

ON POLYHEDRAL APPROXIMATIONS OF COPOSITIVE FORMULATIONS OF CERTAIN QUADRATIC OPTIMIZATION PROBLEMS

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ON POLYHEDRAL APPROXIMATIONS OF COPOSITIVE
FORMULATIONS OF CERTAIN QUADRATIC OPTIMIZATION
PROBLEMS

Koç University

Graduate School of Sciences and Engineering

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*To my family
and
my husband*

ABSTRACT

Copositive optimization is the minimization or maximization of a linear objective function subject to linear equality constraints over the cone of copositive or completely positive matrices. It has been an intriguing area for researchers since the term "copositive programming" was coined in 2000 in the context of standard quadratic optimization. Later, in the seminal work of Burer, it has been shown that mixed-binary quadratic optimization problems can be reformulated as a conic optimization problem over the convex cone of completely positive matrices.

This class of optimization problems draws attention of researchers since it provides a new perspective on various NP-hard problems. As expected, copositive reformulations are also computationally intractable. Therefore, the completely positive cone can be approximated both from the inside and from the outside by two sequences of nested polyhedral cones of increasing accuracy each of which converges to the original intractable cone in the limit. Such a sequence of approximating cones is called an approximation hierarchy. Therefore, replacing the intractable conic constraint in a copositive optimization problem by an inner and an outer approximation hierarchy yields two sequences of increasingly tighter upper and lower bounds on the optimal value of the original problems. We study the sequences of upper and lower bounds on the optimal value arising from these two hierarchies of inner and outer polyhedral approximations.

We focus on two different classes of quadratic optimization problem that can be reformulated as copositive optimization problems. We first consider standard quadratic optimization problems (StQPs). For this class of problems, we focus on the issues of finite convergence of upper and lower bounds as well as convergence of these bounds only in the limit. We give complete algebraic descriptions of the sets

of instances on which upper and lower bounds are exact at any given finite level of the hierarchy. We identify the structural properties of the sets of instances on which upper and lower bounds converge to the optimal value only in the limit. We present several geometric and topological properties of these sets.

Second, we study box constrained quadratic optimization problems (BoxQPs). We consider two alternative copositive reformulations. We study the sequences of upper and lower bounds arising from the aforementioned polyhedral approximation hierarchies on the optimal value of a (BoxQP) problem for both of these formulations. We compare two formulations in terms of both inner and outer polyhedral approximations. We give a characterization of the feasibility of inner polyhedral approximation problems. We present conditions under which outer approximations have a finite or unbounded optimal value. Furthermore, we study error bounds for both approximation hierarchies.

Our results reveal that polyhedral approximation hierarchies can be useful in theory for standard quadratic optimization problems. On the other hand, these hierarchies yield considerably weaker upper and lower bounds for box constrained quadratic optimization problems.

ÖZETÇE

Kopozitif eniyileme, doğrusal bir amaç fonksiyonunun doğrusal eşitlik kısıtları altında kopozitif veya tamamen pozitif matrisler konisi üzerinde enküçükleme ya da enbüyükme problemidir. Kopozitif eniyileme problemleri, "kopozitif programlama" terimi 2000 yılında standart ikinci dereceden eniyileme problemleri bağlamında ilk kez kullanıldığından beri araştırmacılar için ilgi çekici bir alan olmuştur. Daha sonra, Burer son derece önemli bir çalışmada karışık-ikili ikinci dereceden eniyileme problemlerinin tamamen pozitif matris konisi üzerine konik eniyileme problemi olarak formüle edilebileceğini göstermiştir.

Kopozitif eniyileme problem sınıfının araştırmacıların ilgisini çekmesinin nedeni NP-zor problemler için yeni bir bakış açısı sağlamasıdır. Beklenildiği üzere, kopozitif formülasyonlar da hesaplama açısından zorludur. Bu yüzden, tamamen pozitif matrisler konisine, her biri yaklaşıklama doğruluğu giderek artan ve limitte asıl koniye yakınsayan iki çok yüzlü koni dizisi ile içten ve dıştan yaklaşılabılır. Bu şekilde yakınsayan koni dizisi, yaklaşıklama hiyerarşisi olarak adlandırılır. Bu yüzden, kopozitif eniyileme problemindeki zorlu konik kısıtının içten ve dıştan yaklaşıklama hiyerarşisi ile değiştirilmesi asıl problemin eniyi değeri için gittikçe sıkılaştan alt ve üst sınır dizileri vermektedir. Bu tezde içten ve dıştan çok yüzlü yaklaşımların sağladığı alt ve üst sınırlar ele alınmıştır.

Bu tezde, iki farklı ikinci dereceden eniyileme problem sınıfının kopozitif formülasyonları incelenmiştir. İlk olarak standart ikinci dereceden eniyileme problemleri (StQP) ele alınmıştır. Bu problem sınıfı için alt ve üst sınırların sonlu yakınsama koşulları ve bu sınırların yakınsamadığı durumlar sunulmuştur. Alt ve/veya üst sınırın sonlu bir seviyede en iyi değere eşitlendiği ve alt ve/veya üst sınırın en iyi değere ancak limitte yakınsadığı problemlerin bulunduğu kümelerin bütünlüklü tanımları ve-

rilmiştir. Ayrıca, bu kümelerin bazı geometrik ve topolojik özellikleri de sunulmuştur.

İkinci olarak, kutu kısıtlı ikinci dereceden problemler (BoxQP) çalışılmıştır. Bu problem sınıfı için detaylı olarak iki farklı kopozitif yeniden formülasyon incelenmiştir. (BoxQP) probleminin eniyi değeri için bu iki farklı formülasyonun çok yüzlü koniler kullanılarak elde edilen alt ve üst sınırlar dizisi çalışılmıştır. Bu iki farklı formülasyonun içten ve dıştan çok yüzlü yaklaşımları karşılaştırılmıştır. İçten çok yüzlü yaklaşımların olurluluk koşulları verilmiştir. Ayrıca, dıştan çok yüzlü yaklaşımların eniyi değerlerinin sınırlı veya sınırsız olduğu durumlar ortaya konulmuştur. İncelediğimiz konular arasında her iki yaklaşım için hata payları da yer almaktadır.

Bu sonuçlar, çok yüzlü yaklaşımlama hiyerarşilerinin standart ikinci dereceden eniyileme problemleri için teoride yararlı olabileceğini göstermiştir. Bunun yanında, bu yaklaşımlama hiyerarşileri kutu kısıtlı ikinci dereceden eniyileme problemleri için göreceli olarak daha zayıf alt ve üst sınırlar vermektedir.

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NOMENCLATURE

$\mathbb{R}^n$	n -dimensional Euclidean space
$\mathbb{R}_+^n$	Set of n -dimensional nonnegative real vectors (Nonnegative orthant)
$\mathbb{Q}^n$	Set of n -dimensional rational vectors
$\mathbb{N}^n$	Set of n -dimensional nonnegative integer vectors
$\mathcal{S}^n$	Set of n -dimensional real symmetric matrices
$\mathcal{S}_+^n$	Cone of positive semidefinite matrices of order n
$\mathcal{Q}^n$	Set of n -dimensional rational symmetric matrices
$\mathcal{N}^n$	Cone of componentwise nonnegative matrices of order n
I^n	Identity matrix of order n
$\langle \cdot, \cdot \rangle$	Inner product
$\mathcal{CP}^n$	Cone of completely positive matrices of order n
$\mathcal{COP}^n$	Cone of copositive matrices of order n
$\text{Diag}(\cdot)$	Diagonal matrix with a specified diagonal vector
$\text{diag}(\cdot)$	Vector obtained from the diagonal entries of a matrix
e	Vector of all ones
e_i	i th unit vector
E	Matrix of all ones
E_{ij}	The symmetric matrix $\frac{1}{2}(e_i e_j^T + e_j e_i^T)$
(StQP)	Standard quadratic optimization problem
(BoxQP)	Box constrained quadratic optimization problem
(P1)	First copositive reformulation of (BoxQP)

Nomenclature *(continued)*

(P2)	Second copositive reformulation of (BoxQP)
$\text{rank}(\cdot)$	Rank of a matrix
$\text{conv}(\cdot)$	Convex hull of a set
$\text{cone}(\cdot)$	Conic hull of a set
$\text{cl}(\cdot)$	Closure of a set
$\text{int}(\cdot)$	Interior of a set
$\text{bd}(\cdot)$	Boundary of a set
$\alpha(G)$	Stability number of a simple graph G
A_G	Adjacency matrix of a simple graph G

Chapter 1

INTRODUCTION

Copositive optimization is the optimization of a linear objective function subject to linear equality constraints over the cone of copositive or completely positive matrices. It belongs to the class of convex optimization problems. Burer [16] proved that mixed-binary quadratic optimization problems can be reformulated as a conic optimization problem over the convex cone of completely positive matrices. This result reveals that a very large class of nonconvex and NP-hard optimization problems can be equivalently reformulated as an instance of a convex optimization problem.

The convex reformulation of mixed-binary quadratic optimization problems does not change their computational intractability. Therefore, different approximation hierarchies have been proposed to approximate the intractable copositive and completely positive cones. These approximation hierarchies consist of sequences of nested convex cones that approximate the intractable cone both from inside and from outside by sequences of nested convex cones of increasing accuracy as the *level* of the hierarchy increases. By replacing the intractable conic constraint in a copositive optimization problem by tractable conic constraints from an inner and outer approximation hierarchy, we obtain certain sequences of increasingly tighter lower and upper bounds on the optimal value of the problem.

Motivated by these results, we focus on two different quadratic optimization problem classes that can be reformulated as copositive optimization problems: Standard Quadratic Optimization (StQP) and Box Constrained Quadratic Optimization Problems (BoxQP). We study the sequences of upper and lower bounds on the optimal value for these problems arising from two hierarchies of inner and outer polyhedral

approximations. Regarding these sequences, we attempt to shed light on the following questions:

- How fast do the sequences of upper and lower bounds *converge* to the optimal value?
- Under what conditions do the bounds match the optimal value at a *finite* level of the hierarchy?

For (StQP), a tight error bound on the gap between the upper bound and lower bound at a given level of the hierarchy has already been established [74]. Therefore, for this class of problems, we focus on a complete algebraic description of the instances on which upper and lower bounds are already *exact* at a finite level of the hierarchy, and the instances for which upper and lower bounds converge to the optimal value only in the *limit*. For (BoxQP), we analyze the upper and lower bounds provided by inner and outer approximations. We also study the gap between the optimal value and the lower and upper bounds. Therefore, our main goal in this thesis is to shed light on the behavior of inner and outer approximations on copositive reformulations of these two classes of quadratic optimization problems.

In this chapter, we first review some basic definitions from convex analysis. Then, we introduce the conic optimization problem together with the definitions of copositive and completely positive matrices. We present Burer's copositive reformulation for mixed-binary quadratic optimization problems. Finally, we close the chapter by our motivation, contributions and the outline of the dissertation. We use standard notation given in the nomenclature throughout the thesis. Any additional notation will be subsequently introduced in the thesis.

1.1 Preliminaries from Convex Analysis

This section provides some basic definitions from convex analysis.

Definition 1. A set $\mathcal{K} \subseteq \mathbb{R}^n$ is called a cone if for every $x \in \mathcal{K}$ and for every real number $\alpha \geq 0$, we have $\alpha x \in \mathcal{K}$.

Next, we present an elementary theorem about convex cones. Then we introduce the definitions of polyhedral, pointed and full-dimensional cones.

Theorem 1 ([62], Theorem 2.6). *A cone $\mathcal{K} \subseteq \mathbb{R}^n$ is convex if and only if it satisfies the following condition:*

$$x, y \in \mathcal{K} \implies x + y \in \mathcal{K}.$$

Definition 2. *A convex cone $\mathcal{K} \subseteq \mathbb{R}^n$ is a polyhedral cone, if it is in the form of*

$$\mathcal{K} = \{x \in \mathbb{R}^n : Ax \geq 0\},$$

where $A \in \mathbb{R}^{m \times n}$.

Definition 3. *A cone $\mathcal{K} \subseteq \mathbb{R}^n$ is pointed if $\mathcal{K} \cap -\mathcal{K} = \{0\}$.*

Definition 4. *If a cone $\mathcal{K} \subseteq \mathbb{R}^n$ has a nonempty interior, then $\mathcal{K}$ is full-dimensional. In this case, the dimension of $\mathcal{K}$ is equal to n .*

Definition 5. *An inner product space is a vector space $\mathbb{V}$ over $\mathbb{R}^n$ together with an inner product that satisfies the following three axioms for all vectors $x, y, z \in \mathbb{V}$ and all scalars $\alpha \in \mathbb{R}$:*

- *Conjugate symmetry:* $\langle x, y \rangle = \langle y, x \rangle$,
- *Bilinearity:* $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle$ and $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$,
- *Positive-definiteness:* $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0 \iff x = 0$.

Next, we define the dual cone of a set.

Definition 6. *For a set $\mathcal{M} \subseteq \mathbb{R}^n$, the dual cone with respect to the inner product $\langle \cdot, \cdot \rangle$ is given by*

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

Berman [2] showed that if $\mathcal{K}$ is a closed convex cone, then $\mathcal{K}^*$ is also a closed convex cone. Furthermore, we have $(\mathcal{K}^*)^* = \mathcal{K}$.

Definition 7. A set $\mathcal{M} \subseteq \mathbb{R}^n$ is called *self-dual* if $\mathcal{M} = \mathcal{M}^*$.

Some well-known self-dual cones are the nonnegative orthant, the cone of positive semidefinite matrices and the second-order cone. However, self-duality does not always hold. For instance, copositive and completely positive cones which will be introduced shortly are examples of this phenomenon.

For a finite number of points, $x_1, \dots, x_k$, a point of the form $\alpha_1 x_1 + \dots + \alpha_k x_k$, where $\alpha_1, \dots, \alpha_k \geq 0$ and $\alpha_1 + \dots + \alpha_k = 1$, is called a *convex combination*.

Definition 8. The *convex hull* of a set $\mathcal{M} \subseteq \mathbb{R}^n$, denoted by $\text{conv}(\mathcal{M})$, is the set of all convex combinations of points in $\mathcal{M}$, i.e.,

$$\text{conv}(\mathcal{M}) = \{\alpha_1 x_1 + \dots + \alpha_k x_k : x_i \in \mathcal{M}, \alpha_i \geq 0, i = 1, \dots, k, \alpha_1 + \dots + \alpha_k = 1, k \in \mathbb{N}\},$$

which is the smallest convex set with respect to inclusion that contains $\mathcal{M}$.

For a finite number of points, $x_1, \dots, x_k$, a point of the form $\alpha_1 x_1 + \dots + \alpha_k x_k$, where $\alpha_1, \dots, \alpha_k \geq 0$, is called a *conic combination*.

Definition 9. The *conic hull* of a set $\mathcal{M} \subseteq \mathbb{R}^n$ is the set of all conic combinations of points in $\mathcal{M}$, i.e.,

$$\text{cone}(\mathcal{M}) = \{\alpha_1 x_1 + \dots + \alpha_k x_k : x_i \in \mathcal{M}, \alpha_i \geq 0, i = 1, \dots, k, k \in \mathbb{N}\},$$

which is also the smallest convex cone with respect to inclusion that contains $\mathcal{M}$.

In this dissertation, we consider the Euclidean space, with the inner product defined as $\langle x, y \rangle := x^T y = \sum_{i=1}^n x_i y_i$ for vectors and the space of $n \times n$ symmetric matrices with the inner product given by $\langle X, Y \rangle := \text{trace}(XY) = \sum_{i=1}^n \sum_{j=1}^n X_{ij} Y_{ij}$.

1.2 Conic Optimization

We now introduce a general class of optimization problems, referred to as conic optimization and given by

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

where $c \in \mathbb{R}^n$ and $a_i \in \mathbb{R}^n$, $b_i \in \mathbb{R}$ for $i = 1, \dots, m$ are the parameters, $x \in \mathbb{R}^n$ is the decision variable, and $\mathcal{K} \subseteq \mathbb{R}^n$ is a closed convex cone. Linear programming (LP) is a special case of conic optimization. If we replace the cone $\mathcal{K}$ by $\mathbb{R}_+^n$ and use the Euclidean inner product in (P), we obtain a linear programming problem. Similar to a linear programming problem, there is an associated dual problem given by

$$\begin{aligned}
 \text{(D)} \quad & \max \quad \sum_{i=1}^m y_i b_i \\
 & \text{subject to} \quad \sum_{i=1}^m y_i a_i + s = c, \\
 & \quad \quad \quad s \in \mathcal{K}^*.
 \end{aligned}$$

The following lemma presents an important relation, known as *weak duality*, between the primal and dual problems.

Lemma 1. *For all $x \in \text{feas}(P)$ and $y \in \text{feas}(D)$, we have*

$$\langle c, x \rangle \geq \sum_{i=1}^m y_i b_i.$$

Therefore, $\text{opt}(P) \geq \text{opt}(D)$, where $\text{feas}(\cdot)$ and $\text{opt}(\cdot)$ denote the feasible region and the optimal value of the problem, respectively.

Proof. For all $x \in \text{feas}(P)$ and $y \in \text{feas}(D)$,

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

where last inequality follows from the definition of the dual cone. $\square$

By *weak duality*, the objective function value of every feasible solution of the primal problem (P) gives an upper bound for the optimal value of the dual problem (D). For a given $x \in \text{feas}(P)$ and $y \in \text{feas}(D)$, the difference $\langle c, x \rangle - \sum_{i=1}^m y_i b_i$ is called the duality gap. For a general conic optimization problem, if we can find feasible solutions for both (P) and (D) with zero duality gap, then these solutions are optimal for the corresponding problems. In this case, *strong duality* is said to be satisfied. In contrast with linear programming, strong duality does not always hold in general conic optimization. We need some additional conditions to have strong duality, e.g. the Slater's condition. The problem (P) satisfies the Slater's condition, if it has a *strictly feasible solution*, that is, there exists $\bar{x} \in \mathbb{R}^n$ such that

$$\langle a_i, \bar{x} \rangle = b_i, \quad i = 1, \dots, m \text{ and } \bar{x} \in \text{relint}(\mathcal{K}),$$

where $\text{relint}(\cdot)$ denotes the relative interior [14].

Linear programming constitutes an important class of conic optimization since efficient solution methods have been developed both computationally and theoretically. For example, Dantzig [19] introduced the simplex method in 1947 which works fairly efficiently in practice; however, the worst-case time complexity of the algorithm is not polynomial [37]. Later, Khachiyan [36] showed that the ellipsoid algorithm is the first polynomial-time algorithm for solving an LP problem in 1979. However, the practical performance of the ellipsoid method does not seem to be promising [5]. Lastly, Karmarkar [35] developed an algorithm called the interior point method which has a polynomial time worst-case time complexity in 1984. It has been also shown that it has an efficient performance for large-scale linear programming problems [43, 44, 45].

Hence, for over six decades, linear programming remains an important class of optimization problems.

Another well-studied cone is the positive semidefinite cone and the resulting optimization problem is called the semidefinite programming problem (SDP). After Karmarkar's interior point approach to linear programming problem, in 1988 Nesterov and Nemirovski [52] showed that interior point methods can be generalized to all convex optimization problems. This breakthrough discovery implies that an arbitrary linear optimization problem over a convex cone, such as SDP, can be solved in polynomial time using interior point methods, if there is an efficiently computable self-concordant barrier function for the underlying convex cone. As a result, interior point methods are currently accepted as the most efficient way to solve SDP problems.

LP and SDP are among the most well-studied optimization problem classes. Next, we present definitions of two cones that constitute the theme of this thesis work, namely, the cones of copositive and completely positive matrices.

1.3 Copositive and Completely Positive Cones

First, we introduce the definitions of a copositive matrix and a completely positive matrix.

Definition 10. A symmetric matrix $X \in \mathcal{S}^n$ is called *copositive* if

$$u^T X u \geq 0 \text{ for all } u \in \mathbb{R}_+^n.$$

We denote the cone of copositive matrices by

$$\mathcal{COP}^n := \{X \in \mathcal{S}^n : u^T X u \geq 0 \text{ for all } u \in \mathbb{R}_+^n\}. \quad (1.1)$$

Definition 11. A symmetric matrix $X \in \mathcal{S}^n$ is called *completely positive* if

$$X = Y Y^T \text{ for some } Y \in \mathbb{R}_+^{n \times k}.$$

Note that Y is not necessarily a square matrix. The smallest $k \in \mathbb{N}$ for which such a representation is possible is called the cp-rank of X . There are upper bounds on the cp-rank, see some recent papers [12, 13, 66, 67].

We denote the cone of completely positive matrices by

$$\mathcal{CP}^n := \text{conv}\{uu^T : u \in \mathbb{R}_+^n\}. \quad (1.2)$$

The term "copositive" was coined in 1952 by Motzkin [48] who mainly studied the quadratic forms. The completely positive matrices were introduced a bit later in 1958 by Hall [30]. These cones have been studied by mathematicians for over half a century. The early questions of interest were the criteria for copositivity and cp-rank of the completely positive matrices. After the introduction of these cones in optimization, different questions have arisen.

Let us introduce two more familiar convex cones of positive semidefinite matrices and nonnegative matrices:

$$\begin{aligned} \mathcal{S}_+^n &:= \{X \in \mathcal{S}^n : u^T X u \geq 0 \text{ for all } u \in \mathbb{R}^n\}, \\ \mathcal{N}^n &:= \{X \in \mathcal{S}^n : X_{ij} \geq 0, 1 \leq i \leq j \leq n\}. \end{aligned}$$

There are some important relations between these cones and the cones of copositive and completely positive matrices:

$$\mathcal{CP}^n \subseteq \mathcal{S}_+^n \cap \mathcal{N}^n, \quad \mathcal{S}_+^n + \mathcal{N}^n \subseteq \mathcal{COP}^n.$$

In fact, both inclusions above are exact if and only if $n \leq 4$ by [4]. The well-known

Horn matrix [29]

$$Q = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix} \in \mathcal{COP}^5 \setminus (\mathcal{S}_+^5 + \mathcal{N}^5)$$

and

$$P = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 1 & 6 \end{pmatrix} \in (\mathcal{S}_+^5 \cap \mathcal{N}^5) \setminus \mathcal{CP}^5$$

from [4] are the counterexamples for $n = 5$. The interested reader can find further information about the completely positive cone in [4]. Recently, researchers in the optimization community have shown a significant interest in these cones. The main reason of this interest is due to the copositive reformulation of a large class of NP-hard problems over these cones [10, 16, 58, 61]. Next, we present conic optimization problems over these cones.

1.4 Copositive and Completely Positive Optimization

We define the completely positive optimization problem as follows:

$$\begin{aligned} (\text{CoP}) \quad & \min \quad \langle C, X \rangle \\ \text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \dots, m, \\ & X \in \mathcal{CP}^n, \end{aligned} \tag{1.3}$$

where $C \in \mathcal{S}^n$, $A_i \in \mathcal{S}^n$ and $b_i \in \mathbb{R}$ for $i = 1, \dots, m$. The associated dual problem, called a copositive optimization problem, is given by

$$\begin{aligned}
 (\text{CoD}) \quad & \max \quad b^T y \\
 \text{s.t.} \quad & \sum_{i=1}^m y_i A_i + S = C, \\
 & S \in \mathcal{COP}^n,
 \end{aligned} \tag{1.4}$$

where $y \in \mathbb{R}^m$ and $S \in \mathcal{S}^n$ are the decision variables. As we have shown for general conic optimization, weak duality holds between the primal problem (CoP) and the dual problem (CoD). However, strong duality holds under regularity assumptions (e.g., Slater's condition). Since the cones of copositive and completely positive matrices are both convex, (CoP) and (CoD) are convex optimization problems. On the other hand, deciding whether a given symmetric matrix is copositive is co-NP-complete [50]. Furthermore, several NP-hard problems such as standard quadratic optimization, maximum weight clique, graph partitioning, and quadratic assignment problems can be reformulated as an instance of (CoP). It follows that (CoP) and (CoD) are, in general, NP-hard problems [10, 60].

In general, both of these two optimization problems are referred to as copositive optimization problems. Therefore, we adopt this terminology and use *copositive optimization* for both problems. Copositive optimization recently received significant attention from the optimization community [7]. The main reason of this interest is a consequence of an important result presented in the following section.

1.5 Burer's Reformulation

In 2009, Burer [16] established that mixed-binary quadratic optimization problems can be reformulated as conic optimization problems over the cone of completely positive matrices, which constitute the basis of this dissertation. He proposed a relaxation of general quadratic optimization problems with linear equality constraints and continuous and binary variables, which turns out to be an exact reformulation

under some mild assumptions. The general problem he considers is

$$\begin{aligned}
 (\text{QPB}) \quad & \min \quad x^T Q x + 2c^T x \\
 & \text{s.t.} \quad a_i^T x = b_i, \quad i = 1, \dots, m, \\
 & \quad x \geq 0, \\
 & \quad x_j \in \{0, 1\} \quad \forall j \in B,
 \end{aligned}$$

where $Q \in \mathcal{S}^n, c \in \mathbb{R}^n, a_i \in \mathbb{R}^n, b_i \in \mathbb{R}$ for $i = 1, \dots, m$, $x \in \mathbb{R}_+^n$ and $B \subseteq \{1, \dots, n\}$. (QPB) encompasses a huge class of NP-hard problems, e.g., all 0-1 linear integer optimization, all nonconvex (continuous) quadratic optimization, and all unconstrained 0-1 quadratic optimization problems. Assuming that the feasible region of the problem is nonempty, he models this problem as a conic optimization problem over the cone of completely positive matrices:

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

where $(x, X) \in \mathbb{R}^n \times \mathcal{S}^n$. The main result of [16] is given in the next theorem.

Theorem 2 ([16], Theorem 2.6). *The optimization problems (C) and (QPB) have the same optimal value, i.e., $\text{opt}(\text{QPB}) = \text{opt}(\text{C})$. Furthermore, if (x^*, X^*) is optimal for (C), then x^* is in the convex hull of optimal solutions of (QPB).*

Thanks to this result, it has been shown that a huge class of mixed-binary quadratic optimization problems can be reformulated as a copositive optimization problem. Therefore, (CoP) is, in general, computationally intractable. As a result, the conic reformulation moves all the complexity into the convex cone $\mathcal{CP}^n$. Moreover, Bomze

[11] provided a topological interpretation of this result and discussed why the feasibility of the completely positive formulation implies the feasibility of the original mixed-binary quadratic optimization problem. The interested reader is referred to [11, 16] for further details. This conic reformulation of quadratic programs has given rise to various studies about copositive optimization [8, 11, 23, 40, 64, 74].

