EFFICIENT AND CHEAP BOUNDS FOR (STANDARD) QUADRATIC OPTIMIZATION[1]

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ABSTRACT

A standard quadratic optimization problem (StQP) consists in minimizing a quadratic form over a simplex. A number of problems can be transformed into a StQP, including the general quadratic problem over a polytope and the maximum clique problem in a graph.

In this paper we present several polynomial-time bounds for StQP ranging from very simple and cheap ones to more complex and tight constructions. The main tools employed in the conception and analysis of most bounds are Semidefinite Programming and decomposition of the objective function into a sum of two quadratic functions, each of which is easy to minimize.

We provide a complete diagram of the dominance, incomparability, or equivalence relations among the bounds proposed in this and in previous works. In particular, we show that one of our new bounds dominates all the others. Furthermore, a specialization of such bound dominates Schrijver's improvement of Lovász's θ function bound for the maximum size of a clique in a graph.

Key Words: standard quadratic optimization, Semidefinite Programming, Quadratic Programming, maximum clique, resource allocation.

1 Introduction

A standard quadratic optimization problem (StQP) consists of finding (global) minimizers of a quadratic form over the standard simplex, i.e., we consider an optimization problem of the form

$$\ell_Q = \min \left\{ x^\top Q x : x \in \Delta \right\} \;, \tag{1}$$

where Q belongs to the class $\mathcal{M}$ of symmetric $n \times n$ matrices; a $^\top$ denotes transposition; and Δ is the standard simplex in the n-dimensional Euclidean space $\mathbb{R}^n$:

$$\Delta = \{x \in \mathbb{R}^n : e^\top x = 1,\ x \geq o\},$$

where $e = [1, \dots, 1]^\top \in \mathbb{R}^n$.

Note that a non homogeneous quadratic function $x^\top Ax + 2c^\top x$ over Δ can be easily homogenized by considering the rank-two update $Q = A + ec^\top + ce^\top$ in (1). Indeed, $x^\top(A + ec^\top + ce^\top)x = x^\top Ax + 2c^\top x$ over Δ.

While problem (1) seems to be a very special Quadratic Program (QP), it actually retains most of the complexity of the general case where Δ is replaced by any polyhedron P. Indeed, it is well known that (1) is NP-hard.

Furthermore, as shown in Sections 1.2 and 1.3 below, every Quadratic Program with a bounded feasible region can be reformulated as a Standard QP in higher dimension, or relaxed to a Standard QP in the same dimension.

Finally, Bomze also showed that *global* optimality of local solutions of general Quadratic Programs can be characterized by a finite number of copositivity conditions (in fact, not more than the number of non-binding constraints plus one) over polyhedral cones. These copositivity conditions in turn can be reformulated into Standard QPs (generally, in higher dimensions). For details see, e.g., [5] and the references therein.

An important tool for many exact or approximate solution methods for optimization problems is the availability of good and/or efficiently computable bounds on the optimum value of the problem. This well-known fact has induced some authors to propose a number of bounds for the Standard Quadratic Problem [1, 6, 9, 10, 12, 15, 29, 32]. However, in most cases no relation has been provided among the proposed bounds.

In this paper we present several new bounds for StQP and establish dominance, incomparability, or equivalence relations among them, as well as with respect to other previously introduced bounds. In particular, we show that one of our new bounds dominates all the others.

Furthermore, a specialization of such bound dominates Schrijver's improvement of Lovàsz's θ function bound for the maximum size of a clique in a graph.

The paper is organized as follows: after introducing some notation, we describe in more detail some relations between the Standard QP and the general QP. We also illustrate a reformulation of the Quadratic Resource Allocation Problem (including the portfolio selection problem) as a Standard QP, and we describe some connections of StQP with the maximum (weight) clique problem in a graph. Section 2 presents some cheap closed-form bounds while Sections 3, 4 and 5 are devoted to Lagrangian bounds, Convex Underestimation bounds, and Nowak's bound, respectively. Section 6 deals with Copositive bounds, and Section 7 introduces Decomposition bounds. In Section 8, we establish the relations between the previously discussed bounds,while Sections 9 and 10 return to the applications sketched in the Introduction.

1.1 Notation and cones of matrices

We now introduce some notation and present the cones of matrices that will be used in the sequel.

Let A, B $n \times n$ symmetric matrices (i.e., $A, B \in \mathcal{M}$). Recall that the *trace* of a matrix is the sum of its diagonal elements, and that for $A, B \in \mathcal{M}$

$$A \bullet B = \operatorname{trace}(AB) = \sum_{ij} a_{ij} b_{ij}$$

is the standard inner product in $\mathcal{M}$.

If v is a vector in $\mathbb{R}^n$, we denote by Diag (v) the diagonal $n \times n$ matrix A with $a_{ii} = v_i$, for $i = 1, \ldots, n$. Conversely, for an $n \times n$ matrix A, diag (A) denotes the n-dimensional vector formed by the diagonal elements of A. Furthermore, Ddiag (A) denotes the matrix obtained from A by replacing all the off-diagonal entries with 0, i.e., Ddiag $(A) =$ Diag (diag (A)). Note that we have $v^\top \operatorname{diag}(A) = \operatorname{Diag}(v) \bullet A$. We denote by $I_n = \operatorname{Diag}(e)$ the $n \times n$ identity matrix and its ith column (the standard basis vector) by e^i. Further, let $E^{ij} = \frac{1}{2}\left[e^i(e^j)^\top + e^j(e^i)^\top\right] \in \mathcal{M}$ be the matrix all entries of which are zero with the exception of two entries $(E^{ij})_{ij} = (E^{ij})_{ji} = \frac{1}{2}$ if $i \neq j$ while $E^{ii} = \operatorname{Diag}(e^i)$.

In addition to the cone $\mathcal{M}$ of symmetric matrices we will use the following smaller convex cones:

- the cone $\mathcal{P}$ of all positive semidefinite symmetric matrices;
- the cone $\mathcal{N}$ of all nonnegative symmetric matrices;

- the cone $\mathcal{P} \cap \mathcal{N}$ of *doubly nonnegative* matrices;
- the cone of *copositive* matrices
  $\mathcal{C} = \{C \in \mathcal{M} : x^\top C x \geq 0 \text{ for all } x \in \mathbb{R}^n_+\}$;
- the cone of *completely positive* matrices
  $\mathcal{C}^* = \{D \in \mathcal{M} : D = YY^\top,\ Y \text{ some } n \times k \text{ matrix with } Y_{ij} \geq 0,\ \text{all } i, j\}$.

On the set $\mathcal{M}$ of symmetric matrices we will use both the standard partial order $\leq$ defined by componentwise inequalities, i.e., $A \geq B$ whenever $a_{ij} \geq b_{ij}$ for all i and j, and the Löwner partial order $\succeq$ induced on $\mathcal{M}$ by the cone $\mathcal{P}$ of positive semidefinite matrices. Thus we write $A \succeq B$ whenever $A - B \in \mathcal{P}$.

Recall that the (convex) dual cone of a cone $\mathcal{K}$ of matrices with respect to the standard inner product of $\mathcal{M}$ is the cone

$$\mathcal{K}^* = \{Y \in \mathcal{M} : X \bullet Y \geq 0, \text{ for all } X \in \mathcal{K}\}.$$

It is well known that the completely positive cone is the dual of the copositive cone (which justifies the notation $\mathcal{C}^*$), and that the nonnegative and semidefinite cones are self-dual with respect to this inner product.

Recall also that

$$\mathcal{K}_0 = \mathcal{P} + \mathcal{N}$$

is a (zero-order) inner approximation [10] of the copositive cone: $\mathcal{K}_0 \subseteq \mathcal{C}$, with $\mathcal{K}_0 = \mathcal{C}$ if and only if $n \leq 4$ [14]. As $\mathcal{N}^* = \mathcal{N}$ and $\mathcal{P}^* = \mathcal{P}$, we then have

$$\mathcal{C}^* \subseteq \mathcal{K}_0^* = (\mathcal{P} + \mathcal{N})^* = \mathcal{P} \cap \mathcal{N}.$$

1.2 StQP formulation of a general QP over a polytope

If the vertices of a polytope P are known, then the problem of minimizing a function over P can be easily transformed into the problem of minimizing a function on the standard simplex Δ with the change of variables $x = Vy$, where V is the matrix whose column vectors are the vertices $v^1, \ldots, v^N$ of P.

Clearly the transformed problem might have a number of variables that is exponential with respect to the original one. Nevertheless, by means of the above transformation, several theoretical and algorithmic results for StQP can be applied to the problem of minimizing a quadratic function on a more general polytope. In Section 10.1 we use this remark to provide some bounds for the minimum of a quadratic function on the unit ball in the ℓ^1 norm, improving an SDP bound proposed by Nesterov [30] for this problem.

1.3 StQP relaxation of bounded Quadratic Programs

Consider the Quadratic Program

$$\min\{y^\top Cy + 2c^\top y : \; y \in P\} \tag{2}$$

where $P = \{y \in \mathbb{R}^n : Ay = b, \; y \geq o\}$, and A is an $m \times n$ matrix. If P is bounded and $P \neq \{o\}$, there are a vector $p \geq e$ and a number $\pi > 0$ - which can both be obtained by solving a single LP of the size of A - such that P is contained in the intersection of the hyperplane $p^\top y = \pi$ and of the non-negative orthant (see Section 10.2 for details). Thus, by setting

$$D = \pi(\mathrm{Diag}\; p)^{-1} \quad \text{and} \quad Q = DCD + Dce^\top + ec^\top D, \tag{3}$$

we obtain that the Standard QP (1) is a valid relaxation of (2). This obviously implies that any valid lower bound for (1) is also a valid lower bound for (2). This fact will be used in Section 10.2 to provide lower bounds for a general QP with a bounded feasible region.

1.4 Quadratic Resource Allocation and Portfolio Optimization

Given n activities using a common resource R with intensities $a_1, \ldots, a_n$, a *resource allocation problem* consists in finding the levels $x_1, \ldots, x_n$ of these activities that maximize a utility function $f(x_1, \ldots, x_n)$ (see, e.g., [23]). This problem can be formulated as follows

$$\max\left\{f(x) : a^\top x \leq R, \; x \geq o\right\} . \tag{4}$$

Note that a simple scaling of the variables, like in Section 1.3, and the introduction of an additional slack variable allows to transform the constraints of this problem into the form $x \in \Delta$, so that a resource allocation problem with a quadratic utility function is essentially a StQP.

In many applications the utility function f is assumed to be a separable convex function, which considerably simplifies the problem. However, some non-separable and non-convex models are also needed in some cases. An important example is the familiar (Markowitz) mean/variance portfolio selection problem (see, e.g. [26, 27]), which can be formalized as follows: suppose there are n securities to invest in, at an amount expressed in relative shares $x_i \geq 0$ of an investor's budget. Thus, the budget (resource allocation) constraint reads $e^\top x = 1$, and the set of all feasible portfolios is given by Δ. Now, given the expected return m_i of security i during the forthcoming period, and an $n \times n$ covariance matrix

C across all securities, the investor faces the multiobjective problem to maximize expected return $m^\top x$ and simultaneously minimize the risk $x^\top Cx$ associated to her decision x.

One of the most popular approaches to such type of problems is that the user prespecifies a parameter β which in her eyes balances the benefit of high return and low risk. This leads to the parametric QP

$$\max \left\{ f_\beta(x) = m^\top x - \beta x^\top Cx : x \in \Delta \right\} . \tag{5}$$

Note that, for fixed β, this is again a Standard QP.

In theory the matrix C is, as an exact covariance matrix, positive semidefinite (and it could be singular in many applications, see [27]), so that (5) is a convex problem. On the other hand, securities usually are highly correlated, and in time-series analysis one frequently encounters the situation that some of the most reliable estimators $\tilde{C}$ of the unknown covariance matrix C lack semidefiniteness properties [31], [35, pp.134 ff]. Hence, the portfolio optimization problem can be transformed into a (possibly non-convex) parametric Standard QP. Furthermore, Best and Ding [2] show how to reduce the parametric problem to a *single* Standard QP with indefinite Q under some assumptions.

1.5 StQP formulation of the maximum weight clique problem

Consider an undirected graph $\mathcal{G} = (N, \mathcal{E})$ with n nodes. A *clique* S is a subset of the *node set* N which induces a complete subgraph of $\mathcal{G}$ (i.e., any pair of nodes in S is joined by an edge in $\mathcal{E}$, the *edge set*). A clique S is *maximal* if there is no larger clique containing S. A (maximal) clique is a *maximum* clique if it has the largest number of elements among all cliques. In the weighted case we associate weights $w_i > 0$ to the nodes, and define a (separable) *weight function* $W(S) = \sum_{i \in S} w_i$ on the subsets S of nodes. A *maximum weight clique* is then a clique that maximizes the weight function $W(S)$ among all cliques of the graph.

Motzkin and Straus [28] were the first to observe that the maximum clique problem can be formulated as a very special (non-convex) Standard QP. This obviously implies NP-hardness of the general StQP. The StQP formulation of the maximum clique problem has been extended to the weighted case in [18] by exploiting an idea of Lovász. Tardella [40] showed that the same result can also be derived as a consequence of an extension of the Fundamental Theorem of Linear Programming, and proved, in addition, a somewhat converse relation. Indeed, it is shown in [40] that the StQP (1) can be solved by finding a maximal clique in an associated graph that maximizes a suitable non-separable weight function $\widetilde{W}(S)$. Recently, Pavan and Pelillo described a similar reduction of a non-standard maximum weight clique problem used for clustering and image segmentation to StQP [33]. These relations can be obviously exploited to transform results (and, in particular bounds) for Standard QPs into results for the maximum (weight) clique problem, and conversely (see Section 9).

