Analysis of Copositive Optimization Based Linear Programming Bounds on Standard Quadratic Optimization*

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Abstract

The problem of minimizing a quadratic form over the unit simplex, referred to as a standard quadratic optimization problem, admits an exact reformulation as a linear optimization problem over the convex cone of completely positive matrices. This computationally intractable cone can be approximated from the inside and from the outside by two sequences of nested polyhedral cones of increasing accuracy. We investigate the sequences of upper and lower bounds on the optimal value of a standard quadratic optimization problem arising from these two hierarchies of inner and outer polyhedral approximations. We give a complete description of the structural properties of the instances on which upper and lower bounds are exact at a finite level of the hierarchy, and the instances on which upper and lower bounds converge to the optimal value only in the limit.

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1 Introduction

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

$$\text{(StQP)} \quad \nu(Q) := \min_{x \in \Delta_n} x^T Q x, \tag{1}$$

where $Q \in \mathcal{S}$ and $\mathcal{S}$ denotes the set of $n \times n$ real symmetric matrices, $x \in \mathbb{R}^n$, and Δ_n denotes the unit simplex in $\mathbb{R}^n$ given by

$$\Delta_n := \{x \in \mathbb{R}^n_+ : e^T x = 1\}, \tag{2}$$

where $e \in \mathbb{R}^n$ is the vector of all ones and $\mathbb{R}^n_+$ denotes the nonnegative orthant in $\mathbb{R}^n$.

Standard quadratic optimization problems arise in a variety of applications (see, e.g. [2]). 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 be formulated as an instance of (StQP), where the dimension n is equal to the number of vertices of the polytope. Since the maximum stable set problem admits a formulation in the form of (StQP) [14], it follows that (StQP) is in general an NP-hard problem.

The problem (1) can be equivalently reformulated as the following instance of a linear optimization problem over the cone of completely positive matrices [4]:

$$\nu(Q) = \min\{\langle Q, X\rangle : \langle E, X\rangle = 1, \quad X \in \mathcal{C}\}, \tag{3}$$

where $\langle A, B\rangle = \text{trace}(AB) = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}B_{ij}$ for $A, B \in \mathcal{S}$, $E = ee^T \in \mathcal{S}$ is the matrix of all ones, and $\mathcal{C} \subseteq \mathcal{S}$ is the cone of the completely positive matrices given by

$$\mathcal{C} := \text{conv}\{uu^T : u \in \mathbb{R}^n_+\}, \tag{4}$$

where conv$\{\cdot\}$ denotes the convex hull. The dual cone of $\mathcal{C}$ with respect to the trace inner product $\langle\cdot,\cdot\rangle$ is the cone of copositive matrices given by

$$\mathcal{C}^* := \{X \in \mathcal{S} : u^T X u \geq 0 \text{ for all } u \in \mathbb{R}^n_+\}. \tag{5}$$

Since (StQP) is in general an NP-hard problem, the convex optimization problem (3) is in general intractable. Indeed, the computational complexity is now hidden in the conic constraint $X \in \mathcal{C}$, for which the membership problem is NP-hard [10]. Similarly, the membership problem for the dual cone $\mathcal{C}^*$ is also NP-hard [15, 10].

Despite the fact that the convex reformulation (3) 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 convex cones $\mathcal{C}$ and $\mathcal{C}^*$. In fact, Burer [7] established more generally that, under mild assumptions, every optimization problem with a quadratic objective function, linear equality constraints, and a mix of nonnegative and binary variables admits an exact reformulation as a linear optimization problem over the cone $\mathcal{C}$. Therefore, there has recently been a considerable research activity towards a better understanding of the cones $\mathcal{C}$ and $\mathcal{C}^*$. Many of these studies propose different ways of approximating each of these two cones by a sequence of tractable convex cones of increasing accuracy (see, e.g., [16, 12, 8, 3, 17, 6, 21, 18, 5, 13]). Such sequences therefore yield approximation hierarchies for the cones $\mathcal{C}$ and $\mathcal{C}^*$. By replacing the difficult conic constraints with the sequences of increasingly more accurate tractable approximations, one can obtain a sequence of increasingly tighter bounds on the optimal value of a linear optimization problem over the cones of completely positive or copositive matrices.

In this paper, we focus on two approximation hierarchies, each of which is comprised of a sequence of polyhedral cones of increasing accuracy. The first approximation hierarchy, defined originally in the context of standard quadratic optimization by Bomze and de

Klerk [3] and later extended to a hierarchy that consists of nested cones by Yıldırım [21], is motivated by exploiting necessary conditions for copositivity of a matrix. By duality, these conditions translate into a hierarchy of *inner* polyhedral approximations $\mathcal{I}_r,\ r = 0, 1, \ldots$ of the cone $\mathcal{C}$ of completely positive matrices, with the property that $\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \ldots \subseteq \mathcal{C}$ and $\mathrm{cl}\,(\cup_{r\in\mathbb{N}}\mathcal{I}_r) = \mathcal{C}$, where $\mathrm{cl}(\cdot)$ denotes the closure. Exploiting a sequence of sufficient conditions for copositivity of a matrix, de Klerk and Pasechnik [8] proposed another hierarchy, which, by duality, yields a sequence of *outer* polyhedral approximations $\mathcal{O}_r,\ r = 0, 1, \ldots$ of the cone $\mathcal{C}$, with the property that $\mathcal{O}_0 \supseteq \mathcal{O}_1 \supseteq \ldots \mathcal{C}$ and $\cap_{r\in\mathbb{N}}\mathcal{O}_r = \mathcal{C}$.

Since each of the two approximation hierarchies is composed of polyhedral cones, it follows that replacing the conic constraint $X \in \mathcal{C}$ in (3) with $X \in \mathcal{I}_r$ (resp., with $X \in \mathcal{O}_r$), where $r \in \mathbb{N}$, gives rise to a linear programming problem with $O(n^{r+2})$ variables, whose optimal value yields an upper (resp., lower) bound on the optimal value $\nu(Q)$. In this paper, we investigate the upper and lower bounds arising from these inner and outer polyhedral approximations. We give a complete description of the structural properties of the instances of (StQP) for which the upper bound or the lower bound is already exact at a finite level $r \in \mathbb{N}$ of the corresponding hierarchies. Similarly, we completely describe the properties of the instances of (StQP) for which the upper bounds or the lower bounds converge to $\nu(Q)$ only in the limit.

We remark that our perspective in this paper, in general, is not algorithmic in the sense that some of our results 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 identify the relations between the structural properties of instances of (StQP) and the strength of the upper and lower bounds on the optimal value $\nu(Q)$ arising from the inner and outer polyhedral approximations of the cone $\mathcal{C}$. In particular, our results shed light onto the strengths and limitations of the two polyhedral approximation hierarchies 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.

The paper is organized as follows. We define our notation in Section 1.1. In Section 2, we describe the inner and outer polyhedral approximations of the cone of completely positive matrices. Section 3 is devoted to some preliminary results. In Section 4, we present the relations between the structural properties of (StQP) and the behavior of upper bounds. The corresponding relations for lower bounds are discussed in Section 5. We conclude the paper in Section 6.