1.6 Motivation

Various NP-hard problems have been reformulated as a copositive optimization problem [10, 59, 60]. Therefore, it has been possible to treat these nonconvex optimization problems as convex optimization problems. Burer established that copositive reformulation can be applied to a much larger class of optimization problems, i.e., any nonconvex quadratic optimization problem subject to linear constraints with binary and continuous variables [16]. Motivated by this result, we consider copositive reformulations of standard and box constrained quadratic optimization problems in this thesis. Since there is no efficient algorithm for solving these problems, we employ tractable cones to approximate $\mathcal{CP}^n$ from the inside and from the outside. We focus on polyhedral approximation hierarchies. Therefore, resulting optimization problems become LP problems. This provides several advantages for our analysis. First, because of the simpler structure of LP problems, it is easier to analyze theoretically the resulting optimization problems. Furthermore, we have sophisticated optimization tools to solve very large-scale LP problems. Therefore, these polyhedral approximations are more amenable to existing solvers.

In this thesis, we aim to shed light on the quality of approximations arising from the copositive reformulations of certain quadratic optimization problem classes. Hopefully, our results for these problem classes will serve as a basis for approximations of other classes of optimization problems. Moreover, our findings may lead to improved polyhedral approximations using the strengths and limitations of the polyhedral approximations used in this thesis.

1.7 Contributions and Outline

The main contributions of the dissertation are given for the following classes of optimization problems:

Standard Quadratic Optimization

We study the bounds obtained from certain polyhedral approximation hierarchies for the copositive reformulation of this problem. Since a tight error bound exists in the literature [74], we focus on a complete algebraic description of the set of the instances in this class on which upper and lower bounds are already *exact* at a finite level of the hierarchy. We also describe the set of the instances on which the upper and lower bounds converge to the optimal value only in the *limit*. We discuss several geometric and topological properties of these sets. An important result of our analysis is that the upper bounds seem to be more well-behaved in comparison with the lower bounds. Our findings in this part of the thesis were published in [64].

Box Constrained Quadratic Optimization

There are alternative copositive reformulations for (BoxQP). We study two different copositive reformulations. We compare these reformulations with respect to the bounds provided by polyhedral approximation hierarchies. First of all, we derive the necessary and sufficient conditions for the feasibility of inner approximations for both formulations. Next, we provide an exact characterization of the corresponding lower bounds for both formulations. In particular, our results imply that the inner polyhedral approximation hierarchy turns into a *finite* discretization algorithm. We also establish an error bound for the inner polyhedral approximation hierarchy for both formulations. In addition, we present necessary and sufficient conditions for a *finite* upper bound for the first formulation. Our analysis shows that the upper bound of the other formulation is always *finite*. Then, we derive an error bound of the outer polyhedral approximation hierarchy for the instances with nonnegative matrices and vectors. Finally, we give some *pathological* examples to illustrate that large error bounds are possible for the outer approximation of both formulations. Our analysis implies that although copositive reformulations provide equivalent formulations, their

polyhedral approximations behave differently.

The rest of this thesis is organized as follows: Chapter 2 introduces approximation hierarchies and reviews several approximation hierarchies constructed for the copositive and completely positive cones. We focus on standard quadratic optimization problems in Chapter 3. Chapter 4 is dedicated to our results for box constrained quadratic optimization problems. Finally, in Chapter 5, we conclude the dissertation with a brief summary and provide some future research directions.



Chapter 2

APPROXIMATION HIERARCHIES

By Burer's seminal work, a large class of NP-hard problems can be reformulated as copositive optimization problems [16]. This convex reformulation moves all the complexity into the cones of copositive and completely positive matrices. Therefore, there has been a considerable amount of research activity towards a better understanding of the cones $\mathcal{CP}^n$ and $\mathcal{COP}^n$. Many of these studies propose different ways of approximating each of these two cones by a sequence of tractable convex cones of increasing accuracy. Such sequences therefore yield approximation hierarchies for the cones $\mathcal{CP}^n$ and $\mathcal{COP}^n$. For this reason, we first introduce inner and outer approximation hierarchies.

2.1 Introduction

We begin with the formal definition of an *inner approximation hierarchy*.

Definition 12. For a closed convex cone $\mathcal{K} \subseteq \mathcal{S}^n$, a sequence of cones $\mathcal{I}_r \subseteq \mathcal{S}^n$ for all $r \in \mathbb{N}$ that satisfies the following properties

$$\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \dots \subseteq \bigcup_{r \in \mathbb{N}} \mathcal{I}_r \subseteq \mathcal{K} \quad \text{and} \quad \text{cl} \left(\bigcup_{r \in \mathbb{N}} \mathcal{I}_r \right) = \mathcal{K}$$

is called an *inner approximation hierarchy*, where the subscript r denotes the level of the hierarchy.

Similarly, we define an *outer approximation hierarchy*.

Definition 13. For a closed convex cone $\mathcal{K} \subseteq \mathcal{S}^n$, a sequence of cones $\mathcal{O}_r \subseteq \mathcal{S}^n$ for

all $r \in \mathbb{N}$ that satisfies the following properties

$$\mathcal{K} \subseteq \bigcap_{r \in \mathbb{N}} \mathcal{O}_r \subseteq \dots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0 \quad \text{and} \quad \bigcap_{r \in \mathbb{N}} \mathcal{O}_r = \mathcal{K}$$

is called an outer approximation hierarchy.

Hence, we have

$$\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \dots \subseteq \bigcup_{r \in \mathbb{N}} \mathcal{I}_r \subseteq \mathcal{K} \subseteq \bigcap_{r \in \mathbb{N}} \mathcal{O}_r \subseteq \dots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0. \quad (2.1)$$

By duality, these conditions translate into a hierarchy of the dual cone

$$\mathcal{I}_0^* \supseteq \mathcal{I}_1^* \supseteq \dots \supseteq \bigcap_{r \in \mathbb{N}} \mathcal{I}_r^* \supseteq \mathcal{K}^* \supseteq \bigcup_{r \in \mathbb{N}} \mathcal{O}_r^* \supseteq \dots \supseteq \mathcal{O}_1^* \supseteq \mathcal{O}_0^*,$$

where $\mathcal{I}_r^*$ and $\mathcal{O}_r^*$ are the dual cones of $\mathcal{I}_r$ and $\mathcal{O}_r$, respectively. We also have

$$\bigcap_{r \in \mathbb{N}} \mathcal{I}_r^* = \mathcal{K}^*, \quad \text{cl} \left(\bigcup_{r \in \mathbb{N}} \mathcal{O}_r^* \right) = \mathcal{K}^*.$$

Therefore, approximation hierarchies constructed for the copositive cone can also be translated into an approximation hierarchy for the cone of completely positive matrices and vice versa.

We first present inner approximation hierarchies for the cone of completely positive matrices. This is followed by the outer approximation hierarchies for the completely positive cone.

2.2 Inner Approximations

In this section, we review inner approximation hierarchies that are constructed to approximate the cone of completely positive matrices from inside. We begin with a polyhedral approximation approach proposed by Bomze and de Klerk [9], later modified into an outer approximation hierarchy for the cone of copositive matrices

by Yildirim [74] via exploiting necessary conditions for copositivity of a matrix. By duality, this hierarchy yields a sequence of *inner* polyhedral approximations of the cone $\mathcal{CP}^n$. The second part is devoted to non-polyhedral approaches.

2.2.1 Polyhedral Approximations

The first approximation approach was defined originally in the context of standard quadratic optimization by Bomze and de Klerk [9]. Later, Yildirim [74] extended this approach to a hierarchy that consists of a sequence of nested cones by using necessary conditions for copositivity of a matrix. We now describe this outer approximation hierarchy for the cone of copositive matrices.

Recall that a matrix $X \in \mathcal{S}^n$ is copositive if $u^T X u \geq 0$ for all $u \in \mathbb{R}_+^n$. Clearly, we can equivalently state this condition as

$$u^T X u \geq 0, \quad \text{for all } u \in \Delta_n, \quad (2.2)$$

where $\Delta_n \subset \mathbb{R}^n$ is the unit simplex given by

$$\Delta_n := \{x \in \mathbb{R}_+^n : e^T x = 1\}. \quad (2.3)$$

It follows that enforcing the condition (2.2) on any subset of Δ_n yields an outer approximation of $\mathcal{COP}^n$, which, by duality, translates into an inner approximation of the cone of completely positive matrices.

Motivated by these observations, let us define the following regular grid of rational points on the unit simplex (see [9]):

$$\Lambda_n^r := \{x \in \Delta_n : (r+2)x \in \mathbb{N}^n\}, \quad r = 0, 1, \dots \quad (2.4)$$

In order to obtain an increasingly refined sequence of subsets of the unit simplex Δ_n ,

Yıldırım [74] defined

$$\Delta_n^r := \bigcup_{k=0}^r \Lambda_n^k. \quad (2.5)$$

Since $\Delta_n^0 \subset \Delta_n^1 \subset \dots \subset \Delta_n^r$, it follows that enforcing the condition (2.2) only on Δ_n^r yields an increasingly better outer approximation of $\mathcal{COP}^n$ as r increases. Furthermore, since Δ_n^r is a finite set for each $r \in \mathbb{N}$, namely $|\Delta_n^r| = O(n^{r+2})$, it follows that each outer approximation is a polyhedral cone since it is represented by a finite number of linear inequalities in $\mathcal{S}^n$. Clearly, the dual cone is also polyhedral and yields an inner approximation of the cone $\mathcal{CP}^n$. More specifically, the corresponding inner approximations are given by

$$\mathcal{I}_r := \left\{ \sum_{d \in \Delta_n^r} \lambda_d d d^T : \lambda_d \geq 0 \text{ for all } d \in \Delta_n^r \right\}, \quad r = 0, 1, \dots \quad (2.6)$$

It has been shown that this sequence of polyhedral cones satisfies [74]:

$$\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \dots \subseteq \mathcal{CP}^n, \quad \text{and} \quad \text{cl} \left(\bigcup_{r \in \mathbb{N}} \mathcal{I}_r \right) = \mathcal{CP}^n. \quad (2.7)$$

Therefore, this sequence of polyhedral cones constitutes an inner approximation hierarchy for the cone of completely positive matrices. As we increase r , the quality of the approximation gets better and, in the limit, the closure of the union of these polyhedral cones is equal to the completely positive cone.

Another polyhedral approximation scheme is presented by Bundfuss and Dur [15]. They suggested approximation hierarchies for the copositive cone from both inside and outside, which are based on nested simplicial partitions of the standard simplex. They proposed new sufficient conditions for copositivity of a matrix, which ensures that the quadratic form of the matrix is nonnegative over the standard simplex and its simplicial partitions. As the partition consists of more and more points, the conditions eventually capture all strictly copositive matrices. They also provide an algorithmic

implementation of this condition. The outer approximation will be introduced later in the next section.

Note that, both of the inner polyhedral approximation hierarchies are based on discretization. However, there is an important distinction between Bundfuss and Dur's hierarchy, and Yıldırım's hierarchy. The latter one yields a uniform approximation of the cone of copositive matrices. Bundfuss and Dur's hierarchy is refined with respect to the objective function in the copositive optimization problem. Therefore, this hierarchy is better-suited for an algorithmic implementation. On the other hand, since the refinements heavily depend on the particular instance, a theoretical analysis of the behavior of this approximation hierarchy seems to be rather difficult. Therefore, from our point of view, it is not amenable for analysis. As a result, we use the inner polyhedral approximation hierarchy proposed by Yıldırım.

2.2.2 Non-Polyhedral Approximations

Lasserre [40] proposed an outer approximation hierarchy of $\mathcal{COP}^n$ that consists tractable convex cones based on the moments approach. It is a special case of a more general result of [39] about nonnegativity of polynomials on a closed set within the context of quadratic functions. By duality, the corresponding hierarchy of dual cones provides an inner approximation hierarchy for $\mathcal{CP}^n$ converging to $\mathcal{CP}^n$. This approach relies on the Borel measures, e.g., probability distributions. Later, Dickinson and Povh [22] extended this approximation hierarchy by making use of a completely positive constraint. Furthermore, they studied the effect of different choices of Borel measures on the approximation. This approximation hierarchy is also difficult to analyze because of its complicated structure.

2.3 Outer Approximations

In this section, we review outer approximation hierarchies that are constructed to approximate the cone of completely positive matrices from outside. We begin with an inner approximation hierarchy for the cone of copositive matrices proposed by de Klerk

and Pasechnik [20] via exploiting a sequence of sufficient conditions for copositivity of a matrix. By duality this yields a sequence of *outer* polyhedral approximations of the cone $\mathcal{CP}^n$. We again conclude this section with non-polyhedral approximation hierarchies.

2.3.1 Polyhedral Approximations

By duality, outer approximations of the cone $\mathcal{CP}^n$ can be obtained through inner approximations of the cone $\mathcal{COP}^n$. Therefore, by properly exploiting sufficient conditions for copositivity, de Klerk and Pasechnik [20] obtained the following inner approximations of the cone $\mathcal{COP}^n$.

Let us define:

$$\Theta_n^r := \left\{ z \in \mathbb{N}^n : \sum_{i=1}^n z_i = r + 2 \right\} = (r + 2)\Lambda^r, \quad r = 0, 1, 2, \dots \quad (2.8)$$

Using these sets, we can define the following convex cones:

$$\mathcal{O}_r := \left\{ \sum_{z \in \Theta_n^r} \beta_z (zz^T - \text{Diag}(z)) : \beta_z \geq 0 \text{ for all } z \in \Theta_n^r \right\}, \quad r = 0, 1, \dots \quad (2.9)$$

Since $|\Theta_n^r| = O(n^{r+2})$, $\mathcal{O}_r$ is a polyhedral cone for each $r \in \mathbb{N}$. In [20], de Klerk and Pasechnik established that

$$\mathcal{CP}^n \subseteq \dots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0 = \mathcal{N}^n, \quad \text{and} \quad \mathcal{CP}^n = \bigcap_{r \in \mathbb{N}} \mathcal{O}_r. \quad (2.10)$$

Therefore, this sequence of polyhedral cones constitutes an outer approximation hierarchy for the cone of completely positive matrices. As we increase r , the quality of the approximation gets better and, in the limit, the intersection of these polyhedral cones is equal to the completely positive cone.

Bundfuss and Dur also [15] proposed outer approximation hierarchies for the copositive cone. Since this outer approximation hierarchy is also problem specific,

i.e., it is updated according to the objective function, it is also not appropriate for our analysis. As a result, we employ the outer polyhedral approximation hierarchy suggested by de Klerk and Pasechnik.

We next discuss several non-polyhedral outer approximation hierarchies.

2.3.2 Non-Polyhedral Approximations

The idea of approximating the cone of copositive matrices by a sequence of tractable cones was first introduced by Parrilo in 2000 in his thesis [56]. His approximation hierarchy is based on sufficient conditions for nonnegativity of a multivariate polynomial. This is also known as sum-of-squares (SOS) decomposition. Parrilo constructs a hierarchy of tractable convex cones that yields an inner approximation for $\mathcal{COP}^n$, which, by duality, can be translated into an outer approximation for $\mathcal{CP}^n$. We can write SOS condition as a system of Linear Matrix Inequalities (LMIs). Therefore, optimization over these cones can be represented as a semidefinite program. To determine whether a polynomial is SOS requires solving a large instance of the positive semidefinite program. Therefore, the cost of optimizing over these convex cones increases exponentially as the level of the hierarchy increases.

Another approximation hierarchy introduced in 2007 by Pena et al. [57] uses the SOS decomposition as a sufficient condition for the nonnegativity of polynomials with some extra conditions. Thus, they proposed a hierarchy of convex cones to approximate $\mathcal{COP}^n$ from inside and $\mathcal{CP}^n$ from outside. They showed that for each level of the hierarchy, their cones are a subset of the cones constructed by Parrilo. Therefore, they provided a weaker approximation hierarchy for $\mathcal{CP}^n$. Similar to Parrilo's cones, the membership problem of these cones can be rewritten as a system of LMIs. Again, optimizing over these cones amounts to solving a semidefinite program. However, compared to Parrilo's cones, this representation requires a number of smaller SOS conditions. Therefore, verifying membership of these cones for a matrix is computationally cheaper than that of the cones provided by Parrilo.

We want to point out that there exists some other approximation hierarchies to

approximate the completely positive and copositive cone. For further details, we refer the reader to [1, 23, 24].

2.4 Upper and Lower Bounds

By using approximation hierarchies we can approximate a conic optimization problem over an intractable cone by a sequence of easier optimization problems. Recall that the copositive optimization problem is given by

$$\begin{aligned} \text{opt}(\text{CoP}) &:= \min && \langle C, X \rangle \\ \text{s.t.} &&& \langle A_i, X \rangle = b_i, \quad i = 1, \dots, m, \\ &&& X \in \mathcal{CP}^n, \end{aligned}$$

where $C \in \mathcal{S}^n$, $A_i \in \mathcal{S}^n$ and $b_i \in \mathbb{R}$ for $i = 1, \dots, m$. Since no efficient solver is available for this problem, we employ the approximation hierarchies. More precisely, we replace the difficult conic constraint $X \in \mathcal{CP}^n$ by sequences of increasingly more accurate tractable approximations. Hence, one can obtain a sequence of increasingly tighter bounds on $\text{opt}(\text{CoP})$ as the level of the hierarchy increases. If we replace the conic constraint $X \in \mathcal{CP}^n$ by $X \in \mathcal{I}_r$, then we obtain the following problem:

$$\begin{aligned} u_r &:= \min && \langle C, X \rangle \\ \text{s.t.} &&& \langle A_i, X \rangle = b_i, \quad i = 1, \dots, m, \\ &&& X \in \mathcal{I}_r, \end{aligned} \tag{2.11}$$

and by replacing $X \in \mathcal{CP}^n$ by $X \in \mathcal{O}_r$ we have

$$\begin{aligned} l_r &:= \min && \langle C, X \rangle \\ \text{s.t.} &&& \langle A_i, X \rangle = b_i, \quad i = 1, \dots, m, \\ &&& X \in \mathcal{O}_r, \end{aligned} \tag{2.12}$$

where $r = 0, 1, \dots$. Therefore, since (CoP) is a minimization problem, by solving (2.11), we obtain an upper bound on the optimal value. Similarly, the solution of (2.12) yields a lower bound for the optimal value. Because of the relations between each inner and outer cone, as in (2.1), we have

$$l_0 \leq l_1 \leq \dots \leq \text{opt}(\text{CoP}) \leq \dots \leq u_1 \leq u_0.$$

Furthermore, if problems (1.3) and (1.4) are strictly feasible, then we have

$$\lim_{r \rightarrow \infty} l_r = \text{opt}(\text{CoP}) = \lim_{r \rightarrow \infty} u_r.$$

Note that, if the optimization problem given in (1.3) is feasible, then any outer approximation will also be feasible. However, feasibility is not guaranteed for inner approximations. Therefore, we need additional assumptions to ensure the convergence of the sequence of optimal values l_r to $\text{opt}(\text{CoP})$. We refer the reader to [14] for further details.

2.5 Our Scope

Optimization is mainly concerned with finding a minimum or maximum value of a function of several variables subject to a set of constraints. Various necessary and sufficient optimality conditions have been proposed in the literature. For instance, we recommend the books by Horst et al. [33, 34] for the related material. However, it is not always possible to find a global optimal solution for a general optimization problem in a reasonable time. Therefore, researchers usually focus on optimization problems with a special structure.

Quadratic optimization is the minimization or maximization of a quadratic function subject to linear constraints. These problems are widely studied in optimization. It has been shown that a general quadratic optimization problem is NP-hard [50, 65, 71]. Furthermore, a quadratic optimization problem with the Hessian of the objective function having even one negative eigenvalue is NP-hard [55]. There is a

vast amount of literature on quadratic optimization. The interested reader is referred to [26, 27, 28, 42, 51, 54, 70, 73].

In this dissertation, we consider two specific problem classes related to nonconvex quadratic optimization: Standard quadratic optimization and box constrained quadratic optimization problems. These are important problem classes. Even though their structure is simple, they are NP-hard, in general. Furthermore, several well-known NP-hard combinatorial optimization problems can be formulated as quadratic optimization problems. For instance, the maximum stable set problem [49] and the max-cut problem [53, 63] can be reformulated as (StQP) and (BoxQP) problems, respectively. Moreover, these quadratic problems appear frequently in applications, for instance in portfolio selection [6], model predictive control [72], least squares approach [32]. Therefore, we focus on these two classes of optimization problems in this thesis.

Burer's copositive reformulation provides a new research direction for general nonconvex quadratic optimization problems. Therefore, we study copositive reformulations of (StQP) and (BoxQP). Since these convex optimization problems are still intractable due to the intractability of the underlying cones, we focus on using approximation hierarchies for these conic optimization problems. We choose the polyhedral approximation hierarchies proposed by Yıldırım [74] for inner approximation and by de Klerk and Pasechnik [20] for outer approximation. Since each of the two approximation hierarchies is composed of polyhedral cones, it follows that replacing the conic constraint $X \in \mathcal{CP}^n$ in (1.3) by $X \in \mathcal{I}_r$ (resp., by $X \in \mathcal{O}_r$), where $r \in \mathbb{N}$, gives rise to a linear programming problem with $O(n^{r+2})$ variables. For a minimization problem, the optimal value of LP yields an upper (resp., lower) bound on the optimal value. These two polyhedral approximation hierarchies provides approximate solutions with increasing accuracy as r increases. Note that polyhedral approximation hierarchies give rise to a simpler structure that we exploit in our analysis. Moreover, there are powerful computational tools to solve resulting LPs.

In this thesis, for the given problem classes and polyhedral approximation hierarchies, we are interested in two types of questions:

- *Rate of convergence*: How fast do the upper (resp., lower) bounds converge to the optimal value?
- *Finite convergence*: Under what conditions do the upper (resp., lower) bounds match the optimal value at a finite level of the hierarchy?

Our research concentrates on the finite convergence for (StQP) problems in Chapter 3. For (BoxQP) problems, we consider both the finite convergence and the rate of convergence in Chapter 4.



Chapter 3

STANDARD QUADRATIC OPTIMIZATION¹

3.1 Introduction

In this chapter, we study standard quadratic optimization problems given by

$$(\text{StQP}) \quad \nu(Q) := \min_{x \in \Delta_n} x^T Q x, \quad (3.1)$$

where $Q \in \mathcal{S}^n$ and $x \in \mathbb{R}^n$.

Standard quadratic optimization problems arise in a variety of applications (see, e.g. [6]). Despite its seemingly simple structure, the problem (StQP) encompasses several interesting problem classes. For instance, it is well-known that the problem of minimizing a nonhomogeneous quadratic function over the unit simplex can be reformulated in the form of (StQP) using the following identity:

$$x^T Q x + 2c^T x = x^T (Q + ec^T + ce^T)x, \quad \text{for each } x \in \Delta_n.$$

Similarly, any quadratic optimization problem over a polytope can, in theory, be formulated as an instance of (StQP) by representing each feasible point as a convex combination of the vertices of the polytope. In the resulting alternative formulation, each component of x corresponds to the weight of a different vertex. Therefore, the dimension n is equal to the number of vertices of the polytope. Clearly, such a reformulation is not viable if there is an exponential number of vertices as in box-constrained quadratic optimization problems.

¹Published as: [64] G. Sağol and E. A. Yıldırım. Analysis of copositive optimization based linear programming bounds on standard quadratic optimization. *Journal of Global Optimization*, 63(1):37-59, 2015.

Since the maximum stable set problem admits a formulation in the form of (StQP) [49], it follows that (StQP) is in general an NP-hard problem.

An instance of problem (3.1) can be equivalently reformulated as the following instance of a linear optimization problem over the cone of completely positive matrices [10]:

$$\nu(Q) = \min\{\langle Q, X \rangle : \langle E, X \rangle = 1, \quad X \in \mathcal{CP}^n\}. \quad (3.2)$$

Since (StQP) is in general an NP-hard problem, the convex optimization problem (3.2) is in general intractable. Indeed, the computational complexity is now hidden in the conic constraint $X \in \mathcal{CP}^n$, for which the membership problem is NP-hard [21]. Similarly, the membership problem for the dual cone $\mathcal{COP}^n$ is also NP-hard [21, 50].

Despite the fact that the convex reformulation (3.2) of the problem (StQP) does not seem to be helpful from the computational complexity point of view, it offers a new perspective as the difficulty is now shifted to the intractable convex cones $\mathcal{CP}^n$ and $\mathcal{COP}^n$. Therefore, we employ the two particular approximation hierarchies presented in Sections 2.2.1 and 2.3.1 for the following reasons. For standard quadratic optimization, both upper and lower bounds at any level of the hierarchy reduce to an optimization problem over an increasingly larger finite set (see Sections 3.2.2 and 3.2.3). These observations make these two particular approximation hierarchies more amenable to analysis in comparison with the other approximation hierarchies, most of which give rise to semidefinite programming problems (e.g., [38, 40, 56, 57]) that are considerably more difficult to analyze theoretically. Moreover, these two approximation hierarchies lead to a polynomial-time approximation scheme for standard quadratic optimization [9, 74] (see Section 3.2.4). As such, they constitute a natural choice for approximating standard quadratic optimization problems.

In this chapter, we investigate the upper and lower bounds arising from these inner and outer polyhedral approximations in the context of standard quadratic optimization. We give complete algebraic descriptions of the sets of the instances of (StQP) for which the upper bound or the lower bound is already exact at any given finite

level $r \in \mathbb{N}$ of the corresponding hierarchies (see Theorems 4 and 6). We identify the structural properties of the sets of instances on which upper and lower bounds converge to the optimal value only in the limit (see Proposition 2 and Theorem 5). Furthermore, we present several geometric and topological properties of these sets (see Proposition 1, Corollary 1, Propositions 8 and 9).

We remark that our perspective in this chapter, in general, is not algorithmic in the sense that some of our algebraic descriptions may not necessarily translate into an efficient method for deciding, for a given instance of (StQP), whether the upper and/or the lower bound is exact at a given level of the corresponding hierarchies. Rather, our main objective is to further our understanding of the strengths and limitations of these particular inner and outer polyhedral approximations of the cone $\mathcal{CP}^n$ in the context of standard quadratic optimization. We believe that the insights obtained from our results may be useful for the construction of improved polyhedral approximation hierarchies.

