (Dong and Anstreicher, 2013) are given.[1] Except for the graph G_8, the number of bisections is very small and the computed bounds after adding ten cuts are comparable to $\vartheta^{\text{DA}^*}_{\text{mean}}$.

[1] While the author was in the process of finishing this thesis, the final version of the pa-

						Bound values after	
G	α	ϑ'	ϑ^{BFL}	$\vartheta^{\mathrm{DA}^*}_{\mathrm{mean}}$	$\vartheta^{\mathrm{DA}}_{\mathrm{mean}}$	1 cut	10 cuts
C_5	2	2.236	-	-	-	2.000 (5)	2.000 (5)
G_8	3	3.468	3	3.078	3.078	3.461 (148)	3.452 (158)
G_{11}	4	4.694	4.28	4.500	4.362	4.610 (11)	4.544 (23)
G_{14}	5	5.916	5.485	5.722	5.585	5.825 (14)	5.758 (24)
G_{17}	6	7.134	6.657	6.930	6.814	7.065 (17)	6.986 (28)

Table 6.1.: Results on different stable set problems

We tried a different subdivision procedure based on the objective function of problem (6.7) which gives better results but needs significantly more bisections. So we bounded the total number of bisections for each instance by 2000. The strategy is to bisect all edges $\{u, v\}$ for which the value of $\langle I + A_G, uv^T + vu^T\rangle$ is minimal. We denote the set of these edges by $\widehat{E}_{\mathcal{P}}$. To restrict the number of bisections, we then choose those edges for which $uv^T + vu^T$ is close to $\bar{X}$, i.e., all edges $\{u, v\} \in \widehat{E}_{\mathcal{P}}$ for which

$$\|\bar{X} - (uv^T + vu^T)\| \leq (1+q)\cdot \min_{\{u_i,v_i\}\in\widehat{E}_{\mathcal{P}}} \|\bar{X} - (u_i v_i^T + v_i u_i^T)\|$$

for some $q \geq 0$. We reorder these edges such that the values of $\|\bar{X} - (uv^T + vu^T)\|$ increase, and bisect. This bisection procedure is repeated until $\bar{X} \notin \mathcal{I}^*_{\mathcal{P}}$. The computed bounds for $q = 0.1$ after adding one and ten cuts as well as the corresponding number of bisections are shown in columns 4 and 5 of Table 6.2. The results after adding ten cuts are better than for the first strategy. Especially for G_{11} this strategy works very well. For G_8 the number of bisections is even less than when using the first strategy but for all other examples it is significantly larger. For G_{17} the bound on the number of bisections is exceeded, so we did not get a result.

Since the first subdivision strategy only needs few bisections but the second one gives better results, our last strategy is a mix of both. We start with

per (Dong and Anstreicher, 2013) appeared. Since the computed bounds differ from the ones given in the preprint (Dong and Anstreicher, 2011), we decided to include both. In contrast to the preprint, the final version of the paper contains several rounds of cuts, and bounds after each round of cuts are given. We took $\vartheta^{\mathrm{DA}}_{\mathrm{mean}}$ to be the bound after the first round of cuts since this bound seems to correspond best to the one given in the preprint.

	Strategy 1		Strategy 2		Strategy 3	
G	1 cut	10 cuts	1 cut	10 cuts	1 cut	10 cuts
C_5	2.000 (5)	2.000 (5)	2.000 (5)	2.000 (13)	2.000 (10)	2.000 (47)
G_8	3.461 (148)	3.452 (158)	3.427 (78)	3.176 (82)	3.454 (158)	3.213 (237)
G_{11}	4.610 (11)	4.544 (23)	4.610 (39)	4.000 (147)	4.610 (15)	4.260 (141)
G_{14}	5.825 (14)	5.758 (24)	5.825 (68)	5.683 (1197)	5.825 (18)	5.757 (721)
G_{17}	7.065 (17)	6.986 (28)	7.065 (105)	–	7.065 (24)	6.986 (1289)

Table 6.2.: Bound values for different subdivision strategies

the standard simplex and bisect edges $\{u, v\}$ according to the first subdivision strategy until $\bar{X} \notin \mathcal{I}_{\mathcal{P}}^*$. Then we bisect all edges $\{u, v\}$ that meet the condition of the second strategy. After this subdivision procedure, we project $-\bar{X}$ onto $\mathcal{I}_{\mathcal{P}}$, add the resulting cut to (6.7) and compute a new bound on α. The resulting bounds for $p = 0.95$ and $q = 0.1$ as well as the corresponding number of bisections are shown in columns 6 and 7 of Table 6.2. Only for G_8 and G_{11} do the resulting bounds lie between the ones of the first and second subdivision strategy. For G_{14} and G_{17} the number of bisections is less than for the second strategy. However, the resulting bounds for these two instances are not better than those of the first strategy.