In order to describe the relation between the maximum weight clique problem and the Standard QP we need to introduce a subset of the class $\mathcal{M}$ of symmetric matrices called the Motzkin-Straus class of matrices $\mathcal{M}(w,\mathcal{G})$ associated to a graph $\mathcal{G}=(N,\mathcal{E})$ and a vector w in $\mathbb{R}^n$ with $w_i>0$ for all i. We define

$$\mathcal{M}(w,\mathcal{G}) = \{B \in \mathcal{M} : b_{ij} \geq \tfrac{b_{ii}+b_{jj}}{2}, \text{ if } \{i,j\} \notin \mathcal{E}\,; b_{ij}=0, \text{ if } \{i,j\} \in \mathcal{E}\,; \text{ and } b_{ii} = \tfrac{1}{w_i}, \text{ for } i \in N\}\,. \tag{6}$$

In [18] it is shown that the StQP (1) attains the same optimal value for every Q in $\mathcal{M}(w,\mathcal{G})$ and that the inverse of this value coincides with the value of a maximum weight clique on the graph $\mathcal{G}$ with weights w on the nodes, i.e.,

$$\ell_Q = \min\left\{x^\top Qx : x \in \Delta\right\} = 1/W(S^*) \quad \text{for all } Q \in \mathcal{M}(w,\mathcal{G})\,, \tag{7}$$

where S^* is a maximum weight clique of $\mathcal{G}$. Regularization techniques, i.e., modifying the class $\mathcal{M}(w,\mathcal{G})$ may be necessary to extract such an S^* from the solution of (7), see [4].

In the special case where $E=ee^\top$ is the matrix with all ones and $A_\mathcal{G}$ is the node-node adjacency matrix of the graph $\mathcal{G}$, we have $E-A_\mathcal{G} \in \mathcal{M}(e,\mathcal{G})$. Thus, the size $\omega(\mathcal{G})$ of a maximum clique (the *clique number*) of $\mathcal{G}$ is given by

$$\omega(\mathcal{G}) = 1/\ell_{E-A_\mathcal{G}}\,, \tag{8}$$

which is a reformulation of the classical result of Motzkin and Straus [28].

2 Cheap closed-form bounds

Here we describe some basic properties of ℓ_Q and we present two lower bounds that have a simple closed-form representation and can be computed efficiently in $\mathcal{O}(n^2)$ time.

Consider again the all-ones matrix $E=ee^\top$. It is immediate to verify that the minimum ℓ_Q is *shift-equivariant* on $\mathcal{M}$ with respect to E, i.e., we have

$$\ell_{Q+tE} = \ell_Q + t \quad \text{for all } t \in \mathbb{R}.$$

Hence we may and do always assume in the sequel that no entry of Q is negative.

It is straightforward to verify that the minimum ℓ_Q is isotone with respect to both the standard and the Löwner partial orders. In other words if $Q \geq Q'$ or $Q \succeq Q'$ then $\ell_Q \geq \ell_{Q'}$.

Note that every diagonal element of Q is an upper bound for ℓ_Q since $e^i \in \Delta$ and $(e^i)^\top Q\, e^i = q_{ii}$. In the case where Q is a nonnegative diagonal matrix the minimum ℓ_Q has a simple closed-form expression:

$$\ell_Q = \left(\sum_i q_{ii}^{-1} \right)^{-1} .$$

In particular, with the standard extensions $1/0 = \infty$, $t + \infty = \infty$, and $1/\infty = 0$, we have that if $q_{ii} = 0$ for some i, then $\ell_Q = 0$.

From shift-equivariance we immediately deduce that for a matrix Q which has all off-diagonal elements equal to a value $m \leq \min_i q_{ii}$ we have the closed-form expression

$$\ell_Q = m + \left[\sum_i (q_{ii} - m)^{-1} \right]^{-1} . \tag{9}$$

From these preliminary observations we easily derive our first closed-form bounds.

$$\ell_Q^0 = \min_{i,j} q_{ij} \quad \text{and} \quad \ell_Q^{\text{ref}} = \ell_Q^0 + \left[\sum_i (q_{ii} - \ell_Q^0)^{-1} \right]^{-1} ,$$

Lemma 1 *Let $k > 0$, $i \neq j$, and let R be a symmetric matrix with all the off-diagonal entries equal to a value $m < \min_i r_{ii}$. Consider the matrix $R' = R + kE^{ij}$. Then $\ell_{R'} > \ell_R$.*

Proof. By shift-equivariance we can assume, w.l.o.g., that $m = 0$ so that R is a positive-definite diagonal matrix. Therefore the only solution of the strictly convex program defining ℓ_R is given by $x = (e^\top R^{-1} e)^{-1} R^{-1} e$ which is strictly positive. Hence $y^\top R y > x^\top R x = \ell_R$ for all $y \in \Delta \setminus \{x\}$. Next, let $y \in \Delta$ satisfy $y^\top R' y = \ell_{R'}$. If $y_i y_j = 0$, then $y \neq x$ so that $\ell_{R'} = y^\top R' y = y^\top R y > x^\top R x = \ell_R$. On the other hand, if $y_i y_j > 0$, then again $\ell_{R'} = y^\top R' y = y^\top R y + \frac{k}{2} y_i y_j > y^\top R y \geq \ell_R$, and the result follows. □

Theorem 1 *For any $Q \in \mathcal{M}$ we have*

$$\ell_Q^0 \leq \ell_Q^{\text{ref}} \leq \ell_Q.$$

The equality $\ell_Q^0 = \ell_Q^{\rm ref}$ holds if and only if a minimum entry of Q is located on the main diagonal, which is also equivalent to $\ell_Q^0 = \ell_Q$. Furthermore, $\ell_Q^{\rm ref} = \ell_Q$ if and only if all the off-diagonal entries of Q are equal to the value ℓ_Q^0.

Proof. The first inequality, $\ell_Q^0 \le \ell_Q^{\rm ref}$, is trivial. Now put

$$Q' = \mathrm{Ddiag}\,(Q) + \ell_Q^0 (E - I_n)\,.$$

Then the second inequality follows from the isotonicity of ℓ_Q, the matrix inequality $Q' \le Q$, and the closed-form expression (9). Next we characterize the cases where one of the cheap bounds is exact. If $q_{ii} = \min_{ij} q_{ij}$, then $q_{ii} = \ell_Q^0 \le \ell_Q \le {e^i}^\top Q\, e^i = q_{ii}$. Hence $\ell_Q^0 = \ell_Q$. Conversely, if $\ell_Q^{\rm ref} = \ell_Q$, then $\left[\sum_i (q_{ii} - \ell_Q^0)^{-1}\right]^{-1} = 0$, so that $q_{ii} = \ell_Q^0 = \ell_Q$ for some index i. Further, if all the off-diagonal entries of Q are equal to m and $m \ge \min_i q_{ii}$ then we have $\ell_Q^0 = \ell_Q$, which clearly implies $\ell_Q^{\rm ref} = \ell_Q$. On the other hand, if $m < \min_i q_{ii}$, then $\ell_Q^{\rm ref} = \ell_Q$ follows immediately from the closed-form expression (9). Assume now that $\ell_Q^{\rm ref} = \ell_Q$. Then $\ell_{Q'} = \ell_{Q'}^{\rm ref} = \ell_Q^{\rm ref} = \ell_Q$. If $q_{ij} > \ell_Q^0$ for some $i \ne j$ then the matrix $Q'' = Q' + (q_{ij} - \ell_Q^0) E^{ij}$ satisfies $Q' \le Q'' \le Q$ and, by Lemma 1, $\ell_{Q'} < \ell_{Q''}$. This contradicts the equality $\ell_{Q'} = \ell_Q$. Hence all off-diagonal entries of Q must coincide with ℓ_Q^0. $\Box$

Note that the simple bound ℓ_Q^0 has already been identified, e.g., in [29]. However, the refined bound $\ell_Q^{\rm ref}$, which can be computed with only $\mathcal{O}(n)$ additional operations, seems to be new. The two bounds tend to coincide when the dimension n increases. More precisely, the following inequalities hold:

$$\ell_Q^0 + \tfrac{1}{n}\left(\min_k q_{kk} - \ell_Q^0\right) \;\le\; \ell_Q^{\rm ref} \;\le\; \ell_Q^0 + \tfrac{1}{n}\left(\max_k q_{kk} - \ell_Q^0\right)\,.$$

In particular, when all the diagonal entries are equal we have

$$\ell_Q^{\rm ref} \;=\; \ell_Q^0 + \tfrac{1}{n}\left(q_{kk} - \ell_Q^0\right)\,.$$

Nesterov [29, Theorem 2] obtained the following simple closed-form lower bound for ℓ_Q which can also be computed with $\mathcal{O}(n^2)$ operations:

$$\ell_Q^{\rm Ne} = \min_{i,j}\left(q_{ij} + \tfrac{1}{2}(q_{ii} + q_{jj})\right) - \max_k q_{kk}\,. \tag{10}$$

Proposition 1 *The bound defined in (10) is dominated by ℓ_Q^0:*

$$\ell_Q^{\rm Ne} \le \ell_Q^0\,.$$

Proof. The assertion follows immediately from $\frac{1}{2}(q_{ii}+q_{jj}) \le \max_k q_{kk}$. $\square$

3 Lagrangian bounds

The general form of the Lagrange function for (1) is

$$L(x;\nu,u) = x^\top Qx + \nu(1-e^\top x) - u^\top x\,,$$

where $u \in \mathbb{R}^n_+$ and $\nu \in \mathbb{R}$. However, if Q is not positive semidefinite, then

$$\Theta(\nu,u) = \inf\{L(x;\nu,u) : x \in \mathbb{R}^n\} = -\infty$$

for all $(\nu,u) \in \mathbb{R}\times\mathbb{R}^n_+$, so that we are faced with an infinite duality gap, and Lagrange bounds are useless. Similarly, if Q is not positive semidefinite over the hyperplane $e^\perp$, then

$$\Theta_0(u) = \inf\left\{L(x;0,u) = x^\top Qx - u^\top x : x - \tfrac{1}{n}e \in e^\perp\right\} = -\infty\,,$$

and we face the same unfavorable phenomenon. See Section 5 for detailed investigation of convexity over the hyperplane $e^\perp$, wherefrom it can also be easily derived that $Q + tE \notin \mathcal{P}$ for all $t \in \mathbb{R}$, if Q is not positive semidefinite over the hyperplane $e^\perp$, see (17). Thus, also these useless bounds are trivially shift-equivariant.

So the only option for Lagrange approach remains

$$\bar\Theta(\nu) = \inf\left\{L(x;\nu,o) = x^\top Qx + \nu(1-e^\top x) : x \in \mathbb{R}^n_+\right\}\,. \tag{11}$$

We now show that with respect to this dualization, the duality gap is zero regardless of convexity of the objective function:

Theorem 2 *Suppose that Q contains only positive entries. Then for $\bar\Theta$ as in (11), we obtain*

$$\bar\Theta(\nu) = \begin{cases} \nu & \text{if } \nu \le 0\,,\\ \nu - \frac{1}{4\ell_Q}\nu^2 & \text{if } \nu > 0\,, \end{cases} \tag{12}$$

Hence $\max\left\{\bar\Theta(\nu) : \nu \in \mathbb{R}\right\} = \ell_Q$, *and the duality gap is zero.*

Proof. Obviously, for $\nu \le 0$ we obtain $\bar\Theta(\nu) = L(o;\nu,o) = \nu$ by the assumed relation $Q \in \mathcal{N}$. On the other hand, for $\nu > 0$ we get

$$\bar\Theta(\nu) = \nu\left[\min\left\{h(x) = \tfrac{1}{2}x^\top Cx - e^\top x : x \in \mathbb{R}^n_+\right\} + 1\right]\,,$$

where $C = \frac{2}{\nu} Q \in \mathcal{N}$ is strictly copositive. The minimum of h over $\mathbb{R}^n_+$ is attained as a consequence of the Frank-Wolfe theorem (see, e.g., [17]) and, according to Theorem 5 of [4], it takes the value

$$\underline{h}(\nu) = -\left[2\ell_C\right]^{-1} = -\left[\frac{4\ell_Q}{\nu}\right]^{-1} = -\frac{\nu}{4\ell_Q}\,.$$

Hence $\bar{\Theta}(\nu) = \nu\underline{h}(\nu) + \nu = \nu - \frac{1}{4\ell_Q}\nu^2$ if $\nu > 0$, so that we arrive at the form given in (12). Therefore

$$\max\left\{\bar{\Theta}(\nu) : \nu \in \mathbb{R}\right\} = 2\ell_Q - \frac{4\ell_Q^2}{4\ell_Q} = \ell_Q\,,$$

and the result follows. □

Thus the dual Lagrange function $\bar{\Theta}$ is a smooth and (piecewise) quadratic function with curvature proportional to ℓ_Q^{-1}, hence involving the unknown optimal value (and, with exception of its maximum, *not* shift-equivariant). Hence, neither this variant is of any use. Let us note here that [15] considers a wide class of non-convex problems (with possibly positive, finite duality gap) where Lagrangian bounds always are better than convex underestimation bounds, with which we deal in the next subsection.