This chapter is organized as follows. We define our notation in Section 3.1.1. Section 3.2 is devoted to some preliminary results and the polyhedral approximations. In Section 3.3.1, we present algebraic descriptions of the sets of instances on which the upper bound is exact at any given finite level of the hierarchy. We identify the structural properties of the instances on which the upper bound converges to the optimal value in the limit. We also discuss several geometric and topological properties of these sets. The corresponding results for lower bounds are given in Section 3.3.2. We conclude the chapter in Section 3.4.

3.1.1 Notation

In this chapter, there are some additions to the standard notation: We reserve calligraphic uppercase letters to denote subsets of $\mathcal{S}^n$. For a given instance of (StQP), we denote the optimal value by $\nu(Q)$ and the set of optimal solutions by $\Omega(Q) \subseteq \Delta_n$. Let $U \subseteq \{1, \dots, n\}$ and $V \subseteq \{1, \dots, n\}$ be two nonempty index sets with $|U| = u$ and $|V| = v$. Given $x \in \mathbb{R}^n$, we denote by $x_U \in \mathbb{R}^u$ the restriction of x to its components

indexed by U . Similarly, for a given $M \in \mathcal{S}^n$, M_{UV} denotes the $u \times v$ submatrix of M whose rows and columns are indexed by the sets U and V , respectively.

3.2 Preliminaries and Polyhedral Approximations

In this section, we first collect some preliminary results on standard quadratic optimization problems. We then present the two hierarchies of inner and outer polyhedral approximations of the cone of completely positive matrices.

3.2.1 Useful Properties of Standard Quadratic Optimization

We first review the optimality conditions of (StQP).

Theorem 3. *Given an instance of (StQP), let $x^* \in \Omega(Q)$ with the optimal value $\nu(Q) = (x^*)^T Q x^*$. Define*

$$P := \{j \in \{1, \dots, n\} : x_j^* > 0\}, \quad \text{and} \quad Z := \{j \in \{1, \dots, n\} : x_j^* = 0\}. \quad (3.3)$$

Then, x^* satisfies

$$Q_{PP} x_P^* = \nu(Q) e_P, \quad Q_{ZP} x_P^* \geq \nu(Q) e_Z.$$

Proof. The assertion directly follows from the KKT conditions. □

Next, given an instance of (StQP), we present several basic results about the optimal value $\nu(Q)$ and the upper and lower bounds.

Lemma 2. *Let $Q, Q_1, Q_2 \in \mathcal{S}^n$.*

$$(i) \quad l_0(Q) = \min_{1 \leq i \leq j \leq n} Q_{ij}.$$

$$(ii) \quad \text{If } Q \in \mathcal{N}^n, \text{ then } u_r(Q) \geq \nu(Q) \geq l_r(Q) \geq 0 \text{ for each } r = 0, 1, \dots$$

$$(iii) \quad \text{If } Q_1 - Q_2 \in \mathcal{N}^n, \text{ then } \nu(Q_1) \geq \nu(Q_2), \quad u_r(Q_1) \geq u_r(Q_2), \text{ and } l_r(Q_1) \geq l_r(Q_2) \\ \text{for each } r = 0, 1, \dots$$

(iv) For any $\mu \in \mathbb{R}_+$ and any $r \in \mathbb{N}$, $\nu(\mu Q) = \mu\nu(Q)$, $l_r(\mu Q) = \mu l_r(Q)$, and $u_r(\mu Q) = \mu u_r(Q)$.

(v) For any $\lambda \in \mathbb{R}$ and any $r \in \mathbb{N}$, $\nu(Q + \lambda E) = \nu(Q) + \lambda$, $l_r(Q + \lambda E) = l_r(Q) + \lambda$, and $u_r(Q + \lambda E) = u_r(Q) + \lambda$.

Proof. (i) By (2.4), $\Lambda_n^0 = \{e_i : i = 1, \dots, n\} \cup \{(1/2)(e_i + e_j) : 1 \leq i < j \leq n\}$. The assertion follows from this observation and (3.7).

(ii) This is a direct consequence of part (i) and the monotonicity of the lower bounds.

(iii) Let $Q_1 - Q_2 \in \mathcal{N}^n$. For any $x \in \Delta_n$, we have $x^T(Q_1 - Q_2)x \geq 0$, which implies that $x^T Q_1 x \geq x^T Q_2 x$. Therefore,

$$\nu(Q_1) = \min_{x \in \Delta_n} x^T Q_1 x \geq \min_{x \in \Delta_n} x^T Q_2 x = \nu(Q_2).$$

Since $\Delta_n^r \subset \Delta_n$, we can argue similarly for upper bounds by simply replacing $x \in \Delta_n$ above with $d \in \Delta_n^r$ and using (3.5). Considering lower bounds, note that $l_r(Q_1 - Q_2) \geq 0$ by part (ii) for each $r = 0, 1, \dots$. By (3.7),

$$d^T(Q_1 - Q_2)d - \left(\frac{1}{r+2}\right) d^T \text{diag}(Q_1 - Q_2) \geq 0, \quad \text{for all } d \in \Lambda_n^r, \quad r = 0, 1, \dots,$$

which, after rearranging, yields

$$d^T Q_1 d - \left(\frac{1}{r+2}\right) d^T \text{diag}(Q_1) \geq d^T Q_2 d - \left(\frac{1}{r+2}\right) d^T \text{diag}(Q_2),$$

for each $d \in \Lambda_n^r$, $r = 0, 1, \dots$. Minimizing both sides of the inequality over $d \in \Lambda_n^r$, we obtain $l_r(Q_1) \geq l_r(Q_2)$ for each $r = 0, 1, \dots$.

(iv) This is a trivial consequence of (3.7), (3.5), and the hypothesis that $\mu \in \mathbb{R}_+$.

(v) Let $\lambda \in \mathbb{R}$. For any $x \in \Delta_n$, $x^T(Q + \lambda E)x = x^T Q x + \lambda$, which implies that $\nu(Q + \lambda E) = \nu(Q) + \lambda$. Similarly, by (3.5), we obtain $u_r(Q + \lambda E) = u_r(Q) + \lambda$.

since $\Delta_n^r \subset \Delta_n$.

For any $d \in \Delta_n^r$, $r = 0, 1, \dots$, we have

$$\begin{aligned} d^T(Q + \lambda E)d - \left(\frac{1}{r+2}\right) d^T \text{diag}(Q + \lambda E) &= \left(d^T Q d - \left(\frac{1}{r+2}\right) d^T \text{diag}(Q)\right) \\ &\quad + \lambda \left(\frac{r+1}{r+2}\right), \end{aligned}$$

where we used $d^T E d = d^T \text{diag}(E) = e^T d = 1$ by (2.4). It follows from (3.7) that $l_r(Q + \lambda E) = l_r(Q) + \lambda$.

□

3.2.2 Inner Polyhedral Approximations

We define the inner polyhedral approximations in Section 2.2.1. If we replace the difficult conic constraint $X \in \mathcal{CP}^n$ in (3.2) by $X \in \mathcal{I}_r$, we obtain the following linear programming problem whose optimal value yields an upper bound on the optimal value $\nu(Q)$.

$$u_r(Q) := \min\{\langle Q, X \rangle : \langle E, X \rangle = 1, \quad X \in \mathcal{I}_r\}, \quad r = 0, 1, \dots \quad (3.4)$$

As already observed in [74] (see also [9]), it follows directly from the definition of $\mathcal{I}_r$ that $u_r(Q)$ can be equivalently expressed as a minimization problem over a finite set:

$$u_r(Q) = \min_{d \in \Delta_n^r} d^T Q d, \quad r = 0, 1, \dots \quad (3.5)$$

3.2.3 Outer Polyhedral Approximations

In a similar manner, using the outer polyhedral approximations in Section 2.3.1, replacing the difficult conic constraint $X \in \mathcal{CP}^n$ in (3.2) by $X \in \mathcal{O}_r$ gives rise to the following linear programming problem, whose optimal value yields a lower bound on

$\nu(Q)$.

$$l_r(Q) := \min\{\langle Q, X \rangle : \langle E, X \rangle = 1, \quad X \in \mathcal{O}_r\}, \quad r = 0, 1, \dots \quad (3.6)$$

Using the definition of $\mathcal{O}_r$, the lower bound $l_r(Q)$ can similarly be stated as the following minimization problem over a finite set (see also [9, 74]):

$$\begin{aligned} l_r(Q) &= \frac{1}{(r+1)(r+2)} \min_{z \in \Theta_r^n} (z^T Q z - z^T \text{diag}(Q)), \\ &= \left(\frac{r+2}{r+1} \right) \min_{x \in \Lambda^r} \left(x^T Q x - \left(\frac{1}{r+2} \right) x^T \text{diag}(Q) \right), \quad r = 0, 1, \dots, \end{aligned} \quad (3.7)$$

where we used (2.8) in the second line.

3.2.4 Error Bounds and the Maximum Stable Set Problem

Given an instance of (StQP), the two sequences $\{l_r(Q)\}$ and $\{u_r(Q)\}$, $r \in \mathbb{N}$, give rise to increasingly tighter lower and upper bounds, respectively, on the optimal value $\nu(Q)$. Yıldırım [74] established that

$$u_r(Q) - l_r(Q) \leq \frac{1}{r+1} \left(\max_{i=1, \dots, n} Q_{ii} - \nu(Q) \right), \quad r = 0, 1, \dots,$$

which implies that these bounds lead to a polynomial-time approximation scheme for standard quadratic optimization (see also [9] for a slightly different result).

The bounds $l_r(Q)$ and $u_r(Q)$ have closed form expressions for the maximum stable set problem [9, 57, 74], which we review next. Let G be a simple, undirected graph with n vertices and m edges. A subset S of vertices of G is called a stable set if no two vertices in S are connected by an edge. The maximum stable set problem is that of finding the stable set with the largest cardinality in G . The size of the largest stable set, denoted by $\alpha(G)$, is called the stability number of G .

Motzkin and Straus [49] established that the maximum stable set problem can be

formulated as an instance of (StQP) as

$$\frac{1}{\alpha(G)} = \nu(I + A_G) = \min_{x \in \Delta_n} x^T (I + A_G) x, \quad (3.8)$$

where $A_G \in \mathcal{S}$ denotes the vertex adjacency matrix of G .

For the maximum stable set problem, the upper bounds have the following simple closed form expressions [74]:

$$u_r(I + A_G) = \begin{cases} \frac{1}{r+2}, & \text{if } r < \alpha(G) - 2, \\ \frac{1}{\alpha(G)}, & \text{otherwise.} \end{cases} \quad (3.9)$$

Similarly, the lower bounds have the following more complicated closed form expressions [9, 57, 74]:

$$l_r(I + A_G) = \begin{cases} 0, & \text{if } r \leq \alpha(G) - 2, \\ \frac{\binom{s}{2} \alpha(G) + st}{\binom{r+2}{2}}, & \text{otherwise,} \end{cases} \quad (3.10)$$

where s and t are nonnegative integers that satisfy $r+2 = s\alpha(G) + t$ with $0 \leq t < \alpha(G)$ and the convention that $\binom{s}{2} = 0$ if $s = 0$ or $s = 1$.

In the context of the maximum stable set problem, it follows from (3.9) that the upper bound matches the optimal value at level $r = \max\{0, \alpha(G) - 2\}$ of the inner approximation hierarchy. Similarly, if G is a complete graph, then $l_0(Q) = \nu(Q) = 1/\alpha(G) = 1$, where $Q = I + A_G$ by (3.10). It follows that both inner and outer approximations are already exact at level 0 in this case. On the other hand, if $\alpha(G) \geq 2$, then $l_r(Q) < \nu(Q) = 1/\alpha(G)$ for each $r \in \mathbb{N}$ (see [57]), which implies that the lower bound matches the optimal value only in the limit. Therefore, the upper and lower bounds exhibit different behaviors in terms of finite convergence in the context of the maximum stable set problem.

In this chapter, we are interested in understanding the behavior of upper and lower bounds that arise from the completely positive reformulation of general stan-

dard quadratic optimization problems. In particular, we give complete algebraic descriptions of the instances of (StQP) for which $u_r(Q) = \nu(Q)$ (see Theorem 4) or $l_r(Q) = \nu(Q)$ (see Theorem 6) for any given $r \in \mathbb{N}$. We aim to identify structural properties of the instances of (StQP) for which $u_r(Q) > \nu(Q)$ (see Proposition 2) or $l_r(Q) < \nu(Q)$ (see Theorem 5) for all $r \in \mathbb{N}$. Furthermore, we present several geometric and topological properties of these sets (see Proposition 1, Corollary 1, Propositions 8 and 9).

3.3 Analysis of Bounds

In this section, we establish the relations between the structural properties of a given instance of (StQP) and the behavior of upper and lower bounds on its optimal value.

3.3.1 Upper Bounds

In this section, we focus on the upper bounds $u_r(Q)$. We first give a complete algebraic description of the set of instances of (StQP) for which the upper bound matches the optimal value at any given finite level of the inner approximation hierarchy. We next discuss some interesting properties of this set. Finally, we identify the structural properties of the instances for which the upper bound is exact at a finite level of the hierarchy and for which the upper bound converges to the optimal value only in the limit.

Let us define the following sets:

$$\mathcal{U}_r := \{Q \in \mathcal{S}^n : u_r(Q) = \nu(Q)\}, \quad r = 0, 1, \dots \quad (3.11)$$

Due to the monotonicity of the upper bounds, we readily obtain

$$\mathcal{U}_0 \subseteq \mathcal{U}_1 \subseteq \dots \subseteq \mathcal{S}^n.$$

We first give complete algebraic descriptions of the sets $\mathcal{U}_r$.

Theorem 4. For each $r \in \mathbb{N}$, we have

$$\mathcal{U}_r = \bigcup_{d \in \Delta_n^r} \mathcal{V}_d, \quad (3.12)$$

where

$$\mathcal{V}_d := \{Q \in \mathcal{S}^n : d^T Q d \leq x^T Q x, \text{ for each } x \in \Delta_n\}, \quad d \in \Delta_n^r. \quad (3.13)$$

Proof. Let us fix $r \in \mathbb{N}$. By (3.11) and (3.5), $Q \in \mathcal{U}_r$ if and only if

$$\nu(Q) = u_r(Q) = \min_{d \in \Delta_n^r} d^T Q d,$$

which holds if and only if there exists some $d \in \Delta_n^r \cap \Omega(Q)$, or equivalently $Q \in \mathcal{V}_d$ for some $d \in \Delta_n^r$. The relation (3.12) follows. $\square$

The next proposition presents several geometric properties of the sets $\mathcal{U}_r$.

Proposition 1. For each $r \in \mathbb{N}$, $\mathcal{U}_r$ is a closed cone given by the union of a finite number of nonempty, closed, and convex cones. Furthermore, $\mathcal{U}_r$ contains the line $\{\lambda E : \lambda \in \mathbb{R}\}$ for each $r \in \mathbb{N}$.

Proof. For any $x \in \mathbb{R}^n$, note that $x^T Q x = \langle Q, x x^T \rangle$. Therefore, for each $r \in \mathbb{N}$ and each $d \in \Delta_n^r$, $\mathcal{V}_d$ is closed and convex since it is given by the intersection of an infinite number of closed half spaces in $\mathcal{S}^n$. Clearly, $\mathcal{V}_d$ is a cone.

For each $r \in \mathbb{N}$, the set $\mathcal{U}_r$ is a closed cone since it is given by the union of a finite number of closed cones. Finally, for any $\lambda \in \mathbb{R}$ and any $d \in \Delta_n^r$, we have $\lambda E \in \mathcal{V}_d$. Therefore, $\mathcal{U}_r$ contains the line $\{\lambda E : \lambda \in \mathbb{R}\}$ for each $r \in \mathbb{N}$. $\square$

For any $r \in \mathbb{N}$, it follows from Proposition 1 that $Q + \lambda E \in \mathcal{U}_r$ for any $\lambda \in \mathbb{R}$ whenever $Q \in \mathcal{U}_r$. Note, however, that the cones $\mathcal{U}_r$ are in general nonconvex. It is easy to verify that $e_i(e_i)^T \in \mathcal{U}_0$ for each $i = 1, \dots, n$. However, $I = \sum_{i=1}^n e_i(e_i)^T \notin \mathcal{U}_0$ for any $n \geq 3$.

Remark 1. For any $r \in \mathbb{N}$ and any $d \in \Delta_n^r$, the unique global minimizer of the quadratic function $(x-d)^T(x-d)$ is given by d . If we define $Q_d := I - ed^T - de^T \in \mathcal{S}^n$, it follows that $x^T Q_d x = x^T x - 2d^T x = (x-d)^T(x-d) - d^T d \geq -d^T d = d^T Q_d d$ for any $x \in \Delta_n$, with equality if and only if $x = d$. Therefore, $\Omega(Q_d) = \{d\}$ and $Q_d \in \mathcal{V}_d$ by (3.13). Since $\Delta_n^r \subset \Delta_n^{r+1}$ by (2.5), it follows from Proposition 1 that $\mathcal{U}_r \subset \mathcal{U}_{r+1}$ for each $r \in \mathbb{N}$, i.e., the set $\mathcal{U}_{r+1}$ is strictly larger than the set $\mathcal{U}_r$ for each $r \in \mathbb{N}$.

Remark 2. Let $G = (V, E)$ be a simple, undirected graph, where $|V| = n$. Consider the formulation (3.8) of the maximum stable set problem on G as an instance of (StQP), where $Q = I + A_G$. By (3.9), $u_r(I + A_G) = \nu(I + A_G)$ for $r \geq \alpha(G) - 2$, which implies that $I + A_G \in \mathcal{U}_r$ for each $r \geq \alpha(G) - 2$. It follows that, for any simple, undirected graph $G = (V, E)$, we have $I + A_G \in \mathcal{U}_{n-2}$.

Let us next define

$$\mathcal{U} := \bigcup_{r \in \mathbb{N}} \mathcal{U}_r, \quad \text{and} \quad \mathcal{U}_\infty := \mathcal{S}^n \setminus \mathcal{U}. \quad (3.14)$$

Note that the set $\mathcal{U}$ consists of all instances of (StQP) for which the upper bound matches the optimal value at *some* finite level of the inner approximation hierarchy. For instance, it follows from Remark 2 that, for any simple, undirected graph $G = (V, E)$, we have $I + A_G \in \mathcal{U}$. We next present several structural properties of the instances in the sets $\mathcal{U}$ and $\mathcal{U}_\infty$.

Proposition 2. The following relations are satisfied:

$$(i) \quad \mathcal{U} = \{Q \in \mathcal{S}^n : \Omega(Q) \cap \mathbb{Q}^n \neq \emptyset\} \text{ and } \mathcal{U}_\infty = \{Q \in \mathcal{S}^n : \Omega(Q) \cap \mathbb{Q}^n = \emptyset\}.$$

$$(ii) \quad \mathbb{Q}^n \subseteq \mathcal{U}.$$

Proof. (i) The first relation follows from the fact that $Q \in \mathcal{U}_r$ if and only if $\Delta_n^r \cap \Omega(Q) \neq \emptyset$ and the relation $\bigcup_{r \in \mathbb{N}} \Delta_n^r = \mathbb{Q}^n \cap \Delta_n$. The second relation is an immediate consequence of the first one and (3.14).

- (ii) Vavasis [71] proved that any quadratic optimization problem with rational data, which is bounded below, has a rational optimal solution. The assertion directly follows from this result and part (i).

□

For a given $Q \in \mathcal{S}^n$, Proposition 2(i) identifies an important structural property of the corresponding instance of (StQP) in order for the upper bounds to be exact at some finite level of the inner approximation hierarchy. An easy sufficient condition for membership in $\mathcal{U}$ is presented in Proposition 2(ii), which implies that, for a given $Q \in \mathcal{S}^n$, a necessary condition for $Q \in \mathcal{U}_\infty$ is that Q has irrational entries. Note, however, that this condition is not sufficient since, for any $Q \in \mathcal{Q}^n$, we have $\mu Q \in \mathcal{U}$ for any $\mu \in \mathbb{R}_+$ by Proposition 1.

The next corollary presents an important topological property of the set $\mathcal{U}$ and immediately follows from Proposition 2(ii) and the fact that $\text{cl}(\mathcal{Q}^n) = \mathcal{S}^n$.

Corollary 1. *We have $\text{cl}(\mathcal{U}) = \mathcal{S}^n$.*

It follows from Corollary 1 that, for any $Q \in \mathcal{S}^n$, either the upper bound is exact at some finite level of the hierarchy or there exists an arbitrarily small perturbation of Q for which the upper bound is exact at a finite level. Therefore, the set $\mathcal{U}$ is a dense subset of the set $\mathcal{S}^n$. This result reveals the strength of the inner approximation hierarchy of the completely positive cone in the context of standard quadratic optimization.

Finally, the next example illustrates that $\mathcal{U}_\infty \neq \emptyset$ for any $n \geq 2$.

Example 1. *Similar to Remark 1, let $d \in \Delta_n \setminus \mathbb{Q}^n$ and define $Q_d := I - ed^T - de^T \in \mathcal{S}^n$. Then, $\Omega(Q_d) = \{d\}$ and $\Omega(Q_d) \cap \mathbb{Q}^n = \emptyset$. By Proposition 2(i), $Q_d \in \mathcal{U}_\infty$.*

3.3.2 Lower Bounds

In this section, we focus on the behavior of lower bounds $l_r(Q)$. Our analysis of lower bounds is considerably more involved since the expression (3.7) is more complicated in comparison with (3.5).

Similar to $\mathcal{U}_r$, let us define the following sets:

$$\mathcal{L}_r := \{Q \in \mathcal{S}^n : l_r(Q) = \nu(Q)\}, \quad r = 0, 1, \dots \quad (3.15)$$

Since the lower bounds are monotonically nondecreasing, we obtain

$$\mathcal{L}_0 \subseteq \mathcal{L}_1 \subseteq \dots \subseteq \mathcal{S}^n.$$

Similarly, let

$$\mathcal{L} := \bigcup_{r \in \mathbb{N}} \mathcal{L}_r, \quad \text{and} \quad \mathcal{L}_\infty := \mathcal{S}^n \setminus \mathcal{L}. \quad (3.16)$$

This section is organized as follows. First of all, we give a simple algebraic description of the set $\mathcal{L}_0$ (see Proposition 3) and present its geometric properties (see Corollary 2). Then, two auxiliary sets $\mathcal{S}_1$ and $\mathcal{S}_2$ are introduced, which are later used to identify structural properties of the instances in the sets $\mathcal{L}$ and $\mathcal{L}_\infty$ (see Theorem 5 and Proposition 8). Next, we give complete algebraic descriptions of the sets $\mathcal{L}_r$ (see Theorem 6) and present several geometric properties of these sets (see Proposition 9). Finally, we close this section by discussing the relations among the sets $\mathcal{L}_r$, $\mathcal{L}$, $\mathcal{U}_r$, and $\mathcal{U}$ (see Proposition 11).

Characterization of $\mathcal{L}_0$

First, we focus on the set $\mathcal{L}_0$. To that end, given an instance of (StQP) and any $\gamma \in \mathbb{R}$, replacing $Q \in \mathcal{S}^n$ with $Q + \gamma E$ in (StQP) shifts the optimal value by γ by Lemma 2(v), i.e., $\nu(Q + \gamma E) = \nu(Q) + \gamma$, while $\Omega(Q + \gamma E) = \Omega(Q)$. In particular, the shifted matrix obtained with $\gamma = -\min_{1 \leq i \leq j \leq n} Q_{ij} = -l_0(Q)$ will play an important role and we define it below for future reference:

$$Q^s := Q - l_0(Q)E. \quad (3.17)$$

Note that $Q^s \in \mathcal{N}^n$ and $l_0(Q^s) = 0$ by Lemma 2(i).

Next, we give a simple algebraic description of the set $\mathcal{L}_0$.

Proposition 3. $Q \in \mathcal{L}_0$ if and only if there exists an index $k \in \{1, \dots, n\}$ such that $Q_{kk} = \min_{1 \leq i \leq j \leq n} Q_{ij}$. Therefore,

$$\mathcal{L}_0 = \bigcup_{k=1}^n \{Q \in \mathcal{S}^n : Q_{kk} \leq Q_{ij}, \ 1 \leq i \leq j \leq n\}. \quad (3.18)$$

Proof. Suppose that $Q \in \mathcal{L}_0$. Then, $l_0(Q) = \nu(Q) = \min_{1 \leq i \leq j \leq n} Q_{ij}$ by Lemma 2(i). Suppose, for a contradiction, that $Q_{kk} > l_0(Q)$ for each $k = 1, \dots, n$. By (3.17), $\min_{k=1, \dots, n} Q_{kk}^s > 0$. Since $Q^s \in \mathcal{N}^n$, for any $x \in \Delta_n$, we have

$$x^T Q^s x \geq \sum_{j=1}^n Q_{jj}^s x_j^2 \geq \left(\min_{k=1, \dots, n} Q_{kk}^s \right) \left(\sum_{j=1}^n x_j^2 \right) \geq \frac{\min_{k=1, \dots, n} Q_{kk}^s}{n} > 0,$$

where we used $\min_{x \in \Delta_n} \sum_{j=1}^n x_j^2 = 1/n$ to derive the third inequality. Together with Lemma 2(v), we obtain that $\nu(Q^s) = \nu(Q) - l_0(Q) > 0$, contradicting our hypothesis.

Conversely, given $Q \in \mathcal{S}^n$, suppose that there exists an index $k \in \{1, \dots, n\}$ such that $Q_{kk} = \min_{1 \leq i \leq j \leq n} Q_{ij}$. It is easy to verify that $e_k \in \Omega(Q)$. Therefore, $\nu(Q) = Q_{kk} = \min_{1 \leq i \leq j \leq n} Q_{ij} = l_0(Q)$ by Lemma 2(i), which implies that $Q \in \mathcal{L}_0$. $\square$

The following corollary presents some geometric properties of the set $\mathcal{L}_0$ and immediately follows from (3.18).

Corollary 2. *The set $\mathcal{L}_0$ is a closed cone given by the union of n polyhedral cones and contains the line $\{\lambda E : \lambda \in \mathbb{R}\}$.*

We remark that the set $\mathcal{L}_0$ is in general nonconvex since $e_i(e_i)^T \in \mathcal{L}_0$ for each $i = 1, \dots, n$, while $I = \sum_{i=1}^n e_i(e_i)^T \notin \mathcal{L}_0$ for any $n \geq 2$.