1.1 Notation

We denote by $\mathbb{R}^n$ and $\mathbb{R}^n_+$ the n-dimensional Euclidean space and the nonnegative orthant, respectively. We use $\mathbb{N}^n$ and $\mathbb{Q}^n$ for the set of n-dimensional nonnegative integer vectors and the set of rational vectors, respectively. The unit simplex is represented by $\Delta_n \subset \mathbb{R}^n$. The space of $n \times n$ real symmetric matrices is denoted by $\mathcal{S}$. We reserve calligraphic uppercase letters to denote subsets of $\mathcal{S}$. The cones of completely positive and copositive matrices in $\mathcal{S}$ are denoted by $\mathcal{C}$ and $\mathcal{C}^*$, respectively. We use $\mathcal{N}$ to denote the cone of componentwise nonnegative $n \times n$ real symmetric matrices. The set of $n \times n$ symmetric matrices with rational entries is represented by $\mathcal{Q}$. The ith unit vector in $\mathbb{R}^n$ is denoted by $e_i,\ i = 1, \ldots, n$. We use $e = \sum_{i=1}^n e_i$ and $E = ee^T$ to represent the n-dimensional vector of all ones and the $n \times n$ matrix of all ones, respectively. We reserve $I \in \mathcal{S}$ for the identity matrix. Given $x \in \mathbb{R}^n$, $\text{Diag}(x) \in \mathcal{S}$ denotes the diagonal matrix whose diagonal entries are given by the components of x. Similarly, for $M \in \mathcal{S}$, $\text{diag}(M) \in \mathbb{R}^n$ represents the vector composed of the diagonal entries of M. The closure and the convex hull of a set are denoted by $\text{cl}(\cdot)$ and $\text{conv}(\cdot)$, respectively. 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 $U \subseteq \{1, \ldots, n\}$ and $V \subseteq \{1, \ldots, n\}$ 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 $M \in \mathcal{S}$, M_{UV} denotes the $u \times v$ submatrix of M whose rows and columns are indexed by the sets U and V, respectively.

2 Polyhedral Approximation Hierarchies

In this section, we give a detailed description of the two hierarchies of inner and outer polyhedral approximations of the cone of completely positive matrices.

2.1 Inner Polyhedral Approximations

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

$$u^T X u = \langle X, uu^T \rangle \geq 0, \quad \text{for all } u \in \Delta_n. \tag{6}$$

It follows that enforcing the condition (6) on any *finite* subset of Δ_n yields an outer approximation of $\mathcal{C}^*$ by a *polyhedral* cone, which, by duality, translates into an inner polyhedral approximation of the cone of completely positive matrices.

Motivated by these observations, let us define the following sequence of finite subsets of the unit simplex (see [3, 21]):

$$\Delta_n^r := \bigcup_{k=0}^{r} \Lambda_n^k, \quad r = 0, 1, \ldots, \tag{7}$$

where

$$\Lambda_n^k := \{x \in \Delta_n : (k+2)x \in \mathbb{N}^n\}, \quad k = 0, 1, \ldots. \tag{8}$$

Since $\Delta_n^0 \subset \Delta_n^1 \subset \ldots \subset \Delta_n$, it follows that enforcing the condition (6) only on Δ_n^r yields a sequence of increasingly better outer polyhedral approximations of $\mathcal{C}^*$ as r increases. The corresponding dual cones, which are also polyhedral, yield a sequence of increasingly better inner approximations of the cone $\mathcal{C}$. More specifically, the corresponding inner approximations are given by

$$\mathcal{I}_r := \left\{ \sum_{d \in \Delta_n^r} \lambda_d \, dd^T : \lambda_d \geq 0 \text{ for each } d \in \Delta_n^r \right\}, \quad r = 0, 1, \ldots. \tag{9}$$

This sequence of polyhedral cones satisfies [21]

$$\mathcal{I}_0 \subseteq \mathcal{I}_1 \subseteq \ldots \subseteq \mathcal{C}, \quad \text{and} \quad \text{cl}\left(\bigcup_{r \in \mathbb{N}} \mathcal{I}_r \right) = \mathcal{C}. \tag{10}$$

Therefore, replacing the difficult conic constraint $X \in \mathcal{C}$ in (3) with $X \in \mathcal{I}_r$, we obtain the following linear programming problem whose optimal value yields an upper bound on $\nu(Q)$.

$$u_r(Q) := \min\{\langle Q, X\rangle : \langle E, X\rangle = 1, \quad X \in \mathcal{I}_r\}, \quad r = 0, 1, \ldots. \tag{11}$$

As already observed in [21] (see also [3]), 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:

$$u_r(Q) = \min_{d \in \Delta_n^r} d^T Q d, \quad r = 0, 1, \ldots. \tag{12}$$

Since $|\Delta_n^r| = O(n^{r+2})$, $u_r(Q)$ can be computed in polynomial time for each fixed $r \in \mathbb{N}$.

2.2 Outer Polyhedral Approximations

By duality, outer approximations of the cone $\mathcal{C}$ can be obtained through inner approximations of the cone $\mathcal{C}^*$. Therefore, by properly exploiting sufficient conditions for copositivity, de Klerk and Pasechnik [8] obtained the following inner approximations of the cone $\mathcal{C}^*$.

Let us define

$$\Theta_n^r := \left\{ z \in \mathbb{N}^n : \sum_{i=1}^n z_i = r + 2 \right\} = (r+2)\Lambda_n^r, \quad r = 0, 1, 2, \ldots. \tag{13}$$

Consider the following convex cones:

$$\mathcal{O}_r := \left\{ \sum_{z \in \Theta_n^r} \beta_z \left(zz^T - \mathrm{Diag}(z) \right) : \beta_z \geq 0 \text{ for all } z \in \Theta_n^r \right\}, \quad r = 0, 1, \ldots. \tag{14}$$

Since Θ_n^r is a finite set, $\mathcal{O}_r$ is a polyhedral cone for each $r \in \mathbb{N}$. In [8], de Klerk and Pasechnik established that

$$\mathcal{C} \subseteq \ldots \subseteq \mathcal{O}_1 \subseteq \mathcal{O}_0 = \mathcal{N}, \quad \text{and} \quad \mathcal{C} = \bigcap_{r \in \mathbb{N}} \mathcal{O}_r. \tag{15}$$

In a similar manner, replacing the difficult conic constraint $X \in \mathcal{C}$ in (3) with $X \in \mathcal{O}_r$ gives rise to the following linear programming problem, whose optimal value yields a lower bound on $\nu(Q)$.

$$l_r(Q) := \min\{\langle Q, X\rangle : \langle E, X\rangle = 1, \quad X \in \mathcal{O}_r\}, \quad r = 0, 1, \ldots. \tag{16}$$

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 [3, 21]):

$$\begin{aligned} l_r(Q) &= \frac{1}{(r+1)(r+2)} \min_{z \in \Theta_n^r} (z^T Q z - z^T \mathrm{diag}(Q)), \\ &= \left(\frac{r+2}{r+1}\right) \min_{x \in \Lambda_n^r} \left(x^T Q x - \left(\frac{1}{r+2}\right) x^T \mathrm{diag}(Q) \right), \quad r = 0, 1, \ldots, \end{aligned} \tag{17}$$

where we used (13) in the second line. Similarly, for each fixed $r \in \mathbb{N}$, $l_r(Q)$ can be computed in polynomial time since $|\Lambda_n^r| = O(n^{r+2})$.