4 Convex underestimation bounds

Let us again assume that Q has no negative entries. A common method to obtain efficiently computable lower bounds prescribes to use a quadratic convex underestimator $x^\top Sx$ of the function $x^\top Qx$ over Δ. This means that the quadratic form $x^\top Tx$ with $T = Q - S$ takes only non-negative values over Δ, which is equivalent to stipulate that T be copositive. Then, a convex underestimation bound is nothing else than ℓ_S. It is natural to ask if and how can we find the best, i.e., greatest, convex underestimation bound for ℓ_Q. However, the answer to such questions is disappointingly trivial: the best convex underestimation bound is exactly ℓ_Q and is attained by the (constant) convex quadratic form $x^\top Sx$, with $S = \ell_Q E$.

However, the quest for the best convex underestimator can be made much more interesting if we add the restriction that such underestimator should coincide with the original quadratic form $x^\top Qx$ on the vertices of its domain Δ. This additional assumption is based on the consideration that a good convex underestimator should be as close as possible to the original function. In particular, we recall that any function coincides with its *convex envelope* (i.e., its highest convex underestimator) at all vertices of a polyhedral domain (see, e.g. [38]. This also follows from the characterization of convex envelopes in [36, p. 36]).

Thus we define the best (quadratic) convex underestimation bound as follows:

$$\ell_Q^{\rm conv} = \sup\{\ell_S : S \in \mathcal{P}\,,\ Q - S \in \mathcal{N}\,,\ {\rm diag}\,(S) = {\rm diag}\,(Q)\} \qquad (13)$$

(note that any copositive T with diag $(T) = o$ automatically belongs to $\mathcal{N}$, as follows from $2t_{ij} = x^\top T x \geq 0$ for $x = e^i + e^j \in \mathbb{R}^n_+$).

Note that the best convex underestimation bound in the sense of (13) can be obtained in polynomial time by solving a semidefinite program. However, shift-equivariance of $\ell_Q^{\rm conv}$ is not immediate from (13). This property will be established – at least over a shift region for t which ensures $Q + tE \in \mathcal{N}$ – in Section 7.2 by exploiting the coincidence of $\ell_Q^{\rm conv}$ with other bounds.

5 Nowak's bound

It is interesting to investigate what happens if we replace the condition $S \succeq 0$ with the requirement that the function $f_S(x) = x^\top S x$ be convex over the hyperplane $\frac{1}{n}e + e^\perp = \left\{x \in \mathbb{R}^n : e^\top x = 1\right\}$ or, equivalently, over Δ. This approach has been suggested by Nowak [32] who observed (see Lemma 2 in [32]) that $f_S(x) = x^\top S x$ is convex over Δ iff the $(n-1)\times(n-1)$ matrix $\Phi(S)$ defined by $\Phi(S)_{ij} = S_{ij} + S_{nn} - S_{in} - S_{nj}$ is psd.

Nowak's bound is defined as follows:

$$\ell_Q^{\rm No} = \ell_W = \min_{x\in\Delta} x^\top W x\,, x^\top (Q - W)x, \qquad (14)$$

where $W = S$ is a solution of the SDP

$$\min\{E \bullet (Q - S) : S \in \mathcal{M}\,,\ \Phi(S) \succeq 0\,,\ Q - S \in \mathcal{N}\,,\ {\rm diag}\,(S) = {\rm diag}\,(Q)\}\ . \qquad (15)$$

From $\Phi(S + tE) = \Phi(S)$ for all $t \in \mathbb{R}$ it is easy to derive that $\ell_Q^{\rm No}$ is shift-equivariant.

Note that Nowak's bound is related to the convex underestimation bound and seems to improve upon it because of the weaker requirement $\Phi(S) \succeq 0$ instead of $S \succeq 0$. However, we will show in Sections 7.2.2 and 8.6 that Nowak's bound is actually strictly dominated by the convex underestimation bound and by two other equivalent bounds, which can also be obtained with semidefinite programming.

Nowak's transformation Φ is a special case of the following transformation frequently used in the study of Euclidean Distance Matrices (EDM), see, e.g. [19]: fix an arbitrary $v \in \frac{1}{n}e + e^\perp$, i.e., suppose $v^\top e = 1$. Define $P_v = I_n - ve^\top$ and $\Phi_v(S) = P_v^\top S P_v$. Then Nowak's Φ coincides with Φ_v for $v = [0, \ldots, 0, 1]^\top \in \mathbb{R}^n$ (it does not matter that Nowak drops the last row and column of $\Phi(S)$; it could be preferable to choose $v = \frac{1}{n}e$ which renders $P_v = I_n - \frac{1}{n}E$ symmetric – the orthoprojector onto $e^\perp$ – and Φ_v an orthoprojector onto $E^\perp$ w.r.t. $\bullet$).

For later use, we collect some general properties of the map $\Phi_v : \mathcal{M} \to \mathcal{M}$ in the following Lemma.

Lemma 2 *Suppose $v^\top e = 1$ and define $\Phi_v(S) = P_v^\top S P_v$ with $P_v = I_n - ve^\top$. Then $\Phi_v(\mathcal{P}) \subset \mathcal{P}$ and*

$$\Phi_v(S) \in \mathcal{P} \quad \textit{if and only if} \quad \textit{the map } x \mapsto x^\top S x \textit{ is convex over } \Delta\,. \tag{16}$$

Further, for $\Phi_v^{-1}(\mathcal{P}) = \{S \in \mathcal{M} : \Phi_v(S) \succeq 0\}$ we get

$$\Phi_v^{-1}(\mathcal{P}) = \mathcal{P} + \mathit{ker}\ \Phi_v\,,$$

where $\mathit{ker}\ \Phi_v = \{S \in \mathcal{M} : \Phi_v(S) = 0\}$. Finally,

$$\mathit{ker}\ \Phi_v = \mathcal{M} - \Phi_v(\mathcal{M}) = \{ec^\top + ce^\top - (c^\top v)E : c \in \mathbb{R}^n\} \supset \mathbb{R}E\,. \tag{17}$$

Proof. The inclusion $\Phi_v(\mathcal{P}) \subset \mathcal{P}$ is obvious by construction of Φ_v. Assertion (16) is shown, e.g., in [19]. As $P_v^2 = P_v$, also $\Phi_v^2 = \Phi_v$, so that $\ker\ \Phi_v = \mathcal{M} - \Phi_v(\mathcal{M})$ because of $S = S - \Phi_v(S) + \Phi_v(S)$. From this and from $\Phi_v(\mathcal{P}) \subset \mathcal{P}$ we easily infer the identity $\Phi_v^{-1}(\mathcal{P}) = \mathcal{P} + \ker\ \Phi_v$. To prove the second identity in (17), note that from $e^\top v = 1$ we get $Ev = e$ and hence

$$SP_v = ec^\top - (c^\top v)E$$

if $S = ec^\top + ce^\top - (c^\top v)E$. Thus $P_v^\top S P_v = (I - ev^\top)(ec^\top - (c^\top v)E) = 0$, which shows one inclusion. The converse follows by writing down the condition $\Phi_v(S) = 0$ explicitly, which yields

$$S = e(Sv)^\top + (Sv)e^\top - (v^\top Sv)E\,.$$

Then putting $c = Sv$ the result follows. Finally, the last inclusion follows by taking $c = te$ for arbitrary $t \in \mathbb{R}$. $\square$

As a consequence, the new cone

$$\mathcal{K}(v) = \mathcal{N} + \Phi_v^{-1}(\mathcal{P}) = \mathcal{N} + \mathcal{P} + \ker\ \Phi_v = \mathcal{K}_0 + \ker\ \Phi_v$$

contains a ray, i.e., is not pointed any more, so that its dual cone has empty interior. Thus, to avoid any complications with strong duality, we defer a detailed discussion of the domination of Nowak's bound to Section 7.2.2 below.

6 Copositive bounds

6.1 Copositive relaxation

As is well known [9], we can reformulate every StQP of the form (1) into a copositive program:

$$\max\{\lambda : Q - \lambda E \in \mathcal{C}\} = \ell_Q\,, \tag{18}$$

where $\mathcal{C}$ denotes the copositive cone.

A (zero-order) approximation [10] of the copositive cone is given by $\mathcal{K}_0 = \mathcal{P} + \mathcal{N} \subseteq \mathcal{C}$, with $\mathcal{C} = \mathcal{K}_0$ only if $n \leq 4$. Replacing $\mathcal{C}$ with $\mathcal{K}_0$ yields another bound:

$$\ell_Q^{\text{cop}} = \max\{\lambda : Q - \lambda E \in \mathcal{K}_0 = \mathcal{P} + \mathcal{N}\} \leq \ell_Q\,. \tag{19}$$

Obviously, ℓ_Q^{cop} is shift-equivariant. It is also immediately evident that

$$\ell_Q^0 = \max\{\lambda : Q - \lambda E \in \mathcal{N}\} \leq \max\{\lambda : Q - \lambda E \in \mathcal{K}_0 = \mathcal{P} + \mathcal{N}\} = \ell_Q^{\text{cop}}\,.$$

Passing to the dual problems of (18) and (19), we obtain alternative formulations for ℓ_Q and ℓ_Q^{cop}, respectively:

$$\min\{Q \bullet X : E \bullet X = 1\,,\, X \in \mathcal{C}^*\} = \ell_Q\,, \tag{20}$$

with $\mathcal{C}^*$ the completely positive cone, the dual cone of $\mathcal{C}$, and

$$\min\{Q \bullet X : E \bullet X = 1\,,\, X \in \mathcal{P} \cap \mathcal{N}\} = \ell_Q^{\text{cop}}\,, \tag{21}$$

as $\mathcal{K}_0 = \mathcal{P} + \mathcal{N}$ has the dual cone $\mathcal{K}_0^* = \mathcal{P} \cap \mathcal{N}$. In [10], strong duality is established which justifies equality of (20) with (18), and (19) with (21), respectively, and which also guarantees that all extrema there are attained.

A direct argument of why the solution of (21) can never exceed ℓ_Q employs the fact that, for any $x \in \Delta$, the rank-one matrix $X = xx^\top$ satisfies $X \in \mathcal{K}_0^*$ as well as $E \bullet X = (e^\top x)^2 = 1$, along with $Q \bullet X = x^\top Q x$. In the following sections, we offer a new interpretation of this copositive relaxation bound via decompositions.

As an aside, one may wonder what happens if we replace $\mathcal{P} \cap \mathcal{N}$ in the feasible set of (21) by one if its components. Of course, the resulting bounds would be smaller. But, to be more specific, one easily can show that

$$\min\{Q \bullet X : E \bullet X = 1\,,\, X \in \mathcal{N}\} = \ell_Q^0\,, \tag{22}$$

the simplest closed-form bound, whereas

$$\min\{Q \bullet X : E \bullet X = 1\,,\; X \in \mathcal{P}\} = -\infty\,, \tag{23}$$

unless $\Phi(Q) \succeq O$, which characterizes easy instances of the StQP. This follows from the dual of (23),

$$\max \{y \in \mathbb{R} : Q \succeq yE\} \ , \tag{24}$$

since (24) is feasible only if $\Phi(Q) \succeq O$.

6.2 Improving copositive bounds by adding linear cuts

Consider a (finite) set of copositive matrices $\{C_1, \ldots, C_m\}$ and the generated cone

$$\mathcal{D} = \left\{ \sum_{j=1}^{m} y_j C_j : y \in \mathbb{R}^m_+ \right\} \subset \mathcal{C} \, .$$

Since $\mathcal{C}$ is convex, we of course know that $\mathcal{K}_0 + \mathcal{D} \subset \mathcal{C}$, so that we can enlarge the feasible set of (19) and improve the copositive bound ℓ_Q^{cop}, but still get a valid bound:

$$\ell_Q^{\mathcal{D}} = \max \{\lambda : Q - \lambda E \in \mathcal{K}_0 + \mathcal{D}\} \leq \ell_Q \, . \tag{25}$$

Like ℓ_Q^{cop}, also $\ell_Q^{\mathcal{D}}$ is shift-equivariant. It is straightforward to show that the dual of (25) is

$$\min \{Q \bullet X : E \bullet X = 1 \, , C_j \bullet X \geq 0 \, , \text{ all } j \, , \ X \in \mathcal{K}_0^*\} \ , \tag{26}$$

and strong duality still holds since (25) is strictly feasible. Of course, it is not at all clear how many, and which, copositive matrices we should choose to obtain a satisfying bound $\ell_Q^{\mathcal{D}}$. One possibility is to consider matrices $R_i \in \mathcal{M}$ with known exact bounds $\ell_i = \ell_{R_i}$, to form $C_i = R_i - \ell_i E \in \mathcal{C}$. A particular instance of these matrices R_i and bounds ℓ_i would be the following: consider an undirected graph $\mathcal{G}_i$ with adjacency matrix $A_i \in \mathcal{M}$ and known clique number $\omega_i = \omega(\mathcal{G}_i)$. Form $R_i = E - A_i$. Then the Motzkin-Straus theorem (8) ensures $\ell_i = \ell_{R_i} = \frac{1}{\omega_i}$. Specializing further, take just one such graph (i.e., choose $m = 1$), namely a cycle with adjacency matrix A_c and clique number $\omega = 2$, and put $\mathcal{D} = \mathbb{R}_+(\frac{1}{2}E - A_c) = \mathbb{R}_+ D_c$ where $D_c = E - 2A_c$. Section 7.3 will clarify why this choice indeed yields a strict improvement over ℓ_Q^{cop}, and will provide an interpretation as a decomposition bound. Other improvements along these lines still remain to be explored.

7 Decomposition bounds

In this section we present a number of bounds that are based on the simple observation that if $Q = S + (Q - S)$ we always have

$$\beta_Q(S) = \ell_S + \ell_{Q-S} \leq \ell_Q \,. \tag{27}$$

Of course, this trivial property can be used to obtain practical lower bounds for ℓ_Q only if the decomposition $Q = S + (Q - S)$ satisfies the following principle:

(P) *the separate minimization of both pieces in the decomposition can be done efficiently.*

We now describe several ways of obtaining a decomposition satisfying this principle.