From the results in Table 6.2 it can be seen that the subdivision strategy has a crucial influence on the quality of the bounds as well as on the number of bisections. There is a lot of freedom in how an edge is selected and bisected which allows to adapt the approach to different problems and to exploit structural properties. However, it might not be easy to find the optimal strategy.

In all test instances, our results are comparable though slightly weaker than those obtained in Bomze et al. (2010a) and Dong and Anstreicher (2013). This difference is due to the specific procedures used to obtain the cuts. The reader may wonder why so much effort is put into improving bounds of the integer-valued stability number by minor decimal places. As explained in Bomze et al. (2010b), small improvements can be vital in the context of product graphs.

6.4. Cutting planes based on triangle-free subgraphs

We now show how to separate doubly nonnegative matrices that have a triangle-free graph from the completely positive cone. The basic idea of the approach presented in this section is stated in the following theorem.

Theorem 6.4.1 *Let $X \in \mathcal{D}_n \setminus \mathcal{C}_n^*$, and let $K \in \mathcal{C}_n$ be such that $K \circ X \notin \mathcal{C}_n$. Then for every nonnegative $u \in \mathbb{R}^n$ such that $u^T(K \circ X)u < 0$, the copositive matrix $K \circ uu^T$ is a cut separating X from the completely positive cone.*

Proof Suppose that $X \in \mathcal{D}_n \setminus \mathcal{C}_n^*$. By Theorem 2.3.11, there always exists a copositive matrix K such that $K \circ X \notin \mathcal{C}_n$. Now let $u \geq 0$ be such that $u^T(K \circ X)u < 0$. By Theorem 2.2.16, the matrix $K \circ uu^T$ is copositive, and we have

$$\langle K \circ uu^T, X\rangle = u^T(K \circ X)u < 0. \qquad \square$$

If $K \circ X \notin \mathcal{C}_n$, as assumed in the theorem, then by Theorem 2.2.12, $K \circ X$ has a principal submatrix having a positive eigenvector corresponding to a negative eigenvalue. This shows that u can always be chosen as this eigenvector with zeros added to get a vector in $\mathbb{R}^n$.

The following property is obvious but useful, since it allows to construct cutting planes based on submatrices instead of the entire matrix.

Lemma 6.4.2 *Assume that $K \in \mathcal{C}_n$ is a copositive matrix that separates a matrix X from $\mathcal{C}_n^*$. If $A \in \mathbb{R}^{n\times p}$ and $B \in \mathcal{S}_p$ are arbitrary matrices, then the copositive matrix*

$$\begin{pmatrix} K & 0 \\ 0 & 0 \end{pmatrix} \quad \text{is a cut that separates} \quad \begin{pmatrix} X & A \\ A^T & B \end{pmatrix} \quad \text{from } \mathcal{C}_{n+p}^*.$$

Note in the situation of Lemma 6.4.2 it is desirable that K be extreme copositive rather than just copositive, since an extreme matrix will provide a supporting hyperplane and therefore a better (deeper) cut.

6.4.1. Separating a triangle-free doubly nonnegative matrix

Let $X \in \mathcal{D}_n$. We may assume that X has only positive diagonal entries, since otherwise the row and column corresponding to a zero diagonal entry would be zero and we could base our cut on the nonzero submatrix. By applying a suitable scaling if necessary we can also assume that $\operatorname{diag}(X) = e$. Moreover, we will assume that the matrices that we want to separate from the completely positive cone are irreducible, since any reducible matrix can be written as a block diagonal matrix and then the problem can be split into subproblems of smaller dimension where each of the submatrices on the diagonal is considered separately.

Now suppose that X has a triangle-free graph $G(X)$. Note that irreducibility of X is equivalent to $G(X)$ being connected. By the assumptions made above, X is representable as

$$X = I + C, \tag{6.9}$$

where C is a matrix with zero diagonal and $G(C) = G(X)$.

Assume that $X \in \mathcal{D}_n$ is of the form (6.9) but not completely positive. Then, by Corollary 2.3.10, $\rho(C) > 1$. Let u denote the eigenvector of C corresponding to the eigenvalue $\rho(C)$. Since X is nonnegative and irreducible, we have $u > 0$ by Theorem 1.1.1. Recall that the comparison matrix of X is defined by

$$(M(X))_{ij} = \begin{cases} |X_{ij}| & \text{if } i = j \\ -|X_{ij}| & \text{if } i \neq j. \end{cases}$$

We thus have $M(X) = I - C$ and

$$u^T M(X) u = u^T u - u^T C u = u^T u(1 - \rho(C)) < 0.$$

We next construct a copositive matrix A with the property that $M(X) = X \circ A$. It is given by

$$A_{ij} = \begin{cases} -1 & \text{if } \{i, j\} \text{ is an edge of } G(X), \\ +1 & \text{else.} \end{cases} \tag{6.10}$$

Note that by the following theorem, for $n = 5$, the only triangle-free graph $G(X)$ such that $X \in \mathcal{D}_n \setminus \mathcal{C}_n^*$ is the 5-cycle. Thus for $n = 5$, A equals (a permutation of) the Horn matrix.