Two Auxiliary Sets

In this section, we will define two auxiliary sets that will subsequently be helpful in the description of the sets $\mathcal{L}$ and $\mathcal{L}_\infty$. To that end, we first define two index sets.

For a given $Q \in \mathcal{S}^n$, we have $e_k^T Q e_k = Q_{kk} \geq \nu(Q)$ for each $k = 1, \dots, n$. Therefore, each $Q \in \mathcal{S}^n$ induces the following partition of the indices:

$$U := \{k \in \{1, \dots, n\} : Q_{kk} = \nu(Q)\}, \quad V := \{k \in \{1, \dots, n\} : Q_{kk} > \nu(Q)\}. \quad (3.19)$$

We next define the following two auxiliary sets, which partition the set $\mathcal{S}^n$:

$$\mathcal{S}_1 := \left\{ Q \in \mathcal{S}^n : \min_{k=1, \dots, n} Q_{kk} = \nu(Q) \right\} = \{Q \in \mathcal{S}^n : U \neq \emptyset\}, \quad (3.20)$$

$$\mathcal{S}_2 := \left\{ Q \in \mathcal{S}^n : \min_{k=1, \dots, n} Q_{kk} > \nu(Q) \right\} = \{Q \in \mathcal{S}^n : U = \emptyset\}. \quad (3.21)$$

Note that $Q \in \mathcal{S}_1$ if and only if $\Omega(Q) \cap \{e_1, \dots, e_n\} \neq \emptyset$. Therefore,

$$\mathcal{S}_1 = \bigcup_{k=1}^n \mathcal{V}_{e_k}, \quad (3.22)$$

where $\mathcal{V}_{e_k}$ is defined as in (3.13).

The next proposition presents some geometric properties of the set $\mathcal{S}_1$ and its relation with the set $\mathcal{L}_0$.

Proposition 4. $\mathcal{S}_1$ is a closed cone given by the union of a finite number of nonempty, closed, and convex cones. Furthermore,

$$\mathcal{L}_0 \subseteq \mathcal{S}_1. \quad (3.23)$$

Proof. The assertions directly follow from the definition (3.13), (3.22), and Proposition 3. $\square$

We now turn our attention to the set $\mathcal{S}_2$. The following proposition is one of the main results of this section.

Proposition 5. We have $\mathcal{S}_2 \subseteq \mathcal{L}_\infty$, i.e., for a given $Q \in \mathcal{S}$, if $\min_{k=1, \dots, n} Q_{kk} > \nu(Q)$, then $Q \in \mathcal{L}_\infty$.

Proof. Let $Q \in \mathcal{S}_2$ and let $x^* \in \Omega(Q)$. Let the index sets P and Z be defined as in (3.3). Note that $|P| \geq 1$ since $x^* \in \Delta_n$. First, we claim that $|P| \geq 2$. Clearly, $|P| = 1$ if and only if $x^* = e_k$ for some $k \in \{1, \dots, n\}$, in which case $Q \in \mathcal{S}_1$ by (3.22), contradicting our hypothesis.

By Theorem 3,

$$Q_{PP} x_P^* = \nu(Q) e_P. \quad (3.24)$$

Fixing $k \in P$ and considering the corresponding equation above, we obtain

$$\sum_{j \in P} Q_{kj} x_j^* = \nu(Q).$$

Since $Q_{kk} > \nu(Q)$ and $x^* \in \Delta_n$, it follows that there exists some $l \in P$ such that $l \neq k$ and $Q_{kl} < \nu(Q)$.

Let us denote the smallest face of Δ_n that contains x^* by F , i.e., $F = \text{conv}\{e_i : i \in P\}$. We make the following claim. For each $r \in \mathbb{N}$, there exists $q^r \in \Lambda_n^r \cap F$ such that

$$f_r(q^r) := \left(\frac{r+2}{r+1} \right) (q^r)^T Q(q^r) - \left(\frac{1}{r+1} \right) (q^r)^T \text{diag}(Q) < \nu(Q), \quad r = 0, 1, \dots \quad (3.25)$$

We will prove our claim by induction on r . For $r = 0$, we define $q^0 = (1/2)(e_k + e_l)$, where $k \in P$ and $l \in P$ are as defined above. Clearly, $q^0 \in \Lambda_n^0 \cap F$ and

$$f_0(q^0) = 2(q^0)^T Q(q^0) - (q^0)^T \text{diag}(Q) = Q_{kl} < \nu(Q),$$

by the choice of $k \in P$ and $l \in P$. This establishes (3.25) for $r = 0$.

Suppose now that there exists some $q^r \in \Lambda_n^r \cap F$ that satisfies (3.25) for some $r \in \mathbb{N}$. We will show that we can construct $q^{r+1} \in \Lambda_n^{r+1} \cap F$ that satisfies (3.25) for $r + 1$.

Let us define $z^r = (r+2)q^r$. By the induction hypothesis,

$$f_r(q^r) = \frac{1}{(r+1)(r+2)} ((z^r)^T Q(z^r) - (z^r)^T \text{diag}(Q)) < \nu(Q). \quad (3.26)$$

For each $j \in P$, let us define $w^j := z^r + e_j$. We have

$$\left(\frac{1}{r+3}\right) w^j = \left(\frac{r+2}{r+3}\right) q^r + \left(\frac{1}{r+3}\right) e_j \in \Lambda_n^{r+1} \cap F, \quad \text{for each } j \in P.$$

We will show that there exists some $j' \in P$ such that $q^{r+1} = (1/(r+3))w^{j'}$ satisfies (3.25) for $r+1$. To that end,

$$\begin{aligned} (w^j)^T Q(w^j) - (w^j)^T \text{diag}(Q) &= (z^r)^T Q(z^r) + 2(z^r)^T Q e_j \\ &\quad + Q_{jj} - (z^r)^T \text{diag}(Q) - Q_{jj}, \\ &= (z^r)^T Q(z^r) - (z^r)^T \text{diag}(Q) + 2(z^r)^T Q e_j, \quad j \in P. \end{aligned}$$

Let us now focus on the term $(z^r)^T Q e_j$. Observe that $q^r = (1/(r+2))z^r \in F$ by the induction hypothesis and $e_j \in F$ since $j \in P$. Therefore, $(z^r)^T Q e_j = (z_P^r)^T Q_{PP}(e_j)_P$ for each $j \in P$. Multiplying both sides by x_j^* and summing over $j \in P$, we obtain

$$\begin{aligned} \sum_{j \in P} x_j^* ((z_P^r)^T Q_{PP}(e_j)_P) &= (z_P^r)^T Q_{PP} \left(\sum_{j \in P} x_j^* (e_j)_P \right), \\ &= (z_P^r)^T Q_{PP} x_P^*, \\ &= \nu(Q) ((z_P^r)^T e_P), \\ &= (r+2)\nu(Q), \end{aligned}$$

where we used (3.24) in the third line and the definition of z^r in the last line. Since $\sum_{j \in P} x_j^* = 1$ and $x^* \geq 0$, there exists some $j' \in P$ such that $(z_P^r)^T Q_{PP}(e_{j'})_P =$

$(z^r)^T Q e_{j'} \leq (r+2)\nu(Q)$. By defining $q^{r+1} = (1/(r+3))w^{j'}$, we obtain

$$\begin{aligned}
 f_{r+1}(q^{r+1}) &= \left(\frac{r+3}{r+2}\right) (q^{r+1})^T Q (q^{r+1}) - \left(\frac{1}{r+2}\right) (q^{r+1})^T \text{diag}(Q), \\
 &= \frac{1}{(r+2)(r+3)} \left((w^{j'})^T Q (w^{j'}) - (w^{j'})^T \text{diag}(Q) \right), \\
 &= \frac{1}{(r+2)(r+3)} \left((z^r)^T Q (z^r) - (z^r)^T \text{diag}(Q) + 2(z^r)^T Q e_{j'} \right), \\
 &\leq \frac{1}{(r+2)(r+3)} \left((z^r)^T Q (z^r) - (z^r)^T \text{diag}(Q) + 2(r+2)\nu(Q) \right), \\
 &< \frac{1}{(r+2)(r+3)} \left((r+1)(r+2)\nu(Q) + 2(r+2)\nu(Q) \right), \\
 &= \left(\frac{r+1}{r+3}\right) \nu(Q) + \left(\frac{2}{r+3}\right) \nu(Q), \\
 &= \nu(Q),
 \end{aligned}$$

where we used the choice of j' in the first inequality and the induction hypothesis (3.26) in the second one. Since $l_r(Q) \leq f_r(q^r)$ by (3.7), it follows from (3.25) that $l_r(Q) < \nu(Q)$ for each $r \in \mathbb{N}$. Therefore, $Q \in \mathcal{L}_\infty$. $\square$

Example 2. Consider an instance of (StQP) in which Q^s is a diagonal matrix with strictly positive diagonal entries. Note that this class includes all instances of (StQP) in which Q itself is a strictly positive diagonal matrix. Let $\beta = \sum_{i=1}^n (1/Q_{ii}^s)$. It is easy to verify that the unique optimal solution $x^* \in \Omega(Q)$ is given by $x_j^* = (1/Q_{jj}^s)/\beta$, $j = 1, \dots, n$. Therefore, by (3.22), $Q \notin \mathcal{S}_1$ for any $n \geq 2$. It follows from Proposition 5 that $Q \in \mathcal{L}_\infty$ for any $n \geq 2$.

Remark 3. Let $G = (V, E)$ be a simple, undirected graph, where $|V| = n$. Consider the formulation (3.8) of the maximum stable set problem on G as an instance of (StQP), where $Q = I + A_G$. If G is a complete graph, then $Q = E$, which implies that $Q \in \mathcal{L}_0$ by Corollary 2. Therefore, $l_0(Q) = 1/\alpha(G) = 1$. On the other hand, if $\alpha(G) \geq 2$, then $\min_{k=1, \dots, n} Q_{kk} = 1 > \nu(Q) = 1/\alpha(G)$, which implies that $Q \in \mathcal{S}_2$ by (3.21). By Proposition 5, $Q \in \mathcal{L}_\infty$. It follows that the relation $l_r(Q) < \nu(Q)$ established in [57] is a special case of Proposition 5.

The following result, which is an immediate consequence of Proposition 5 and

(3.22), presents an important relation between the sets $\mathcal{L}$ and $\mathcal{S}_1$.

Corollary 3. *We have $\mathcal{L} \subseteq \mathcal{S}_1$, where $\mathcal{L}$ and $\mathcal{S}_1$ are defined as in (3.16) and (3.20), respectively. Therefore, for a given $Q \in \mathcal{S}^n$, if $Q \in \mathcal{L}$, then $\Omega(Q) \cap \{e_1, \dots, e_n\} \neq \emptyset$.*

Corollary 3 presents a necessary condition for $Q \in \mathcal{L}$. An interesting question is whether this condition is sufficient, i.e., whether we have $\mathcal{L} = \mathcal{S}_1$. The next two examples answer this question in the negative for different reasons.

Example 3. *Consider an instance of (StQP), where*

$$Q = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix}.$$

One can verify that $\nu(Q) = 1$ and $\Omega(Q) = \{e_1, (e_2 + e_3)/2\}$, which implies that $Q \in \mathcal{S}_1$ by (3.22). In this example, $U = \{1\}$ and $V = \{2, 3\}$. Let us focus on Q_{VV} . Note that $\nu(Q_{VV}) = 1$, which implies that, for $n = 2$, $Q_{VV} \in \mathcal{L}_\infty$ by Proposition 5. Therefore, for any $r \in \mathbb{N}$, $l_r(Q_{VV}) < \nu(Q_{VV}) = 1$. It follows that

$$\begin{aligned} l_r(Q) &= \left(\frac{r+2}{r+1} \right) \min_{d \in \Lambda_n^r} \left(d^T Q d - \left(\frac{1}{r+2} \right) d^T \text{diag}(Q) \right), \\ &\leq \left(\frac{r+2}{r+1} \right) \min_{d \in \Lambda_n^r: d_1=0} \left(d^T Q d - \left(\frac{1}{r+2} \right) d^T \text{diag}(Q) \right), \\ &= l_r(Q_{VV}) < 1, \end{aligned}$$

for any $r \in \mathbb{N}$. Therefore, $Q \in \mathcal{L}_\infty$, i.e., $Q \in \mathcal{S}_1 \setminus \mathcal{L}$.

Example 4. *Consider an instance of (StQP), where*

$$Q = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 3 & 0 \\ 1 & 0 & 3 \end{bmatrix}.$$

Q is positive definite. It is easy to verify that $\nu(Q) = 1$ and $\Omega(Q) = \{e_1\}$, which implies that $Q \in \mathcal{S}_1$ by (3.22). Similarly, $U = \{1\}$ and $V = \{2, 3\}$. We claim that

$Q \notin \mathcal{L}$. Let us fix $r \in \mathbb{N}$ and define $d_r := \left(\frac{1}{r+2}\right) [r, 1, 1]^T \in \Lambda_n^r$. By (3.7),

$$\begin{aligned} l_r(Q) &\leq \left(\frac{r+2}{r+1}\right) \left(d_r^T Q d_r - \left(\frac{1}{r+2}\right) d_r^T \text{diag}(Q) d_r\right), \\ &= \frac{r^2 + 4r + 6 - (r+6)}{(r+1)(r+2)}, \\ &= \frac{r^2 + 3r}{r^2 + 3r + 2} < 1, \end{aligned}$$

which implies that $l_r(Q) < \nu(Q)$ for each $r \in \mathbb{N}$. Therefore, $Q \in \mathcal{L}_\infty$, i.e., $Q \in \mathcal{S}_1 \setminus \mathcal{L}$.

Note that $\nu(Q_{VV}) = 3/2 > 1 = \nu(Q)$ on this instance.

Structural Properties of $\mathcal{L}$ and $\mathcal{L}_\infty$

In this section, our goal is to identify the structural properties of the instances in the sets $\mathcal{L}$ and $\mathcal{L}_\infty$. We first generalize Examples 3 and 4 in an attempt to further our understanding of the set $\mathcal{S}_1 \setminus \mathcal{L}$ (see Propositions 6 and 7). We then use these observations to present our main result in Theorem 5, which establishes the structural properties of the instances in $\mathcal{L}$ and $\mathcal{L}_\infty$. Finally, Proposition 8 presents a relation between the sets $\mathcal{L}$ and $\mathcal{S}_1$.

We first present a useful property of the instances in the set $\mathcal{S}_1 \setminus \mathcal{L}$.

Lemma 3. *For any $Q \in \mathcal{S}_1 \setminus \mathcal{L}$, there exists $k \in \{1, \dots, n\}$ such that $Q_{kk} > \nu(Q)$, i.e., we have $V \neq \emptyset$, where V is defined as in (3.19).*

Proof. Let $Q \in \mathcal{S}_1 \setminus \mathcal{L}$. Suppose, for a contradiction, that $V = \emptyset$. Then, $\{e_1, \dots, e_n\} \subseteq \Omega(Q)$ since $U = \{1, \dots, n\}$. By Theorem 3, we have $Q_{ij} \geq Q_{ii} = \nu(Q)$ for each $1 \leq i \leq j \leq n$. Therefore, $Q \in \mathcal{L}_0$ by Proposition 3, which contradicts our hypothesis since $\mathcal{L}_0 \subseteq \mathcal{L}$. $\square$

It follows from the proof of Lemma 3 that

$$Q_{ij} \geq \nu(Q) \quad \text{for each } i \in U, j = 1, \dots, n. \quad (3.27)$$

The next proposition gives a sufficient condition for membership in $\mathcal{S}_1 \setminus \mathcal{L}$ and generalizes Example 3.

Proposition 6. *Let $Q \in \mathcal{S}_1$ be such that $V \neq \emptyset$. If $\nu(Q_{VV}) = \nu(Q)$, where V is defined as in (3.19), then $Q \in \mathcal{S}_1 \setminus \mathcal{L}$.*

Proof. The assertion follows from the observation that $Q_{VV} \in \mathcal{L}_\infty$ for $n = |V|$ by Proposition 5 and a similar argument as in Example 3. $\square$

The next proposition presents another sufficient condition for membership in $\mathcal{S}_1 \setminus \mathcal{L}$, thereby generalizing Example 4.

Proposition 7. *Let $Q \in \mathcal{S}_1$ be such that $|V| \geq 2$, where V is defined as in (3.19). Suppose that there exist indices $i \in U$, $j \in V$, $k \in V$, and $j \neq k$ such that*

$$Q_{ij} = Q_{ik} = \nu(Q), \quad Q_{jk} < \nu(Q). \quad (3.28)$$

Then, $Q \in \mathcal{S}_1 \setminus \mathcal{L}$.

Proof. Suppose that $Q \in \mathcal{S}_1$ satisfies the hypothesis and let us fix $r \in \mathbb{N}$. We define $d \in \Lambda_n^r$ as follows:

$$d_i = \frac{r}{r+2}, \quad d_j = \frac{1}{r+2}, \quad d_k = \frac{1}{r+2},$$

and all remaining entries of d are set to 0. By (3.7),

$$\begin{aligned} l_r(Q) &\leq \left(\frac{r+2}{r+1} \right) \left(d^T Q d - \left(\frac{1}{r+2} \right) d^T \text{diag}(Q) d \right), \\ &= \frac{\nu(Q)(r^2 + 3r) + 2Q_{jk}}{r^2 + 3r + 2} < \nu(Q), \end{aligned}$$

where we used (3.28) to derive the last inequality. It follows that $Q \notin \mathcal{L}$. $\square$

We remark that the sufficient conditions of Propositions 6 and 7, in general, are not implied by one another. Indeed, the instance in Example 3 satisfies only the

sufficient condition of Proposition 6, whereas the instance in Example 4 satisfies only that of Proposition 7 with $i = 1$, $j = 2$, and $k = 3$.

Recall that $Q \in \mathcal{S}_1$ if and only if $\Omega(Q) \cap \{e_1, \dots, e_n\} \neq \emptyset$. Motivated by the sufficient conditions of Propositions 6 and 7, let us define the following subset of $\mathcal{S}_1$.

$$\begin{aligned} \mathcal{S}'_1 := & \{Q \in \mathcal{S}_1 : V \neq \emptyset \text{ and } \nu(Q_{VV}) = \nu(Q)\} \cup \{Q \in \mathcal{S}_1 : \exists i \in U, \\ & \exists j \in V, \exists k \in V \text{ such that } j \neq k, Q_{ij} = Q_{ik} = \nu(Q), Q_{jk} < \nu(Q)\}. \end{aligned} \quad (3.29)$$

The next theorem, which is one of the main results of Section 3.3.2, establishes the relationships between the sets $\mathcal{L}$ and $\mathcal{L}_\infty$ and the sets $\mathcal{S}_1$, $\mathcal{S}'_1$, and $\mathcal{S}_2$.

Theorem 5. *The following relations are satisfied:*

1. $\mathcal{L} = \mathcal{S}_1 \setminus \mathcal{S}'_1 = \{Q \in \mathcal{S}^n : \Omega(Q) \cap \{e_1, \dots, e_n\} \neq \emptyset\} \setminus \mathcal{S}'_1$,
2. $\mathcal{L}_\infty = \mathcal{S}_2 \cup \mathcal{S}'_1 = \{Q \in \mathcal{S}^n : \Omega(Q) \cap \{e_1, \dots, e_n\} = \emptyset\} \cup \mathcal{S}'_1$,

where $\mathcal{S}'_1$ is defined as in (3.29).

Proof. Note that $\mathcal{S}_1 \cup \mathcal{S}_2 = \mathcal{L} \cup \mathcal{L}_\infty = \mathcal{S}$ and $\mathcal{S}_1 \cap \mathcal{S}_2 = \mathcal{L} \cap \mathcal{L}_\infty = \emptyset$ by (3.16), (3.20), and (3.21). By Propositions 5, 6 and 7, we obtain $\mathcal{S}'_1 \cup \mathcal{S}_2 \subseteq \mathcal{L}_\infty$. Taking the complements of both sides yields $\mathcal{L} \subseteq \mathcal{S}_1 \setminus \mathcal{S}'_1$. Therefore, both assertions will be proved by showing that any one of these two inclusions in fact holds with equality. We will show that the latter inclusion holds with equality by showing that the reverse inclusion $\mathcal{S}_1 \setminus \mathcal{S}'_1 \subseteq \mathcal{L}$ is satisfied.

Let $Q \in \mathcal{S}_1 \setminus \mathcal{S}'_1$. Let us define the following index sets:

$$W_1 := \{(j, k) : j \in V, k \in V, j \neq k, Q_{jk} < \nu(Q)\}, \quad (3.30)$$

$$W_2 := \{(j, k) : j \in V, k \in V, j \neq k, Q_{jk} \geq \nu(Q)\}. \quad (3.31)$$

If $W_1 = \emptyset$, then it follows from (3.27), (3.31), and (3.29) that $Q_{ij} \geq \nu(Q)$ for $1 \leq i \leq j \leq n$ and $Q_{kk} = \nu(Q)$ for some $k = 1, \dots, n$. Therefore, $Q \in \mathcal{L}_0$ by Proposition 3, which implies that $Q \in \mathcal{L}$, establishing the reverse inclusion.

We will henceforth assume that $W_1 \neq \emptyset$. In this case, it follows from (3.29) that

$$\beta_{ijk} := \max\{Q_{ij}, Q_{ik}\} > \nu(Q), \quad \text{for each } i \in U, (j, k) \in W_1.$$

We also define

$$\beta := \min_{i \in U; (j,k) \in W_1} \beta_{ijk} > \nu(Q), \quad \text{and} \quad \rho := \beta - \nu(Q) > 0. \quad (3.32)$$

Next, we will establish a lower bound on $l_r(Q)$ for each $r \in \mathbb{N}$. Let us fix $r \in \mathbb{N}$. Recall that $l_r(Q)$ is given by

$$l_r(Q) = \frac{1}{(r+1)(r+2)} \min_{z \in (r+2)\Lambda_n^r} (z^T Q z - z^T \text{diag}(Q)), \quad r = 0, 1, \dots$$

We can rewrite the expression in the parentheses on the right-hand side as

$$\begin{aligned} z^T Q z - z^T \text{diag}(Q) &= \sum_{i \in U} \sum_{j \in U} Q_{ij} z_i z_j - \sum_{i \in U} Q_{ii} z_i + 2 \sum_{i \in U} \sum_{k \in V} Q_{ik} z_i z_k \\ &\quad + \sum_{j \in V} \sum_{k \in V} Q_{jk} z_j z_k - \sum_{j \in V} Q_{jj} z_j. \end{aligned} \quad (3.33)$$

Next, we will derive lower bounds on the terms on the right-hand side of (3.33). For a given $z \in (r+2)\Lambda_n^r$, let us define

$$\sum_{j \in V} z_j = \eta,$$

so that $\sum_{i \in U} z_i = r+2-\eta$.

By (3.27),

$$\begin{aligned} \sum_{i \in U} \sum_{j \in U} Q_{ij} z_i z_j - \sum_{i \in U} Q_{ii} z_i &= \sum_{i \in U} Q_{ii} z_i (z_i - 1) + \sum_{i \in U} \sum_{j \in U \setminus \{i\}} Q_{ij} z_i z_j, \\ &\geq \nu(Q) \left(\left(\sum_{i \in U} z_i \right)^2 - \sum_{i \in U} z_i \right), \\ &= (r+2-\eta)(r+1-\eta)\nu(Q), \end{aligned} \quad (3.34)$$

where we used $z \in \mathbb{N}^n$ to derive the inequality.

Similarly,

$$\sum_{j \in V} \sum_{k \in V} Q_{jk} z_j z_k - \sum_{j \in V} Q_{jj} z_j = \sum_{j \in V} Q_{jj} z_j (z_j - 1) + \sum_{(j,k) \in W_1} Q_{jk} z_j z_k + \sum_{(j,k) \in W_2} Q_{jk} z_j z_k.$$

By (3.30) and (3.31), we obtain the following lower bounds.

$$\sum_{j \in V} \sum_{k \in V} Q_{jk} z_j z_k - \sum_{j \in V} Q_{jj} z_j \geq \begin{cases} \nu(Q)\eta(\eta - 1), & \text{if } z_j z_k = 0 \\ & \text{for all } (j, k) \in W_1, \\ \eta(\eta - 1)l_{\eta-2}(Q_{VV}), & \text{otherwise,} \end{cases} \quad (3.35)$$

where the second part follows from the definition of $l_r(Q_{VV})$ and the fact that $z_V \in (r + 2)\Lambda_{|V|}^{\eta-2}$. Note that, in the second case, z_V should have at least two positive components, which implies that $\eta \geq 2$.

Finally,

$$\sum_{i \in U} \sum_{k \in V} Q_{ik} z_i z_k = \sum_{i \in U} z_i \left(\sum_{k \in V} Q_{ik} z_k \right).$$

Note that $Q_{ik} \geq \nu(Q)$ for each $i \in U$ and $k \in V$ by (3.27). Furthermore, if there exists $(j', k') \in W_1$ such that $z_{j'} z_{k'} > 0$, then

$$\sum_{k \in V} Q_{ik} z_k = \sum_{k \in V \setminus \{j', k'\}} Q_{ik} z_k + Q_{i,j'} z_{j'} + Q_{i,k'} z_{k'} \geq \nu(Q)\eta + \rho, \quad \text{for each } i \in U,$$

since $\max\{Q_{i,j'}, Q_{i,k'}\} \geq \nu(Q) + \rho$ by (3.32) for each $i \in U$. Therefore,

$$\sum_{i \in U} \sum_{k \in V} Q_{ik} z_i z_k \geq \begin{cases} (r + 2 - \eta)(\nu(Q)\eta + \rho), & \text{if } z_j z_k > 0 \\ & \text{for some } (j, k) \in W_1, \\ \nu(Q)(r + 2 - \eta)\eta, & \text{otherwise,} \end{cases} \quad (3.36)$$

Using these lower bounds, we consider the following five cases:

Case 1: If $\sum_{j \in V} z_j = \eta = 0$, then $z_j = 0$ for each $j \in V$. By (3.33) and (3.34),

$$z^T Q z - z^T \text{diag}(Q) \geq (r+2)(r+1)\nu(Q).$$

Case 2: If $\sum_{j \in V} z_j = \eta = 1$, then it follows from (3.33), (3.34), (3.35), and (3.36) that

$$z^T Q z - z^T \text{diag}(Q) \geq (r+2)(r+1)\nu(Q).$$

Case 3: If $\sum_{j \in V} z_j = \eta = r+2$, then $z_i = 0$ for each $i \in U$. By (3.33) and (3.35),

$$z^T Q z - z^T \text{diag}(Q) \geq (r+2)(r+1) \min\{\nu(Q), l_r(Q_{VV})\}.$$

Case 4a: If $2 \leq \sum_{j \in V} z_j = \eta \leq r+1$ and $z_j z_k = 0$ for each $(j, k) \in W_1$, then it follows from (3.33), (3.34), (3.35), and (3.36) that

$$z^T Q z - z^T \text{diag}(Q) \geq (r+2)(r+1)\nu(Q).$$

Case 4b: If $2 \leq \sum_{j \in V} z_j = \eta \leq r+1$ and there exists $(j, k) \in W_1$ such that $z_j z_k > 0$, then, by (3.33), (3.34), (3.35), and (3.36),

$$z^T Q z - z^T \text{diag}(Q) \geq (r+2-\eta)(r+1+\eta)\nu(Q) + \eta(\eta-1)l_{\eta-2}(Q_{VV}) + 2\rho(r+2-\eta).$$

It follows from the five cases above that

$$l_r(Q) \geq \min \left\{ \nu(Q), l_r(Q_{VV}), \min_{\eta \in \{2, \dots, r+1\}} h(Q, \eta, r) \right\}, \quad (3.37)$$

where

$$h(Q, \eta, r) := (1 - \lambda_{\eta, r})\nu(Q) + \lambda_{\eta, r}l_{\eta-2}(Q_{VV}) + \frac{2\rho(r+2-\eta)}{(r+1)(r+2)}, \quad (3.38)$$

and

$$\lambda_{\eta,r} := \frac{\eta(\eta-1)}{(r+1)(r+2)}.$$

We next establish that the second and the third terms in (3.37) are at least as large as $\nu(Q)$ for all sufficiently large values of r .