7.1 Difference-of-convex decomposition bounds

A possible way, pioneered by Tuy [21, 41] for general nonconvex problems, and specialized in [1, 6, 12] for the case of standard quadratic optimization, is to employ a difference-of-convex decomposition (dcd), i.e., $Q = S + T$ where $S \succeq O$ and $O \succeq T$. Both the minimizations required to compute the lower bound ℓ_S and ℓ_T are "easy" ones. Indeed, the first one is a convex problem and the optimal value of the second one is simply the lowest entry of T along the diagonal, due to concavity of the quadratic form $x^\top T x$. There are many possible dcd's and recently Anstreicher and Burer [1] have characterized the best possible bound of this type, i.e.,

$$\ell_Q^{\mathrm{dcd}} = \sup\left\{\beta_Q(S) = \ell_S + \ell_{Q-S} : S \in \mathcal{P}^Q\right\} \tag{28}$$

where

$$\mathcal{P}^Q = \{S \in \mathcal{P} : S - Q \in \mathcal{P}\} \,. \tag{29}$$

One of the key techniques used in [1] is the so-called Shor relaxation of the StQP (1). Consider the semidefinite program (SDP)

$$\nu_Q = \min\left\{Q \bullet X : X \succeq xx^\top \text{ for some } x \in \Delta\right\} \,. \tag{30}$$

As already noted in Section 6 (just put $X = xx^\top$), we always have $\nu_Q \leq \ell_Q$. But, as observed in [1], $\nu_Q = -\infty$ unless $Q \succeq O$, similar to the Lagrangian bounds above. Furthermore, for $S \in \mathcal{P}$ the Shor relaxation is exact: $\ell_S = \nu_S$. For convenient reference, we repeat the argument here: if $S \in \mathcal{P}$ and $X \succeq xx^\top$, then $S \bullet X \geq S \bullet xx^\top = x^\top S x$, whence

$\nu_S \geq \ell_S$ follows. The reverse inequality always holds. Hence ℓ_S can be found by solving an SDP.
By employing the modified dual $\mathrm{SQPS}'_{\mathrm{DC}}$ in [1],

$$\ell_Q^{\mathrm{dcd}} = \min\left\{Q \bullet X : E \bullet X = 1\,,\; Xe \geq o\,,\; \mathrm{Diag}\,(Xe) \succeq X \succeq O\right\}\,, \quad (31)$$

one sees that also this bound is shift-equivariant. Indeed, $(Q+tE)\bullet X = Q \bullet X + t$ if $E \bullet X = 1$.

One of the main assertions of [1] is the dominance of the copositive relaxation bound over the dcd bound. This result will emerge quite naturally in the next Section from a characterization of ℓ_Q^{cop} as another decomposition bound which uses an enlargement of the feasible set $\mathcal{P}^Q$ in (28).

7.2 Convex/vertex-optimal decomposition bounds

A natural question is: why should we restrict to dcd's? The main point with decomposition bounds is to decompose the objective function in such a way that property (P) holds. A larger set of possible decompositions follows by the simple observation that, in dcd decompositions, we only use the condition $T \preceq O$ to guarantee that

$$\ell_T = \min_i t_{ii} = \min_{j,k} t_{jk} = \ell_T^0\,.$$

Hence, we can trivially enlarge $\mathcal{P}^Q$ to

$$\mathcal{S}^Q = \left\{S \in \mathcal{P} : T = Q - S \text{ satisfies } \min_i t_{ii} = \ell_T^0\right\}\,. \quad (32)$$

For obvious reasons, the resulting bound

$$\ell_Q^{\mathrm{cvd}} = \sup\left\{\beta_Q(S) = \ell_S + \ell_{Q-S} : S \in \mathcal{S}^Q\right\} \quad (33)$$

is called *convex/vertex-optimal decomposition (cvd) bound.*

We now proceed to show that $\ell_Q^{\mathrm{cvd}} = \ell_Q^{\mathrm{cop}} = \ell_Q^{\mathrm{conv}}$, i.e., that the cvd bound, the copositive relaxation bound, and the convex underestimation bounds all give the same value.

We first need to show that the cvd bound is unchanged if we replace $\mathcal{S}^Q$ in (33) with its subset $\mathcal{T}^Q = \bigcup_{\delta\in\mathbb{R}} \mathcal{T}^Q(\delta)$, where

$$\mathcal{T}^Q(\delta) = \left\{S \in \mathcal{P} : \mathrm{diag}\,(Q - S) = -\delta e \text{ and } \ell_{Q-S}^0 = -\delta\right\}\,,\; \delta \in \mathbb{R}\,. \quad (34)$$

Lemma 3 (Diagonal homogenization)

$$\ell_Q^{\mathrm{cvd}} = \sup\left\{\beta_Q(S) : S \in \mathcal{T}^Q\right\}\,.$$

Proof. The inequality $\ell_Q^{\mathrm{cvd}} \geq \sup\left\{\beta_Q(S) : S \in \mathcal{T}^Q\right\}$ is trivial by $\mathcal{T}^Q \subseteq \mathcal{S}^Q$. To prove the reverse inequality, take any $S \in \mathcal{S}^Q$, so that $T = Q - S$ has a minimum entry ℓ_T^0 on its main diagonal, so that $\ell_T = \ell_T^0$. Put $d = \mathrm{diag}\ (T) - \ell_T^0 e$, $S' = S + \mathrm{Diag}\ (d)$, and $T' = Q - S' = T - \mathrm{Diag}\ (d)$. Then we have $d \geq o$, thus $S' \succeq S$ and $\mathrm{diag}\ (T') = \ell_T^0 e$ as well as $\ell_{T'}^0 = \ell_T^0$ by construction. Therefore $\ell_{T'} = \ell_T^0 = \ell_T$, and hence $S' \in \mathcal{T}^Q$ with $\beta_Q(S') = \ell_{S'} + \ell_{T'} \geq \ell_S + \ell_T = \beta_Q(S)$. □

Remark 1 *Note that a similar diagonal homogenization result can be also proved, with the same argument, for the dcd bound. In other words we have*

$$\ell_Q^{\mathrm{dcd}} = \sup\left\{\beta_Q(S) : S \in \mathcal{P}^Q\,,\ \mathrm{diag}(Q - S) = \lambda e\,,\ \textit{some } \lambda \in \mathbb{R}\right\}\,.$$

To calculate ℓ_S in (33), one could use Shor's relaxation (30), which is an SDP in minimization form. However, we search for the largest such ℓ_S. Hence, to avoid a maximin problem, one can first dualize for $\nu_S = \ell_S$ with $S \in \mathcal{T}^Q(\delta)$ fixed. So we obtain

$$\ell_S = \max\{\mu - \sigma : \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s + \mu e \leq o\,,\ s \in \mathbb{R}^n\,,\ \mu, \sigma \in \mathbb{R}\}\,, \tag{35}$$

since the duality gap between (30) with $Q = S$ and its SDP dual (35) is zero [1]. We prove a slight generalization of this duality result in Proposition 4 in Section 7.2.2 below.

Now, as we have seen, the second part of the bound is $-\delta$, if $\mathrm{diag}\ (T) = -\delta e$ and $-\delta \leq t_{ij}$ for all i, j. Hence finding the *cvd* bound means searching for a solution $(\delta, \mu, \sigma, s, S)$ of

$$\begin{aligned} \ell_Q^{\mathrm{cvd}} = \max\{\mu - \sigma - \delta : \quad & \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s + \mu e \leq o\,, \\ & S \in \mathcal{T}^Q(\delta)\,,\ s \in \mathbb{R}^n,\ \mu, \sigma, \delta \in \mathbb{R}\}\,. \end{aligned} \tag{36}$$

Now we are in a position to establish equivalence between the cvd and the copositive relaxation bound.

Theorem 3 *For any $Q \in \mathcal{M}$, we have*

$$\ell_Q^{\mathrm{cvd}} = \ell_Q^{\mathrm{cop}}\,.$$

Proof. We start with an equivalent reformulation of (36):

$$\begin{aligned} \ell_Q^{\mathrm{cvd}} = \max\{\mu - \sigma - \delta : \quad & \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s + \mu e \leq o\,, \\ & S - Q \leq \delta E\,,\ s \in \mathbb{R}^n,\ \mu, \sigma, \delta \in \mathbb{R}\}\,, \end{aligned} \tag{37}$$

and, similar to the argument in the diagonal homogenization Lemma 3, we take a feasible solution $(\delta, \mu, \sigma, s, S)$ of (37). Then of course diag $(S - Q) \le \delta e$, and $S' = S + \mathrm{Ddiag}\,[\delta I_n - S + Q)] \succeq S$. Hence $S' \in \mathcal{T}^Q(\delta)$ and $(\delta, \mu, \sigma, s, S')$ is now feasible for (36) without changing the objective. The dual of (37) and therefore of (36) is, similarly to $\mathrm{SQPS_{DC}}$ in [1],

$$\min\{Q \bullet X : E \bullet X = 1\,,\ X \in \mathcal{N}\,,\ X \succeq xx^\top\,,\ x \in \Delta\}\,. \tag{38}$$

Observe that (38)-feasibility of (X, x) implies $Xe = x$, as argued in [1]. This follows from the chain of (in)equalities

$$1 = e^\top Xe = E \bullet X \ge E \bullet xx^\top = (e^\top x)^2 = e^\top (xx^\top) e = 1$$

whence $e \in \ker\,(X - xx^\top)$ or $Xe = x(x^\top e) = x$. Therefore (38) is equivalent to

$$\min\{Q \bullet X : E \bullet X = 1\,,\ X \in \mathcal{N}\,,\ X \succeq (Xe)(Xe)^\top\}\,. \tag{39}$$

Now $X - (Xe)(Xe)^\top$ is always psd for any $X \in \mathcal{K}_0^* = \mathcal{P} \cap \mathcal{N}$ with $E \bullet X = 1$, which follows from (cf. Lemma 1 of [1])

$$\begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} = \begin{bmatrix} e^\top \\ I_n \end{bmatrix} X\,[e\ I_n] \succeq O \quad \text{and} \quad x = Xe\,.$$

Hence (39) is indeed equivalent to

$$\min\{Q \bullet X : E \bullet X = 1\,,\ X \in \mathcal{K}_0^*\} = \ell_Q^{\mathrm{cop}}\,, \tag{40}$$

which establishes the asserted equality. □

We now prove the equivalence between the copositive bound and the convex underestimation bound introduced in Section 4.

Theorem 4 *For any $Q \in \mathcal{M}$, we have*

$$\ell_Q^{\mathrm{conv}} = \ell_Q^{\mathrm{cop}}\,. \tag{41}$$

Proof. Since $\ell_{Q-S} = 0$ for all $S \in \mathcal{T}^Q(0)$, we have

$$\ell_Q^{\mathrm{conv}} = \sup\left\{\beta_Q(S) : S \in \mathcal{T}^Q(0)\right\} \le \sup\left\{\beta_Q(S) : S \in \mathcal{S}^Q\right\} = \ell_Q^{\mathrm{cvd}} = \ell_Q^{\mathrm{cop}}\,.$$

To show the reverse inequality, observe that $Q \in \mathcal{N}$ implies that $\lambda = 0$ is feasible for (19), so that $\lambda^* = \ell_Q^{\mathrm{cop}} \ge 0$. This means that for some $S^* \in \mathcal{P}$ and $T^* \in \mathcal{N}$ we have $Q = S^* + \lambda^* E + T^*$. Now define again $S' = S^* + \lambda^* E + \mathrm{Ddiag}\,(T^*)$ and $T' = T^* - \mathrm{Ddiag}\,(T^*)$. Then $S' \in \mathcal{P}$ since $\lambda^* \ge 0$; $T' \in \mathcal{N}$ with diag $(T') = o$, so that S' is feasible to (13). Therefore, $\ell_Q^{\rm conv} \geq \ell_{S'}$. But $C = S^* + \mathrm{Ddiag}\,(T^*) \in \mathcal{P}$, so $S' = \lambda^* E + C \succeq \lambda^* E$, hence $\ell_{S'} \geq \ell_{\lambda^* E} = \lambda^* = \ell_Q^{\rm cop}$. □

As an immediate consequence of Theorem 3, we obtain the dominance of $\ell_Q^{\rm cop}$ and of the other equivalent bounds over the refined closed-form bound of Section 2.

Theorem 5 *For any $Q \in \mathcal{M}$, we have*

$$\ell_Q^{\rm ref} \leq \ell_Q^{\rm cop}\,. \tag{42}$$

Proof. First observe that, by Theorem 1 and by equation (9), we have $\ell_Q^{\rm ref} = \beta_Q(S)$ for $S = \mathrm{Ddiag}\,(Q - \ell_Q^0 I_n) \in \mathcal{T}^Q(-\ell_Q^0) \subset \mathcal{S}^Q$. Hence, $\ell_Q^{\rm ref} \leq \ell_Q^{\rm cvd} = \ell_Q^{\rm cop}$. □

The next two subsections analyze possible natural approaches to improve the copositive bound. However, in both cases it turns out that no real improvement can be obtained. As a by-product of our analysis we discover that also the $\ell_Q^{\rm No}$ bound by Nowak is dominated by the copositive bound. On the other hand, we present a concrete improvement of this bound in Section 7.3, under the form of a new decomposition bound.