Theorem 6.4.3 (Berman and Shaked-Monderer (2003, Corollary 2.6)) *Let G be a graph. Then the following are equivalent:*

(i) *Every doubly nonnegative matrix X whose graph is G is completely positive.*

(ii) *G does not contain an odd cycle of length ≥ 5.*

Let $G_{-1}(A)$ be the graph on n vertices with $i \neq j$ being adjacent if and only if $A_{ij} = -1$. According to the following theorem, the matrix A is copositive. If, in addition, the diameter of $G_{-1}(A)$ equals 2, then A is even extreme.

Theorem 6.4.4 (Haynsworth and Hoffman (1969, Theorem 3.1)) *Let $A \in \mathcal{S}_n$ be such that every entry is 1 or -1 and each diagonal entry is 1. Then*

(i) *A is copositive if and only if $G_{-1}(A)$ is triangle-free.*

(ii) *A is extreme copositive if and only if $G_{-1}(A)$ is triangle-free and of diameter 2.*

It is easy to see that indeed $M(X) = X \circ A$. With u as above, we derive

$$0 > u^T M(X) u = u^T (X \circ A) u = \langle uu^T, X \circ A \rangle = \langle A \circ uu^T, X \rangle. \tag{6.11}$$

Since $u > 0$, the matrix $K = A \circ uu^T$ is copositive, which combined with the above gives that K is a cut that separates X from the completely positive cone.

Cyclic graphs

Cyclic graphs are special triangle-free graphs. When a matrix $X \in \mathcal{D}_n$ of the form (6.9) has a cyclic graph, then the above results can be strengthened. First note that by Theorem 6.4.3, if $G(X)$ is an even cycle, then $X \in \mathcal{C}_n^*$.

If $G(X)$ is an odd cycle, then for $n = 5$ let H denote the Horn matrix, and for $n \geq 7$ let H denote the Hoffman–Pereira matrix. This matrix has been introduced in Hoffman and Pereira (1973) for $n = 7$ but can easily be generalized to other dimensions, see Appendix A.

By the same arguments as above, the matrix $K := H \circ uu^T$ provides a cut separating X from the completely positive cone. In this case, H is an extreme copositive matrix. For $n = 5$, H is the Horn matrix which is extreme copositive, and for $n \geq 7$, H is a Hoffman–Pereira matrix. These matrices are also extreme which can be seen by applying Hoffman and Pereira (1973, Theorem 4.1). For a detailed proof see Appendix A. By Theorem 2.2.17, K is extreme as well, and therefore provides a deeper cut than the matrix A constructed above would.

6.4.2. Numerical results for some stable set problems

We next illustrate the separation procedure by applying it to some instances of the stable set problem. After stating the results, we compare them in Section 6.4.2.1 and Section 6.4.2.2 to the results of other separation procedures.

We use the following conic reformulation of the stable set problem which is due to de Klerk and Pasechnik (2002):

$$\alpha = \max\{\langle E, X \rangle : \langle I, X \rangle = 1,\ \langle A_G, X \rangle = 0,\ X \in \mathcal{C}_n^*\}. \tag{6.12}$$

As in Section 6.3.2, relaxing $\mathcal{C}_n^*$ to $\mathcal{D}_n$ results in the Lovász–Schrijver bound:

$$\vartheta' = \max\{\langle E, X \rangle : \langle I, X \rangle = 1,\ \langle A_G, X \rangle = 0,\ X \in \mathcal{D}_n\}. \tag{6.13}$$

We consider some instances for which $\vartheta' \neq \alpha$ and try to get better bounds by adding cuts to the doubly nonnegative relaxation. The cuts are computed as described in Section 6.4.1.

Let $\bar{X}$ denote the optimal solution we get by solving (6.13). If $\vartheta' \neq \alpha$, then $\bar{X} \in \mathcal{D}_n \setminus \mathcal{C}_n^*$. We want to find cuts that separate $\bar{X}$ from the feasible set of (6.12). To do so, we determine all 5×5 principal submatrices of $\bar{X}$ that have a connected triangle-free graph. Let Y denote such a submatrix. In general, $\operatorname{diag}(Y) \neq e$ as in (6.9). Therefore, we consider the scaled matrix DYD, where D is a diagonal matrix with $D_{ii} = \frac{1}{\sqrt{Y_{ii}}}$. Since Y is a doubly nonnegative matrix having a triangle-free graph, the same holds for DYD. Furthermore, DYD can be written as $DYD = I + C$, where C is a matrix with zero diagonal and $G(C)$ a triangle-free graph. Let ρ denote the spectral radius of C and let u be the eigenvector of C corresponding to the eigenvalue ρ. Let A be as in Section 6.4.1, i.e., for $n = 5$, the matrix A is the Horn matrix. If $\rho > 1$, then according to (6.11), we have

$$0 > \langle A \circ uu^T, DYD \rangle = \langle D(A \circ uu^T)D, Y \rangle.$$

Therefore, $D(A \circ uu^T)D$ defines a cut that separates Y from the completely positive cone.