2.3 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 [21] established that

$$u_r(Q) - l_r(Q) \leq \frac{1}{r+1} \left(\max_{i=1,\ldots,n} Q_{ii} - \nu(Q) \right), \quad r = 0, 1, \ldots. \tag{18}$$

which implies that these bounds lead to a polynomial-time approximation scheme for standard quadratic optimization (see also [3] for a slightly different result).

The bounds $l_r(Q)$ and $u_r(Q)$ have a closed form expression for the maximum stable set problem [3, 17, 21], 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 [14] established that the maximum stable set problem can be formulated as an instance of (StQP) as

$$\frac{1}{\alpha(G)} = \min_{x \in \Delta_n} x^T (I + A_G) x, \tag{19}$$

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 [21]:

$$u_r(I + A_G) = \begin{cases} \frac{1}{r+2}, & \text{if } r < \alpha(G) - 2, \\ \frac{1}{\alpha(G)}, & \text{otherwise.} \end{cases} \tag{20}$$

Similarly, the lower bounds have more complicated closed form expressions [3, 17]. In particular, we have

$$l_r(I + A_G) = 0, \quad \text{if } r \leq \alpha(G) - 2, \quad \text{and} \quad l_r(I + A_G) > 0, \quad \text{if } r > \alpha(G) - 2. \tag{21}$$

It follows from the closed form expressions for the maximum stable set problem that the error bound in (18) is tight and, in general, cannot be improved [21].

In this paper, we are interested in the description of the structural properties of the instances of (StQP) for which $l_r(Q) = \nu(Q)$ or $u_r(Q) = \nu(Q)$ for some finite value of $r \in \mathbb{N}$. Similarly, we aim to identify structural properties of the instances of (StQP) for which $l_r(Q) < \nu(Q)$ or $u_r(Q) > \nu(Q)$ for all $r \in \mathbb{N}$.

3 Preliminaries

In this section, we collect some preliminary results about (StQP). We then establish some basic properties of upper and lower bounds.

We first review the optimality conditions of (StQP).

Theorem 3.1 *Given an instance of (StQP), let $x^* \in \Omega(Q)$ with the optimal value $\nu(Q) = (x^*)^T Q x^*$. Define*

$$P := \{j \in \{1, \ldots, n\} : x_j^* > 0\}, \quad \textit{and} \quad Z := \{j \in \{1, \ldots, n\} : x_j^* = 0\}. \tag{22}$$

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 3.1 *Let $Q, Q_1, Q_2 \in \mathcal{S}$.*

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

(ii) If $Q \in \mathcal{N}$, then $u_r(Q) \ge \nu(Q) \ge l_r(Q) \ge 0$ for each $r = 0, 1, \ldots$.

(iii) If $Q_1 - Q_2 \in \mathcal{N}$, then $\nu(Q_1) \ge \nu(Q_2)$, $u_r(Q_1) \ge u_r(Q_2)$, and $l_r(Q_1) \ge l_r(Q_2)$ for each $r = 0, 1, \ldots$.

(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 (13), $\Theta_n^0 = \{2e_i : i = 1, \ldots, n\} \cup \{e_i + e_j : 1 \le i < j \le n\}$. The assertion follows from this observation and (17).

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

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

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

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 (12). Considering lower bounds, note that $l_r(Q_1 - Q_2) \ge 0$ for each $r = 0, 1, \ldots$, by part (ii). By (17),

$$z^T(Q_1 - Q_2)z - z^T \mathrm{diag}(Q_1 - Q_2) \ge 0, \quad \text{for all } z \in \Theta_n^r,\ r = 0, 1, \ldots,$$

which, after rearranging, yields

$$z^T Q_1 z - z^T \text{diag}(Q_1) \geq z^T Q_2 z - z^T \text{diag}(Q_2), \quad \text{for all } z \in \Theta_n^r,\ r = 0, 1, \ldots.$$

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

(iv) This is a trivial consequence of (17), (12), 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 (12), we obtain $u_r(Q + \lambda E) = u_r(Q) + \lambda$ since $\Delta_n^r \subset \Delta_n$.

For any $z \in \Theta_n^r,\ r = 0, 1, \ldots$, we have

$$z^T(Q + \lambda E)z - z^T \text{diag}(Q + \lambda E) = \left(z^T Q z - z^T \text{diag}(Q)\right) + \lambda(r + 2)(r + 1),$$

where we used $z^T E z = (r + 2)^2$ and $z^T \text{diag}(E) = e^T z = r + 2$ by (13). It follows from (17) that $l_r(Q + \lambda E) = l_r(Q) + \lambda$.

□

4 Upper Bounds

In this section, we establish the relations between the structural properties of a given instance of (StQP) and the behavior of upper bounds $u_r(Q)$. Let us define the following sets:

$$\mathcal{U}_r := \{Q \in \mathcal{S} : u_r(Q) = \nu(Q)\}, \quad r = 0, 1, \ldots. \tag{23}$$

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

$$\mathcal{U}_0 \subseteq \mathcal{U}_1 \subseteq \ldots \subseteq \mathcal{S}.$$

We first present necessary and sufficient conditions for membership in $\mathcal{U}_r$ for each $r \in \mathbb{N}$.

Lemma 4.1 *$Q \in \mathcal{U}_r$ for some $r \in \mathbb{N}$ if and only if $\Omega(Q) \cap \Delta_n^r \neq \emptyset$.*

Proof. The assertion follows immediately from (23) and (12). $\square$

The next proposition presents an algebraic description of the sets $\mathcal{U}_r$.

Proposition 4.1 *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. More specifically,*

$$\mathcal{U}_r = \bigcup_{d \in \Delta_n^r} \mathcal{V}_d, \tag{24}$$

where

$$\mathcal{V}_d := \{Q \in \mathcal{S} : d^T Q d \leq x^T Q x, \quad \textit{for each } x \in \Delta_n\}, \quad d \in \Delta_n^r. \tag{25}$$

Furthermore, $\mathcal{U}_r$ contains the line $\{\lambda E : \lambda \in \mathbb{R}\}$.

Proof. Let us fix $r \in \mathbb{N}$. Note that $Q \in \mathcal{V}_d$ if and only if $d \in \Omega(Q)$. The relation (24) follows immediately from Lemma 4.1.

For 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 $\mathcal{S}$. Clearly, $\mathcal{V}_d$ is a cone.