7.2.1 Iterating copositive bounds does not improve

Now let us take a fresh look at vertex optimality. As before, we start with a decomposition $Q = S + T$. Observe that the minimum ℓ_T is attained at vertex i if and only if

$$t_{ii} \leq t_{ij} \quad \text{for all } j \tag{43}$$

and, putting $T_i = [t_{jk}]_{j\neq i, k\neq i}$,

$$t_{ii} \leq \ell_{T_i}\,.$$

Now ℓ_{T_i} is (almost) as difficult to obtain as ℓ_Q itself, hence we need a lower bound for ℓ_{T_i} to guarantee for vertex-optimality.

The trivial lower bound is $\ell_{T_i}^0 = \min\{t_{jk} : j \neq i, k \neq i\}$, with which the above conditions reduce to $t_{ii} = \min_{j,k} t_{jk} = \ell_T^0$, and we arrive at the cvd bound $\ell_Q^{\rm cvd} = \ell_Q^{\rm cop}$ as above. One may wonder if we can improve by using refined bounds for ℓ_{T_i}. For instance, one may take $\beta_{T_i}(S_i)$ for some (optimal) $S_i \in \mathcal{S}^Q$ as a lower bound, i.e., employ the copositive bound $\ell_{T_i}^{\rm cop}$. Hence the idea is to iterate bounds for vertex optimality. However, as it will turn out, there is no strict improvement possible here. We specify an explicit proof also to elucidate the duality arguments which led to the dual formulations previously employed. The arguments needed there are rather similar.

Theorem 6 *The best cvd bound employing the relations $t_{ii} \le \ell^{\rm cop}_{T_i}$ and (43) to ensure $\ell_T = t_{ii}$, is again equal to $\ell^{\rm cop}_Q$. In particular, this bound does not depend on the choice of vertex i.*

Proof. We start with a decomposition $Q = S + T$, putting

$$S = \begin{bmatrix} s_{ii} & s_i^\top \\ s_i & S_i \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} q_{ii} & q_i^\top \\ q_i & Q_i \end{bmatrix}. \tag{44}$$

Next, we use (19) to rewrite the condition $t_{ii} \le \ell^{\rm cop}_{T_i}$:

$$\begin{array}{rcl} t_{ii} & \le & \lambda \\ Q_i - S_i - \lambda E_i & \in & \mathcal{P}_i + \mathcal{N}_i \\ \lambda & \in & \mathbb{R}\,, \end{array} \tag{45}$$

where all expressions $\mathcal{A}_i$ result from $\mathcal{A}$ by dropping coordinate i. Now we can combine the conditions in (45) with (43), to arrive at

$$\begin{array}{rcl} -\lambda - s_{ii} & \le & -q_{ii} \\ s_i - s_{ii}e & \le & q_i - q_{ii}e \\ S_i + R_i + \lambda E_i & \le & Q_i \\ \lambda & \in & \mathbb{R}\,,\ R_i \in \mathcal{P}_i\,. \end{array} \tag{46}$$

Employing again the Shor relaxation formulation (35), we arrive at the following SDP, noting that $\ell_T = q_{ii} - s_{ii}$ under (46):

$$\begin{array}{l} \max\{\mu - \sigma + q_{ii} - s_{ii} : \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s + \mu e \le o\,, \\ \qquad\qquad S \text{ satisfies } (46)\,,\ s \in \mathbb{R}^n,\ \mu, \sigma, \lambda \in \mathbb{R}\}\,. \end{array} \tag{47}$$

Denoting the Lagrange multipliers of the inequality constraints in (46) by $\nu \ge 0$, $2u \in \mathbb{R}^{n-1}_+$, and $U \in \mathcal{N}_i$, respectively, while $x \in \mathbb{R}^n_+$ corresponds to the explicit inequality constraint in (47), we arrive at the following Lagrange function, where we convert maximization into usual minimization multiplying by (-1):

$$\begin{array}{rcl} L(\lambda, \mu, \sigma, s, S, R_i; x, \nu, u, U) & = & \sigma - \mu + s_{ii} - q_{ii} + x^\top(2s + \mu e) + \\ & & + \nu(q_{ii} - \lambda - s_{ii}) + 2u^\top(s_i - s_{ii}e - q_i + q_{ii}e) \\ & & + U \bullet (S_i + R_i + \lambda E_i - Q_i) \\ & = & \mu(e^\top x - 1) + \lambda(U \bullet E_i - \nu) + R_i \bullet U + \\ & & + q_{ii}(2u^\top e + \nu - 1) - 2q_i^\top u - Q_i \bullet U + \\ & & + \begin{bmatrix} \sigma & s^\top \\ s & \begin{bmatrix} s_{ii} & s_i^\top \\ s_i & S_i \end{bmatrix} \end{bmatrix} \bullet \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \end{array} \tag{48}$$

with

$$X = \begin{bmatrix} 1 - \nu - 2u^\top e & u^\top \\ u & U \end{bmatrix} . \tag{49}$$

In a bit more compact form, using (44), we arrive at

$$\begin{aligned} L(\lambda, \mu, \sigma, s, S, R_i; x, \nu, u, U) &= \mu(e^\top x - 1) + \lambda(U \bullet E_i - \nu) + R_i \bullet U + \\ &+ \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \bullet \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} - Q \bullet X . \end{aligned} \tag{50}$$

Now, the Lagrange dual function

$$\begin{aligned} \Theta(x, \nu, u, U) = \inf \{ L(\lambda, \mu, \sigma, s, S, R_i; x, \nu, u, U) : \quad & \lambda, \mu, \sigma \in \mathbb{R} , \; s \in \mathbb{R}^n , \\ & \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O , \; R_i \in \mathcal{P}_i \, \} \end{aligned}$$

can be finite only if $e^\top x = 1$ (which together with $x \in \mathbb{R}^n_+$ gives $x \in \Delta$); $U \bullet E_i = \nu$; $U \in \mathcal{P}_i$ (which together with $U \in \mathcal{N}_i$ gives $U \in \mathcal{P}_i \cap \mathcal{N}_i$); and

$$\begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \succeq O . \tag{51}$$

Note that by (49), the relation $U \bullet E_i = \nu$ is equivalent to $E \bullet X = 1$. Of course, also $X \in \mathcal{P}$ must hold, so that by the same arguments as used in the proof of Theorem 3, we see that under $E \bullet X = 1$, (51) is equivalent to $X \in \mathcal{K}_0^*$. Note that by this way, we respect the additional linear constraints originating from nonnegativity conditions for Lagrange multipliers ν, u, U. This is obvious for u and U, while nonnegativity of ν is equivalent to $x_{11} + 2\sum_{j>1} x_{1j} \leq 1$, which is guaranteed anyhow by $E \bullet X = 1$ and $x_{jk} \geq 0$ for all $j, k > 1$. Summarizing, we arrive at

$$\sup \Theta(x, \nu, u, U) = -\inf \{ Q \bullet X : X \in \mathcal{K}_0^* \} ,$$

and hence the iterated copositive relaxation bound equals ℓ_Q^{cop}. Note that no strict feasibility condition is needed here, as we already know that strong duality holds for (19). □

7.2.2 Cvd bounds with convexity over the hyperplane $e^\perp$

Here we show that the copositive bound will not be improved if we combine the optimal decomposition bound approach with Nowak's idea in refining the bounds by requiring convexity of $x^\top Sx$ merely over the hyperplane $e^\perp$ rather than over the whole $\mathbb{R}^n$.

Indeed, we actually show, with an extension of Shor's relaxation, that copositive bounds always dominate Nowak's bound (strict domination can be established, e.g., by means of Example (68) of Section 8 where $\ell_Q^{\rm No} < \ell_Q^0 \le \ell_Q^{\rm cop}$).

From Lemma 2 we know that a $W \in \mathcal{M}$ yields a convex quadratic form over Δ if and only if $\Phi_v(W) \succeq O$ for a fixed vector $v \in \Delta$, or equivalently, if and only if

$$W = S + G \quad \text{with} \quad S \succeq O \quad \text{and} \quad G = ec^\top + ce^\top - (c^\top v)E$$

for some vector $c \in \mathbb{R}^n$. Now by shift-equivariance, we may and do absorb the constant $(-c^\top v)$ into the matrix T in a decomposition $Q = W + T$. This way, we get rid of the dependence on v.

Lemma 4 *Suppose $S \in \mathcal{P}$ and put $\overline{S}(c) = S + ec^\top + ce^\top$ as well as*

$$\gamma(S, c) = \min\left\{S \bullet X + 2c^\top x \ : \ x \in \Delta\,,\ X \succeq xx^\top\right\}. \tag{52}$$

Then

$$\ell_{\overline{S}(c)} = \min\left\{x^\top Sx + 2c^\top x : x \in \Delta\right\} = \gamma(S, c)\,. \tag{53}$$

Moreover, by dualization we get

$$\gamma(S, c) = \max\left\{\mu - \sigma \ : \ \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s + \mu e \le 2c\right\}. \tag{54}$$

Proof. First observe that the quadratic form $x^\top \overline{S}(c)x = x^\top Sx + 2c^\top x$ is equivalent to a linear term over the standard simplex, i.e., $x^\top Gx = 2c^\top x - c^\top v$ for all $x \in \Delta$. This establishes the leftmost equality of (53). To prove the rightmost one of (53), put $X = xx^\top$ to show $\ell_{\overline{S}(c)} \ge \gamma(S, c)$. The converse inequality follows again from $S \succeq O$ which yields

$$S \bullet X + 2c^\top x \ge S \bullet xx^\top + 2c^\top x = x^\top Sx + 2c^\top x$$

whenever $X \succeq xx^\top$. Next we establish the dual formulation (54). Abbreviate by

$$Y = \begin{bmatrix} X & x \\ x^\top & \eta \end{bmatrix},$$

consider the constraint $\eta = 1$ with multiplier $\sigma \in \mathbb{R}$, the constraint $1 - e^\top x = 0$ with multiplier $\mu \in \mathbb{R}$, the constraints $-x \le o$ with multiplier $2u \in \mathbb{R}^n_+$, to form the Lagrange function

$$\begin{aligned} L(Y; \mu, \sigma, u) &= S \bullet X + 2c^\top x \ + \sigma(\eta - 1) + \mu(1 - e^\top x) - 2u^\top x \\ &= \begin{bmatrix} X & x \\ x^\top & \eta \end{bmatrix} \bullet \begin{bmatrix} S & c - u - \frac{\mu}{2}e \\ (c - u - \frac{\mu}{2}e)^\top & \sigma \end{bmatrix} + \mu - \sigma \\ &= Y \bullet \begin{bmatrix} S & s \\ s^\top & \sigma \end{bmatrix} + \mu - \sigma\,, \end{aligned} \tag{55}$$

where $s = c - u - \frac{\mu}{2}e$. Then $\Theta(\mu, \sigma, u) = \inf \{L(Y; \mu, \sigma, u) : Y \succeq O\}$ can be finite only if

$$\begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O$$

and $2s + \mu e \leq 2c$ by construction of s, since $2u \in \mathbb{R}^n_+$ as multiplier of $x \geq o$. Hence

$$\sup \left\{ \Theta(\mu, \sigma, u) : u \in \mathbb{R}^n_+ \,,\ \mu, \sigma \in \mathbb{R} \right\}$$

is as specified at the right-hand side of (54), and strong duality guarantees the assertion. □

Now we look for an optimal decomposition bound

$$\ell_Q^{\mathrm{cop},c} = \sup \left\{ \gamma(S, c) + \ell_T : S \in \mathcal{P}\,, T = Q - \overline{S}(c) \text{ has } \ell_T = \ell_T^0 \right\} . \quad (56)$$

Lemma 5 *For all $c \in \mathbb{R}^n$,*

$$\begin{aligned} \ell_Q^{\mathrm{cop},c} = \max\{\mu - \sigma - \delta : &\begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ \overline{S}(c) \in \mathcal{T}^Q(\delta)\,, \\ &2s + \mu e \leq 2c\,,\ s \in \mathbb{R}^n,\ \mu, \sigma, \delta \in \mathbb{R}\} . \end{aligned} \quad (57)$$

Proof. We employ again a diagonal homogenization argument: let $S \in \mathcal{P}$ and $T = Q - \overline{S}(c)$, and put $\delta = -\ell_T = -\ell_T^0$. Then $\delta E + T \in \mathcal{N}$, and we have

$$S' = S + \mathrm{Ddiag}\ (\delta E + T) \succeq S\,.$$

Moreover,

$$\overline{S'}(c) = S' + ce^\top + ec^\top = S + ce^\top + ec^\top + \mathrm{Ddiag}\ (\delta E + T) = \overline{S}(c) + \mathrm{Ddiag}\ (\delta E + T)\,,$$

and $\mathrm{diag}\ (\overline{S'}(c) - Q) = \delta e$ by construction, i.e., $\overline{S'}(c) \in \mathcal{T}^Q(\delta)$, while still

$$\begin{bmatrix} \sigma & s^\top \\ s & S' \end{bmatrix} \succeq \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,.$$

Hence feasibility with respect to (54) is maintained without changing the objective there, and the claim is proven via the observation that for T and $T' = Q - \overline{S'}(c)$, we have $\ell_T = \ell_T^0 = -\delta = \ell_{T'}^0 = \ell_{T'}$. □

Recall that, by definition, $\ell_Q^{\mathrm{No}} = \ell_W$ for any solution $W = S$ to (15). Since for any such solution we also have $\ell_{Q-W} = \ell_{Q-W}^0 = 0$, we immediately obtain that $\ell_Q^{\mathrm{No}} = \ell_W + \ell_{Q-W}$, i.e., Nowak's bound is a decomposition bound. Furthermore, the next result shows that it is dominated by the copositive bound and that nothing can be gained by relaxing convexity from the whole space to the $e^\perp$ hyperplane.