As in Section 6.3.2, we consider as test instances the 5-cycle C_5 and the graphs G_8, G_{11}, G_{14} and G_{17} from Peña et al. (2007). For every 5×5 principal submatrix of the optimal solution $\bar{X}$ of (6.13) that has a triangle-free graph, we compute a cut. Note that for these instances none of the computed matrices $\bar{X}$ has a triangle-free subgraph of size greater than 5. We then solve the doubly nonnegative relaxation after adding each of these cuts and after adding all computed cuts. The results are shown in Table 6.3. We denote by ϑ^K_{min} and ϑ^K_{max} the minimal respectively maximal bound we get by adding a single cut to the doubly nonnegative relaxation (6.13), and ϑ^K_{all} denotes the bound we get after adding all computed cuts. The last column indicates the reduction of the optimality gap when all cuts are added.

6.4.2.1. Comparison with cuts based on subgraphs with known clique number

In this section, we compare our cuts to the ones introduced by Bomze, Frommlet and Locatelli (2010a), since the basic structure is quite similar. In Bomze et al. (2010a), the maximum clique problem is considered and cuts are computed to improve the bound resulting from solving the doubly nonnegative

Graph	α	ϑ'	ϑ^K_{min}	ϑ^K_{max}	ϑ^K_{all}	# cuts	reduction
C_5	2	2.236	2.0000	2.0000	2.0000	1	100%
G_8	3	3.468	3.3992	3.3992	3.2163	4	54%
G_{11}	4	4.694	4.6273	4.6672	4.4307	10	38%
G_{14}	5	5.916	5.8533	5.8977	5.6460	20	29%
G_{17}	6	7.134	7.0745	7.1227	6.8615	35	24%

Table 6.3.: Results on different stable set problems

relaxation of that problem. These cuts are based on subgraphs with known clique number.

To make it easier to compare the results, we assume that we want to compute the clique number ω of the complement of a graph G, i.e., that we want to determine $\omega(\bar{G})$, which is equivalent to the problem of computing the stability number α of G. As we have seen above (see (6.12)), the problem can be stated as

$$\omega(\bar{G}) = \alpha(G) = \max\{\langle E, X\rangle : \langle I, X\rangle = 1,\ \langle A_G, X\rangle = 0,\ X \in \mathcal{C}_n^*\}. \qquad (6.14)$$

Let ϑ' denote the bound on α that we get by solving the doubly nonnegative relaxation of (6.14). De Klerk and Pasechnik (2002, Corollary 2.4) have shown that by simplifying and dualizing (6.14), the stable set problem can also be stated as a copositive program

$$\alpha(G) = \min\{\lambda : \lambda(I + A_G) - E \in \mathcal{C}_n\}.$$

By $I + A_G = E - A_{\bar{G}}$, we get

$$\omega(\bar{G}) = \alpha(G) = \min\{\lambda : \lambda(E - A_{\bar{G}}) - E \in \mathcal{C}_n\}. \qquad (6.15)$$

The construction of cuts in Bomze et al. (2010a) is based on the observation that for any optimal solution $\bar{X}$ of the doubly nonnegative relaxation of (6.14), we have $\bar{X}_{ij} = 0$ for all $\{i, j\} \in E(G)$. This means that $\bar{X}_{ij} > 0$ implies $i = j$ or $\{i, j\} \in E(\bar{G})$. The cuts introduced in Bomze et al. (2010a) are based on subgraphs H of $\bar{G}$ with known clique number $\omega(H)$. According to (6.15), the matrix $\omega(H)(E - A_H) - E$ is copositive. Since $\omega(H) > 0$, this implies that the matrix

$$C'_H = (1 - \frac{1}{\omega(H)})E - A_H$$

is copositive, and consequently also

$$C_H = \begin{pmatrix} C'_H & 0 \\ 0 & 0 \end{pmatrix}$$

is copositive.

In Bomze et al. (2010a), a heuristic approach is used to find subgraphs H of $\bar{G}$ with known clique number $\omega(H)$ such that the matrix C_H is a cut that separates $\bar{X}$ from the feasible set of (6.14). For the computational results, subgraphs with clique number $\omega(H) = 2$ or 3 are considered. We will concentrate on the case that H is a subgraph with $\omega(H) = 2$, i.e., H is a triangle-free subgraph of $\bar{G}$.