For any $\hat{Q} \in \mathcal{S}_1$ with $V \neq \emptyset$, we have

$$\nu(\hat{Q}_{VV}) = \min\{x^T \hat{Q} x : e^T x = 1, x \geq 0, x_i = 0, i \in U\} \geq \nu(\hat{Q}).$$

By (3.29), we therefore have $\nu(Q_{VV}) > \nu(Q)$ for any $Q \in \mathcal{S}_1 \setminus \mathcal{S}'_1$. Since $\lim_{r \rightarrow \infty} l_r(Q_{VV}) = \nu(Q_{VV})$, there exists $\hat{r} \in \mathbb{N}$ such that

$$l_r(Q_{VV}) \geq \nu(Q), \quad \text{for all } r > \hat{r}. \quad (3.39)$$

Therefore, the second term in (3.37) is at least as large as $\nu(Q)$ for all $r > \hat{r}$. Let us next focus on the third term in (3.37) for $r > \hat{r}$. Note that it suffices to consider only $\eta \in \{2, \dots, \hat{r} + 2\}$ for the range of the minimum since $h(Q, \eta, r) > \nu(Q)$ for all $\eta > \hat{r} + 2$ by (3.39).

Let us now fix $\eta \in \{2, \dots, \hat{r} + 2\}$ and consider the last term in (3.37) as a function of r . We claim that there exists $r_\eta \in \mathbb{N}$ such that

$$h(Q, \eta, r) \geq \nu(Q), \quad \text{for all } r \geq r_\eta, \quad (3.40)$$

where h is defined as in (3.38). Indeed, $h(Q, \eta, r)$ can be rewritten as

$$\nu(Q) + \frac{2\rho(r+2-\eta) - \eta(\eta-1)(\nu(Q) - l_{\eta-2}(Q_{VV}))}{(r+1)(r+2)}.$$

Therefore, there exists $r_\eta \in \mathbb{N}$ such that the second term is nonnegative for all $r \geq r_\eta$, which establishes (3.40).

It follows from (3.39), (3.40), and (3.37) that

$$l_r(Q) = \nu(Q), \quad \text{for all } r \geq r^*,$$

where

$$r^* := \max \left\{ \hat{r} + 1, \max_{\eta \in \{2, \dots, \hat{r}+2\}} r_\eta \right\} < \infty.$$

Therefore, $Q \in \mathcal{L}$, which implies that $\mathcal{S}_1 \setminus \mathcal{S}'_1 \subseteq \mathcal{L}$. The proof is complete. $\square$

For illustrative purposes, we present the following example.

Example 5. *Let*

$$Q(\rho) := \begin{bmatrix} 1 & 1+\rho & 1+\rho \\ 1+\rho & 3 & 0 \\ 1+\rho & 0 & 3 \end{bmatrix}.$$

For any $\rho \geq 0$, $\nu(Q(\rho)) = 1$ and $\Omega(Q(\rho)) = e_1$, which implies that $Q(\rho) \in \mathcal{S}_1$. We have $U = \{1\}$ and $V = \{2, 3\}$. Note that $Q(0) \in \mathcal{S}'_1$ by Example 4. On the other hand, for any $\rho > 0$, $Q(\rho) \in \mathcal{S}_1 \setminus \mathcal{S}'_1$, which implies that $Q \in \mathcal{L}$ by Theorem 5. Our computational experiments reveal that $Q(1) \in \mathcal{L}_5$ and $Q(0.1) \in \mathcal{L}_{48}$.

Example 5 illustrates that $\mathcal{L}$, in general, is not a closed set. Our next result gives a description of the closure of $\mathcal{L}$.

Proposition 8. *We have*

$$\text{cl}(\mathcal{L}) = \mathcal{S}_1 = \{Q \in \mathcal{S} : \Omega(Q) \cap \{e_1, \dots, e_n\} \neq \emptyset\}.$$

Proof. By Corollary 3, $\mathcal{L} \subseteq \mathcal{S}_1$. Note that $\mathcal{S}_1$ is a closed set by Proposition 4. Therefore, $\text{cl}(\mathcal{L}) \subseteq \mathcal{S}_1$.

Conversely, let $Q \in \mathcal{S}_1$. Therefore, there exists some $i \in \{1, \dots, n\}$ such that

$e_i \in \Omega(Q)$. Let us define the following sequence:

$$Q_k := Q + \frac{1}{k} (ee^T - e_i(e_i)^T), \quad k = 1, 2, \dots$$

Clearly, $\lim_{k \rightarrow \infty} Q_k = Q$. We will show that $Q_k \in \mathcal{L}$ for each $k = 1, 2, \dots$. Let us fix k . Since $Q_k - Q \in \mathcal{N}$, $\nu(Q_k) \geq \nu(Q)$ by Lemma 2(iii). Furthermore, $(e_i)^T Q_k e_i = \nu(Q) \geq \nu(Q_k)$, which implies that $\nu(Q_k) = \nu(Q)$ and $e_i \in \Omega(Q_k)$. Therefore, $Q_k \in \mathcal{S}_1$ for each $k = 1, 2, \dots$. Since $e_i \in \Omega(Q)$, we have $Q_{ij} \geq \nu(Q)$ and $Q_{jj} \geq \nu(Q)$ for each $j = 1, \dots, n$. By the definition of Q_k , $U = \{i\}$, $V = \{1, \dots, n\} \setminus \{i\}$. We have

$$\nu((Q_k)_{VV}) = \min_{x \in \Delta_n: x_i=0} \left\{ x^T Q_k x + \frac{1}{k} \right\} \geq \nu(Q) + \frac{1}{k} > \nu(Q) = \nu(Q_k),$$

which implies that the condition of Proposition 6 cannot be satisfied. Since $(Q_k)_{ij} > \nu(Q)$ for each $j \in V$, the condition of Proposition 7 cannot be satisfied either. Therefore, $Q_k \notin \mathcal{S}'_1$, i.e., $Q_k \in \mathcal{S}_1 \setminus \mathcal{S}'_1$. By Theorem 5, $Q_k \in \mathcal{L}$ for each $k = 1, 2, \dots$, which implies that $Q \in \text{cl}(\mathcal{L})$. $\square$

By Proposition 8, $Q(0) \in \text{cl}(\mathcal{L}) \setminus \mathcal{L}$ in Example 5. Note that $\text{cl}(\mathcal{L}) \subset \mathcal{S}$ in general. For instance, $I \notin \text{cl}(\mathcal{L})$ since $I \notin \mathcal{S}_1$ for any $n \geq 2$.

Description of $\mathcal{L}_r$

In this section, we give complete algebraic descriptions of the sets $\mathcal{L}_r$. In particular, our next result generalizes Proposition 3.

Theorem 6. *For any $r = 0, 1, \dots$, we have*

$$\mathcal{L}_r := \bigcup_{k=1}^n \mathcal{L}_r^k, \tag{3.41}$$

where

$$\mathcal{L}_r^k := \left\{ Q \in \mathcal{S}^n : Q_{kk} \leq \frac{1}{(r+1)(r+2)} (z^T Q z - z^T \text{diag}(Q)) , \quad \text{for all } z \in (r+2)\Delta_n^r \right\},$$

for $k = 1, \dots, n$.

Proof. Let us fix $r \in \mathbb{N}$ and let $Q \in \mathcal{L}_r$. By Corollary 3 and (3.16), $\mathcal{L}_r \subseteq \mathcal{S}_1$, which implies that

$$\nu(Q) = \min_{k=1, \dots, n} Q_{kk} = l_r(Q) = \frac{1}{(r+1)(r+2)} \min_{z \in (r+2)\Delta_n^r} (z^T Q z - z^T \text{diag}(Q)).$$

Therefore, $Q \in \mathcal{L}_r$ if and only if $Q \in \mathcal{L}_r^k$ for some $k \in \{1, \dots, n\}$. □

Our next result establishes some geometric properties of the sets $\mathcal{L}_r$.

Proposition 9. *For any $r = 0, 1, \dots$, the set $\mathcal{L}_r$ is given by the union of n polyhedral cones.*

Proof. Since Λ_n^r is a finite set, $\mathcal{L}_r^k$ is a polyhedral cone for each $r \in \mathbb{N}$ and $k = 1, \dots, n$. The assertion directly follows from (3.41). □

Recall that $\mathcal{L}_r^k$ is defined by $O(n^{r+2})$ inequalities for each $k = 1, \dots, n$. Therefore, it follows from Theorem 6 that, for any fixed $r \in \mathbb{N}$, one can check in polynomial time if $Q \in \mathcal{L}_r$. On the other hand, Theorem 5 does not yield an algorithmic procedure for checking if $Q \in \mathcal{L}$.

We next establish an interesting connection between the behavior of lower bounds and the stability number of a certain associated graph. By Proposition 3, $Q \in \mathcal{L}_0$ if and only if all the diagonal elements of the shifted matrix $Q^s \in \mathcal{N}^n$ given by (3.17) are equal to zero. Therefore, for each $Q \notin \mathcal{L}_0$, $\min_{k=1, \dots, n} Q_{kk}^s > 0$ and Q^s has at least one off-diagonal entry which is equal to zero.

Given $M \in \mathcal{N}^n$, we define the sparsity graph G_M associated with M as follows. There are n vertices labeled $1, \dots, n$ and vertex i and vertex j are connected by an edge if $M_{ij} > 0$, $1 \leq i < j \leq n$. The next result establishes a connection between

the stability number of the sparsity graph of the matrix Q^s and the behavior of lower bounds $l_r(Q)$.

Proposition 10. *Let $Q \in \mathcal{S}^n \setminus \mathcal{L}_0$ and let $G = G_{Q^s}$ denote the sparsity graph of Q^s with stability number $\alpha(G)$. Then, $l_r(Q) = \min_{1 \leq i \leq j \leq n} Q_{ij} < \nu(Q)$ for each $r = 0, 1, \dots, \alpha(G) - 2$ and $l_r(Q) > \min_{1 \leq i \leq j \leq n} Q_{ij}$ for each $r \geq \alpha(G) - 1$. Therefore,*

$$Q \notin \mathcal{L}_r, \quad \text{for each } r = 0, 1, \dots, \alpha(G) - 2. \quad (3.42)$$

Proof. Given $Q \in \mathcal{S}^n \setminus \mathcal{L}_0$, let $G = G_{Q^s}$ denote the sparsity graph of Q^s and let $A_G \in \mathcal{S}^n$ denote the adjacency matrix of G . By the discussion preceding the proposition, there exists some $1 \leq i < j \leq n$ such that $Q_{ij}^s = 0$. Therefore, $\alpha(G) \geq 2$ by definition of the sparsity graph.

We now define the following two matrices.

$$Q_* := \left(\min_{1 \leq i \leq j \leq n: Q_{ij}^s > 0} Q_{ij}^s \right) (I + A_G), \quad Q^* := \left(\max_{1 \leq i \leq j \leq n} Q_{ij}^s \right) (I + A_G).$$

Clearly, we have $Q_* \in \mathcal{N}^n$, $Q^* \in \mathcal{N}^n$, $Q^s - Q_* \in \mathcal{N}^n$, and $Q^* - Q^s \in \mathcal{N}^n$. By Lemma 2(iii),

$$l_r(Q_*) \leq l_r(Q^s) \leq l_r(Q^*), \quad \text{for each } r = 0, 1, \dots$$

Note that each of Q^* and Q_* is a positive multiple of $I + A_G$. By Lemma 2(iv), we have

$$\left(\min_{1 \leq i \leq j \leq n: Q_{ij}^s > 0} Q_{ij}^s \right) l_r(I + A_G) \leq l_r(Q^s) \leq \left(\max_{1 \leq i \leq j \leq n} Q_{ij}^s \right) l_r(I + A_G).$$

The assertion now follows directly from (3.17), Lemma 2(v), and (3.10). The relation (3.42) follows immediately. $\square$

Example 6. Consider an instance of (StQP) in which

$$Q = Q^s = \begin{bmatrix} 1 & 2 & 2 & \dots & 2 \\ 2 & n & 0 & \dots & 0 \\ 2 & 0 & n & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 2 & 0 & 0 & \dots & n \end{bmatrix}$$

is an $n \times n$ arrowhead matrix, where $n \geq 3$. It is easy to verify that $\nu(Q) = 1$ and $\Omega(Q) = \{e_1\}$. Therefore, $U = \{1\}$ and $V = \{2, \dots, n\}$. By (3.29) and Theorem 5, $Q \in \mathcal{L}$. We have $\alpha(G) = n - 1$, where $G = G_Q$ denotes the sparsity graph of Q . By Proposition 10, we have $l_r(Q) = \min_{1 \leq i \leq j \leq n} Q_{ij} = 0$ for each $r = 0, 1, \dots, n - 3$ and $l_r(Q) > 0$ for each $r \geq n - 2$. It follows that $Q \notin \mathcal{L}_r$ for each $r = 0, 1, \dots, n - 3$.

Relations Among Different Sets

In this section, we summarize the relations among all the important sets defined in the previous sections.

Proposition 11. The following relations are satisfied:

$$\mathcal{L}_0 \subseteq \mathcal{L}_1 \subseteq \dots \subseteq \mathcal{L} \subseteq \text{cl}(\mathcal{L}) = \mathcal{S}_1 \subseteq \mathcal{U}_0 \subseteq \mathcal{U}_1 \subseteq \dots \subseteq \mathcal{U} \subseteq \text{cl}(\mathcal{U}) = \mathcal{S}^n,$$

where $\mathcal{L}_r$, $\mathcal{L}$, $\mathcal{S}_1$, $\mathcal{U}_r$, and $\mathcal{U}$ are defined as in (3.15), (3.16), (3.20), (3.11), and (3.14), respectively.

Proof. By Corollary 3, Proposition 4, and Proposition 1, we obtain $\mathcal{L} \subseteq \mathcal{S}_1 \subseteq \mathcal{U}_0$ since $\{e_1, \dots, e_n\} \subseteq \Delta_n^0$. The last equality follows from Corollary 1. The remaining inclusions follow from the definitions (3.15), (3.16), (3.11), and (3.14). $\square$

It is worth noticing the significant difference between the sets $\mathcal{L}$ and $\mathcal{U}$. For any $n \geq 2$, $\text{cl}(\mathcal{L})$ is strictly contained in the set $\mathcal{U}_0$, which is the smallest set in the sequence of the sets $\mathcal{U}_r$. On the other hand, recall that $\text{cl}(\mathcal{U}) = \mathcal{S}^n$ by Corollary 1.

It follows that upper and lower bounds exhibit quite different behaviors in terms of finite convergence in the context of standard quadratic optimization. In particular, our results reveal that inner polyhedral approximations, which give rise to upper bounds, are considerably stronger than outer polyhedral approximations in terms of finite convergence in the context of standard quadratic optimization.

We close this section by briefly commenting on the instances of (StQP) for which the upper and lower bounds coincide at a finite level of the hierarchy. From a computational point of view, this class of instances is especially important since equality of upper and lower bounds yields a certificate of optimality. We therefore define the following sets:

$$\mathcal{E}_r := \{Q \in \mathcal{S}^n : l_r(Q) = u_r(Q)\} = \mathcal{L}_r \cap \mathcal{U}_r = \mathcal{L}_r, \quad r = 0, 1, \dots,$$

where the last equality follows from Proposition 11. Therefore, the algebraic description of such instances are precisely given by Theorem 6.

3.4 Concluding Remarks

In this chapter, we investigated the sequences of copositive optimization based upper and lower bounds on the optimal value of a standard quadratic optimization problem. We gave complete algebraic descriptions of the sets of instances for which the upper and/or the lower bound is exact at a finite level of the hierarchy. We identified the structural properties of the sets of instances for which the upper and/or the lower bound converges to the optimal value only in the limit. We discussed several geometric and topological properties of these sets.

An important consequence of our analysis is that the upper bounds seem to be more well-behaved in comparison with the lower bounds. Note that the extreme rays of inner polyhedral approximations $\mathcal{I}_r$, which give rise to upper bounds, are given by dd^T , where $d \in \Delta_n^r$ and the extreme rays of the cone $\mathcal{CP}^n$ of completely positive matrices are given by rank one matrices xx^T , where $x \in \mathbb{R}_+^n \setminus \{0\}$ (see, e.g., [4]). It

follows that the set of extreme rays of $\mathcal{I}_r$ is a subset of the set of extreme rays of $\mathcal{CP}^n$. On the other hand, the outer polyhedral approximations $\mathcal{O}_r$ are generated by the matrices $(r+2)dd^T - \text{Diag}(d)$, where $d \in \Lambda_n^r$. For $d = e_i \in \Lambda_n^r$, the corresponding matrix is a multiple of $e_i(e_i)^T$, $i = 1, \dots, n$, which is also an extreme ray of $\mathcal{CP}^n$. However, for each $d \in \Lambda_n^r \setminus \{e_i : i = 1, \dots, n\}$, it is easy to construct a $w \in \mathbb{R}^n \setminus \{0\}$ such that $w^T d = 0$ and $\langle (r+2)dd^T - \text{Diag}(d), ww^T \rangle < 0$, which implies that $(r+2)dd^T - \text{Diag}(d) \notin \mathcal{CP}^n$. Together with our analysis, this observation suggests that only a few faces of $\mathcal{O}_r$ in fact coincide with those of $\mathcal{CP}^n$ whereas most of the faces of $\mathcal{O}_r$ do not support the cone $\mathcal{CP}^n$. Our results, combined with the recent progress on the facial structure of the cone $\mathcal{CP}^n$ (see, e.g., [21, 25]), may serve as a basis for the construction of tighter polyhedral outer approximations.

Chapter 4

BOX CONSTRAINED QUADRATIC OPTIMIZATION

4.1 Introduction

In this chapter, we consider the box constrained quadratic optimization problem defined as follows:

$$\text{(BoxQP)} \quad \nu(Q, c) := \max \{ (1/2)x^T Q x + c^T x : 0 \leq x \leq e, x \in \mathbb{R}^n \}, \quad (4.1)$$

where $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$ are the parameters. Box constrained quadratic optimization problems include all optimization problems with a quadratic objective function and upper and lower bound constraints, i.e.,

$$\begin{aligned} \max \quad & \frac{1}{2}y^T Q y + c^T y \\ \text{s.t.} \quad & l \leq y \leq u, \\ & y \in \mathbb{R}^n, \end{aligned}$$

where $Q \in \mathcal{S}^n$ and c , l , and u are given vectors in $\mathbb{R}^n$. We can easily convert this problem to (BoxQP) problem using a simple change of variable. This is an important problem class since it is a fundamental NP-hard global optimization problem which has applications in a wide variety of areas including optimal control, numerical analysis, and operations research. Therefore, there has been a considerable amount of research activity towards understanding and solving these problems (see, e.g., [17, 18, 31, 46, 47, 68, 69]).

In this chapter, our study focuses on the copositive perspective for the box constrained quadratic optimization problems. The problem (4.1) can be equivalently

reformulated as the following instance of a conic optimization problem over the cone of completely positive matrices [16]:

$$\begin{aligned}
 \text{(P1)} \quad \nu(Q, c) := \max \quad & \frac{1}{2} \langle Q, X \rangle + c^T x \\
 \text{s.t.} \quad & x_i + s_i = 1, \quad i = 1, \dots, n, \\
 & X_{ii} + 2R_{ii} + S_{ii} = 1, \quad i = 1, \dots, n, \\
 & \begin{bmatrix} 1 & x^T & s^T \\ x & X & R \\ s & R^T & S \end{bmatrix} \in \mathcal{CP}^{2n+1}.
 \end{aligned}$$

The copositive reformulation of the box constrained quadratic optimization problem, (P1), is not unique. Due to Burer [16], we can eliminate the variables x and s from (P1) and obtain another copositive reformulation in a lower dimension:

$$\begin{aligned}
 \text{(P2)} \quad \nu(Q, c) := \max \quad & \frac{1}{2} \langle Q, X \rangle + \frac{1}{n} c^T (X + R)e \\
 \text{s.t.} \quad & e_i^T (X + R)e + e_i^T (R^T + S)e = n, \quad i = 1, \dots, n, \\
 & X_{ii} + 2R_{ii} + S_{ii} = 1, \quad i = 1, \dots, n, \\
 & \begin{bmatrix} X & R \\ R^T & S \end{bmatrix} \in \mathcal{CP}^{2n}.
 \end{aligned}$$

Burer established that these two copositive reformulations are equivalent in the sense that their optimal values coincide. For the sake of completeness, we present the equivalence of the copositive formulations in the context of (BoxQP) in the following proposition.

Proposition 12. *(P1) and (P2) are equivalent completely positive formulations for the box constrained quadratic optimization problem denoted by (BoxQP).*

Proof. To prove the claim, we will show that any feasible solution of each formulation can be converted into a feasible solution of the other formulation with the same objective function value. Therefore, we first show that an arbitrary feasible solution of (P1) can be transformed into a feasible solution of (P2) with the same objective

function value. Secondly, we will construct a feasible solution of (P1) for any arbitrary feasible solution of (P2) with the same objective function value. Therefore, we will conclude that the optimal values of (P1) and (P2) agree.

Let $\hat{Y}$ be a feasible solution for the problem (P1). Alternative definition of the cone of completely positive matrices is given by

$$\mathcal{CP}^n = \left\{ \sum_i x_i x_i^T : x_i \in \mathbb{R}_+^n \text{ for all } i \right\}.$$

Therefore, we use this definition and restrict $\hat{Y}$ to be a convex combination of rank one matrices such that $x^t, s^t \in \mathbb{N}^n$ for all $t = 1, \dots, k$:

$$\hat{Y} = \begin{bmatrix} 1 & \hat{x}^T & \hat{s}^T \\ \hat{x} & \hat{X} & \hat{R} \\ \hat{s} & \hat{R}^T & \hat{S} \end{bmatrix} = \sum_{t=1}^k \lambda_t \begin{bmatrix} 1 \\ x^t \\ s^t \end{bmatrix} [1 \ (x^t)^T \ (s^t)^T], \quad (4.2)$$

where $\sum_{t=1}^k \lambda_t = 1$, $\hat{x} = \sum_{t=1}^k \lambda_t(x^t)$, $\hat{s} = \sum_{t=1}^k \lambda_t(s^t)$, $\hat{X} = \sum_{t=1}^k \lambda_t(x^t)(x^t)^T$, $\hat{R} = \sum_{t=1}^k \lambda_t(x^t)(s^t)^T$, and $\hat{S} = \sum_{t=1}^k \lambda_t(s^t)(s^t)^T$. Let us also define the following submatrix of $\hat{Y}$:

$$\hat{Z} = \begin{bmatrix} \hat{X} & \hat{R} \\ \hat{R}^T & \hat{S} \end{bmatrix}.$$

First, we will show that $\hat{Z}$ is feasible for (P2). We can rearrange the first constraint set of (P2) and using (4.2), we can conclude for all $i = 1, \dots, n$ that

$$\begin{aligned} n &\stackrel{!}{=} \sum_{j=1}^n \hat{X}_{ij} + \sum_{j=1}^n \hat{S}_{ij} + \sum_{j=1}^n \hat{R}_{ij} + \sum_{j=1}^n \hat{R}_{ji}, \\ &= \sum_{j=1}^n \sum_{t=1}^k \lambda_t (x^t)_i (x^t)_j + \sum_{j=1}^n \sum_{t=1}^k \lambda_t (s^t)_i (s^t)_j + \sum_{j=1}^n \sum_{t=1}^k \lambda_t (x^t)_i (s^t)_j + \sum_{j=1}^n \sum_{t=1}^k \lambda_t (s^t)_i (x^t)_j, \end{aligned}$$

$$\begin{aligned}
&= \underbrace{\sum_{t=1}^k \lambda_t(x^t)_i}_{\hat{x}_i} \sum_{j=1}^n (x^t)_j + \underbrace{\sum_{t=1}^k \lambda_t(s^t)_i}_{\hat{s}_i} \sum_{j=1}^n (s^t)_j + \underbrace{\sum_{t=1}^k \lambda_t(x^t)_i}_{\hat{x}_i} \sum_{j=1}^n (s^t)_j + \underbrace{\sum_{t=1}^k \lambda_t(s^t)_i}_{\hat{s}_i} \sum_{j=1}^n (x^t)_j, \\
&= \hat{x}_i \left(\sum_{j=1}^n (x^t)_j + \sum_{j=1}^n (s^t)_j \right) + \hat{s}_i \left(\sum_{j=1}^n (s^t)_j + \sum_{j=1}^n (x^t)_j \right), \\
&= n\hat{x}_i + n\hat{s}_i, \\
&= n(\hat{x}_i + \hat{s}_i) = n.
\end{aligned}$$

Hence, the first constraint set of (P2) is satisfied. Again by using the definition of $\hat{X}$, $\hat{R}$, and $\hat{S}$, it is clear that $\hat{Z}$ is also a completely positive matrix:

$$\begin{bmatrix} \hat{X} & \hat{R} \\ \hat{R}^T & \hat{S} \end{bmatrix} = \sum_{t=1}^k \lambda_t \begin{bmatrix} (x^t)(x^t)^T & (x^t)(s^t)^T \\ (s^t)(x^t)^T & (s^t)(s^t)^T \end{bmatrix} = \sum_{t=1}^k \lambda_t \begin{bmatrix} (x^t) \\ (s^t) \end{bmatrix} [(x^t)^T \ (s^t)^T],$$

where $x^t, s^t \in \mathbb{N}^n$ for all $t = 1, \dots, k$.