Theorem 7 *For all $c \in \mathbb{R}^n$,*

$$\ell_Q^{\rm No} \le \ell_Q^{\rm cop} = \ell_Q^{{\rm cop},c}$$

Proof. We calculate the dual of (57) and show it coincides with (40). The Lagrange function can be expressed in a now already familiar way:

$$\begin{array}{rcl} L(\delta,\mu,\sigma,s,S;u,U,w) & = & \sigma - \mu + \delta + u^\top(2s + \mu e - 2c) + \\ & & + w^\top {\rm diag}\,(S + ce^\top + ec^\top - Q - \delta E) \\ & & + U \bullet (S + ce^\top + ec^\top - Q - \delta E) \\ & = & \left[\begin{array}{cc} \sigma & s^\top \\ s & S \end{array}\right] \bullet \left[\begin{array}{cc} 1 & u^\top \\ u & U + {\rm Diag}\, w \end{array}\right] \\ & & + \mu(e^\top u - 1) + \delta(1 - U \bullet E - w^\top e) \\ & & - 2u^\top c + (U + {\rm Diag}\, w) \bullet (ce^\top + ec^\top - Q) \end{array} \quad (58)$$

with $u \in \mathbb{R}^n_+$; $U \in \mathcal{N}$; and $w \in \mathbb{R}^n$ without sign restrictions. As argued previously, only those (u,U,w) are relevant for a finite value of the dual function

$$\Theta(u,U,w) = \inf\left\{L(\delta,\mu,\sigma,s,S;u,U,w) : \begin{array}{l} \delta,\mu,\sigma \in \mathbb{R}\,,\ s \in \mathbb{R}^n\,, \\ \left[\begin{array}{cc} \sigma & s^\top \\ s & S \end{array}\right] \succeq O \end{array}\right\}$$

which satisfy $u \in \Delta$; $X = U + {\rm Diag}\, w \in \mathcal{N} \cap \mathcal{P}$ with $E \bullet X = 1$; and

$$Z = \left[\begin{array}{cc} 1 & u^\top \\ u & X \end{array}\right] \succeq O\,,$$

wherefrom we can infer $u = Xe$, so that we can remove the last psd condition because it is already implied by $X \in \mathcal{N} \cap \mathcal{P}$ and $E \bullet X = 1$. Thus

$$\begin{array}{rl} & \sup\{\Theta(u,U,w) : X \in \mathcal{K}_0^*\,,\ E \bullet X = 1\,,\ Z \succeq 0\} \\ = & \sup\left\{X \bullet (ce^\top + ec^\top - Q) - 2(Xe)^\top c : X \in \mathcal{K}_0^*\,,\ E \bullet X = 1\right\} \\ = & \sup\{-Q \bullet X : X \in \mathcal{K}_0^*\,,\ E \bullet X = 1\} \\ = & -\ell_Q^{\rm cop}\,, \end{array}$$

since $X \bullet (ce^\top + ec^\top) = 2(Xe)^\top c$, and the equality $\ell_Q^{\rm cop} = \ell_Q^{{\rm cop},c}$ follows. Next we establish $\ell_Q^{\rm No} \le \ell_Q^{\rm cop}$. To this end, observe that as argued before, $\ell_Q^{\rm No} = \ell_W + \ell_{Q-W}$, with $W = S + ce^\top + ec^\top$ chosen as the optimal solution of (15). Hence $\ell_Q^{\rm No} = \mu - \sigma - \delta$ for some (57)-feasible constellation (δ,μ,σ,s,S). Thus, $\ell_Q^{\rm No} \le \ell_Q^{{\rm cop},c} = \ell_Q^{\rm cop}$. □

Remark 2 *This theoretical result conflicts with the empirical evidence reported in [32], that on a relative efficiency scale, the quality of* $\ell_Q^{\rm No}$ *exceeds that of* $\ell_Q^{\rm cop}$ *by a factor of 100 roughly, averaged over a randomly drawn sample of Q instances. We are indebted to Florian Frommlet (personal communication) who repeated the same experiment (albeit on a smaller scale), and his results also confirmed validity of Theorem 7, contrasting [32].*

7.3 Convex/edge-optimal decomposition bounds

We now further extend the class of decompositions by relaxing the vertex optimality condition on one of the two quadratic forms to the condition of vertex or *edge* optimality. A simple sufficient condition guaranteeing vertex or edge optimality for a quadratic form $x^\top Tx$ on the standard simplex can be easily rephrased from the results of Tardella [39, Corollary 2.2.1 and Proposition 3.1] and [40, Theorem 5]. Indeed, these results can be restated by saying that *vertex or edge optimality is guaranteed for a quadratic function on a polyhedron if the set of edges along which the function is strictly convex induces a triangle-free graph over the vertices of the polyhedron.*

So we start by requiring concavity (thus preventing strict convexity) along a set of edges that complements the edge set of a simple triangle-free graph like a cycle. Of course, this is not the only triangle-free graph and possibly not even the best one for our purposes, but it is already sufficient to provide an improvement over the cvd bound. Note that different choices of the triangle-free graph can give rise to different bounds, see Remark 3 in Section 9 below. For ease of exposition, consider the "canonical" cycle

$$\mathcal{I} = \{\{i, i+1\} : 1 \leq i \leq n-1\} \cup \{\{1, n\}\}$$

with adjacency matrix $A_c = \mathrm{tridiag}(e, o, e) + 2E^{1n}$, where $\mathrm{tridiag}(e, o, e)$ is the tridiagonal matrix with all zeros on the main diagonal and all ones on the adjacent diagonals.

Again, we restrict our attention to decompositions $Q = S + T$ where T satisfies the diagonal homogeneity condition $\mathrm{diag}\, T = -\delta e$. Hence the values of $x^\top Tx$ coincide at all vertices of Δ, and the concavity condition along edge $\{k, l\}$ reads $t_{kl} \geq -\delta = t_{kk} = t_{ll}$. On the other hand, the minimum $\tau = \ell_T$ must be attained at an edge $\{i, j\} \in \mathcal{I}$, which means

$$\tau \leq \frac{t_{ii}t_{jj} - t_{ij}^2}{t_{ii} + t_{jj} - 2t_{ij}} = \frac{t_{ij}^2 - \delta^2}{2(t_{ij} + \delta)} = \frac{t_{ij} - \delta}{2}\,,$$

and, of course, $\tau \leq -\delta$. Summarizing, we obtain the conditions

$$\begin{aligned} t_{ij} - \delta - 2\tau &\geq 0 \quad \text{for all } \{i,j\} \in \mathcal{I} \\ t_{kl} + \delta &\geq 0 \quad \text{for all } \{k,l\} \notin \mathcal{I} \\ -\delta - \tau &\geq 0 \\ \operatorname{diag} T + \delta e &= o\,. \end{aligned} \tag{59}$$

Now, the best convex/edge-optimal decomposition (cved) bound of this type is given by

$$\begin{aligned} \ell_Q^{\mathrm{cved}} &= \sup\{\beta_Q(S) : S \in \mathcal{P}\,,\ T = Q - S \text{ satisfies (59) for some } \delta, \tau \in \mathbb{R}\} \\ &= \sup\{\ell_S + \tau : S \in \mathcal{P}\,,\ \delta, \tau \in \mathbb{R}\,,\ T = Q - S \text{ satisfies (59)}\}\,. \end{aligned} \tag{60}$$

Theorem 8 *The best convex/edge-optimal decomposition (cved) bound coincides with* $\ell_Q^{\mathcal{D}}$ *where* $\mathcal{D} = \mathbb{R}_+ D_c$ *and* $D_c = E - 2A_c$. *This bound is not worse than the copositive (cvd, conv) bound:*

$$\ell_Q^{\mathrm{cved}} = \ell_Q^{\mathcal{D}} \geq \ell_Q^{\mathrm{cvd}} = \ell_Q^{\mathrm{cop}} = \ell_Q^{\mathrm{conv}}.$$

Proof. By using the matrix D_c, we can summarize the first two constraints in (59) as $T + \delta D_c - 2\tau A_c \in \mathcal{N}$. Let us denote the corresponding Lagrange multiplier with $V \in \mathcal{N}$. Likewise, the third constraint in (59) gets a scalar multiplier $\nu \geq 0$, while the last one there gets a vector $v \in \mathbb{R}^n$, unrestricted in sign. As before in (48), we calculate the Lagrangian function:

$$\begin{aligned} L(\tau,\delta,\mu,\sigma,s,S;x,\nu,v,V) &= \sigma - \mu - \tau + x^\top(2s + \mu e) + \\ &\quad + \nu(\delta + \tau) + v^\top \operatorname{diag}(S - Q - \delta E) \\ &\quad + V \bullet (S - Q - \delta D_c + 2\tau A_c) \\ &= \sigma + \mu(e^\top x - 1) + \delta(\nu - v^\top e - V \bullet D_c) + 2x^\top s \\ &\quad + \tau(2V \bullet A_c + \nu - 1) + (\operatorname{Diag} v + V) \bullet (S - Q)\,, \end{aligned} \tag{61}$$

or, written more compactly, introducing $X = V + \operatorname{Diag} v$,

$$\begin{aligned} L(\tau,\delta,\mu,\sigma,s,S;x,\nu,v,V) &= \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \bullet \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} - Q \bullet X + \mu(e^\top x - 1) \\ &\quad + \delta(\nu - v^\top e - V \bullet D_c) + \tau(2V \bullet A_c + \nu - 1)\,. \end{aligned} \tag{62}$$

Next, the condition that the Lagrange dual function

$$\Theta(x,\nu,v,V) = \inf\left\{L(\tau,\delta,\mu,\sigma,s,S;x,\nu,v,V) :\ \tau,\delta,\mu,\sigma \in \mathbb{R}\,,\ s \in \mathbb{R}^n\,,\ \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\right\}$$

takes a finite value amounts to, again, $e^\top x = 1$ (which together with $x \in \mathbb{R}^n_+$ gives $x \in \Delta$); further, to the two conditions

$$\begin{aligned} v^\top e + V \bullet D_c - \nu &= 0 \\ 2V \bullet A_c + \nu &= 1\,, \end{aligned} \tag{63}$$

and, again,

$$\begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \succeq O\,. \tag{64}$$

First, we add the two equations from (63), to arrive at

$$v^\top e + V \bullet (2A_c + D_c) = 1\,,$$

and obtain

$$E \bullet X = E \bullet (V + \mathrm{Diag}\ v) = E \bullet V + v^\top e = (2A_c + D_c) \bullet V + v^\top e = 1\,.$$

Now, as in the proof of Theorem 6, we argue that the conditions necessary for finiteness of Θ are equivalent to $X = V + \mathrm{Diag}\ v \in \mathcal{P} \cap \mathcal{N}$ (note that nonnegativity of diagonal entries follows from semidefiniteness of $X \succeq xx^\top \succeq O$ while nonnegativity of the off-diagonal entries originates from $V \in \mathcal{N}$), and $x = Xe$. However, this time we also have to take into account the dual feasibility condition $\nu \geq 0$, which gives, from the second equation in (63),

$$A_c \bullet X = A_c \bullet V \leq \tfrac{1}{2}\,.$$

Hence we arrive at

$$\ell_Q^{\mathrm{cved}} = \min\left\{Q \bullet X : E \bullet X = 1\,,\ A_c \bullet X \leq \tfrac{1}{2}\,,\ X \in \mathcal{K}_0^*\right\} \geq \ell_Q^{\mathrm{cop}}\,, \tag{65}$$

and, by definition of $\mathcal{D} = \mathbb{R}_+ D_c$, $\ell_Q^{\mathrm{cved}} = \ell_Q^{\mathcal{D}}$, as argued in Section 6.2. □

7.4 Decomposition bounds with more than two parts

Up to now we have only considered decompositions of Q into two matrices. However, nothing prevents us from considering decompositions into more than two matrices. A careful reading of Section 6.2 actually reveals that bounds based on decompositions into three matrices have been already introduced there. Indeed, in that section bound $\ell_Q^{\mathcal{D}}$ is the best possible bound for three-part decompositions

$$Q = R + S + T,$$

where R is some *fixed* matrix whose minimum along Δ is known, while $S \in \mathcal{P}$ and T satisfies the usual condition

$$\min_i \ t_{ii} \leq \min_{i,j} \ t_{ij}.$$

We also remark again that the choice $R \in \mathbb{R}_+ D_c$ adopted in Section 6.2 is by no means the only possible one, and rules for an appropriate choice of R are an interesting subject for future research.