$\mathcal{U}_r$ is closed since it is given by the union of a finite number of closed sets. Finally, for any $\lambda \in \mathbb{R}$ and any $d \in \Delta_n^r$, we have $\lambda E \in \mathcal{V}_d$. $\square$

For any $r \in \mathbb{N}$, it follows from Proposition 4.1 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 $i = 1, \ldots, n$. 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 $Q_d := I - ed^T - de^T \in \mathcal{S}$, 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 (25). Since $\Delta_n^r \subset \Delta_n^{r+1}$ by (7), it follows from Proposition 4.1 that $\mathcal{U}_r \subset \mathcal{U}_{r+1}$ for each $r \in \mathbb{N}$.*

Remark 2 *Let $G = (V, E)$ be a simple, undirected graph, where $|V| = n$. Consider the formulation (19) of the maximum stable set problem on G as an instance of (StQP), where*

$Q = I + A_G$. By (20), $u_r(I + A_G) = \nu(I + A_G)$ 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 $G = (V, E)$, $I + A_G \in \mathcal{U}_{n-2}$.

Let us next define

$$\mathcal{U} := \bigcup_{r \in \mathbb{N}} \mathcal{U}_r, \quad \text{and} \quad \mathcal{U}_\infty := \mathcal{S} \backslash \mathcal{U}. \tag{26}$$

The next lemma presents a structural property of the set $\mathcal{U}$.

Lemma 4.2 *We have*

$$\mathcal{U} = \{Q \in \mathcal{S} : \Omega(Q) \cap \mathbb{Q}^n \neq \emptyset\}. \tag{27}$$

Proof. The relation (27) follows from Lemma 4.1, (26), and the fact that $\cup_{r \in \mathbb{N}} \Delta_n^r = \mathbb{Q}^n \cap \Delta_n$. □

The following corollary presents an easy sufficient condition for membership in $\mathcal{U}$.

Corollary 4.1 *We have $\mathcal{Q} \subseteq \mathcal{U}$.*

Proof. Vavasis [20] proved that any quadratic optimization problem with rational data, which is not unbounded below, has a rational optimal solution. The assertion directly follows from this result and Lemma 4.2. □

Since $\text{cl}(\mathcal{Q}) = \mathcal{S}$, the next result is a direct consequence of Corollary 4.1.

Corollary 4.2 *We have*

$$cl(\mathcal{U}) = \mathcal{S}. \tag{28}$$

By Corollary 4.1, for a given $Q \in \mathcal{S}$, 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 $Q \in \mathcal{Q}$, we have $\mu Q \in \mathcal{U}$ for any $\mu \in \mathbb{R}_+$ by Proposition 4.1.

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

Example 4.1 *Similar to Remark 1, let $d \in \Delta_n \backslash \mathbb{Q}^n$ and define $Q_d := I - ed^T - de^T \in \mathcal{S}$. Then, $\Omega(Q_d) = \{d\}$ and $\Omega(Q_d) \cap \mathbb{Q}^n = \emptyset$. By Lemma 4.2, $Q_d \in \mathcal{U}_\infty$.*

5 Lower Bounds

In this section, we focus on the relations between the structural properties of a given instance of (StQP) and the behavior of lower bounds $l_r(Q)$. Our analysis of lower bounds is considerably more involved since the expression (17) is more complicated in comparison with (12).

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

$$\mathcal{L}_r := \{Q \in \mathcal{S} : l_r(Q) = \nu(Q)\}, \quad r = 0, 1, \ldots. \tag{29}$$

Since the lower bounds are monotonically nondecreasing, we obtain

$$\mathcal{L}_0 \subseteq \mathcal{L}_1 \subseteq \ldots \subseteq \mathcal{S}.$$

5.1 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 $Q \in \mathcal{S}$ with $Q + \gamma E$ in (StQP) shifts the optimal value by γ, i.e., $\nu(Q + \gamma E) = \nu(Q) + \gamma$, by Lemma 3.1(v), 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:

$$Q^s := Q - l_0(Q)E. \tag{30}$$

Note that $Q^s \in \mathcal{N}$ and $l_0(Q^s) = 0$. By Lemma 3.1(ii),

$$\nu(Q^s) = \nu(Q) - l_0(Q) \geq 0. \tag{31}$$

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

Proposition 5.1 *$Q \in \mathcal{L}_0$ if and only if there exists an index $k \in \{1, \ldots, n\}$ such that $Q_{kk} = \min_{1 \leq i \leq j \leq n} Q_{ij}$. Therefore, $\mathcal{L}_0$ is a closed cone given by the union of n polyhedral cones, i.e.,*

$$\mathcal{L}_0 = \bigcup_{k=1}^{n} \{Q \in \mathcal{S} : Q_{kk} \leq Q_{ij},\ 1 \leq i \leq j \leq n\}. \tag{32}$$

Proof. Suppose that $Q \in \mathcal{L}_0$. Then, $l_0(Q) = \nu(Q) = \min_{1 \le i \le j \le n} Q_{ij}$ by Lemma 3.1(i). Suppose, for a contradiction, that $Q_{kk} > l_0(Q)$ for each $k = 1, \ldots, n$. By (30), $\min_{k=1,\ldots,n} Q^s_{kk} > 0$. Since $Q^s \in \mathcal{N}$, for any $x \in \Delta_n$, we have

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

where we used $\min_{x \in \Delta_n} \sum_{j=1}^n (x_j)^2 = 1/n$ to derive the third inequality. Together with (31), we obtain that $\nu(Q^s) = \nu(Q) - l_0(Q) > 0$, contradicting our hypothesis.

Conversely, given $Q \in \mathcal{S}$, suppose that there exists an index $k \in \{1, \ldots, n\}$ such that $Q_{kk} = \min_{1 \le i \le j \le n} Q_{ij}$. It is easy to verify that $e_k \in \Omega(Q)$. Therefore, $\nu(Q) = Q_{kk} = \min_{1 \le i \le j \le n} Q_{ij} = l_0(Q)$, where we used Lemma 3.1(i). Therefore, $Q \in \mathcal{L}_0$.

The relation (32) follows immediately. □

As an immediate consequence of the characterization in Proposition 5.1, the set $\mathcal{L}_0$ is in general nonconvex since $e_i(e_i)^T \in \mathcal{L}_0$ for each $i = 1, \ldots, n$, while $I = \sum_{i=1}^n e_i(e_i)^T \notin \mathcal{L}_0$ for any $n \ge 2$.

Let us define

$$\mathcal{L} := \bigcup_{r \in \mathbb{N}} \mathcal{L}_r, \quad \text{and} \quad \mathcal{L}_\infty := \mathcal{S} \backslash \mathcal{L}. \tag{33}$$

The next two sections lay the groundwork for the description of the sets $\mathcal{L}_r$, $\mathcal{L}$, and $\mathcal{L}_\infty$.

5.2 Two Auxiliary Sets

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

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

$$U := \{k \in \{1, \ldots, n\} : Q_{kk} = \nu(Q)\}, \quad V := \{k \in \{1, \ldots, n\} : Q_{kk} > \nu(Q)\}. \tag{34}$$

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

$$\mathcal{S}_1 \;\; := \;\; \left\{Q \in \mathcal{S} : \min_{k=1,\ldots,n} Q_{kk} = \nu(Q)\right\} = \{Q \in \mathcal{S} : U \ne \emptyset\}, \tag{35}$$

$$\mathcal{S}_2 := \left\{ Q \in \mathcal{S} : \min_{k=1,\ldots,n} Q_{kk} > \nu(Q) \right\} = \{Q \in \mathcal{S} : U = \emptyset\}. \tag{36}$$

First, we present an algebraic description of the set $\mathcal{S}_1$.