We will next show that the objective function values of $\hat{Y}$ in (P1) and $\hat{Z}$ in (P2) are the same. The objective function value of (P1) for the feasible solution $\hat{Y}$ is given by

$$\frac{1}{2} \langle Q, \hat{X} \rangle + c^T \hat{x}. \tag{4.3}$$

Let us rearrange the second part of the objective function of (P2), that is $(\frac{1}{n}) c^T (\hat{X} + \hat{R})e$:

$$\begin{aligned}
\left(\frac{1}{n}\right) c^T (\hat{X} + \hat{R})e &= \left(\frac{1}{n}\right) \sum_{i=1}^n c_i \sum_{j=1}^n (\hat{X}_{ij} + \hat{R}_{ij}), \\
&= \left(\frac{1}{n}\right) \sum_{i=1}^n c_i \sum_{j=1}^n \left[\sum_{t=1}^k \lambda_t(x^t)_i (x^t)_j + \sum_{t=1}^k \lambda_t(x^t)_i (s^t)_j \right],
\end{aligned}$$

$$\begin{aligned}
&= \left(\frac{1}{n} \right) \sum_{i=1}^n c_i \left[\underbrace{\sum_{t=1}^k \lambda_t(x^t)_i}_{\hat{x}_i} \left(\sum_{j=1}^n (x^t)_j \right) + \underbrace{\sum_{t=1}^k \lambda_t(x^t)_i}_{\hat{x}_i} \left(\sum_{j=1}^n (s^t)_j \right) \right], \\
&= \left(\frac{1}{n} \right) \sum_{i=1}^n c_i [\hat{x}_i n] = \sum_{i=1}^n c_i \hat{x}_i = c^T \hat{x}.
\end{aligned}$$

Therefore, the objective function value of (P2) for the feasible solution $\hat{Z}$ is given by

$$\frac{1}{2} \langle Q, \hat{X} \rangle + c^T \hat{x},$$

which is equal to (4.3). Hence, we showed that the lower submatrix of any feasible solution of (P1) is a feasible solution of (P2) with the same objective function value.

Conversely, now assume that $\hat{Z}$ is feasible for (P2). Next, we will show that there exist $\hat{x}, \hat{s} \in \mathbb{R}^n$ such that $\hat{Y}$ is feasible for (P1). Let us define

$$\hat{x} = \left(\frac{1}{n} \right) (\hat{X} + \hat{R})e.$$

Then, the objective functions become the same, $\frac{1}{2} \langle Q, X \rangle + c^T x$. Now, let $s = \left(\frac{1}{n} \right) (S + R^T)e$, then,

$$n = e_i^T (\hat{X} + \hat{R})e + e_i^T (\hat{R}^T + \hat{S})e, \quad i = 1, \dots, n,$$

$$n = n\hat{x}_i + n\hat{s}_i, \quad i = 1, \dots, n,$$

$$1 = \hat{x}_i + \hat{s}_i, \quad i = 1, \dots, n.$$

Finally, we need to show that $\hat{Y}$ is a completely positive matrix. We know that $\hat{Z}$ is completely positive. Therefore, $\hat{Z}$ can be decomposed as

$$\begin{bmatrix} \hat{X} & \hat{R} \\ \hat{R}^T & \hat{S} \end{bmatrix} = \sum_{i=1}^k \begin{bmatrix} a_i \\ b_i \end{bmatrix} [(a_i)^T \ (b_i)^T],$$

where $a_i, b_i \in \mathbb{N}^n$ for all $i = 1, \dots, k$. We will show that the following relation is

satisfied for some nonnegative real number $\alpha_1, \dots, \alpha_k$:

$$\begin{bmatrix} 1 & \hat{x}^T & \hat{s}^T \\ \hat{x} & \hat{X} & \hat{R} \\ \hat{s} & \hat{R}^T & \hat{S} \end{bmatrix} = \sum_{i=1}^k \begin{bmatrix} \alpha_i \\ a_i \\ b_i \end{bmatrix} [\alpha_i \ (a_i)^T \ (b_i)^T]. \quad (4.4)$$

Note that, the parameters α_i , $i = 1, \dots, k$ should satisfy:

$$\sum_{i=1}^k (\alpha_i)^2 = 1, \quad \sum_{i=1}^k (\alpha_i) a_i = \hat{x}, \quad \sum_{i=1}^k (\alpha_i) b_i = \hat{s}.$$

Recall that

$$\hat{x} = \left(\frac{1}{n} \right) (\hat{X} + \hat{R})e$$

and

$$\hat{s} = \left(\frac{1}{n} \right) (\hat{S} + \hat{R}^T)e.$$

Therefore, by setting $\alpha_i = \left(\frac{1}{n} \right) ((a_i)^T + (b_i)^T)e$, $i = 1, \dots, k$, we see that the equation in (4.4) is satisfied. Note that $\alpha_i \geq 0$, $i = 1, \dots, k$. Finally, we will show that $\sum_{i=1}^k (\alpha_i)^2 = 1$ is satisfied. Using the properties of the trace inner product, we derive the assertion as follows:

$$\begin{aligned} \sum_{i=1}^k (\alpha_i)^2 &= \sum_{i=1}^k [(a_i)^T + (b_i)^T] e e^T (a_i + b_i), \\ &= \sum_{i=1}^k \langle e e^T, (a_i + b_i)(a_i + b_i)^T \rangle, \\ &= \sum_{i=1}^k \langle e e^T, (a_i)(a_i)^T + (a_i)(b_i)^T + (b_i)(a_i)^T + (b_i)(b_i)^T \rangle, \end{aligned}$$

$$\begin{aligned}
&= \left\langle ee^T, \sum_{i=1}^k (a_i)(a_i)^T + \sum_{i=1}^k (a_i)(b_i)^T + \sum_{i=1}^k (b_i)(a_i)^T + \sum_{i=1}^k (b_i)(b_i)^T \right\rangle, \\
&= \left(\frac{1}{n^2} \right) \left\langle ee^T, \hat{X} + \hat{R} + \hat{R}^T + \hat{S} \right\rangle, \\
&= \left(\frac{1}{n^2} \right) \left\langle e \left[\sum_{i=1}^n (e_i)^T \right], \hat{X} + \hat{R} + \hat{R}^T + \hat{S} \right\rangle, \\
&= \left(\frac{1}{n^2} \right) \sum_{i=1}^n (e_i)^T (\hat{X} + \hat{R} + \hat{R}^T + \hat{S}) e, \\
&= \left(\frac{1}{n^2} \right) \left[\sum_{i=1}^n \underbrace{(e_i)^T (\hat{X} + \hat{R}) e}_{n\hat{x}_i} + \sum_{i=1}^n \underbrace{(e_i)^T (\hat{R}^T + \hat{S}) e}_{n\hat{s}_i} \right] = \left(\frac{1}{n^2} \right) n^2 = 1.
\end{aligned}$$

It follows that (P1) and (P2) are equivalent completely positive formulations for the box constrained quadratic optimization problem given by (BoxQP). $\square$

Our focus in this chapter is the analysis of inner and outer polyhedral approximations of the completely positive formulations of a box constrained quadratic optimization problem. This chapter consists of five sections. In Section 4.2, we provide the characterization of the feasibility of the inner polyhedral approximations proposed by Yıldırım [74] for completely positive formulations of (BoxQP). Then, Section 4.3 presents the necessary and sufficient conditions for obtaining a finite optimal value of the outer polyhedral approximations for (P1) and (P2) introduced by de Klerk and Pasechnik [20]. We analyze the error bounds of the inner and outer polyhedral approximations in Section 4.4. Section 4.5 summarizes our results on (BoxQP).

4.1.1 Notation

We use the following notation: Subscripts are used to refer to the elements of a vector. We start the indexing from zero for vectors in $\mathbb{R}^{n+1}$, i.e., if $v \in \mathbb{R}^{n+1}$, then $v^T = [v_0 \ v_1 \ \dots \ v_n]$ with the following exception. The i th unit vector in $\mathbb{R}^n$ is denoted by e_i , $i = 1, \dots, n$. Letter subscripts are used to denote the subvectors of a vector. We use $u_r^{(k)}(\cdot)$ to denote the upper bound arising from the r th level of outer approximation hierarchy for the k th copositive reformulation, $k = 1, 2$. If the outer

approximation is unbounded, we define the upper bound as $+\infty$. Similarly, $l_r^{(k)}(\cdot)$ is used for the lower bound arising from the r th level of the inner approximation hierarchy for the k th copositive reformulation, $k = 1, 2$. If the inner approximation is infeasible, we define the lower bound as $-\infty$.

4.2 Inner Polyhedral Approximations

In this section, we focus on the inner approximations of both copositive reformulations (P1) and (P2). In our analysis, we employ the particular inner polyhedral approximation introduced in Section 2.2.1. We first present the feasibility conditions of the inner polyhedral approximations for (P1) and (P2). Next, we give the exact characterization of the lower bounds for both formulations. Then, we identify the instances whose lower bounds match the optimal value at a finite level of the hierarchy. Finally, we show that the lower bounds provided using (P2) outperforms their counterparts obtained from (P1).

The next two propositions provide the necessary and sufficient conditions of the feasibility of the inner approximations of (P1) and (P2), respectively.

Proposition 13. *For a given instance of (BoxQP), $l_r^{(1)}(Q, c)$ is finite if and only if $r \geq n - 1$.*

Proof. Let us fix $r \in \mathbb{N}$. We need to show that the inner polyhedral approximation has a nonempty feasible region if and only if $r \geq n - 1$. Let us assume $\hat{Y} = \sum_{d \in \Delta_{2n+1}^r} \lambda_d d d^T$ is an arbitrary feasible solution, where Δ_{2n+1}^r is defined in (2.5). Assume $d^T = [d_0 \ d_U^T \ d_L^T]$, where $d_0 \in \mathbb{R}$, $d_U \in \mathbb{R}^n$, and $d_L \in \mathbb{R}^n$. We partition Δ_{2n+1}^r into two subsets as:

$$\Delta_{2n+1}^r = \Psi_0 \cup \Psi_1,$$

where $\Psi_0 = \{d \in \Delta_{2n+1}^r : d_0 > 0\}$ and $\Psi_1 = \{d \in \Delta_{2n+1}^r : d_0 = 0\}$. Now we consider

the feasible solution of inner approximation of (P1) using these new sets:

$$\begin{aligned} \hat{Y} = \begin{bmatrix} 1 & x^T & s^T \\ x & X & R \\ s & R^T & S \end{bmatrix} &= \sum_{d \in \Psi_0} \lambda_d \begin{bmatrix} 1 \\ \left(\frac{1}{d_0}\right) d_U \\ \left(\frac{1}{d_0}\right) d_L \end{bmatrix} \begin{bmatrix} 1 & \left(\frac{1}{d_0}\right) d_U^T & \left(\frac{1}{d_0}\right) d_L^T \end{bmatrix} \\ &+ \sum_{d \in \Psi_1} \mu_d \begin{bmatrix} 0 \\ d_U \\ d_L \end{bmatrix} [0 \ d_U^T \ d_L^T]. \end{aligned} \quad (4.5)$$

By definition of the inner approximation, we have $d_0 + e^T d_U + e^T d_L = 1$. By (4.5), we obtain

$$\sum_{d \in \Psi_0} \lambda_d = 1, \quad (4.6)$$

and

$$x = \sum_{d \in \Psi_0} \lambda_d \left(\frac{1}{d_0}\right) d_U, \quad s = \sum_{d \in \Psi_0} \lambda_d \left(\frac{1}{d_0}\right) d_L.$$

We next consider the constraints of the problem. First, we have $x_i + s_i = 1, i = 1, \dots, n$, which implies that

$$\sum_{d \in \Psi_0} \lambda_d \left[\left(\frac{1}{d_0}\right) (d_U)_i + \left(\frac{1}{d_0}\right) (d_L)_i \right] = 1, \quad i = 1, \dots, n.$$

If we let $\left(\frac{1}{d_0}\right) (d_U)_i + \left(\frac{1}{d_0}\right) (d_L)_i = 1 + (w_d)_i, \quad \forall d \in \Psi_0, \quad i = 1, \dots, n$, then

$$\sum_{d \in \Psi_0} \lambda_d (1 + (w_d)_i) = \sum_{d \in \Psi_0} \lambda_d + \sum_{d \in \Psi_0} \lambda_d (w_d)_i = 1, \quad i = 1, \dots, n,$$

which, by (4.6), yields

$$\sum_{d \in \Psi_0} \lambda_d ((w_d)_i) = 0, \quad i = 1, \dots, n. \quad (4.7)$$

Now, let us focus on the second set of constraints in (P2), i.e., $X_{ii} + 2R_{ii} + S_{ii} = 1$, $i = 1, \dots, n$, which can be rewritten as

$$\sum_{d \in \Psi_0} \lambda_d \left(\frac{1}{d_0} \right)^2 ((d_U)_i + (d_L)_i)^2 + \sum_{d \in \Psi_1} \mu_d ((d_U)_i + (d_L)_i)^2 = 1, \quad i = 1, \dots, n.$$

After some modifications, we have the following equality:

$$\underbrace{\sum_{d \in \Psi_0} \lambda_d}_1 + 2 \underbrace{\sum_{d \in \Psi_0} \lambda_d (w_d)_i}_0 + \underbrace{\sum_{d \in \Psi_0} \lambda_d ((w_d)_i)^2}_{\geq 0} + \underbrace{\sum_{d \in \Psi_1} \mu_d ((d_U)_i + (d_L)_i)^2}_{\geq 0} = 1, \quad i = 1, \dots, n. \quad (4.8)$$

Using (4.6) and (4.7), $\lambda_d \geq 0$ for all $d \in \Psi_0$, $\mu_d \geq 0$ for all $d \in \Psi_1$ and $d_U \geq 0, d_L \geq 0$ for all $d \in \Delta_{2n+1}^r$; we can satisfy the equality in (4.8) if and only if $\sum_{d \in \Psi_0} \lambda_d ((w_d)_i)^2 = 0$ and $\sum_{d \in \Psi_1} \mu_d ((d_U)_i + (d_L)_i)^2 = 0$. Since $\lambda_d \geq 0$, $\sum_{d \in \Psi_0} \lambda_d (w_d)_i^2 = 0$ implies that

$$w_d = 0, \quad \forall d \in \Psi_0. \quad (4.9)$$

As a result, using the previous assumption and (4.9),

$$(d_U)_i + (d_L)_i = d_0, \quad \forall d \in \Psi_0, \quad i = 1, \dots, n. \quad (4.10)$$

If we sum the equation in (4.10) over all i 's, we obtain

$$\sum_{i=1}^n ((d_U)_i + (d_L)_i) = n d_0,$$

$$1 - d_0 = n d_0.$$

Finally we have

$$d_0 = \frac{1}{n+1}, \quad d \in \Delta_{2n+1}^r,$$

and together with (4.10)

$$(d_U)_i + (d_L)_i = \frac{1}{n+1}, \quad i = 1, \dots, n, \quad d \in \Delta_{2n+1}^r.$$

For each $d \in \Delta_{2n+1}^r$, $(r+2)d \in \mathbb{N}^{2n+1}$ is satisfied if $r+2$ is integer when multiplied by $(n+1)$ or its positive multiplication. Therefore, the lowest level of the hierarchy that satisfies this condition is given by $r+2 = n+1$, equivalently $r = n-1$. This proves the assertion. $\square$

Similarly, we present the feasibility condition of the inner polyhedral approximation for (P2).

Proposition 14. *For a given instance of (BoxQP), $l_r^{(2)}(Q, c)$ is finite if and only if $r \geq n-2$.*

Proof. The proof is very similar to that of Proposition 13 and is therefore omitted. $\square$

The important results of this section are given in the subsequent theorems. Both of the theorems present exact characterizations of the lower bounds arising from each copositive reformulation, (P1) and (P2), respectively.

Theorem 7. *For a given $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$,*

$$l_r^{(1)}(Q, c) = \max_{x \in \{\bigcup_{l=1}^k V_l\}} \left\{ \frac{1}{2} x^T Q x + c^T x \right\}, \quad k(n+1) - 2 \leq r \leq (k+1)(n+1) - 3,$$

for all $k, l \geq 1$ and $k, l \in \mathbb{N}$, where $V_l = \{0 \leq x \leq e : l \cdot x \in \mathbb{N}^n\}$.

Proof. As it has been shown in the proof of Proposition 13, inner polyhedral approximation optimization problem is feasible if and only if all the entries of $d \in \Delta_{2n+1}^r$ is integer when multiplied by $(n+1)$ or its positive multiplication. Since for each $d \in \Delta_{2n+1}^r$ satisfies $(r+2)d \in \mathbb{N}^{2n+1}$ when only $r+2 = k(n+1)$ for $k \geq 1$ and $k \in \mathbb{N}$, new solutions would be added only in this case. Furthermore, since the objective function is linear, the optimal value is given by one of these solutions. Therefore, the claim is true. $\square$

Theorem 8. For a given $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$,

$$l_r^{(2)}(Q, c) = \max_{x \in \{\bigcup_{i=1}^k V_i\}} \left\{ \frac{1}{2} x^T Q x + c^T x \right\}, \quad kn - 2 \leq r \leq (k+1)n - 3,$$

for all $k, l \geq 1$ and $k, l \in \mathbb{N}$.

Proof. The proof is similar to the proof of Theorem 7 and is therefore omitted. $\square$

Theorems 7 and 8 present the major results of this chapter, since they reveal that the lower bounds can be computed by maximizing the objective function over a *finite* set. Particularly, for both formulations (P1) and (P2), this inner approximation hierarchy is reduced to a finite discretization algorithm. In fact, a recent paper [75] shows that the inner approximations of the completely positive cone generated by nonnegative rank one matrices turns into an optimization problem over a subset of feasible points from the original feasible region in the context of (QPB), which generalizes the results given in Theorems 7 and 8.

Now, we turn our attention to the characterization of the instances whose lower bounds are *exact* at a finite level of the hierarchy. The following lemma presents an exact characterization of the instances for which lower bounds provided by the inner approximations of (P1) and (P2) are equal to the optimal value $\nu(Q, c)$:

Lemma 4. The lower bounds of both reformulations, (P1) and (P2), are exact at some finite level $r^* \in \mathbb{N}$ if and only if $\Omega(Q, c) \cap \mathbb{Q}^n \neq \emptyset$.

Proof. Under the assumption $\Omega(Q, c) \cap \mathbb{Q}^n \neq \emptyset$, there exists an optimal solution satisfying $x^* \in \mathbb{Q}^n$. Therefore, there is also $l \in \mathbb{N}$ satisfying $l \cdot x^* \in \mathbb{N}^n$. In this case, since $x^* \in V_l$, by using Theorems 7 and 8, we can conclude that both lower bounds match the optimal value for some finite $r^* \in \mathbb{N}$.

Conversely, assume that the lower bounds of both reformulations, (P1) and (P2), are exact at some finite level $r^* \in \mathbb{N}$. Then, we claim that there exists $x^* \in \Omega(Q, c)$ such that it satisfies $x^* \in \mathbb{Q}^n$ and $l \cdot x^* \in \mathbb{N}^n$ for $l \in \mathbb{N}$. Assume to the contrary, $\Omega(Q, c) \cap \mathbb{Q}^n = \emptyset$, i.e., for all $x^* \in \Omega(Q, c)$, we have $x^* \in \mathbb{R}^n \setminus \mathbb{Q}^n$. However, in this

case we cannot satisfy $l \cdot x^* \in \mathbb{N}^n$ for any $l \in \mathbb{N}$. Therefore, the lower bounds of (P1) and (P2) do not match the optimal value at any finite level $r^* \in \mathbb{N}$, which contradicts our assumption. Hence, the result follows. $\square$

By Lemma 4, we obtain an exact characterization of the instances whose lower bounds are exact at a finite level of the hierarchy. The next corollary provides an easily verifiable sufficient condition for such an instance.

Corollary 4. *If $Q \in \mathcal{Q}^n$ and $c \in \mathbb{Q}^n$, then the lower bounds of both reformulations, (P1) and (P2), are exact at some finite level $r^* \in \mathbb{N}$.*

Proof. Vavasis [71] proved that if the problem has rational data, which is bounded below, then it has a rational optimal solution. Therefore, this statement follows from Vavasis' result and Lemma 4. $\square$

Next, we focus on instances of (BoxQP) in which Q is a positive semidefinite matrix. For these instances, we can guarantee that the lower bound is *exact* at a finite level of hierarchy depending on the size of the original (BoxQP) problem.

Corollary 5. *If $Q \in \mathcal{S}^n$ is a positive semidefinite matrix, then the lower bound of (P1) is exact for $r \geq n - 1$.*

Proof. Since the objective function is convex, the maximum is attained at a vertex of the feasible region, i.e., $x^* \in \mathbb{N}^n$. Therefore, $x^* \in V_1$. Hence by Theorem 7, the lower bound of (P1) matches the optimal value $\nu(Q, c)$ when $r = n - 1$, which completes the proof. $\square$

Corollary 6. *If $Q \in \mathcal{S}^n$ is a positive semidefinite matrix, then the lower bound of (P2) is exact for $r \geq n - 2$.*

Proof. The proof is similar to the proof of Corollary 5 and is therefore omitted. $\square$

The following table summarizes the feasibility conditions of inner polyhedral approximations of two formulations.

The next proposition directly follows from Theorems 7 and 8.

	Infeasible	Feasible
(P1)	$r \leq n - 2$	$r \geq n - 1$
(P2)	$r \leq n - 3$	$r \geq n - 2$

Table 4.1: Threshold r Values for the Feasibility of Inner Approximations

Proposition 15. *For any given $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$,*

$$l_r^{(2)}(Q, c) \geq l_r^{(1)}(Q, c), \quad \text{for all } r \geq 0,$$

i.e., lower bounds arising from the inner approximation of (P2) are at least as tight as those arising from (P1).

Proof. For $r \leq n - 3$, we have $l_r^{(2)}(Q, c) = l_r^{(1)}(Q, c) = -\infty$ by Propositions 13 and 14 (with the convention that the optimal value of an infeasible maximization problem is $-\infty$). For $r = n - 2$, as a result of mentioned propositions, $l_r^{(2)}(Q, c) > -\infty$ and $l_r^{(1)}(Q, c) = -\infty$. Therefore, for $r \leq n - 2$, the claim holds. Now, we focus on $r \geq n - 1$. Using the result of Theorems 7 and 8, the assertion also follows. $\square$

This is a critical result since it reveals that the inner approximations of (P2) always give tighter bounds than those of (P1) on the optimal value of the (BoxQP) problem.

4.3 Outer Polyhedral Approximations

We analyze the upper bounds based on the approximation hierarchy proposed by de Klerk and Pasechnik [20] for both of the reformulations (P1) and (P2). Note that any instance of (BoxQP) has a finite optimal value since the feasible region is compact and the objective function is continuous. However, the feasible region of any outer approximation of (P1) and (P2) is at least as large as that of (P1) and (P2). Therefore, the corresponding upper bounds may not necessarily be finite.

In this section, we first focus on necessary and sufficient conditions that should

be satisfied by an instance of (BoxQP) so that the upper bound arising from the first formulation (P1) would be finite. Then, we establish that the upper bound arising from (P2) is finite at any level of the hierarchy. Finally, for a given level of the hierarchy, we compare the upper bounds arising from both formulations (P1) and (P2).

The next proposition presents necessary and sufficient conditions for a finite $u_0^{(1)}(Q, c)$ with its closed-form solution.

Proposition 16. *Given an instance of (BoxQP) with $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$, $u_0^{(1)}(Q, c)$ is finite if and only if $Q_{ij} \leq 0$ for all $1 \leq i < j \leq n$. Furthermore, in this case, the upper bound is given by*

$$u_0^{(1)}(Q, c) = \sum_{i: c_i > 0} c_i + \frac{1}{2} \sum_{j: Q_{jj} > 0} Q_{jj}.$$

Proof. Since $\mathcal{O}_0 = \mathcal{N}^{2n+1}$, the constraints of outer approximation optimization problem are given by the following:

$$\begin{aligned} \begin{bmatrix} 1 & x^T & s^T \\ x & X & R \\ s & R^T & S \end{bmatrix} &\in \mathcal{N}^{2n+1}, \\ x_i + s_i &= 1, \quad i = 1, \dots, n, \\ X_{ii} + 2R_{ii} + S_{ii} &= 1, \quad i = 1, \dots, n. \end{aligned}$$

If there exists some (i, j) pair such that $1 \leq i < j \leq n$ and $Q_{ij} > 0$, then we let $X_{ij} = \alpha$ and as $\alpha \rightarrow +\infty$, we get $\frac{1}{2}Q_{ij}X_{ij} \rightarrow +\infty$. Otherwise, we set $x_i = 1$ for all i such that $c_i > 0$ and set $X_{jj} = 1$ for all j such that $Q_{jj} > 0$. The result follows. $\square$

The next result generalizes the previous proposition. To simplify the notation, we define a function $M(\cdot)$ from $\mathbb{R}_+^n$ to $\mathcal{N}^n$:

$$M(z) := zz^T - \text{Diag}(z), \quad z \in \Theta_n^r. \quad (4.11)$$

Proposition 17. *Given an instance of (BoxQP) with $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$, suppose that there exists $1 \leq i < j \leq n$ such that $Q_{ij} > 0$. Then, for each $r \leq n - 2$, the outer approximation of (P1) is unbounded.*

Proof. Let us fix $r = n - 2$. Then, we choose any arbitrary feasible solution, $\hat{Y} \in \mathcal{S}^{2n+1}$, of the outer approximation of (P1). Next, we consider the following direction for $r = n - 2$:

$$\xi = M \begin{pmatrix} 0 \\ e_i + e_j \\ e - e_i - e_j \end{pmatrix},$$

where $M(\cdot)$ is defined in (4.11). We claim that $\hat{Y} + \lambda \xi$ is feasible for any $\lambda \geq 0$ and ξ is an ascent direction since it increases the objective function value, $\langle Q, \xi \rangle = 2Q_{ij} > 0$; it is feasible, $\xi \in \mathcal{O}^r$; and it satisfies the constraints, $\xi_{0,k} + \xi_{0,n+k} = 0$ and $\xi_{k,k} + 2\xi_{k,n+k} + \xi_{n+k,n+k} = 0, k = 1, \dots, n$. Therefore, we show that there exists an ascent direction for $r = n - 2$. Also by the monotonicity of the bounds, it follows that we can also find ascent directions for $r \leq n - 3$. Hence, the claim is proved. $\square$

Therefore, for $r \leq n - 2$, the upper bound arising from the formulation (P1) is finite if and only if the matrix Q has nonpositive off-diagonal entries. Note that this condition is satisfied by diagonal matrices. We provide a closed-form solution of the upper bound for the latter case in the following lemma.