In the approach described in Section 6.4.1, we consider (scaled) submatrices $Y = I + C$ of $\bar{X}$ that have a triangle-free graph $G(C)$. Since $\bar{X}_{ij} > 0$ implies $i = j$ or $\{i, j\} \in E(\bar{G})$, we can conclude that $G(C)$ is a subgraph of $\bar{G}$. Considering the definition of A in (6.10), it becomes clear that the negative entries of the cut correspond to the edges of $G(C)$. The same holds for the cuts C_H, i.e., the negative entries of C_H correspond to the edges of H which is a subgraph of $\bar{G}$. Therefore, the basic structure of the cuts is the same in the sense that the negative entries of the constructed matrices represent edges of a subgraph of $\bar{G}$. In Section 6.4.1, we consider triangle-free graphs which is a special case of the cuts in Bomze et al. (2010a). The main difference is how the cuts are constructed. While the entries of C'_H are either $(1 - \frac{1}{\omega(H)})$ or $-\frac{1}{\omega(H)}$, the cut K in Section 6.4.1 combines the basic matrix A with the eigenvector u.

Next, we compare both constructions. In order to do so, we consider the same instances as before and compute cuts of the form C_H for all 5×5 principal submatrices of the optimal solution $\bar{X}$ of the doubly nonnegative relaxation of (6.14) that have a triangle-free graph H. As for the cuts K, we then add these cuts to the doubly nonnegative relaxation and compute new bounds on $\omega(\bar{G}) = \alpha(G)$. We denote by $\vartheta^H_{\min}$ and $\vartheta^H_{\max}$ the minimal respectively maximal bound we get by adding a single cut, and by ϑ^H_{all} the bound resulting from adding all computed cuts. The results are shown in Table 6.4.

The results show that the bounds based on the cuts K from Section 6.4.1 are better than the bounds based on the cuts C_H from Bomze et al. (2010a). This comes from the fact that the construction of the cuts K is more specific. The cuts K do not only reflect which entries of $\bar{X}$ are positive but also the entries of $\bar{X}$ themselves play a role, in form of the eigenvector u. On the other hand, the cuts in Bomze et al. (2010a) are more general since they also apply to subgraphs with higher clique number, and the subgraphs do not have to be induced subgraphs. Moreover, if those cuts are not restricted to triangle-

Graph	α	ϑ'	ϑ^K_{min}	ϑ^H_{min}	ϑ^K_{max}	ϑ^H_{max}	ϑ^K_{all}	ϑ^H_{all}
C_5	2	2.236	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000
G_8	3	3.468	3.3992	3.4149	3.3992	3.4149	3.2163	3.2609
G_{11}	4	4.694	4.6273	4.6508	4.6672	4.6712	4.4307	4.5097
G_{14}	5	5.916	5.8533	5.8805	5.8977	5.9023	5.6460	5.7506
G_{17}	6	7.134	7.0745	7.1038	7.1227	7.1263	6.8615	6.9843

Table 6.4.: Comparison with the cuts from Bomze et al. (2010a)

free subgraphs, then better bounds are obtained as the results in Bomze et al. (2010a) show.

6.4.2.2. Comparison with other cutting planes

Finally, we want to compare our results to the results from Dong and Anstreicher (2013) and to the results presented in Section 6.3.2. For the sake of completeness, we also include the results from Bomze et al. (2010a) although these cuts have already been considered in Section 6.4.2.1. Furthermore, as in Section 6.3.2, we also consider the results of Dong and Anstreicher (2011).

The different bounds are stated in Table 6.5. The bound from Bomze et al. (2010a) is denoted by ϑ^{BFL}, the bound from Dong and Anstreicher (2011) by $\vartheta^{\text{DA}^*}_{\text{mean}}$, the bound from Dong and Anstreicher (2013) by $\vartheta^{\text{DA}}_{\text{mean}}$, and ϑ^{SD} denotes the bound from Section 6.3.2 when using the third subdivision strategy.

Note that ϑ^{BFL} is different from the bound ϑ^H presented in the previous section. This is because for the computation of ϑ^H only triangle-free subgraphs were considered, whereas for the computation of ϑ^{BFL} also cuts based on subgraphs with higher clique number are added to the doubly nonnegative relaxation of (6.14).

As can be seen from the table, the bound ϑ^K_{all} is comparable to the bounds $\vartheta^{\text{DA}^*}_{\text{mean}}$ and ϑ^{SD}. For some of the instances the cuts from Dong and Anstreicher (2011) and Section 6.3.2 give better results, whereas for other instances the cuts introduced here yield a better bound. The results from Dong and Anstreicher (2013) are slightly better in all cases. The same holds for the results from Bomze et al. (2010a), which comes from the fact that these cuts are more general in the sense that they are not only based on triangle-free subgraphs but also use subgraphs with clique number 3. Nevertheless, we have seen in Section 6.4.2.1 that our construction gives better results when the underlying

Graph	α	ϑ'	ϑ^K_{all}	ϑ^{BFL}	$\vartheta^{\text{DA}^*}_{\text{mean}}$	$\vartheta^{\text{DA}}_{\text{mean}}$	ϑ^{SD}
G_8	3	3.468	3.216	3.000	3.078	3.078	3.213
G_{11}	4	4.694	4.431	4.280	4.500	4.362	4.260
G_{14}	5	5.916	5.646	5.485	5.722	5.585	5.757
G_{17}	6	7.134	6.862	6.657	6.930	6.814	6.986

Table 6.5.: Comparison with other cuts

subgraph is the same.