Proposition 5.2 *$Q \in \mathcal{S}_1$ if and only if $\Omega(Q) \cap \{e_1, \ldots, e_n\} \neq \emptyset$. Furthermore, $\mathcal{S}_1$ is a closed cone given by the union of a finite number of nonempty, closed, and convex cones. More specifically,*

$$\mathcal{S}_1 = \bigcup_{k=1}^{n} \mathcal{V}_{e_k}, \tag{37}$$

where $\mathcal{V}_{e_k}$ is defined as in (25).

Proof. The assertions directly follow from (35) and the definition (25). □

The following inclusion follows immediately from Proposition 5.1 and (35):

$$\mathcal{L}_0 \subseteq \mathcal{S}_1. \tag{38}$$

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

Proposition 5.3 *$\mathcal{S}_2 \subseteq \mathcal{L}_\infty$.*

Proof. Let $Q \in \mathcal{S}_2$ and let $x^* \in \Omega(Q)$. Let the index sets P and Z be defined as in (22). First, we remark that $|P| \geq 2$. Note that $|P| = 1$ if and only if $x^* = e_k$ for some $k \in \{1, \ldots, n\}$, in which case $Q \in \mathcal{S}_1$ by Proposition 5.2, contradicting our hypothesis.

By Theorem 3.1,

$$Q_{PP}\, x^*_P = \nu(Q) e_P. \tag{39}$$

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

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

Since $Q_{kk} > \nu(Q)$, it follows that there exists $l \in P$ 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

$$f_r(q^r) := \left(\frac{r+2}{r+1}\right)(q^r)^T Q(q^r) - \left(\frac{1}{r+1}\right)(q^r)^T \text{diag}(Q) < \nu(Q), \quad r = 0, 1, \ldots. \tag{40}$$

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

$$f_0(q^0) = 2(q^0)^T Q(q^0) - (q^0)^T \text{diag}(Q) = Q_{kl} < \nu(Q), \tag{41}$$

by the choice of $k \in P$ and $l \in P$. This establishes (40) for $r = 0$.

Suppose now that there exists $q^r \in \Lambda_n^r \cap F$ that satisfies (40) 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 (40) for $r + 1$.

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

$$f_r(q^r) = \frac{1}{(r+1)(r+2)}\left((z^r)^T Q(z^r) - (z^r)^T \text{diag}(Q)\right) < \nu(Q). \tag{42}$$

For each $j \in P$, let us define $w^j := z^r + e_j \in \Theta_n^{r+1}$. 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 $j' \in P$ such that $q^{r+1} = (1/(r+3))w^{j'}$ satisfies (40) 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 get

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

where we used (39) in the third line and the definition of z^r in the last line. Therefore, there exists $j' \in P$ such that $(z^r_P)^T Q_{PP} (e_{j'})_P = (z^r)^T Q e_{j'} \leq (r+2)\nu(Q)$. By defining $q^{r+1} = (1/(r+3)) w^{j'}$, we obtain

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

where we used the choice of j' in the first inequality and the induction hypothesis (42) in the second one. Since $l_r(Q) \leq f_r(q^r)$ by (17), it follows from (40) that $l_r(Q) < \nu(Q)$ for each $r \in \mathbb{N}$. Therefore, $Q \in \mathcal{L}_\infty$. □

Example 5.1 *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 $\beta = \sum_{i=1}^n (1/Q^s_{ii})$. It is easy to verify that the unique optimal solution $x^* \in \Omega(Q)$ is given by $x^*_j = (1/Q^s_{jj})/\beta$, $j = 1, \ldots, n$. Therefore, by Proposition 5.2, $Q \notin \mathcal{S}_1$ for any $n \geq 2$. It follows from Proposition 5.3 that $Q \in \mathcal{L}_\infty$ for any $n \geq 2$.*

The following result is an immediate consequence of Proposition 5.3.

Corollary 5.1 $\mathcal{L} \subseteq \mathcal{S}_1$.

It follows from Proposition 5.2 and Corollary 5.1 that a necessary condition for $Q \in \mathcal{L}$ is that $\Omega(Q) \cap \{e_1, \ldots, e_n\} \neq \emptyset$. An interesting question is whether this necessary condition is in fact sufficient. The next two examples answer this question in the negative for different reasons.

Example 5.2 *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 $Q \in \mathcal{S}_1$. In this example, $U = \{1\}$ and $V = \{2, 3\}$. Let us focus on Q_{VV}. Note that, for $n = 2$, $Q_{VV} \in \mathcal{L}_\infty$ by Example 5.1. Therefore, for any $r \in \mathbb{N}$, $l_r(Q_{VV}) < \nu(Q_{VV}) = 1$. It follows that

$$\begin{aligned} l_r(Q) &= \frac{1}{(r+1)(r+2)} \min_{z \in \Theta_n^r} \left(z^T Q z - z^T diag(Q) \right), \\ &\leq \frac{1}{(r+1)(r+2)} \min_{z \in \Theta_n^r : z_1 = 0} \left(z^T Q z - z^T diag(Q) \right), \\ &= l_r(Q_{VV}) < 1, \end{aligned}$$

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

Example 5.3 *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 $Q \in \mathcal{S}_1$. Similarly, $U = \{1\}$ and $V = \{2, 3\}$. We claim that $Q \notin \mathcal{L}$. Let us fix $r \in \mathbb{N}$ and define $z_r := [r, 1, 1]^T \in \Theta_n^r$. By (17),

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

which implies that $l_r(Q) < \nu(Q)$ *for each* $r \in \mathbb{N}$. *Therefore,* $Q \in \mathcal{L}_\infty$, *i.e.,* $Q \in \mathcal{S}_1 \backslash \mathcal{L}$. *Note that* $\nu(Q_{VV}) = 3/2 > 1 = \nu(Q)$ *on this instance.*

5.3 Description of $\mathcal{S}_1 \backslash \mathcal{L}$

Our next goal is to generalize Examples 5.2 and 5.3 in order to obtain a complete description of the set $\mathcal{S}_1 \backslash \mathcal{L}$.

The next lemma presents useful properties of the set $\mathcal{S}_1 \backslash \mathcal{L}$.

Lemma 5.1 *For any* $Q \in \mathcal{S}_1 \backslash \mathcal{L}$, *we have* $V \neq \emptyset$, *where* V *is defined as in (34).*

Proof. Let $Q \in \mathcal{S}_1 \backslash \mathcal{L}$. Suppose, for a contradiction, that $V = \emptyset$. Then, $\{e_1, \ldots, e_n\} \subseteq \Omega(Q)$ since $U = \{1, \ldots, n\}$. By Theorem 3.1, 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 5.1, which contradicts our hypothesis since $\mathcal{L}_0 \subseteq \mathcal{L}$. $\square$

It follows from the proof of Lemma 5.1 that

$$Q_{ij} \geq \nu(Q) \quad \text{for each} \quad i \in U, \; j = 1, \ldots, n. \tag{43}$$

The next proposition gives a sufficient condition for membership in $\mathcal{S}_1 \backslash \mathcal{L}$ and generalizes Example 5.2.