8 Relations between bounds

In this section we summarize the relations between the different bounds introduced in this paper (see also Figure 1). In what follows $\rightarrow$ denotes

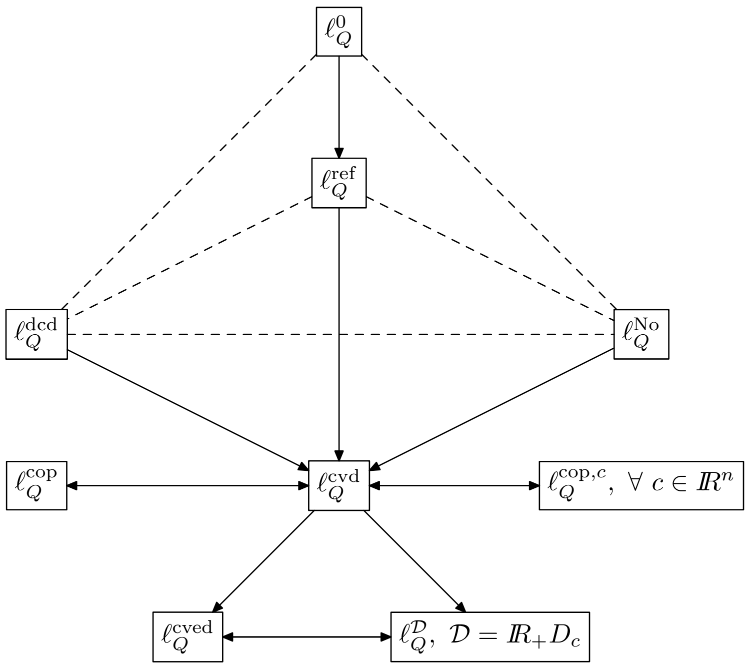

Figure 1: Relations between different bounds: $\rightarrow$ denotes strict domination, $\leftrightarrow$ denotes equivalence, the dashed line denotes no domination.

strict domination (the bound on the right of the arrow is always at least as good and in some cases strictly better than the bound on the left), $\leftrightarrow$ denotes *equivalence* between bounds, $\cdots$ denotes the case of no domination between bounds, i.e., on some instances one bound is better than the other but on other instances the reverse is true.

8.1 The relation $\ell_Q^0 \to \ell_Q^{\text{ref}}$

The fact that ℓ_Q^{ref} is always at least as good as ℓ_Q^0 follows immediately from the definitions (see also Theorem 1). Strict domination is also trivially verified when Q is the identity matrix ($\ell_{I_n}^0 = 0 < \frac{1}{n} = \ell_{I_n}^{\text{ref}} = \ell_{I_n}$ by Theorem 1). Another example is provided by the matrix

$$Q = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}. \tag{66}$$

for which $-1 = \ell_Q^0 < \ell_Q^{\text{ref}} = -\frac{1}{3} < \ell_Q$, where the last strict inequality follows again by Theorem 1.

8.2 The relations ℓ_Q^0 , $\ell_Q^{\text{ref}} \cdots \ell_Q^{\text{dcd}}$

Instance (66) also shows that ℓ_Q^{dcd} (equal to 0 on this instance) can be strictly better than ℓ_Q^0 and ℓ_Q^{ref}, while for

$$Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{67}$$

we have that $\ell_Q^{\text{dcd}} = -\frac{1}{8}$ (as computed in [1]) is strictly worse than $\ell_Q^0 = \ell_Q^{\text{ref}} = 0$.

8.3 The relations ℓ_Q^0 , $\ell_Q^{\text{ref}} \cdots \ell_Q^{\text{No}}$

Again instance (66) shows that ℓ_Q^{No} (equal to 0 on this instance) can be strictly better than ℓ_Q^0 and ℓ_Q^{ref}, while on the instance

$$Q = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \tag{68}$$

simple but tedious computations show that $\ell_Q^{\text{No}} = -\frac{9}{8}$ and is thus worse than $\ell_Q^0 = \ell_Q^{\text{ref}} = -1$.

8.4 The relation $\ell_Q^{\mathrm{No}} \quad \cdots \quad \ell_Q^{\mathrm{dcd}}$

On instance (67) $\ell_Q^{\mathrm{No}} = 0$ (matrix W in the definition of ℓ_Q^{No} is equal to the O matrix in this case) is better than $\ell_Q^{\mathrm{dcd}} = -\frac{1}{8}$, while on instance (68) $\ell_Q^{\mathrm{dcd}} = -1$ is better than $\ell_Q^{\mathrm{No}} = -\frac{9}{8}$.

8.5 The relations $\ell_Q^{\mathrm{cvd}} \leftrightarrow \ell_Q^{\mathrm{cop}} \leftrightarrow \ell_Q^{\mathrm{cop},c}\ \forall\ c \in \mathbb{R}^n$

The first equivalence has been established in Theorem 3, the second one in Theorem 7, both in Section 7.2.

8.6 The relations ℓ_Q^{ref}, ℓ_Q^{dcd}, $\ell_Q^{\mathrm{No}} \longrightarrow \ell_Q^{\mathrm{cvd}}$

The fact that ℓ_Q^{cvd} ia at least as good as ℓ_Q^{dcd} has been established in [1], while for ℓ_Q^{ref} and ℓ_Q^{No} this has been established in Theorem 5, and Theorem 7, respectively. Strict domination immediately follows from the previous examples, since each one of the three bounds $\ell_Q^{\mathrm{ref}}, \ell_Q^{\mathrm{dcd}}, \ell_Q^{\mathrm{No}}$ is on some instances strictly worse than at least one of the other two.

8.7 The relation $\ell_Q^{\mathrm{cvd}} \longrightarrow \ell_Q^{\mathrm{cved}}$

The fact that ℓ_Q^{cved} is at least as good as ℓ_Q^{cvd} has been established in Theorem 8, while strict improvement follows, e.g., by considering the 5×5-matrix

$$Q = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix},$$

(observe $Q = D_c$ from section 6.2) for which the copositive bound can not be exact (this is an example of a copositive matrix Q which can not be written as the sum of a semidefinite positive and a nonnegative matrix, as shown in [14]). Hence $\ell_Q^{\mathrm{cvd}} < 0$, whereas the cved bound is exact: $\ell_Q^{\mathrm{cved}} = 0$. More precisely, from [10] $\ell_Q^{\mathrm{cvd}} = \ell_Q^{\mathrm{cop}} = \frac{2}{\sqrt{5}} - 1 \approx -0.1056$.

8.8 The relation $\ell_Q^{\mathrm{cved}} \leftrightarrow \ell_Q^{\mathcal{D}}$ with $\mathcal{D} = \mathbb{R}_+ D_c$

The equivalence has been established in Theorem 8.

9 Bounding the (weighted) clique number: θ numbers and improvements

In this section, we apply the previously derived bounds to the maximum weight clique problem (or, equivalently, to the maximum weight stable set problem). In particular, we obtain new reformulations and improvements of the θ numbers by Lovász [25] and Schrijver [37] for the unweighted case. Recall that the maximum weight clique problem for the graph $\mathcal{G} = (N, \mathcal{E})$ with weights w is exactly the maximum stable set problem for the complement graph $\bar{\mathcal{G}} = (N, \bar{\mathcal{E}})$ with the same weights w, where $\{i,j\} \in \bar{\mathcal{E}}$ if and only if ($i \neq j$ and) $\{i,j\} \notin \mathcal{E}$. Hence the Motzkin-Straus Theorem (8) can also be written as

$$\frac{1}{\alpha(\overline{\mathcal{G}}, w)} = \frac{1}{\omega(\mathcal{G}, w)} = \ell_B \quad \text{for any } B \in \mathcal{M}(w, \mathcal{G}) \, ,$$

where $\omega(\mathcal{G}, w)$ and $\alpha(\overline{\mathcal{G}}, w)$ denote the weighted versions of the clique number for $\mathcal{G}$, and of the independence number for $\overline{\mathcal{G}}$, respectively. If $\ell_B^{\rm gen} \leq \ell_B$ denotes any generic valid lower bound for ℓ_B, then the following numbers provide an upper bound for $\alpha(\overline{\mathcal{G}}, w)$:

$$\bar{\theta}_B^{\rm gen} = \frac{1}{\ell_B^{\rm gen}} \geq \alpha(\overline{\mathcal{G}}, w) = \omega(\mathcal{G}, w) \quad \text{for any } B \in \mathcal{M}(w, \mathcal{G}) \, .$$

Now for the unweighted case $w = e$, the well known θ number by Lovász and its improvement θ' by Schrijver satisfy the sandwich theorem (we use $\bar{\theta}$ to stress conversion to the complement graph)

$$\alpha(\overline{\mathcal{G}}, e) \leq \bar{\theta}' \leq \bar{\theta} \leq \chi(\mathcal{G}) \, , \tag{69}$$

where $\chi(\mathcal{G})$ is the coloring number of $\mathcal{G}$. In [13] it is observed that

$$\bar{\theta}' = \bar{\theta}^{\rm cop}_{E - A_{\mathcal{G}}} = \frac{1}{\ell^{\rm cop}_{E - A_{\mathcal{G}}}} \, ,$$

and we recall that $E - A_{\mathcal{G}} \in \mathcal{M}(e, \mathcal{G})$.

By exploiting the previous equivalence results on cvd bounds, we arrive at seemingly new reformulations for $\bar{\theta}'$:

Theorem 9 *The inverse value of Schrijver's $\bar{\theta}'$ number (for the complement graph) can be written as the optimal value of the following SDPs:*

$$\left[\bar{\theta}'\right]^{-1} = \max \left\{ \ell_S : S \in \mathcal{P} \, , \, \textit{diag}\ (S) = e \, , \, s_{ij} \leq 0 \textit{ for all } \{i,j\} \in \mathcal{E} \right\} \, , \tag{70}$$

and also

$$\left[\bar\theta'\right]^{-1} = \max\{\mu-\sigma-\delta : \begin{bmatrix} \sigma & s^\top \\ s & S \end{bmatrix} \succeq O\,,\ 2s+\mu e \le o\,,\ \mathit{diag}\,(S) = (\delta+1)e\,,$$
$$s_{ij} \le \delta \text{ for all } \{i,j\} \in \mathcal{E}\,,\ s \in \mathbb{R}^n,\ \mu,\sigma,\delta \in \mathbb{R}\}\,. \tag{71}$$

Proof. The results follow by recalling (13) and (36) and invoking Theorems 3 and 4, for $Q = A_{\overline{\mathcal{G}}} + I_n$. Indeed, for establishing (71), note that $S \in \mathcal{P}$, and diag $(S) = (\delta+1)e$ implies $s_{ij} \le \delta+1$ for any $i \neq j$, so that for $\{i,j\} \in \bar{\mathcal{E}}$ the condition $s_{ij} - \delta \le q_{ij}$ is void. The same argument, replacing δ with zero, yields (70). □

We now present an improvement of the $\bar\theta'$ number, based on the cved bound.

Theorem 10 *Let $A_{\mathcal{G}}$ be the adjacency matrix of a graph $\mathcal{G}$, and define*

$$\bar\theta^{\text{cved}} = \frac{1}{\ell^{\text{cved}}_{E-A_{\mathcal{G}}}}\,.$$

Then

$$\omega(\mathcal{G}) = \alpha(\bar{\mathcal{G}}) \le \bar\theta^{\text{cved}} \le \bar\theta' \le \chi(\mathcal{G})\,, \tag{72}$$

and the middle inequality can be strict for some graphs $\mathcal{G}$. Furthermore, we have the following SDP characterization of the inverse value of this new number:

$$\left[\bar\theta^{\text{cved}}\right]^{-1} = \max\{\ \ell_S + \tau : \quad \mathit{diag}\,(S) = (\delta+1)e\,,\ S \in \mathcal{P}\,, \delta+\tau \le 0\,,\ \delta,\tau \in \mathbb{R}\,,$$
$$s_{ij} - \delta(D_c)_{ij} + 2\tau(A_c)_{ij} \le 0 \text{ for all } \{i,j\} \in \mathcal{E}\ \}\ . \tag{73}$$

Proof. The new version of the Sandwich Theorem (72) follows from (69) and Theorem 8. Next we establish strict dominance of the $\bar\theta^{\text{cved}}$ numbers in graph instances. To this end, let $\mathcal{G}$ be the 5-cycle with 5×5 adjacency matrix A_c. Then derive

$$E - A_c = \tfrac{1}{2}(E + D_c) = \tfrac{1}{2}(E + Q)$$

where Q is the instance in Section 8.7. Therefore

$$\bar\theta^{\text{cved}} = 1/\ell^{\text{cved}}_{E-A_{\mathcal{G}}} = 1/\tfrac{1}{2}(1+\ell^{\text{cved}}_Q) = 2 = \omega(\mathcal{G})$$

whereas

$$\bar\theta' = 1/\tfrac{1}{2}(1+\ell^{\text{cvd}}_Q) > 2\,,$$

since $\ell_Q^{\rm cvd} < 0$ as argued in Section 8.7. Finally, to prove (73), we employ definition (60), recalling the definition of $A_{\mathcal{G}}$. Thus we can write

$$\begin{aligned} \ell_{E-A_{\mathcal{G}}}^{\rm cved} &= \max\{\,\ell_S+\tau:\ \mathrm{diag}\,(S)=(\delta+1)e\,,\ S\in\mathcal{P}\,,\delta+\tau\le 0\,,\ \delta,\tau\in\mathbb{R}\,, \\ &\qquad s_{ij}-\delta(D_c)_{ij}+2\tau(A_c)_{ij}\le 1 \text{ for all } \{i,j\}\in\bar{\mathcal{E}}\,, \\ &\qquad s_{ij}-\delta(D_c)_{ij}+2\tau(A_c)_{ij}\le 0 \text{ for all } \{i,j\}\in\mathcal{E}\ \}\,, \end{aligned} \tag{74}$$

where A_c and D_c are again of general size $n\times n$. Clearly, for any feasible point (S,δ,τ) to (74), it must hold $\delta+1\ge 0$ and $s_{ij}\le\delta+1$ for all i,j, by semidefiniteness of S. Then we derive from $\delta\le-\tau$ the condition $s_{ij}\le\delta+1\le-\delta-2\tau+1$, which is exactly $s_{ij}-\delta(D_c)_{ij}+2\tau(A_c)_{ij}\le 1$ if $\{i,j\}\in\bar{\mathcal{E}}\cap\mathcal{I}$. Even simpler is the condition $s_{kl}-\delta(D_c)_{kl}+2\tau(A_c)_{kl}\le 1$ if $\{k,l\}\in\bar{\mathcal{E}}\setminus\mathcal{I}$, as this amounts to $s_{kl}\le\delta+1$. Hence we can safely ignore the conditions for $\{i,j\}\in\bar{\mathcal{E}}$, and (73) follows. □

Remark 3 *If we replace the canonical cycle matrix A_c by the adjacency matrix $A_{\mathcal{H}}$ of a different triangle-free graph $\mathcal{H}$, we arrive at a variant $\ell_Q^{\rm cved'}$ of the cved bound.*

Consider the graph $\mathcal{G}$ with adjacency matrix $A_{\mathcal{G}}=A_c\otimes I_5+E\otimes A_c$, where A_c is the adjacency matrix of the five-cycle C_5, and $\otimes$ denotes the Kronecker product. For this graph we have

$$\omega(\mathcal{G})=4=\lfloor 1/0.2236\rfloor=\lfloor\bar{\theta}^{\rm cved'}\rfloor=\lfloor 1/\ell_{E-A_{\mathcal{G}}}^{\rm cved'}\rfloor<5=\bar{\theta}'\,, \tag{75}$$

as computed by Florian Frommlet (personal communication) who used as $\mathcal{H}$ a graph resulting from $\mathcal{G}$ by dropping some of the 150 edges there, namely the triangle-free graph with adjacency matrix $A_{\mathcal{H}}=E\otimes A_c$. Hence the cved(') improvement even survives truncation in some instances, a phenomenon rarely observed in other SDP improvements of Schrijver's bound.