Lemma 5. *Given an instance of (BoxQP) with $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$, suppose $Q_{ij} = 0$ for all $1 \leq i < j \leq n$ and $c \in \mathbb{R}^n$. Then,*

$$u_0^{(1)}(Q, c) = u_1^{(1)}(Q, c) = \dots = u_n^{(1)}(Q, c) = \sum_{i: c_i > 0} c_i + \frac{1}{2} \sum_{j: Q_{jj} > 0} Q_{jj}.$$

Proof. For $r = 0$, we know that the claim is true by Proposition 16. Suppose, without loss of generality, that the vector c satisfies the following relation:

$$c_1 \geq c_2 \geq \dots \geq 0 > c_{k+1} \geq \dots \geq c_n.$$

Let us fix $r = n$ (or $r + 2 = n + 2$). Now, we construct the following solution:

$$\begin{aligned} \hat{Y} = & \frac{1}{(r+1)(r+2)} \left(\sum_{i: Q_{ii} > 0} M \left((r+2) \begin{bmatrix} 0 \\ e_i \\ 0 \end{bmatrix} \right) \right) \\ & + \frac{1}{(r+1)(r+2)} \left(\sum_{i: Q_{ii} \leq 0} M \left((r+2) \begin{bmatrix} 0 \\ 0 \\ e_i \end{bmatrix} \right) \right) + \frac{1}{2} M \left(\begin{bmatrix} 2 \\ 1_k \\ 0_{n-k} \\ 0_k \\ 1_{n-k} \end{bmatrix} \right), \end{aligned}$$

where $M(\cdot)$ is defined in (4.11). $\hat{Y}$ is a feasible solution for outer approximation of (P1), since

- $\hat{Y}_{00} = 1$,
- $\hat{Y}_{0i} + \hat{Y}_{0,n+i} = 1, \quad i = 1, \dots, n$,
- $\hat{Y}_{ii} + 2\hat{Y}_{i,n+i} + \hat{Y}_{n+i,n+i} = 1, \quad i = 1, \dots, n$.

Consequently, it is clear that $\hat{Y}_{ii} = 1$ if $Q_{ii} > 0$ and $\hat{Y}_{n+i,n+i} = 1$ if $Q_{ii} \leq 0$. Note that, $\hat{Y}$ provides the same objective function value as $u_0^{(1)}(Q, c)$. Therefore, by the monotonicity of the bounds, it is an optimal solution. Note that, again by the monotonicity of the bounds, the upper bounds for $1 \leq r \leq n-1$ are also the same. Hence, the claim is proved. $\square$

Our next result gives a characterization of the levels of the hierarchy for which the outer approximation of (P1) has a finite optimal value for any given instance of (BoxQP).

Proposition 18. *For all $r \geq n-1$, the outer approximation of (P1) has a finite optimal value for any given instance of (BoxQP).*

Proof. We claim that the feasible region of the outer approximation of (P1) is bounded for all $r \geq n - 1$. We will show that it is not possible to find an ascent direction for $r \geq n - 1$. Assume that ξ is a feasible ascent direction. Therefore it should satisfy $\xi_{00} = \xi_{0,i} = \xi_{0,n+i} = \xi_{ii} = \xi_{i,n+i} = \xi_{n+i,i} = \xi_{n+i,n+i} = 0$ for $i = 1, \dots, n$, where

$$\xi = \sum_{z \in \Theta_{2n+1}^r} \lambda_z M \begin{pmatrix} 0 \\ z_U \\ z_L \end{pmatrix},$$

and $M(\cdot)$ is defined in (4.11). By the assumption, $e^T z_U + e^T z_L = r + 2 \geq n + 1$. If there exists some $i \in \{1, \dots, n\}$ such that $(z_U)_i \geq 2$, then it follows that $\xi_{ii} > 0$, which contradicts the feasibility of ξ to be an ascent direction. Similarly, for $(z_L)_i \geq 2$, ξ is also not a feasible ascent direction. Hence, $(z_U)_i \leq 1$ and $(z_L)_i \leq 1$ for all $i = 1, \dots, n$. Since $e^T z_U + e^T z_L = n + 1$ for $r = n - 1$, there should be an index $i^* \in \{1, \dots, n\}$ such that $(z_U)_{i^*} = (z_L)_{i^*} = 1$. We therefore obtain

$$\xi_{i^*,n+i^*} = \xi_{n+i^*,i^*} > 0,$$

which contradicts the feasibility of an ascent direction. It follows that there is no ascent direction. Hence, upper bounds arising from (P2) are always finite. $\square$

So far we provided the necessary and sufficient conditions for having a finite upper bound of (P1). The next result shows that the upper bounds provided by (P2) are always finite.

Proposition 19. *For any given instance of (BoxQP), we have $u_r^{(2)}(Q, c) < +\infty$ for all $r \in \mathbb{N}$.*

Proof. Since $\mathcal{O}_0 = \mathcal{N}^{2n}$, we need to satisfy the following constraints for the feasibility

of the outer approximation of (P2):

$$\begin{aligned} \begin{bmatrix} X & R \\ R^T & S \end{bmatrix} &\in \mathcal{N}^{2n}, \\ e_i^T(X + R)e + e_i^T(R^T + S)e &= n, \quad i = 1, \dots, n, \\ X_{ii} + 2R_{ii} + S_{ii} &= 1, \quad i = 1, \dots, n. \end{aligned}$$

We can sum the second constraint over all i 's:

$$\begin{aligned} e^T(X + R)e + e^T(R^T + S)e &= n^2, \\ [e^T \ e^T] \begin{bmatrix} X & R \\ R^T & S \end{bmatrix} \begin{bmatrix} e \\ e \end{bmatrix} &= n^2. \end{aligned}$$

Therefore, the sum of all elements of any feasible solution for $r = 0$ is equal to n^2 . Since each component of a feasible solution is also nonnegative, it follows that the feasible region of the outer approximation for $r = 0$ is bounded. As a result, the upper bound for $r = 0$ is finite. By the monotonicity of upper bounds, the result follows. $\square$

To summarize our results on the upper bounds arising from both reformulations (P1) and (P2), we present the following table.

	$0 \leq r \leq n - 2$	$r \geq n - 1$
(P1)	Finite if and only if $Q_{ij} \leq 0$ for all $1 \leq i < j \leq n$	Finite
(P2)	Finite	Finite

Table 4.2: Conditions for a Finite Upper Bound of (P1) and (P2)

We conclude the section with the discussion of the comparison of the upper bounds

provided by (P1) and (P2). In the following cases, we show that the outer approximation of (P2) is tighter than that of (P1).

Lemma 6. *For any given instance of (BoxQP), we have*

$$u_0^{(1)}(Q, c) \geq u_0^{(2)}(Q, c).$$

Proof. We will show this argument as follows: We can construct a feasible solution for the outer approximation of (P1) using a feasible solution of (P2) with the same objective function value. Therefore, it suffices to choose x and s for the outer approximation of (P1) as follows:

$$x = \frac{1}{n}(X + R)e, \quad s = \frac{1}{n}(R^T + S)e.$$

It is clear that the constraints are satisfied with the same objective function for $r = 0$. Therefore, $u_0^{(1)}(Q, c) \geq u_0^{(2)}(Q, c)$. $\square$

We can generalize this result for a subset of the levels of outer approximation hierarchy of completely positive formulations, (P1) and (P2).

Lemma 7. *Given an instance of (BoxQP) with $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$, we have*

$$u_{k(n+1)-1}^{(1)}(Q, c) \geq u_{kn-1}^{(2)}(Q, c), \text{ for all } k \geq 1 \text{ and } k \in \mathbb{N}.$$

Proof. We will use a constructive proof technique such that we will find a feasible solution for outer approximation of (P1) for a given feasible solution of (P2) with the same objective function value at different levels of the hierarchy. Since we compare two different levels of the hierarchies for each formulation, we need to differentiate the levels of the hierarchies for them. Therefore, we denote the level of the hierarchy of (P2) by r and that of (P1) by r' . Then, recall the definition of $M(\cdot)$ given in (4.11).

We take a feasible solution for the outer approximation of (P2):

$$\begin{bmatrix} X & R \\ R^T & S \end{bmatrix} = \sum_{z \in \Theta_{2n}^r} \beta_z M \left(\begin{bmatrix} z_U \\ z_L \end{bmatrix} \right). \quad (4.12)$$

Now, we construct a feasible solution for the outer approximation of (P1) using (4.12):

$$\begin{bmatrix} 1 & x^T & s^T \\ x & X & R \\ s & R^T & S \end{bmatrix} = \sum_{z \in \Theta_{2n+1}^{r'}} \beta_z M \left(\begin{bmatrix} z_0 \\ z_U \\ z_L \end{bmatrix} \right) + \alpha M \left(\begin{bmatrix} r' + 2 \\ 0 \\ 0 \end{bmatrix} \right), \quad (4.13)$$

where $\alpha \geq 0$. Our aim to use above equality to derive an expression for a feasible z_0 . Therefore, we first construct x as follows:

$$x = \frac{1}{n}(X + R)e = \left(\frac{r+1}{n} \right) \sum_{z \in \Theta_{2n}^r} \beta_z z_U. \quad (4.14)$$

By using the constraints, we can easily find that

$$\sum_{z \in \Theta_{2n}^r} \beta_z = \frac{n^2}{(r+1)(r+2)}.$$

Note that x appears in (4.13) and (4.14). Therefore by combining these equations, we obtain

$$\left(\frac{r+1}{n} \right) \sum_{z \in \Theta_{2n}^r} \beta_z z_U = \sum_{z \in \Theta_{2n}^r} \beta_z z_0 z_U,$$

which gives

$$z_0 = \frac{r+1}{n}.$$

Now, we focus on the first entry of the matrix of (P1) given in (4.13).

$$\sum_{z \in \Theta_{2n+1}^{r'}} \beta_z z_0 (z_0 - 1) + \alpha(r' + 2)(r' + 1) = 1.$$

Since we have $\sum_{z \in \Theta_{2n}^r} \beta_z = \sum_{z \in \Theta_{2n+1}^{r'}} \beta_z$ for each feasible solution, by using equivalences, we get

$$\begin{aligned} \frac{n^2}{(r+1)(r+2)} \left(\frac{r+1}{n} \right) \left(\frac{r+1}{n} - 1 \right) + \alpha(r' + 2)(r' + 1) &= 1, \\ \left(\frac{r+1-n}{r+2} \right) + \alpha(r' + 2)(r' + 1) &= 1. \end{aligned}$$

Since $\left(\frac{r+1-n}{r+2} \right) \leq 1$, the above equation can be satisfied. Let $r+1 = kn$, where $k \in \mathbb{N}$ and clearly, $z_0 = k$, then

$$[1 \ e^T \ e^T] \begin{bmatrix} z_0 \\ z_U \\ z_L \end{bmatrix} = k + r + 2.$$

Hence, $u_{k+r}^{(1)}(Q, c) \geq u_r^{(2)}(Q, c)$ for all $k \geq 1$ since we are able to find a feasible solution for outer approximation of (P1) for a given feasible solution of (P2) with the same objective function value. If we use $r+1 = kn$, then we have the desired result. $\square$

4.4 Error Bounds

In this section, we study the gap between the bounds provided by the inner and the outer approximations and the optimal value of (BoxQP). We try to bound this gap by an *error bound*. We start with the error bounds of (P1) and (P2) obtained via inner polyhedral approximations. Then, we focus on the error bounds obtained from outer polyhedral approximations for both reformulations.

4.4.1 Inner Approximations

We first consider some properties of the objective function. Then, we derive the error bound by using these results.

Lemma 8. *Let $f(x) = x^T Qx + 2c^T x$. Then,*

$$|f(y) - f(x)| \leq L\|y - x\|_\infty, \text{ for any } x, y \in \mathbb{R}^n,$$

where

$$L = \max_{0 \leq y \leq e} \|Qy + c\|_1. \quad (4.15)$$

Proof. Let $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$ be two feasible solutions for a given (BoxQP) problem. Then by the Mean Value Theorem, there exists $\gamma \in (0, 1)$ such that the following equality holds:

$$f(y) - f(x) = \nabla f(x + \gamma(y - x))^T (y - x) = (Q(x + \gamma(y - x)) + c)^T (y - x).$$

Therefore,

$$|f(y) - f(x)| \leq \|Q(x + \gamma(y - x)) + c\|_1 \|y - x\|_\infty.$$

The claim is proved since $\nabla f(x + \gamma(y - x))^T = Q(x + \gamma(y - x)) + c$ and $y \in [0, 1]^n$ is a convex set. $\square$

The next two lemmas constitute a basis for constructing the error bound for inner polyhedral approximations.

Lemma 9. *If $|f(y) - f(x)| \leq L\|y - x\|_\infty$ and we evaluate f on all the points such that $\left(\frac{i_1}{p}, \frac{i_2}{p}, \dots, \frac{i_n}{p}\right)$, where $i_j \in \{0, 1, \dots, p\}$ and return the best point $\bar{x}$, then*

$$f(x^*) - f(\bar{x}) \leq \frac{L}{2p},$$

where $f(x^*)$ is the maximum value of the function given by x^* and L is given in (4.15).

Proof. This assertion follows from the fact that the largest distance between the optimal solution and the closest sample point can be $\frac{1}{2p}$. $\square$

Our aim is to establish a connection between Lemma 9 and the inner approximation hierarchy. As a result, we can derive an error bound for the inner approximation. We first discuss the inner approximation of (P2). Recall, we define

$$V_l = \{0 \leq x \leq e : l \cdot x \in \mathbb{N}^n\}$$

in Theorem 7. Now, suppose that we want to have points of the form $\left(\frac{i_1}{p}, \frac{i_2}{p}, \dots, \frac{i_n}{p}\right)$, where $i_j \in \{0, 1, \dots, p\}$ in the feasible region of inner approximation of (P2). Then, a sufficient condition is

$$\begin{bmatrix} x \\ s \end{bmatrix} = n \begin{bmatrix} d_U \\ d_L \end{bmatrix}, \text{ for some } \begin{bmatrix} d_U \\ d_L \end{bmatrix} \in \Delta_{2n}^r,$$

for all choices of points, i.e., $x \in V_l$ and $s \in V_l$. Note that $e^T x + e^T s = n$ and $e^T d_U + e^T d_L = 1$. We know that

$$(r+2) \begin{bmatrix} d_U \\ d_L \end{bmatrix} \in \mathbb{N}^{2n},$$

which implies

$$\frac{(r+2)}{n} \begin{bmatrix} x \\ s \end{bmatrix} \in \mathbb{N}^{2n},$$

or $\frac{r+2}{np} [i_1 \dots i_n (p-i_1) \dots (p-i_n)]^T \in \mathbb{N}^{2n}$. This is true if $\frac{r+2}{np}$ is an integer, i.e., $r+2 = npt$ for some positive integer t . Smallest value of r is $np-2$. If $p=1$, then $r+2=n$; if $p=2$, then $r+2=2n$. In general, we need $r = np-2$.

We can present the main outcomes of this section with next theorems.

Theorem 9. Consider the inner approximation of (P2) for given $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$. Then,

$$\nu(Q, c) - l_r^{(2)}(Q, c) \leq \frac{L}{2 \lfloor \frac{r+2}{n} \rfloor}, \quad r \geq n-2,$$

where L is defined as in (4.15).

Proof. We showed that we need $r = np-2$ for integer valued points. If we set $p = \frac{r+2}{n}$, then, by using Lemma 9, we obtain the claim. $\square$

Similar argument can be applied to (P1).

Theorem 10. Consider the inner approximation of (P1) for given $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$. Then,

$$\nu(Q, c) - l_r^{(1)}(Q, c) \leq \frac{L}{2 \lfloor \frac{r+2}{n+1} \rfloor}, \quad r \geq n-1,$$

where L is defined as in (4.15).

Proof. The proof is similar to the proof of Theorem 9 and is therefore omitted. $\square$

It is worth noticing that these error bounds are valid after different threshold values for the level of the hierarchy for (P1) and (P2). These threshold values are consequences of Propositions 13 and 14. Another conclusion that can be drawn from Theorems 9 and 10 is that the error bound derived for the inner approximation of (P2) is always as tight as that of (P1) since $\lfloor \frac{r+2}{n} \rfloor \geq \lfloor \frac{r+2}{n+1} \rfloor$. Therefore, in practice, (P2) would be the reasonable choice for finding a lower bound for (BoxQP) compared to (P1). However, we remark that solving the inner approximation problems of (P2) is still not practical for large instances since $|\Delta_n^r| = O(n^{r+2})$.

4.4.2 Outer Approximations

In this section, we first consider an easy class of box constrained quadratic optimization problems with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$. Then, we use these results to derive error bounds for general matrices and vectors.

Nonnegative Case

In this section, we consider instances of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$. This class encompasses easy instances of (BoxQP) since an optimal solution is $e \in \Omega(Q, c)$. Therefore, the optimal value of the problem is given by

$$\nu(Q, c) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n Q_{ij} + \sum_{i=1}^n c_i. \quad (4.16)$$

Our analysis starts with the outer approximation of (P2). The next lemma simplifies our analysis, since it presents a useful property of an optimal solution of the outer approximation of (P2).

Lemma 10. *Given an instance of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$, assume the optimal solution of the outer approximation of (P2) is given by the following:*

$$\begin{bmatrix} X & R \\ R^T & S \end{bmatrix} = \sum_{z \in \Theta_{2n}^r} \beta_z M \left(\begin{bmatrix} z_U \\ z_L \end{bmatrix} \right), \quad (4.17)$$

where $M(\cdot)$ given in (4.11). Then, there exists an optimal solution such that $z_L = 0$ for all $z \in \Theta_{2n}^r$ such that $\beta_z > 0$.

Proof. We take any arbitrary optimal solution of the outer approximation of (P2) and convert it to an optimal solution satisfying the given condition. Now, suppose that (4.17) is an arbitrary optimal solution. Then we have,

$$X = \sum_{z \in \Theta_{2n}^r} \beta_z (z_U z_U^T - \text{Diag}(z_U)), \quad R = \sum_{z \in \Theta_{2n}^r} \beta_z z_U z_L^T.$$

We construct x as follows

$$x = \frac{1}{n} (X + R)e = \frac{(r+1)}{n} \sum_{z \in \Theta_{2n}^r} \beta_z z_U.$$

Now, we can compute the upper bound as follows:

$$\begin{aligned}
u_r^{(2)}(Q, c) &= \frac{1}{2} \langle Q, X \rangle + \frac{1}{n} c^T (X + R) e, \\
&= \frac{1}{2} \left\langle Q, \sum_{z \in \Theta_{2n}^r} \beta_z (z_U z_U^T - \text{Diag}(z_U)) \right\rangle + \frac{(r+1)}{n} \sum_{z \in \Theta_{2n}^r} \beta_z c^T z_U, \\
&= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j + \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n Q_{ii} ((z_U)_i ((z_U)_i - 1)) \\
&\quad + \frac{(r+1)}{n} \sum_{z \in \Theta_{2n}^r} \beta_z c^T z_U.
\end{aligned}$$

Also, we have the following constraints,

$$\sum_{z \in \Theta_{2n}^r} \beta_z ((z_U)_i + (z_L)_i) = \frac{n}{(r+1)}, \quad i = 1, 2, \dots, n, \quad (4.18)$$

and

$$\begin{aligned}
&\sum_{z \in \Theta_{2n}^r} \beta_z (((z_U)_i)^2 - (z_U)_i) + 2 \sum_{z \in \Theta_{2n}^r} \beta_z (z_U)_i (z_L)_i \\
&\quad + \sum_{z \in \Theta_{2n}^r} \beta_z ((z_L)_i)^2 - (z_L)_i = 1, \quad i = 1, 2, \dots, n.
\end{aligned} \quad (4.19)$$

We can construct a new solution as follows:

$$(\hat{z}_U)_i = (z_U)_i + (z_L)_i, \quad (\hat{z}_L)_i = 0, \quad i = 1, 2, \dots, n, \quad \forall z \in \Theta_{2n}^r.$$

It is clear that the new solution satisfies the constraints (4.18) and (4.19). In addition, the objective function value for the upper bound does not decrease since $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$. Hence the claim follows. $\square$

Therefore, it suffices to consider $z \in \Theta_{2n}^r$ such that $z_L = 0$ and $e^T z_U = r+2$ for the outer approximation of an instance of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$, satisfying the simplified constraints:

- $\sum_{z \in \Theta_{2n}^r} \beta_z (z_U)_i = \frac{n}{(r+1)}, \quad i = 1, 2, \dots, n,$
- $\sum_{z \in \Theta_{2n}^r} \beta_z (z_U)_i ((z_U)_i - 1) = 1, \quad i = 1, 2, \dots, n.$

Now, we can simplify the upper bound using the simplified constraints:

$$\begin{aligned}
 u_r^{(2)}(Q, c) &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j + \frac{1}{2} \sum_{i=1}^n Q_{ii} \underbrace{\sum_{z \in \Theta_{2n}^r} \beta_z ((z_U)_i ((z_U)_i - 1))}_{=1} \\
 &\quad + \underbrace{\frac{(r+1)}{n} \sum_{z \in \Theta_{2n}^r} \beta_z c^T z_U}_{c^T e}, \\
 &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j + \frac{1}{2} \sum_{i=1}^n Q_{ii} + c^T e,
 \end{aligned}$$

where cancellations are derived from the simplified constraints. The optimal value is given in (4.16). Therefore, the difference between the upper bound and the optimal value is given by

$$u_r^{(2)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij}. \quad (4.20)$$

We employ a decomposition of $Q \in \mathcal{N}^n$ which will be helpful in our analysis. Let us define the decomposition as follows:

$$Q = \gamma E + D + F, \quad (4.21)$$

where $\gamma = \min_{i,j} Q_{ij}$, D is a diagonal matrix, and $\text{diag}(F) = 0$. Note that, $E, D, F \in \mathcal{N}^n$. Clearly, this decomposition is unique. Our purpose is to use this decomposition in (4.20) so that the error bound reduces to an easily computable expression. The next lemma simplifies the equality in (4.20).

Lemma 11. *Suppose we use the decomposition provided in (4.21) for $Q \in \mathcal{N}^n$ and*

$c \in \mathbb{R}_+^n$. Then,

$$u_r^{(2)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n F_{ij} X_{ij} - \frac{1}{2} e^T F e,$$

where $X_{ij} = \sum_{z \in \Theta_{2n}^r} \beta_z (z_U)_i (z_U)_j$ for $i = 1, \dots, n$ and $j = 1, \dots, n$ and X is given in (4.17).

Proof. Using (4.20) and (4.21), we obtain

$$\begin{aligned} u_r^{(2)}(Q, c) - \nu(Q, c) &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n (\gamma + F_{ij}) (z_U)_i (z_U)_j \\ &\quad - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n (\gamma + F_{ij}), \\ &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \gamma \sum_{i=1}^n (z_U)_i \underbrace{\sum_{j=1, j \neq i}^n (z_U)_j}_{(r+2) - (z_U)_i} \\ &\quad + \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n F_{ij} (z_U)_i (z_U)_j \\ &\quad - \frac{1}{2} \gamma n(n-1) - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n F_{ij}, \\ &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n F_{ij} (z_U)_i (z_U)_j - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n F_{ij}, \\ &= \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z z_U^T F z_U - \frac{1}{2} e^T F e. \end{aligned}$$

Since $X_{ij} = \sum_{z \in \Theta_{2n}^r} \beta_z (z_U)_i (z_U)_j$ for $i = 1, \dots, n$ and $j = 1, \dots, n$, we can conclude

$$u_r^{(2)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n F_{ij} X_{ij} - \frac{1}{2} e^T F e.$$

□

Next, we present an error bound for the first level of the hierarchy of the outer approximation of (P2), using Lemma 11 and (4.21).

Proposition 20. *Suppose we use the decomposition given in (4.21) for $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$. Then,*

$$u_0^{(2)}(Q, c) - \nu(Q, c) \leq \frac{1}{2}(n-1) \sum_{i=1}^n \max_{j \neq i} F_{ij} - \frac{1}{2} e^T F e.$$

Proof. We aim to find an upper bound for X_{ij} for $i = 1, \dots, n$ and $j = 1, \dots, n$ in Lemma 11, so that we can bound the expression in the right hand side of the equation in Lemma 11. Therefore, we use the constraints and objective function that enforce the following conditions on X :

- $X_{ii} = 1$ for $i = 1, \dots, n$, since $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$,
- $X_{ij} \leq n-1$ for all i, j such that $i \neq j$, since the elements of each row of X, R, R^T , and S given in (4.17) sum up to n and by subtracting the diagonal element, we obtain this inequality.

Since $\mathcal{O}_0 = \mathcal{N}^{2n}$, for each $i = 1, \dots, n$,

$$\sum_{j=1}^n F_{ij} X_{ij} \leq (n-1) \max_{j \neq i} F_{ij}.$$

Using the above inequality,

$$u_0^{(2)}(Q, c) - \nu(Q, c) \leq \frac{1}{2}(n-1) \sum_{i=1}^n \max_{j \neq i} F_{ij} - \frac{1}{2} e^T F e.$$

□

As a consequence of Proposition 20, for the instances of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$, the upper bound arising from (P2) at $r = 0$ only depends on the matrix F given in (4.21).

Corollary 7. *For given $Q \in \mathcal{N}^n$, if $F = 0$ in (4.21) and $c \in \mathbb{R}_+^n$, then*

$$u_0^{(2)}(Q, c) = \nu(Q, c),$$

i.e., the upper bound at level 0 is exact.