Proposition 5.4 *Let* $Q \in \mathcal{S}_1$ *be such that* $V \neq \emptyset$. *If* $\nu(Q_{VV}) = \nu(Q)$, *where* V *is defined as in (34), then* $Q \in \mathcal{S}_1 \backslash \mathcal{L}$.

Proof. The assertion follows from the observation that $Q_{VV} \in \mathcal{L}_\infty$ for $n = |V|$ and a similar argument as in Example 5.2. $\square$

The next proposition presents another sufficient condition for membership in $\mathcal{S}_1 \backslash \mathcal{L}$, thereby generalizing Example 5.3.

Proposition 5.5 *Let* $Q \in \mathcal{S}_1$ *be such that* $|V| \geq 2$, *where* V *is defined as in (34). Suppose that there exist indices* $i \in U$, $j \in V$, $k \in V$, *and* $j \neq k$ *such that*

$$Q_{ij} = Q_{ik} = \nu(Q), \quad Q_{jk} < \nu(Q). \tag{44}$$

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

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

$$z_i = r, \quad z_j = 1, \quad z_k = 1,$$

and all remaining entries of z are set to 0. By (17),

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

where we used (44) to derive the last inequality. It follows that $Q \notin \mathcal{L}$. □

We remark that the sufficient conditions of Propositions 5.4 and 5.5, in general, are not implied by one another. Indeed, the instance in Example 5.2 satisfies only the sufficient condition of Proposition 5.4, whereas the instance in Example 5.3 satisfies only that of Propositon 5.5 with $i = 1$, $j = 2$, and $k = 3$.

Motivated by these sufficient conditions, let us define the following subset of $\mathcal{S}_1$.

$$\begin{aligned} \mathcal{S}_1' \;:=\; & \{Q \in \mathcal{S}_1 : V \neq \emptyset \text{ and } \nu(Q_{VV}) = \nu(Q)\} \cup \{Q \in \mathcal{S}_1 : \exists\, i \in U,\ \exists\, j \in V, \\ & \exists\, k \in V \text{ such that } j \neq k,\ Q_{ij} = Q_{ik} = \nu(Q),\ Q_{jk} < \nu(Q)\}. \end{aligned} \tag{45}$$

By Propositions 5.4 and 5.5, $\mathcal{S}_1' \subseteq \mathcal{L}_\infty$. Let us define

$$\mathcal{S}_1'' := \mathcal{S}_1 \backslash \mathcal{S}_1'. \tag{46}$$

Our next goal is to establish that the sufficent conditions of Propositions 5.4 and 5.5 completely describe the instances in $\mathcal{S}_1 \backslash \mathcal{L}$, i.e., $\mathcal{S}_1' = \mathcal{S}_1 \backslash \mathcal{L}$. We will prove this assertion by showing that $\mathcal{S}_1'' \subseteq \mathcal{L}$.

We now focus on instances of (StQP) for which $Q \in \mathcal{S}_1''$. For a given $Q \in \mathcal{S}_1''$, the following index sets will be useful.

$$W_1 := \{(j,k) : j \in V,\ k \in V,\ j \neq k, \quad Q_{jk} < \nu(Q)\}, \tag{47}$$

$$W_2 := \{(j,k) : j \in V,\ k \in V,\ j \neq k, \quad Q_{jk} \geq \nu(Q)\}. \tag{48}$$

For $Q \in \mathcal{S}_1''$, if $W_1 = \emptyset$, it follows from (43), (48), and (46) that $Q_{ij} \geq \nu(Q)$ for $1 \leq i \leq j \leq n$ and $Q_{kk} = \nu(Q)$ for some $k = 1, \ldots, n$. Therefore, $Q \in \mathcal{L}_0$ by Proposition 5.1, which implies that $Q \in \mathcal{L}$. We will henceforth assume that $W_1 \neq \emptyset$. In this case, it follows from (45) and (46) that

$$\beta_{ijk} := \max\{Q_{ij}, Q_{ik}\} > \nu(Q), \quad \text{for each } i \in U,\ (j,k) \in W_1. \tag{49}$$

We also define

$$\beta := \min_{i \in U;\ (j,k) \in W_1} \beta_{ijk} > \nu(Q), \quad \text{and} \quad \rho := \beta - \nu(Q) > 0. \tag{50}$$

For a given $Q \in \mathcal{S}_1''$, we will next 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

$$l_r(Q) = \frac{1}{(r+1)(r+2)} \min_{z \in \Theta_n^r} (z^T Q z - z^T \mathrm{diag}(Q)), \quad r = 0, 1, \ldots.$$

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

$$\begin{aligned} z^T Q z - z^T \mathrm{diag}(Q) &= \sum_{i \in U} \sum_{j \in U} Q_{ij} z_i z_j - \sum_{i \in U} Q_{ii} z_i + 2 \sum_{i \in U} \sum_{k \in V} Q_{ik} z_i z_k \\ &\quad + \sum_{j \in V} \sum_{k \in V} Q_{jk} z_j z_k - \sum_{j \in V} Q_{jj} z_j. \end{aligned} \tag{51}$$

Next, we will derive lower bounds on the terms on the right-hand side of (51). For a given $z \in \Theta_n^r$, let us define

$$\sum_{j \in V} z_j = \eta, \tag{52}$$

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

By (43),

$$\begin{aligned} \sum_{i \in U} \sum_{j \in U} Q_{ij} z_i z_j - \sum_{i \in U} Q_{ii} z_i &= \sum_{i \in U} Q_{ii} z_i (z_i - 1) + \sum_{i \in U} \sum_{j \in U \setminus \{i\}} Q_{ij} z_i z_j, \\ &\geq \nu(Q) \left(\left(\sum_{i \in U} z_i \right)^2 - \sum_{i \in U} z_i \right), \\ &= (r + 2 - \eta)(r + 1 - \eta) \nu(Q), \end{aligned} \tag{53}$$

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

Similarly,

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

By (47) and (48), we obtain the following lower bounds.

$$\sum_{j\in V}\sum_{k\in V} Q_{jk}z_jz_k - \sum_{j\in V} Q_{jj}z_j \geq \begin{cases} \nu(Q)\eta(\eta-1), & \text{if } z_jz_k = 0 \\ & \text{for all } (j,k)\in W_1, \\ \eta(\eta-1)l_{\eta-2}(Q_{VV}), & \text{otherwise,} \end{cases} \tag{54}$$

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

Finally,

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

Note that $Q_{ik} \geq \nu(Q)$ for each $i \in U$ and $k \in V$ by (43). 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 (50) for each $i \in U$. Therefore,

$$\sum_{i\in U}\sum_{k\in V} Q_{ik}z_iz_k \geq \begin{cases} (r+2-\eta)\left(\nu(Q)\eta+\rho\right), & \text{if } z_jz_k > 0 \\ & \text{for some } (j,k)\in W_1, \\ \nu(Q)(r+2-\eta)\eta, & \text{otherwise,} \end{cases} \tag{55}$$