Summary and outlook

We considered several aspects of copositive programming. In Chapter 4, we showed how to project a matrix onto the copositive and the completely positive cone. These projections can be used to compute factorizations of completely positive matrices. To compute the copositive projections, we used inner and outer approximations of the copositive cone that are based on simplicial partitions of the standard simplex (cf. Bundfuss and Dür (2009)). There is a lot of freedom in how the simplicial partition is refined. Since the subdivision strategy has a crucial influence on the performance of the presented algorithms, it would be desirable to guide the partitioning in an efficient way. Although this seems to be a difficult problem, it could be worthwhile to study the influence of the subdivision strategy in more detail.

In Chapter 5, we considered the conic reformulation of the standard quadratic optimization problem. We showed that for several classes of objective functions, the relaxation resulting from replacing the copositive or the completely positive cone by a tractable cone is exact. These results lead to two algorithms for solving standard quadratic optimization problems. In these algorithms, the problem is repeatedly split into subproblems of smaller dimension. Consequently, the number of iterations quickly increases with the problem size. For one of the algorithms, we presented an extension that allows to considerably reduce the number of iterations. However, it would be desirable to further reduce the number of iterations in order to apply the algorithm to larger instances. Therefore, a topic of further research is the inclusion of a bounding procedure.

Another interesting question is how the presented algorithm performs when it is applied to problems having a separable objective function, since for this class Bomze and Locatelli (2012) developed an algorithm of worst-case complexity $\mathcal{O}(n \log n)$, whereas general standard quadratic optimization problems are NP-hard.

In Chapter 6, we studied cutting planes to separate a matrix from the completely positive cone. Two new approaches were presented. In the first approach, we showed how the copositive projections introduced in Chapter 4 can be used to compute cuts. It is an interesting open question how the approach can be adapted to different problems by exploiting structural properties.

Besides the cuts based on copositive projection, we showed how to separate a triangle-free doubly nonnegative matrix from the completely positive cone. We illustrated the method by applying it to some stable set problems in order to improve the Lovász–Schrijver bound ϑ'. If $\vartheta' \neq \alpha$ for a graph G, then G is not perfect which implies that it has an odd hole or antihole. We consider an optimal solution $\bar{X}$ of the semidefinite relaxation. There is a scaling D such that $D\bar{X}D = I + X$. $G(X)$ is a subgraph of $\bar{G}$ since $\bar{X}_{ij} > 0$ implies $i = j$ or $\{i, j\} \in E_{\bar{G}}$. Consequently, if G has an odd antihole, then there is a submatrix $Y = I + C$ of $D\bar{X}D$ such that $G(Y)$ is triangle-free. In this case, we can compute a cut as we have seen in Section 6.4. It is an open question what can we conclude if G has an odd hole and if we can construct a cut in that case.

A. Hoffman–Pereira matrices

Let A denote the Hoffman–Pereira matrix. This matrix has been introduced in Hoffman and Pereira (1973) for $n = 7$ and has the following form

$$A = \begin{pmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{pmatrix}.$$

The matrix can easily be extended to higher dimensions by increasing the number of diagonal bands of zeros. For odd $n \geq 7$, we will call these matrices $(n \times n)$ Hoffman–Pereira matrices. For $n = 7$, Hoffman and Pereira (1973) showed that A is an extreme copositive matrix. We will show that the same holds for every odd $n \geq 7$.

We will use the terminology of Hoffman and Pereira (1973). Let $\mathcal{E}$ denote the set of symmetric matrices in which every entry is 0, 1 or -1 and each diagonal entry is 1. To each $n \times n$ matrix $X \in \mathcal{E}$, we associate four graphs, $G_{-1}(X)$, $G_0(X)$, $G_1(X)$ and $L^*(X)$. The graph $G_{-1}(X)$ (respectively $G_0(X)$, $G_1(X)$) is a graph on n vertices with $i \neq j$ being adjacent if and only if $X_{ij} = -1$ (respectively $X_{ij} = 0$, $X_{ij} = 1$). The vertices of $L^*(X)$ are the edges of $G_0(X)$ with two vertices being adjacent if and only if the corresponding edges in $G_0(X)$ have a common vertex and the third edge of the associated triangle is an edge in $G_{-1}(X)$.

To illustrate the definitions, the graphs associated to the matrix A are given in Figure A.1.

Hoffman and Pereira used the following theorem to show that A is extreme copositive.