It can be readily observed that Corollary 7 presents a sufficient condition for $u_0^{(2)}(Q, c)$ to match the optimal value. It follows that the upper bound for instances of (BoxQP) in which Q can be expressed as a sum of a nonnegative multiple of all ones matrix and a nonnegative diagonal matrix is exact at the first level of the hierarchy for (P2).

We will next illustrate the tightness of the bound provided in Proposition 20. We will employ the following lemma, in which we characterize the optimal value of the (BoxQP) instances in which Q is a diagonal matrix. The problem (BoxQP) decomposes for this class of instances. Consequently, we can derive a closed-form solution of the problem.

Lemma 12. *Given an instance of (BoxQP) with $Q \in \mathcal{N}^n$ is diagonal, then the optimal solution $\nu(Q, c)$ is given by a closed-form expression.*

Proof. When $Q \in \mathcal{S}^n$ is diagonal, we can rewrite (BoxQP) problem in a simplified version:

$$\max_{0 \leq x \leq e} \frac{1}{2} \sum_{i=1}^n Q_{ii}(x_i)^2 + \sum_{i=1}^n c_i x_i.$$

We can decompose the problem above as follows::

$$(P_i) \quad \max_{0 \leq x_i \leq 1} \frac{1}{2} Q_{ii}(x_i)^2 + c_i x_i, \quad i = 1, \dots, n.$$

We can easily find the optimal value of (P_i) :

- Case 1: If $Q_{ii} \geq 0$, then the objective function is convex. Therefore, an optimal solution is one of the vertices, which implies that the optimal value of the problem is given by $\max \{0, \frac{1}{2}Q_{ii} + c_i\}$ for all $i = 1, \dots, n$.
- Case 2: If $Q_{ii} < 0$, then we take the derivative and obtain $x_i = -\frac{c_i}{Q_{ii}}$. Note that $x_i \in [0, 1]$ is not guaranteed, therefore we need to consider $x_i < 0$ and $x_i > 1$

for all $i = 1, \dots, n$. The optimal values for these different cases are presented below.

Finally, we have the following result:

$$\max_{0 \leq x_i \leq 1} \frac{1}{2} Q_{ii} (x_i)^2 + c_i x_i = \begin{cases} \max \{0, \frac{1}{2} Q_{ii} + c_i\}, & \text{if } Q_{ii} \geq 0. \\ -\frac{(c_i)^2}{2Q_{ii}}, & \text{if } 0 \leq -\frac{c_i}{Q_{ii}} \leq 1 \text{ and } Q_{ii} < 0. \\ 0, & \text{if } -\frac{c_i}{Q_{ii}} < 0 \text{ and } Q_{ii} < 0. \\ \frac{1}{2} Q_{ii} + c_i, & \text{if } -\frac{c_i}{Q_{ii}} > 1 \text{ and } Q_{ii} < 0. \end{cases}$$

□

We show that the bound provided in Proposition 20 is tight for reverse diagonal matrices with $n = 2k$, where $k \geq 2$. We use the optimal value given in Lemma 12.

Example 7. Consider the following instance of (BoxQP). $Q \in \mathcal{S}^n$ is reverse diagonal matrix, i.e., $Q_{1n} = \alpha_1, Q_{2(n-1)} = \alpha_2, \dots, Q_{n1} = \alpha_n$ and $n = 2k$, where $k \geq 2$ and $c \in \mathbb{R}^n$. Then, it is easy to verify that

$$u_0^{(2)}(Q, c) = \frac{1}{2}(n-1) \sum_{j=1}^n \alpha_j + c^T e$$

and the optimal value of (BoxQP) is

$$\nu(Q, c) = \frac{1}{2} \sum_{j=1}^n \alpha_j + c^T e.$$

by Lemma 12. Hence,

$$u_0^{(2)}(Q, c) - \nu(Q, c) = \left(\frac{n}{2} - 1\right) \sum_{j=1}^n \alpha_j,$$

which is equal to the bound provided in Proposition 20.

Next, we extend this result to all levels of the outer approximation hierarchies of (P2) for the instances with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$.

Proposition 21. *Given an instance of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$, we have*

$$u_r^{(2)}(Q, c) - \nu(Q, c) \leq \frac{n}{2(r+1)} e^T F e,$$

where F is defined as in (4.21).

Proof. To derive an error bound, we will bound X_{ij} for $1 \leq i < j \leq n$ from above in Lemma 11. Note that, the following relations are satisfied for all $z \in \Theta_{2n}^r$ for fixed $1 \leq i \leq n$ and $r \in \mathbb{N}$:

- (a) $\sum_{z \in \Theta_{2n}^r} \beta_z(z_U)_i = \frac{n}{(r+1)},$
- (b) $\sum_{z \in \Theta_{2n}^r} \beta_z(z_U)_i ((z_U)_i - 1) = 1.$

By (a) and (b), we have:

$$\sum_{z \in \Theta_{2n}^r} \beta_z((z_U)_i)^2 = \frac{n}{(r+1)} + 1. \quad (4.22)$$

We can find an upper bound on X_{ij} for $1 \leq i < j \leq n$ using the above equality:

$$\begin{aligned} X_{ij} &= \sum_{z \in \Theta_{2n}^r} \beta_z(z_U)_i (z_U)_j, \\ &\leq \frac{1}{2} \sum_{z \in \Theta_{2n}^r} \beta_z(((z_U)_i)^2 + ((z_U)_j)^2), \\ &= \frac{1}{2} \left[2 \left(1 + \frac{n}{(r+1)} \right) \right], \\ &= 1 + \frac{n}{(r+1)}, \end{aligned}$$

where we used the fact that $(z_U)_i (z_U)_j \leq \frac{1}{2} (((z_U)_i)^2 + ((z_U)_j)^2)$ in the second line, derived from

$$((z_U)_i - (z_U)_j)^2 = [((z_U)_i)^2 + ((z_U)_j)^2 - 2(z_U)_i (z_U)_j] \geq 0.$$

Hence,

$$X_{ij} \leq 1 + \frac{n}{(r+1)}, \quad 1 \leq i < j \leq n. \quad (4.23)$$

By Lemma 11 and (4.23), we have

$$u_r^{(2)}(Q, c) - \nu(Q, c) \leq \frac{n}{2(r+1)} e^T F e.$$

□

Now, we continue our study on the error bound provided by the outer approximation of (P1) for the instances of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$. We construct a similar result for (P1) as in Lemma 10.

Lemma 13. *Given an instance of (BoxQP) with $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$, assume that the optimal solution of the outer approximation of (P1) is given by*

$$\begin{bmatrix} 1 & x^T & s^T \\ x & X & R \\ s & R^T & S \end{bmatrix} = \sum_{z \in \Theta_{2n+1}^r} \beta_z M \left(\begin{bmatrix} z_0 \\ z_U \\ z_L \end{bmatrix} \right), \quad (4.24)$$

where $M(\cdot)$ given in (4.11). Then, there exists an optimal solution such that $z_L = 0$ for all $z \in \Theta_{2n+1}^r$ with $\beta_z > 0$.

Proof. The proof is similar to proof of Lemma 10. □

We can therefore restrict our attention to those $z \in \Theta_{2n+1}^r$, such that $z_L = 0$ and $e^T z_U = r + 2 - z_0$ for $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$ which satisfy the following constraints:

- $\sum_{z \in \Theta_{2n+1}^r} \beta_z z_0 (z_U)_i = 1, \quad i = 1, 2, \dots, n,$
- $\sum_{z \in \Theta_{2n+1}^r} \beta_z (z_U)_i ((z_U)_i - 1) = 1, \quad i = 1, 2, \dots, n,$
- $\sum_{z \in \Theta_{2n+1}^r} \beta_z ((z_0)^2 - z_0) = 1.$

Using the simplified constraints, we derive a simplified objective function of the outer approximation of (P1):

$$\begin{aligned}
 u_r^{(1)}(Q, c) &= \frac{1}{2} \sum_{z \in \Theta_{2n+1}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j + \frac{1}{2} \sum_{i=1}^n Q_{ii} \underbrace{\sum_{z \in \Theta_{2n+1}^r} \beta_z ((z_U)_i ((z_U)_i - 1))}_{=1} \\
 &\quad + \underbrace{\sum_{z \in \Theta_{2n+1}^r} \beta_z z_0^T c^T z_U}_{c^T e}.
 \end{aligned}$$

Therefore, by using the optimal value given in (4.16) the difference becomes

$$u_r^{(1)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{z \in \Theta_{2n+1}^r} \beta_z \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (z_U)_i (z_U)_j - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij}. \quad (4.25)$$

In the next lemma, we use $X_{ij} = \sum_{z \in \Theta_{2n+1}^r} \beta_z (z_U)_i (z_U)_j$ for $i = 1, \dots, n$ and $j = 1, \dots, n$. Therefore, we reduce the problem to the question of finding an upper bound on X_{ij} for $i = 1, \dots, n$ and $j = 1, \dots, n$.

Lemma 14. For given $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$,

$$u_r^{(1)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (X_{ij} - 1),$$

where $X_{ij} = \sum_{z \in \Theta_{2n+1}^r} \beta_z (z_U)_i (z_U)_j$ for $i = 1, \dots, n$ and $j = 1, \dots, n$ and X is given in (4.24).

Proof. Since $X_{ij} = \sum_{z \in \Theta_{2n+1}^r} \beta_z (z_U)_i (z_U)_j$ for $i = 1, \dots, n$ and $j = 1, \dots, n$ and by (4.25), we can conclude

$$\begin{aligned}
 u_r^{(1)}(Q, c) - \nu(Q, c) &= \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} X_{ij} - \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij}, \\
 &= \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (X_{ij} - 1).
 \end{aligned}$$

□

To derive an error bound for outer approximation of (P1) we employ Lemma 14. Then, we find upper bound on $X_{ij} = \sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i(z_U)_j$ for $1 \leq i < j \leq n$ in the following proposition.

Proposition 22. For $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$,

$$u_r^{(1)}(Q, c) - \nu(Q, c) \leq \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} \left(\frac{n^2}{r+2-n} \right), \quad r \geq n-1.$$

Proof. We have shown that

$$u_r^{(1)}(Q, c) - \nu(Q, c) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} (X_{ij} - 1)$$

in Lemma 14, where $X_{ij} = \sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i(z_U)_j$ for $1 \leq i < j \leq n$. We will find an upper bound on $\sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i$, so that an upper bound on X_{ij} . Combining with Lemma 14, we will derive an error bound for (P1). We first focus on the constraints:

$$\begin{aligned} \sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i((z_U)_i - 1) &= 1, \quad i = 1, 2, \dots, n, \\ \sum_{z \in \Theta_{2n+1}^r} \beta_z \sum_{i=1}^n (z_U)_i((z_U)_i - 1) &= n, \\ \sum_{z \in \Theta_{2n+1}^r} \beta_z \left(\sum_{i=1}^n ((z_U)_i)^2 - \sum_{i=1}^n (z_U)_i \right) &= n, \\ \sum_{z \in \Theta_{2n+1}^r} \beta_z \left(n \left(\frac{r+2}{n} \right)^2 - (r+2) \right) &\leq n. \end{aligned}$$

Finally, we obtain

$$\sum_{z \in \Theta_{2n+1}^r} \beta_z \leq \left(\frac{n^2}{(r+2)(r+2-n)} \right), \quad \text{if } r \geq n-1. \quad (4.26)$$

We can find an upper bound on $\sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i$ by (4.26) and the fact that $(z_U)_i \leq$

$r + 2$ for all $i = 1, 2, \dots, n$:

$$\sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i \leq \left(\frac{n^2}{r+2-n} \right), \quad i = 1, 2, \dots, n, \quad \text{if } r \geq n-1.$$

We know that $\sum_{z \in \Theta_{2n+1}^r} \beta_z((z_U)_i)^2 = \sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i + 1$ for all $i = 1, 2, \dots, n$ by the constraints. Therefore,

$$\sum_{z \in \Theta_{2n+1}^r} \beta_z((z_U)_i)^2 \leq 1 + \frac{n^2}{r+2-n}, \quad i = 1, 2, \dots, n. \quad (4.27)$$

We can find an upper bound on X_{ij} for $1 \leq i < j \leq n$ using (4.27):

$$\begin{aligned} X_{ij} &= \sum_{z \in \Theta_{2n+1}^r} \beta_z(z_U)_i(z_U)_j, \\ &\leq \frac{1}{2} \sum_{z \in \Theta_{2n+1}^r} \beta_z(((z_U)_i)^2 + ((z_U)_j)^2), \\ &\leq \frac{1}{2} \left[2 \left(1 + \frac{n^2}{r+2-n} \right) \right], \\ &= 1 + \frac{n^2}{r+2-n}. \end{aligned}$$

Hence, for $Q \in \mathcal{N}^n$ and $c \in \mathbb{R}_+^n$,

$$u_r^{(1)}(Q, c) - \nu(Q, c) \leq \frac{1}{2} \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} \left(\frac{n^2}{r+2-n} \right), \quad r \geq n-1.$$

□

Note that the error bound of (P1) is not defined for $0 \leq r \leq n-2$, since the upper bound of (P1) is $+\infty$ for some instances given in Proposition 17.

Now we use these results to derive an error bound for a general instance of (BoxQP).

General Case

Now let us construct a bound for general matrices and vectors. Initially, we present the following auxiliary lemma:

Lemma 15. *Given an instance of (BoxQP), let $Q = Q_1 - Q_2$ and $c = c_1 - c_2$, where $Q_2 \in \mathcal{N}^n$ and $c_2 \in \mathbb{R}_+^n$. Then,*

$$u_0^{(2)}(Q, c) \leq u_0^{(2)}(Q_1, c_1).$$

Proof. As a result of $\mathcal{O}_0 = \mathcal{N}^{2n}$ and the assumptions. □

In light of this observation, we present the relation of the upper bounds for the following decomposition of matrices and vectors.

Corollary 8. *Given an instance of (BoxQP), let $Q = Q_+ - Q_-$, where $(Q_+)_{ij} = \max\{Q_{ij}, 0\}$ and $(Q_-)_{ij} = \max\{-Q_{ij}, 0\}$ for all i, j . Similarly, let $c = c_+ - c_-$, where $(c_+)_{ij} = \max\{c_{ij}, 0\}$ and $(c_-)_{ij} = \max\{-c_{ij}, 0\}$ for all j . Then,*

$$u_0^{(2)}(Q, c) \leq u_0^{(2)}(Q_+, c_+).$$

Proof. The proof follows from Lemma 15. □

$\nu(Q, c)$ denotes the optimal value of (BoxQP) with $Q \in \mathcal{S}^n$ and $c \in \mathbb{R}^n$, $\nu(Q_+, c_+)$ denotes the optimal value of (BoxQP) with $Q_+ \in \mathcal{N}^n$ and $c_+ \in \mathbb{R}^n$ and $\nu(Q_-, c_-)$ is defined similarly. The following relation between the optimal values holds:

$$\nu(Q, c) \geq \frac{1}{2}e^T Q e + c^T e = \nu(Q_+, c_+) - \nu(Q_-, c_-),$$

where the first inequality follows from the fact that $e \in \mathbb{R}^n$ is a feasible solution and the inequality is a consequence of the fact that $e \in \Omega(Q_+, c_+)$ and $e \in \Omega(Q_-, c_-)$.

Then,

$$\begin{aligned}
u_0^{(2)}(Q, c) - \nu(Q, c) &\leq u_0^{(2)}(Q, c) - \nu(Q_+, c_+) + \nu(Q_-, c_-), \\
&\leq u_0^{(2)}(Q_+, c_+) - \nu(Q_+, c_+) + \nu(Q_-, c_-), \\
&\leq \left(\frac{n-1}{2}\right) \sum_{i=1}^n \max_j F(Q_+)_{ij} - \frac{1}{2} e^T F(Q_+) e + \nu(Q_-, c_-),
\end{aligned}$$

where $F(Q_+)$ is given by the corresponding decomposition of Q_+ defined in (4.21) and Proposition 20.

Another bound is given by using Corollary 8:

$$\begin{aligned}
u_0^{(2)}(Q, c) - \nu(Q, c) &\leq u_0^{(2)}(Q_+, c_+) - \nu(Q, c), \\
&\leq \left(\frac{n-1}{2}\right) \sum_{i=1}^n \max_j F(Q_+)_{ij} - \frac{1}{2} e^T F(Q_+) e + \nu(Q_+, c_+) - \nu(Q, c), \\
&\leq \left(\frac{n-1}{2}\right) \sum_{i=1}^n \max_j F(Q_+)_{ij} - \frac{1}{2} e^T F(Q_+) e + \nu(Q_+, c_+)
\end{aligned}$$

since $\nu(Q, c) \geq 0$.

Hence,

$$u_0^{(2)}(Q, c) - \nu(Q, c) \leq \left(\frac{n-1}{2}\right) \sum_{i=1}^n \max_j F(Q_+)_{ij} - \frac{1}{2} e^T F(Q_+) e + \min\{\nu(Q_+, c_+), \nu(Q_-, c_-)\}. \quad (4.28)$$

Pathological Examples

In this section, we construct some examples to illustrate the behavior of outer polyhedral approximations of (P1) and (P2). We also define another error bound measure to evaluate the quality of the bound given by the approximations.

Example 8. Let $Q = (2M + \varepsilon)I$ and $c = -Me$, where $M > 0$ and $\varepsilon > 0$. Then the

optimal value is given by

$$\nu(Q, c) = n \frac{\varepsilon}{2},$$

which follows from by Lemma 12. The upper bound is

$$u_0^{(1)}(Q, c) = n \left(M + \frac{\varepsilon}{2} \right)$$

by Proposition 16. Therefore, the difference between $u_0^{(1)}(Q, c)$ and $\nu(Q, c)$ becomes

$$u_0^{(1)}(Q, c) - \nu(Q, c) = Mn.$$

We can also construct the following feasible solution of outer approximation of (P2) :

$$\left[\begin{array}{c|c} I & 0 \\ \hline 0 & ee^T - I \end{array} \right],$$

therefore the upper bound of (P2) is

$$u_0^{(2)}(Q, c) \geq n \frac{\varepsilon}{2} + M(n - 1).$$

The gap between $u_0^{(2)}(Q, c)$ and $\nu(Q, c)$ is bounded by the following expression:

$$u_0^{(2)}(Q, c) - \nu(Q, c) \geq M(n - 1).$$

Note that, the error bound is a function of n . Therefore, for large instances the error bound is weaker.

The next corollaries directly follow from by Example 8.

Corollary 9. For any real number $M > 0$, there exists an instance of (BoxQP) such

that

$$u_n^{(1)}(Q, c) - \nu(Q, c) = Mn.$$

Proof. Follows from Lemma 5 and Example 8. $\square$

Corollary 9 implies that the upper bound of (P1) does not improve until $r = n$.

Corollary 10. *For any real number $M > 0$, there exists an instance of (BoxQP) such that*

$$u_{(n-2)}^{(2)}(Q, c) - \nu(Q, c) \geq M(n-1).$$

Proof. We will construct a feasible solution for the outer approximation of (P2) for $r = n - 2$. Let us choose the following matrix:

$$\left[\begin{array}{c|c} I & 0 \\ \hline 0 & ee^T - I \end{array} \right] = \sum_{i=1}^n \frac{1}{n(n-1)} (z^i (z^i)^T - \text{Diag}(z^i)) + (\bar{z} \bar{z}^T - \text{Diag}(\bar{z})),$$

where z^i is a vector whose i^{th} component is n and others are 0; $\bar{z}$ has zeros for first n components, and ones for the last n entries. Note that, this matrix satisfies the constraints and its objective function value is $n\frac{\varepsilon}{2} + M(n-1)$ for Example 8. Therefore, the assertion follows. $\square$

Corollary 10 implies that the upper bound of (P2) *may not* improve until $r = n - 1$. Now, we proceed to another example where the error bound measure is defined as the ratio between the upper bound and the optimal value.

Example 9. *Let $Q = -mI$ and $c = e$, where $m > 1$. Then, the optimal value is*

$$\nu(Q, c) = \sum_{i=1}^n - \left\{ \frac{(c_i)^2}{2Q_{ii}} \right\} = \frac{n}{2m},$$

which follows from Lemma 12. We can find the upper bound using Proposition 16:

$$u_0^{(1)}(Q, c) = \sum_{i: c_i > 0} c_i = n.$$

We use the following feasible solution:

$$\left[\begin{array}{c|c} 0^n & \frac{1}{2}ee^T \\ \hline \frac{1}{2}ee^T & 0^n \end{array} \right],$$

where 0^n denotes the zero matrix. Therefore, we can find a lower bound on $u_0^{(2)}(Q, c)$:

$$u_0^{(2)}(Q, c) \geq \frac{n}{2}.$$

Hence, we can analyze the ratio between optimal values of the two approximations and the optimal value of the original problem.

$$\frac{u_0^{(1)}(Q, c)}{\nu(Q, c)} = \frac{n}{\frac{n}{2m}} = 2m$$

and

$$\frac{u_0^{(2)}(Q, c)}{\nu(Q, c)} \geq \frac{\frac{n}{2}}{\frac{n}{2m}} = m.$$

The next corollaries follow from Example 9.

Corollary 11. *For any real number $m > 0$, there exists an instance of (BoxQP) such that*

$$\frac{u_0^{(2)}(Q, c)}{\nu(Q, c)} \geq m.$$

Proof. This is a direct consequence of Example 9. □

Corollary 12. *For any real number $m > 0$, there exists an instance of (BoxQP) such*

that

$$\frac{u_0^{(1)}(Q, c)}{\nu(Q, c)} = \frac{u_1^{(1)}(Q, c)}{\nu(Q, c)} = \dots = \frac{u_n^{(1)}(Q, c)}{\nu(Q, c)} = 2m.$$

Proof. As a result of Lemma 5 and Example 9. □

Example 9 shows that both of the formulations can give poor results in terms of the ratio of the upper bound to the optimal value. Another consequence of this example is that the upper bound provided by (P1) can be weaker than that of (P2). Moreover, $u_r^{(2)}(Q, c)$ may decrease as we increase r in numerical studies, despite $u_r^{(1)}(Q, c)$ does not change until $r = n - 1$. To conclude, for both examples, the error bounds for the outer approximations of (P2) provide tighter bounds than those of (P1).

4.5 Conclusion

In this chapter, we analyzed the box constrained quadratic optimization problem. We focused on the copositive reformulations due to Burer [16]. We studied two different copositive reformulations for (BoxQP). Initially, we presented the equivalence of the formulations (P1) and (P2) using the results in [16]. Next, we analyzed the lower and upper bounds for both formulations using the polyhedral hierarchies defined in Sections 2.2.1 and 2.3.1. Inner polyhedral approximation problems of (P1) and (P2) are infeasible for $r \leq n - 2$ and $r \leq n - 3$, respectively. Also, we showed that the lower bounds provided by (P2) outperform those of (P1). For outer polyhedral approximations, we presented necessary and sufficient conditions for having a finite optimal value for (P1). Additionally, we showed that upper bounds obtained from (P2) are always finite. We presented some partial results about the comparison of upper bounds provided by (P2) and (P1). Then, we focused on the error bounds provided by inner and outer approximations. Using the Lipschitz constant, we were able to give a bound for the gap between the optimal value and the lower bound for both of the formulations (see Theorem 10 and 9). For outer approximations, we provided error bounds for the instances of (BoxQP) with nonnegative matrices and

vectors (see Section 4.4.2). Finally, we gave some *pathological examples* to show the cases in which error bounds can be arbitrarily large.

Note that, besides the completely positive formulations provided by Burer, there is another completely positive formulation due to Bomze [8] and Lieder [41]. Although this is another equivalent reformulation of (BoxQP), we do not consider this formulation in our analysis of inner and outer polyhedral approximations since it gives weaker bounds compared to (P1).

We conclude this chapter with some future research directions. For instance, can we show that the outer approximation of (P2) gives always tighter bounds than that of (P1)? Another research direction is to provide an error bound for general matrices and vectors for the outer polyhedral approximations of both formulation which tends to *zero* as r goes to infinity.

Chapter 5

CONCLUSION AND FURTHER RESEARCH

In conclusion, we briefly summarize our main contributions and list some possible future research directions.

5.1 *Conclusion*

In this dissertation, we studied the behavior of specific polyhedral approximations for copositive reformulations of standard quadratic optimization and box constrained quadratic optimization problems.

In the introduction, we presented the most related results from convex analysis and conic optimization. In Chapter 2, we introduced the approximation hierarchies developed for the cones of copositive and completely positive matrices. Our motivation for studying these approximations was based on the new copositive reformulations of a large class of optimization problems [16]. Therefore, our aim was to investigate the copositive reformulation of different problem classes and to analyze the bounds provided by polyhedral approximation hierarchies. Note that our aim was not to present an algorithmic framework to solve the copositive optimization problems. Rather, we contribute to the theoretical results for the behavior of bounds provided by polyhedral approximations of these problems.

We provided new results about the standard quadratic optimization problem in Chapter 3, which consists of the complete algebraic description of the sets consisting of the instances for which the upper and/or the lower bound is already exact at a finite level of the hierarchy and the instances for which the upper and/or the lower bound converges to the optimal value only in the limit. We also showed the geometrical and topological properties of these sets.

In Chapter 4, we analyzed and compared the bounds provided by the polyhedral approximations of two copositive reformulations of box constrained quadratic optimization. We showed that the lower bounds provided by (P2) outperforms that of (P1). A similar result holds for a subset of $r \in \mathbb{N}$ is valid for upper bounds. Moreover, we gave an error bound for inner approximations. The error bound for outer approximations is derived for the instances of (BoxQP) with nonnegative matrices and vectors. We also extended our results by presenting several *pathological* examples. Finally, our analysis showed that although copositive reformulations are equivalent, their polyhedral approximations behave differently.

5.2 Future Work and Open Questions

We first aim to find an error bound for outer polyhedral approximations of general box constrained quadratic optimization problems. Specifically, we studied the error bounds for outer approximations for both formulations (P1) and (P2). We have the desired results for nonnegative matrices and vectors, however, we intend to generalize these results for general matrices and vectors.

Another natural direction of research is to study the behavior of non-polyhedral approximation hierarchies for different or general quadratic optimization problems. It would be interesting to see how effective each approximation hierarchy is on different classes of optimization problems. Therefore, this analysis would shed some light on the question of solving copositive optimization problems efficiently in a problem specific context. Furthermore, we can use these results gained from different problem classes to construct improved inner and outer approximations for these specific problems.

Finally, a recent paper reviews several open questions for the cones of copositive and completely positive matrices [3]. For solving a copositive optimization problem, every improvement for understanding the structure of these cones would be useful.

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