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 (51) and (53),

$$z^TQz - z^T\text{diag}(Q) \geq (r+2)(r+1)\nu(Q). \tag{56}$$

Case 2: If $\sum_{j\in V} z_j = \eta = 1$, then it follows from (51), (53), (54), and (55) that

$$z^TQz - z^T\text{diag}(Q) \geq (r+2)(r+1)\nu(Q). \tag{57}$$

Case 3: If $\sum_{j\in V} z_j = \eta = r+2$, then $z_i = 0$ for each $i \in U$. By (51) and (54),

$$z^TQz - z^T\text{diag}(Q) \geq (r+2)(r+1)\min\{\nu(Q), l_r(Q_{VV})\}. \tag{58}$$

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 (51), (53), (54), and (55) that

$$z^TQz - z^T\text{diag}(Q) \geq (r+2)(r+1)\nu(Q). \tag{59}$$

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 (51), (53), (54), and (55),

$$z^TQz - z^T\text{diag}(Q) \geq (r+2-\eta)(r+1+\eta)\nu(Q) + \eta(\eta-1)l_{\eta-2}(Q_{VV}) + 2\rho(r+2-\eta). \tag{60}$$

It follows from the five cases above that

$$l_r(Q) \geq \min\left\{\nu(Q),\ l_r(Q_{VV}),\ \min_{\eta\in\{2,\ldots,r+1\}} h(Q,\eta,r)\right\}, \tag{61}$$

where

$$h(Q,\eta,r) := (1-\lambda_{\eta,r})\nu(Q) + \lambda_{\eta,r} l_{\eta-2}(Q_{VV}) + \frac{2\rho(r+2-\eta)}{(r+1)(r+2)}, \tag{62}$$

and

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

We next establish that the second and the third terms in (61) are at least as large as $\nu(Q)$ for all sufficiently large values of r.

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

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

By (45) and (46), we therefore have $\nu(Q_{VV}) > \nu(Q)$ for any $Q \in \mathcal{S}_1''$. Since $\lim_{r\to\infty} l_r(Q_{VV}) = \nu(Q_{VV})$, there exists $\hat{r} \in \mathbb{N}$ such that

$$l_r(Q_{VV}) \geq \nu(Q), \quad \text{for all } r > \hat{r}. \tag{63}$$

Therefore, the second term in (61) is at least as large as $\nu(Q)$ for all $r > \hat{r}$. Let us next focus on the third term in (61) for $r > \hat{r}$. Note that it suffices to consider only $\eta \in \{2,\ldots,\hat{r}+2\}$ for the range of the minimum since $h(Q,\eta,r) > \nu(Q)$ for all $\eta > \hat{r}+2$ by (63).

Let us now fix $\eta \in \{2, \dots, \hat{r}+2\}$ and consider the last term in (61) as a function of r. We claim that there exists $r_\eta \in \mathbb{N}$ such that

$$h(Q, \eta, r) \geq \nu(Q), \quad \text{for all } r \geq r_\eta, \tag{64}$$

where h is defined as in (62). 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 (64).

It follows from (63), (64), and (61) 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, $Q \in \mathcal{L}$.

5.4 Descriptions of $\mathcal{L}$ and $\mathcal{L}_\infty$

The following main result provides a complete description of the sets $\mathcal{L}$ and $\mathcal{L}_\infty$.

Theorem 5.1 *The following relations are satisfied:*

1. $\mathcal{L} = \mathcal{S}_1''$.

2. $\mathcal{L}_\infty = \mathcal{S}_1' \cup \mathcal{S}_2$.

where $\mathcal{S}_1', \mathcal{S}_1''$ and $\mathcal{S}_2$ are defined as in (45), (46), and (36), respectively.

For illustrative purposes, we present the following example.

Example 5.4 *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 5.3. On the other hand, for any $\rho > 0$, $Q(\rho) \in \mathcal{S}_1''$. Our computational experiments reveal that $Q(1) \in \mathcal{L}_5$ and $Q(0.1) \in \mathcal{L}_{48}$.

Example 5.4 illustrates that $\mathcal{L}$, in general, is not a closed set. Our next result gives a description of the closure of $\mathcal{L}$.

Proposition 5.6 *$cl(\mathcal{L}) = \mathcal{S}_1$.*

Proof. By Theorem 5.1 and (46), $\mathcal{L} \subseteq \mathcal{S}_1$. Note that $\mathcal{S}_1$ is a closed set by Proposition 5.2. Therefore, $\text{cl}(\mathcal{L}) \subseteq \mathcal{S}_1$.

Conversely, let $Q \in \mathcal{S}_1$. By Proposition 5.2, there exists some $i \in \{1, \ldots, n\}$ such that $e_i \in \Omega(Q)$. Let us define the following sequence.

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

Clearly, $\lim_{k\to\infty} Q_k = Q$. We will show that $Q_k \in \mathcal{L}$ for each $k = 1, 2, \ldots$. Let us fix k. Since $Q_k - Q \in \mathcal{N}$, $\nu(Q_k) \geq \nu(Q)$ by Lemma 3.1(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 $k = 1, 2, \ldots$. Since $e_i \in \Omega(Q)$, we have $Q_{ij} \geq \nu(Q)$ and $Q_{jj} \geq \nu(Q)$ for each $j = 1, \ldots, n$. By the definition of Q_k, $U = \{i\}$, $V = \{1, \ldots, n\}\backslash\{i\}$. We have

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

which implies that the condition of Proposition 5.4 cannot be satisfied. Since $(Q_k)_{ij} > \nu(Q)$ for each $j \in V$, the condition of Proposition 5.5 cannot be satisfied either. Therefore, $Q_k \notin \mathcal{S}_1'$, i.e., $Q_k \in \mathcal{S}_1''$. By Theorem 5.1, $Q_k \in \mathcal{L}$ for each $k = 1, 2, \ldots$. Therefore, $Q \in \text{cl}(\mathcal{L})$. □

By Proposition 5.6, $Q(0) \in \text{cl}(\mathcal{L})\backslash\mathcal{L}$ in Example 5.4. It is worth noticing 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 $n \geq 2$.

5.5 Description of $\mathcal{L}_r$

In this section, we give an algebraic description of the sets $\mathcal{L}_r$. In particular, our next result generalizes Proposition 5.1.

Theorem 5.2 *For any $r = 0, 1, \ldots$, $\mathcal{L}_r$ is given by the union of n polyhedral cones. More specifically, we have*

$$\mathcal{L}_r := \bigcup_{k=1}^{n} \mathcal{L}_r^k, \tag{65}$$

where

$$\mathcal{L}_r^k := \left\{ Q \in \mathcal{S} : Q_{kk} \leq \frac{1}{(r+1)(r+2)} \left(z^T Q z - z^T \, diag(Q) \right), \quad \text{for all } z \in \Theta_n^r \right\}, \tag{66}$$

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

Proof. Let us fix $r \in \mathbb{N}$ and let $Q \in \mathcal{L}_r$. By Corollary 5.1 and (33), $\mathcal{L}_r \subseteq \mathcal{S}_1$, which implies that

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

Therefore, $Q \in \mathcal{L}_r$ if and only if $Q \in \mathcal{L}_r^k$ for some $k \in \{1, \ldots, n\}$. Since Θ_n^r is a finite set, $\mathcal{E}_r^k$ is a polyhedral cone and the result follows. □

Recall that $\mathcal{L}_r^k$ is defined by $O(n^{r+2})$ inequalities for each $k = 1, \ldots, n$. Therefore, it follows from Theorem 5.2 that, for any fixed $r \in \mathbb{N}$, one can check in polynomial time if $Q \in \mathcal{L}_r$.