Now let us return to the weighted case and the generic θ numbers $\bar{\theta}_B^{\rm gen}=\frac{1}{\ell_B^{\rm gen}}$ for any $B\in\mathcal{M}(w,\mathcal{G})$. Obviously, we may further improve any such bound by noting that every $B\in\mathcal{M}(w,\mathcal{G})$ yields the same value $\ell_B=\frac{1}{\omega(\mathcal{G},w)}$. Since the bounds $\ell_B^{\rm gen}$ may vary with B, it may pay to use

$$\bar{\theta}^{\rm gen}=\left[\sup\{\ell_B^{\rm gen}:B\in\mathcal{M}(w,\mathcal{G})\}\right]^{-1} \tag{76}$$

as a valid upper bound for $\omega(\mathcal{G},w)$. Observe that $\mathcal{M}(w,\mathcal{G})$ forms a shifted polyhedral matrix cone with apex $B(\mathcal{G},w)$ given by $b_{ij}(\mathcal{G},w)=0$ if $\{i,j\}\in\mathcal{E}$ and $b_{ij}(\mathcal{G},w)=\frac{1}{2w_i}+\frac{1}{2w_j}$, else. If $\ell_B^{\rm gen}$ results from an LP or SDP, then also (76) amounts to solving an LP or SDP, respectively, by adding a linear constraint for every edge in $\bar{\mathcal{E}}$. Note that the bounds treated in Section 2 are of little use here as $\ell_B^0 = 0$ for all $B \in \mathcal{M}(w, \mathcal{G})$ unless $\mathcal{E} = \emptyset$, and similarly $\bar{\theta}_B^{\text{ref}} = W(N)$ for all $B \in \mathcal{M}(w, \mathcal{G})$ in that case.

Further improvements of θ numbers along the approach outlined in Section 6.2, as well as empirical comparison of these bounds with each other and with further, very recently proposed SDP-based bounds [16, 34], remain to be investigated as an interesting subject of research in the near future.

10 Bounding a general Quadratic Program on a Polytope

10.1 Bounding a quadratic function over a polytope with known vertices: the ℓ^1 ball

As anticipated in Section 1.2, when we know the vertices of a polytope P, the problem of minimizing a function $g(y)$ over P can be easily transformed into the problem of minimizing the function $f(x) = g(Vx)$ on the standard simplex Δ with the simple change of variables $y = Vx$, where V is the matrix whose column vectors are the vertices $v^1, \dots, v^N$ of P.

In the case of a quadratic function, $g(y) = y^\top Cy + 2c^\top y$, the transformed function becomes $f(x) = x^\top V^\top CVx + 2c^\top Vx$. Again, we can further reduce this problem to a Standard QP of the form (1) by taking $Q = Q(C, c) = V^\top CV + ec^\top V + V^\top ce$. Thus, all the bounds for $\ell_{Q(C,c)}$ yield corresponding bounds for the minimum of $g(y)$ over P.

As an example of application of this simple but important remark we consider the problem

$$\ell_C^{B_1} = \min \left\{ y^\top Cy : y \in B_1 \right\} \quad \text{where} \quad B_1 = \left\{ x \in \mathbb{R}^m : \sum_i |x_i| \le 1 \right\}. \tag{77}$$

Problem (77) has been analyzed, e.g., by Nesterov [30] who proposes a lower bound for it but without establishing its relative accuracy.

By reducing this problem to a StQP we are able to show that Nesterov's bound is dominated by the cvd bound for the latter problem. Furthermore, we obtain simple $\mathcal{O}(m^2)$ closed-form bounds for the minimum on B_1, by rephrasing the analogous bounds for the StQP.

It is simple to check that the vertices of the ℓ^1 ball B_1 are the $2n$ vectors $\pm e^i$, $i \in \{1, \dots, n\}$. Hence the reduction from B_1 to the standard simplex can be performed with the matrix $V = [I_n|-I_n]$. Thus $\ell_C^{B_1} = \ell_Q$, where

$$Q = \begin{bmatrix} C & -C \\ -C & C \end{bmatrix}. \tag{78}$$

We recall that Nesterov [30, pag. 387] established the validity of the following lower bound[2] for $\ell_C^{B_1}$

$$\bar{\ell}_C^{B_1} = \sup_{S,\lambda} \{\lambda : \lambda e = -\mathrm{diag}\,(S),\ S + C \succeq O,\ S \succeq O\}\,. \tag{79}$$

By taking $S' = -S$ we obtain the equivalent formulation

$$\bar{\ell}_C^{B_1} = \sup_{S',\lambda} \{\lambda : \lambda e = \mathrm{diag}\,(S'),\ C - S' \succeq O,\ S' \preceq O\}\,. \tag{80}$$

When $S' \preceq O$ and $C - S' \succeq O$, we have that both

$$-T = \begin{bmatrix} -S' & S' \\ S' & -S' \end{bmatrix} \quad \text{and} \quad Q - T = \begin{bmatrix} C - S' & S' - C \\ S' - C & C - S' \end{bmatrix} \tag{81}$$

are positive-semidefinite. Hence, $\ell_{Q-T} \geq 0$ and $\ell_T = \lambda$, since diag $(S') = \lambda e$. Therefore, taking into account Remark 1 and Section 8.6, we obtain

$$\bar{\ell}_C^{B_1} \leq \sup\{\beta_Q(T) : Q - T \succeq O,\ T \succeq O,\ \mathrm{diag}\,(T) = \lambda e\} = \ell_Q^{dcd} \leq \ell_Q^{cvd}\,,$$

with strict inequality between the two extremes above in some instances. The latter result has also been established, by a completely different argument, in [11], where some empirical evidence on the quality of the improvement is provided. Now, to obtain simple closed-form lower bounds for (77) we just need to apply the results of Section 2 to the matrix Q defined in (78). Thus we obtain (the leftmost inequality below can also be derived directly from the triangle inequality)

$$\hat{\ell}_C^{B_1} = -\max_{i,j} |c_{ij}| \leq \ell_C^{B_1} \quad \text{and} \quad \check{\ell}_C^{B_1} = \hat{\ell}_C^{B_1} + \left[2 \sum_i (c_{ii} - \hat{\ell}_C^{B_1})^{-1}\right]^{-1} \leq \ell_C^{B_1}.$$

10.2 Bounding the StQP relaxation of a Quadratic Program over a polytope

Consider a polytope in standard LP form

$$P = \{y \in \mathbb{R}^n : Ay = b,\ y \geq o\},$$

[2] In fact Nesterov stated an equivalent upper bound for a maximization problem.

where A is an $m \times n$ matrix and $b \in \mathbb{R}^m$. It is obvious that if for some index i we have $b_i \neq 0$ and $a_{ij} b_i > 0$ for all j, then $S_i = \{x \in \mathbb{R}^n : \sum_j a_{ij} x_j = b_i, x \geq o\}$ is a (non-standard) simplex and P is bounded and contained in S_i.

On the other hand, we now show that *every* non-trivial bounded polytope in standard LP form is contained in a (non-standard) simplex, which can be determined by solving a Linear Program.

Lemma 6 *Let P be bounded and different from $\{o\}$, then the polyhedron*

$$R = \{z \in \mathbb{R}^m : A^\top z \geq e\} \tag{82}$$

is nonempty. Furthermore, setting $p^z = A^\top z$ and $\pi^z = b^\top z$, for every $z \in R$ we have that $\pi^z > 0$ as well as $p^z \geq e$, and P is contained in the simplex $S^z = \left\{y \in \mathbb{R}^n : (p^z)^\top y = \pi^z,\ y \geq o\right\}$.

Proof. The inclusion $P \subseteq S^z$ and the inequality $p^z \geq e$ for every $z \in R$ follow immediately from the definitions. Hence, we only need to prove that R is nonempty and that $\pi^z > 0$ for every z in R. Since P is bounded, the function $e^\top y$ attains its maximum on P. Hence, by LP duality, R is nonempty. Since P is bounded and different from $\{o\}$, we must have $b \neq o$. Hence, from $Ay = b$ and $A^\top z \geq e$ we also obtain $\pi^z > 0$. □

With this result, it is easy to establish closed-form bounds for the general QP over P:

Proposition 2 *Consider the problem of minimizing a quadratic function $f(y) = y^\top C y + 2c^\top y$ over a nontrivial polytope P. Let R be defined as in (82) and select an arbitrary $z \in R$. Put $\pi = b^\top z > 0$ and $p = A^\top z \geq e$. Then with $D = \pi(\mathrm{Diag}\, p)^{-1}$ and $Q = DCD + Dce^\top + ec^\top D$ we have*

$$\ell_Q^0 = \min_{i,j} \left[c_{ij} \frac{\pi^2}{p_i p_j} + c_i \frac{\pi}{p_i} + c_j \frac{\pi}{p_j} \right] \leq \min\{f(y) : y \in P\}\ ,$$

and

$$\ell_Q^{\mathrm{ref}} = \ell_Q^0 + \left[\sum_i (c_{ii} \frac{\pi^2}{p_i} + 2c_i \frac{\pi}{p_i} - \ell_Q^0)^{-1} \right]^{-1} \leq \min\{f(y) : y \in P\}\ .$$

Proof. By Lemma 6 we have $P \subseteq \left\{y \in \mathbb{R}^n_+ : p^\top y = \pi\right\}$. Hence, in Section 1.3, by the variable transformation $y = Dx$ we see that $x^\top Q x = f(y)$ and $x \in \Delta$, so that the StQP (1) with Q as specified above provides a lower bound for f on P, i.e., precisely,

$$\min\left\{x^\top Q x : x \in \Delta\right\} \leq \min\{f(y) : y \in P\}\ . \tag{83}$$

Hence, every lower bound for ℓ_Q provides a lower bound for f on P. In particular we obtain the claimed closed-form bounds from Section 2. □

Remark 4 *In view of Lemma 6, for* every *function f on S^z we have*

$$\min\{f(y) : y \in P\} \geq \min\{f(y) : y \in S^z\} . \tag{84}$$

Thus any lower bound for f on S^z is also a valid lower bound for f on P. We now apply this simple remark to obtain efficiently computable lower bounds in the case where f is quasi-concave. In this case we know that the minimum of $f(x)$ on S^z is attained at a vertex of S^z, so that

$$\min\{f(y) : y \in P\} \geq \; h(z) = \min_i f(\frac{\pi^z}{p_i^z}\, e^i) . \tag{85}$$

At this point one might be tempted to find the best possible bound of this type $h^* = \max\{h(z) : z \in R\}$. Unfortunately, $h(z)$ is a nonlinear and nonconcave function in general. However, we can easily find an upper bound for h^* by solving the quasi-concave one-dimensional problems $\sup_{t\geq 0} f^i(t)$, where $f^i(t) = f(te^i)$, and setting

$$\bar{h} = \min_i \sup_{t\geq 0} f^i(t) .$$

Clearly, $h^* \leq \bar{h}$. Furthermore, since the functions f_i are quasi-concave, the sets $T^i(\alpha) = \{t \geq 0 : f^i(t) \geq \alpha\}$ are intervals, and it is, in general, simple to determine their extremes $L_i(\alpha), U_i(\alpha)$ so that $T^i(\alpha) = [L_i(\alpha), U_i(\alpha)]$. Now the problem of checking whether $\alpha = \bar{h}$ - or any lower value of α - is a lower bound for $\min_{x\in P} f(x)$ reduces to the feasibility of the system of inequalities:

$$L_i(\alpha) \leq \frac{\pi^z}{p_i^z} \leq U_i(\alpha),\; i = 1, \ldots, n,\; z \in R . \tag{86}$$

Recalling the definitions of π_i^z, p_i^z and R we can rewrite (86) as the following system of linear *inequalities*

$$A^\top z \geq e, \quad L_i(\alpha) a_i^\top z \leq b^\top z \leq U_i(\alpha) a_i^\top z,\; i = 1, \ldots, n,\; z \in \mathbb{R}^m , \tag{87}$$

where a_i denotes the i^{th} column of A. By construction, feasibility of (87) guarantees the validity of the lower bound

$$\alpha \leq \min\{f(y) : y \in P\} .$$

However, it should also be clear that the above bound might hold even when system (87) is infeasible.

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