Theorem A.1 (Hoffman and Pereira (1973, Theorem 4.1)) *Let $X \in \mathcal{E}$. Then X is extreme copositive if and only if each of the following holds*

(i) $G_{-1}(X)$ *is connected and contains no triangles.*

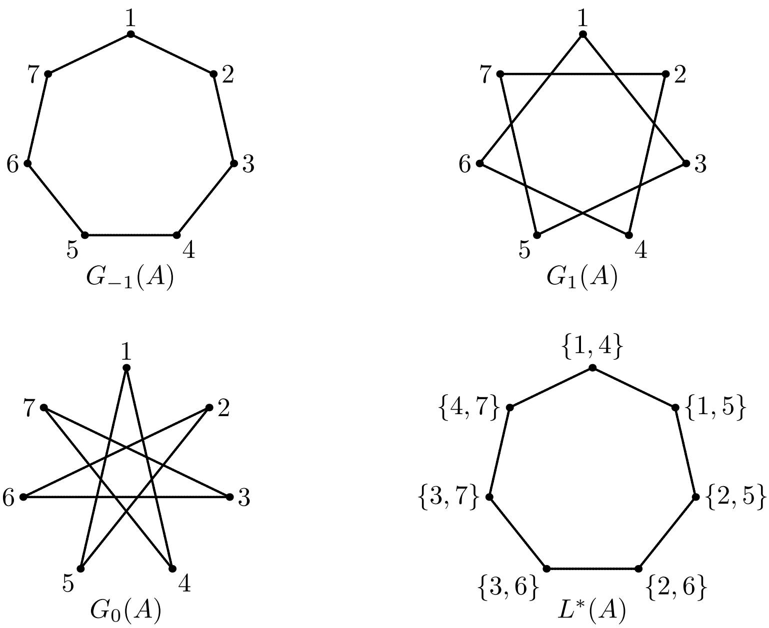

Figure A.1.: $G_{-1}(A)$, $G_1(A)$, $G_0(A)$ and $L^*(A)$

(ii) *$G_1(X)$ contains precisely those edges $\{i, j\}$ where i and j are at distance 2 in $G_{-1}(X)$.*

(iii) *$L^*(X)$ has no isolated vertices and no connected component that is bipartite.*

Applying Theorem A.1, we want to show the following.

Theorem A.2 *Let $n \geq 7$ be odd. Then the $n \times n$ Hoffman–Pereira matrix is extreme copositive.*

Proof Let B be an $n \times n$ Hoffman–Pereira matrix for $n \geq 7$ be odd. We will check the conditions of Theorem A.1 to show that B is an extreme copositive matrix.

(i): It is easy to see that $G_{-1}(B)$ is a cycle of length n, i.e., $G_{-1}(B) = (1, 2, \ldots, n, 1)$. Thus $G_{-1}(B)$ is connected and triangle-free.

(ii): The graph $G_1(B)$ is the n-cycle $(1, 3, \ldots, n-2, n, 2, 4, \ldots, n-1, 1)$, hence it contains precisely those edges that are at distance 2 in $G_{-1}(B)$.

(iii): The vertices of $L^*(B)$ are the edges of $G_0(B)$, i.e., the set of vertices can be described as

$$V(L^*(B)) = \{\{i,j\} : \mathrm{d}_{G_{-1}(B)}(i,j) \geq 3,\ i,j = 1,\ldots,n\}.$$

Two vertices $\{i,j\}$ and $\{i',j'\}$ are adjacent if and only if

$$\begin{aligned}
&\big(i = i' \quad \text{and} \quad \{j,j'\} \in E(G_{-1}(B))\big)\\
\text{or}\quad &\big(i = j' \quad \text{and} \quad \{j,i'\} \in E(G_{-1}(B))\big)\\
\text{or}\quad &\big(j = i' \quad \text{and} \quad \{i,j'\} \in E(G_{-1}(B))\big)\\
\text{or}\quad &\big(j = j' \quad \text{and} \quad \{i,i'\} \in E(G_{-1}(B))\big).
\end{aligned}$$

From the description of the vertex and edge set, it can be seen that the n-cycle

$$\begin{aligned}C = \big(&\{1,4\},\{1,5\},\ldots,\{1,n-2\},\\ &\{2,n-2\},\{2,n-1\},\{3,n-1\},\{3,n\},\{4,n\},\{1,4\}\big)\end{aligned}$$

is a subgraph of $L^*(B)$. For $n = 7$, the cycle contains all vertices of $L^*(B)$ showing the result.

For $n \geq 9$, the graph has more vertices and we will first show that the other vertices of $L^*(B)$ are all connected to C. The vertices $\{2,5\},\{2,6\},\ldots,\{2,n-3\}$ lie on a path which is connected to C since $\{2,n-3\}$ is adjacent to $\{2,n-2\}$. Similarly, the vertices $\{3,6\},\{3,7\},\ldots,\{3,n-2\}$ and the vertices $\{4,7\},\ldots,\{4,n-1\}$ form paths, and $\{3,n-2\}$ is adjacent to $\{3,n-1\}$ and $\{4,n-1\}$ is adjacent to $\{4,n\}$. Thus both paths are connected to the cycle. The remaining vertices of the graph lie on the paths

$$\begin{aligned}
&\big(\{5,8\},\{5,9\},\ldots,\{5,n\}\big)\\
&\quad\vdots\\
&\big(\{n-4,n-1\},\{n-4,n\}\big)\\
&\big(\{n-3,n\}\big).
\end{aligned}$$