We next establish an interesting connection between the behavior of lower bounds and the stability number of a certain associated graph. By Proposition 5.1, $Q \in \mathcal{L}_0$ if and only if all the diagonal elements of the shifted matrix $Q^s \in \mathcal{N}$ given by (30) are equal to zero. Therefore, for each $Q \notin \mathcal{L}_0$, $\min_{k=1,\ldots,n} Q_{kk}^s > 0$ and Q^s has at least one off-diagonal entry which is equal to zero.

Given $M \in \mathcal{N}$, we define the sparsity graph G_M associated with M as follows. There are n vertices labeled $1, \ldots, n$ 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 5.7 *Let $Q \in \mathcal{S}\backslash\mathcal{L}_0$ and let $G = G_{Q^s}$ denote the sparsity graph of Q^s with stability number $\alpha(G)$. Then, $l_r(Q) = \min_{1 \le i \le j \le n} Q_{ij} < \nu(Q)$ for each $r = 0, 1, \ldots, \alpha(G) - 2$ and $l_r(Q) > \min_{1 \le i \le j \le n} Q_{ij}$ for each $r \ge \alpha(G) - 1$. Therefore,*

$$Q \notin \mathcal{L}_r, \quad r = 0, 1, \ldots, \alpha(G) - 2. \tag{67}$$

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

We now define the following two matrices.

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

Clearly, we have $Q_* \in \mathcal{N}$, $Q^* \in \mathcal{N}$, $Q^s - Q_* \in \mathcal{N}$, and $Q^* - Q^s \in \mathcal{N}$. By Lemma 3.1(iii),

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

Note that each of Q^* and Q_* is a positive multiple of $I + A_G$. By Lemma 3.1(iv), we have

$$\left(\min_{1 \le i \le j \le n : Q^s_{ij} > 0} Q_{ij} \right) l_r(I + A_G) \le l_r(Q^s) \le \left(\max_{1 \le i \le j \le n} Q^s_{ij} \right) l_r(I + A_G). \tag{68}$$

The assertion now follows directly from (19), (30), Lemma 3.1(v), and (21). The relation (67) follows immediately. □

Example 5.5 *Consider an instance of (StQP) in which*

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

is an $n \times n$ arrowhead matrix, where $n \ge 3$. It is easy to verify that $\nu(Q) = 1$ and $\Omega(Q) = \{e_1\}$. Therefore, $U = \{1\}$ and $V = \{2, \ldots, n\}$. By (45), (46), and Theorem 5.1, $Q \in \mathcal{L}$. We have $\alpha(G) = n - 1$, where $G = G_Q$ denotes the sparsity graph of Q. By Proposition 5.7, we have $l_r(Q) = \min_{1 \le i \le j \le n} Q_{ij} = 0$ for each $r = 0, 1, \ldots, n - 3$ and $l_r(Q) > 0$ for each $r \ge n - 2$. It follows that $Q \notin \mathcal{L}_r$ for each $r = 0, 1, \ldots, n - 3$.

5.6 Relations Among Different Sets

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

Proposition 5.8 *The following relations are satisfied:*

$$\mathcal{L}_0 \subseteq \mathcal{L}_1 \subseteq \ldots \subseteq \mathcal{L} \subseteq cl(\mathcal{L}) = \mathcal{S}_1 \subseteq \mathcal{U}_0 \subseteq \mathcal{U}_1 \subseteq \ldots \subseteq \mathcal{U} \subseteq cl(\mathcal{U}) = \mathcal{S}. \tag{69}$$

Proof. By Corollary 5.1, Proposition 5.2, and Proposition 4.1, we obtain $\mathcal{L} \subseteq \mathcal{S}_1 \subseteq \mathcal{U}_0$ since $\{e_1, \ldots, e_n\} \subseteq \Delta_n^0$. The last equality follows from Corollary 4.2. The remaining inclusions follow from the definitions (29), (33), (23), and (26). □

It is worth noticing the significant difference between the sets $\mathcal{L}$ and $\mathcal{U}$. For any $n \geq 2$, while $\mathrm{cl}(\mathcal{L})$ is strictly contained in the set $\mathcal{U}_0$, which is the smallest set in the sequence of the sets $\mathcal{U}_r$, we have $\mathrm{cl}(\mathcal{U}) = \mathcal{S}$.

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:

$$\mathcal{E}_r := \{Q \in \mathcal{S} : l_r(Q) = u_r(Q)\} = \mathcal{L}_r \cap \mathcal{U}_r = \mathcal{L}_r, \quad r = 0, 1, \ldots, \tag{70}$$

where the last equality follows from Proposition 5.8. Therefore, the algebraic description of such instances are precisely given by Theorem 5.2.

6 Concluding Remarks

In this paper, we investigated the sequences of copositive optimization based upper and lower bounds on the optimal value of a standard quadratic optimization problem. We gave a complete description of the instances for which the upper and/or the lower bound is 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.

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 $\mathcal{C}$ of completely positive matrices are given by rank one matrices xx^T, where $x \in \mathbb{R}_+^n \backslash \{0\}$ (see, e.g., [1]). It follows that the set of extreme rays of $\mathcal{I}_r$ is a subset of the set of extreme rays of $\mathcal{C}$. On the other hand, the outer polyhedral approximations $\mathcal{O}_r$ are generated by the matrices $(1/((r+1)(r+2))(zz^T - \text{Diag}(z))$, where $z \in \Theta_n^r$. For $z = (r+2)e_i \in \Theta_n^r$, the corresponding matrix is given by $e_i(e_i)^T$, $i = 1, \ldots, n$, which are also extreme rays of $\mathcal{C}$. However, for each $z \in \Theta_n^r \backslash \{(r+2)e_i : i = 1, \ldots, n\}$, it is easy to construct a $w \in \mathbb{R}^n \backslash \{0\}$ such that $w^T z = 0$ and $\langle zz^T - \text{Diag}(z), ww^T \rangle < 0$, which implies that $zz^T - \text{Diag}(z) \notin \mathcal{C}$. Together with our analysis, this observation suggests that a few faces of $\mathcal{O}_r$ in fact coincide with those of $\mathcal{C}$ whereas most of the faces of $\mathcal{O}_r$ do not support the cone $\mathcal{C}$. Our results, combined with the recent progress on the facial structure of the cone $\mathcal{C}$ (see, e.g., [11, 9]), may serve as a basis for the construction of tighter polyhedral outer approximations.

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