Since the end vertices of these paths form the path

$$\big(\{5,n\},\ldots,\{n-4,n\},\{n-3,n\}\big),$$

all vertices of these paths are connected, and since $\{5,8\}$ and $\{4,8\}$ are adjacent, the vertices are also all connected to C. Consequently, the graph $L^*(B)$ consists of only one component. Thus, the graph has no isolated vertices. Furthermore, the only component of $L^*(B)$ is not bipartite since it contains an odd cycle. $\square$

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Notation

Vectors

$\mathbb{R}^n_+$	Set of nonnegative real n-vectors.
$\mathbb{R}^n_{++}$	Set of positive real n-vectors.
e	Vector of all-ones.
e_i	i-th unit vector.
$\operatorname{diag}(D)$	For $D \in \mathbb{R}^{n\times n}$, $\operatorname{diag}(D)$ is the vector $d \in \mathbb{R}^n$ with $d_i = D_{ii}$, $i = 1, \dots, n$.

Matrices

$\mathcal{C}_n$	Set of copositive $n \times n$ matrices.
$\mathcal{C}_n^*$	Set of completely positive $n \times n$ matrices.
$\mathcal{C}_\mathcal{K}$	Set of $\mathcal{K}$-semidefinite matrices.
$\mathcal{D}_n$	Set of doubly nonnegative $n \times n$ matrices
$\mathcal{N}_n$	Set of nonnegative symmetric $n \times n$ matrices.
$\mathcal{S}_n$	Set of symmetric $n \times n$ matrices.
$\mathcal{S}_n^+$	Set of positive semidefinite symmetric $n \times n$ matrices.
$\mathcal{S}_n^{++}$	Set of positive definite symmetric $n \times n$ matrices.
$\|A\|$	Frobenius norm of A, i.e., $\|A\| = \sqrt{\sum_{i,j=1}^n \lvert A_{ij}\rvert^2}$.
$\langle A, B\rangle$	Inner product of $A, B \in \mathbb{R}^{m\times n}$, i.e., $\langle A, B\rangle = \operatorname{trace}(B^T A)$.

$A \circ B$	Hadamard product of $A, B \in \mathbb{R}^{m \times n}$, i.e., $A \circ B$ is the matrix with entries $(A \circ B)_{ij} = A_{ij} B_{ij}$.
$A \geq 0$	A is entrywise nonnegative (and symmetric).
$A \succ 0$	A is positive definite (and symmetric).
$A \succeq 0$	A is positive semidefinite (and symmetric).
E	Matrix of all-ones.
I	Identity matrix.
$M(A)$	Comparison matrix of A, page 20.
$\mathrm{Diag}(d)$	For $d \in \mathbb{R}^n$, $\mathrm{Diag}(d)$ is the diagonal matrix $D \in \mathbb{R}^{n \times n}$ with $D_{ii} = d_i$, $i = 1, \ldots, n$.
$\mathrm{rank}(A)$	Rank of A.
$\mathrm{trace}(A)$	Trace of A.
$\rho(A)$	Spectral radius of A.

Sets

$\mathrm{aff}(M)$	Affine hull of M.
$\mathrm{cl}(M)$	Closure of M.
$\mathrm{cone}(M)$	Conic hull of M.
$\mathrm{conv}(M)$	Convex hull of M.
$\mathrm{int}(M)$	Interior of M.
$\mathrm{relint}(M)$	Relative interior of M.
$\mathrm{span}(M)$	Linear hull of M.
$\mathrm{Ext}(\mathcal{K})$	Set of vectors generating extreme rays of the cone $\mathcal{K}$.
$\mathcal{K}^*$	Dual cone of $\mathcal{K}$.
$\mathcal{K}^\circ$	Polar cone of $\mathcal{K}$.

$\mathrm{pr}(\mathcal{K}, x)$	Projection of x onto $\mathcal{K}$.
Feas(P)	Feasible set of problem (P).

Simplices

Δ^S	Standard simplex.
$\mathcal{P}$	Simplicial partition.
$\delta(\mathcal{P})$	Diameter of $\mathcal{P}$.

Graphs

$\alpha(G)$	Stability number of G.
$\chi(G)$	Chromatic number of G.
$\omega(G)$	Clique number of G.
$\vartheta'(G)$	Lovász–Schrijver bound for G, page 84.
A_G	Adjacency matrix of G.
C_n	Cycle of length n.
$d_G(i, j)$	Distance of the vertices i, j in G.
$E(G)$	Edge set of G.
$G(X)$	Graph of the matrix X, page 7.
K_n	Complete graph on n vertices.
$V(G)$	Vertex set of G.
$\bar{G}$	Complementary graph of G.

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