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D.C. Versus Copositive Bounds for Standard QP

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Abstract. The *standard quadratic program* (QPS) is $\min_{x\in\Delta} x^T Qx$, where $\Delta\subset\Re^n$ is the simplex $\Delta=\{x\geqslant 0 \mid \sum_{i=1}^n x_i=1\}$. QPS can be used to formulate combinatorial problems such as the maximum stable set problem, and also arises in global optimization algorithms for general quadratic programming when the search space is partitioned using simplices. One class of 'd.c.' (for 'difference between convex') bounds for QPS is based on writing $Q=S-T$, where S and T are both positive semidefinite, and bounding $x^T Sx$ (convex on Δ) and $-x^T Tx$ (concave on Δ) separately. We show that the maximum possible such bound can be obtained by solving a semidefinite programming (SDP) problem. The dual of this SDP problem corresponds to adding a simple constraint to the well-known Shor relaxation of QPS. We show that the max d.c. bound is dominated by another known bound based on a copositive relaxation of QPS, also obtainable via SDP at comparable computational expense. We also discuss extensions of the d.c. bound to more general quadratic programming problems. For the application of QPS to bounding the stability number of a graph, we use a novel formulation of the Lovasz ϑ number to compare ϑ, Schrijver's ϑ', and the max d.c. bound.

1. Introduction

Consider the *quadratic program on the simplex*

$$\begin{aligned} \text{QPS}: \quad \min \quad & x^T Qx \\ \text{s.t.} \quad & x\in\Delta, \end{aligned}$$

where Q is symmetric, $\Delta=\{x\in\Re^n_+ \mid e^T x=1\}$, $\Re^n_+$ denotes the non-negative orthant, and e is the vector of ones. The problem QPS is often refered to as the *standard quadratic program*. It is easy to show that in the general case QPS is NP-Hard; for example the problem of computing the maximum stable set in a graph can be posed as an instance of QPS. QPS also arises naturally in global optimization algorithms for general quadratic programming when simplices, rather than upper and lower bounds on variables, are used to partition the search space.

A number of recent papers have considered the construction of approximate solutions and/or lower bounds for QPS. Let v_{QPS} denote the solution

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value in QPS, and let $\bar{v}_{\text{QPS}} = \max_{x\in\Delta} x^T Qx$. Nesterov [7] constructs an approximate solution x satisfying

$$x^T Qx - v_{\text{QPS}} \leqslant \epsilon(\bar{v}_{\text{QPS}} - v_{\text{QPS}}) \tag{1}$$

for some $0 \leqslant \epsilon \leqslant 1$. In [7] two approaches yield approximations with $\epsilon = \frac{2}{3}$ and $\epsilon = \frac{1}{2}$. Bomze and de Klerk [2] consider families of linear programming (LP) and semidefinite programming (SDP) relaxations of QPS based on approximations of the cone of copositive matrices. For $r = 0, 1, \ldots$ either approach obtains a lower bound $v^r \leqslant v_{\text{QPS}}$ such that

$$v_{\text{QPS}} - v^r \leqslant \frac{1}{r+1}(\bar{v}_{\text{QPS}} - v_{\text{QPS}}). \tag{2}$$

In [2] it is also shown that a discretization of Δ, closely related to the LP bound, obtains a feasible solution $x \in \Delta$ satisfying (1) with $\epsilon = \frac{1}{r+2}$.

Bomze [1] suggests the use of 'd.c.' (for 'difference between convex') bounds for QPS, based on writing $Q = S - T$, where $S \succeq 0$, $T \succeq 0$. It is then obvious that a lower bound for QPS is given by

$$v(S, T) = \min_{x\in\Delta} x^T Sx + \min_{x\in\Delta} -x^T Tx, \tag{3}$$

where the first minimization is convex and the second is concave. For any (S, T) the value of $v(S, T)$ is efficiently computable; in fact obtainable in polynomial time in the case where the entries of Q are rational [8]. Bomze considers several approaches for choosing a good (S, T), including maximizing a certain SDP approximation of $v(S, T)$.

In this paper we describe further results for the d.c. bounds considered by Bomze [1]. In the next section we show that for a given Q the bound $v(S, T)$ can be directly maximized by solving an SDP, resulting in an optimal bound of this type. The required SDP is no more complex than that used as an approximation of $v(S, T)$ in [1]. We also show that the dual of the SDP that gives the max d.c. bound has a surprising interpretation as a strengthening of the well-known Shor relaxation of QPS. In Section 3 we show that the optimal d.c. bound is itself dominated by the $r = 0$ SDP bound from [2], which can be obtained at comparable computational effort. In Section 4 we discuss the extension of the results obtained for QPS to the general quadratic programming problem over linear constraints. In Section 5 we consider in more detail the application of QPS to bound the size of the maximum stable set in a graph. We give a novel formulation of the Lovasz ϑ number that illustrates the relationship between ϑ, Schrijver's ϑ', and the max d.c. bound. In the last section we give some computational results, using a set of test problems considered in [2].

Notation. All matrices are symmetric. For matrices A and B we use $A \succeq B$ to denote that $A - B$ is positive semidefinite, and $A \geqslant 0$ to denote that A is componentwise nonnegative. The matrix inner product is written $A \bullet B = \mathrm{tr}(AB)$, where $\mathrm{tr}(\cdot)$ denotes the trace. For a matrix A, $\underline{\lambda}(A)$ and $\overline{\lambda}(A)$ denote the minimal and maximal eigenvalues, respectively. We use e to denote a vector of arbitrary dimension with each component equal to one, and $E = ee^T$. If A is a matrix and a is a vector, then $\mathrm{diag}(A)$ is the vector of diagonal components of A, and $\mathrm{Diag}(a)$ is the diagonal matrix with $\mathrm{diag}(\mathrm{Diag}(a)) = a$. The nonnegative orthant in $\Re^n$ is denoted $\Re^n_+$, and $\mathcal{S}^n_+$ is the cone of $n \times n$ symmetric positive semidefinite matrices.

2. An Optimal D.C. Bound

The class of 'd.c.' bounds for QPS considered in [1] is based on writing $Q = S - T$, where $S \succeq 0$ and $T \succeq 0$. A lower bound on v_{QPS} is then given by $v(S, T)$, from (3). In [1] it is suggested that to obtain a good choice of (S, T) one could use the fact that

$$v(S,T) \geqslant v'(S,T) = \frac{1}{n}\underline{\lambda}(S) - \overline{\lambda}(T).$$

The problem of maximizing $v'(S, T)$ can be posed as an SDP. This SDP can be approximately solved to yield matrices $S \succeq 0$ and $T \succeq 0$ which can then be used to compute $v(S, T)$.

In this section we will show that the use of $v'(\cdot,\cdot)$ as a surrogate for $v(\cdot,\cdot)$ is unnecessary, and instead $v(\cdot,\cdot)$ can be directly maximized by solving an SDP. To obtain the required SDP we will use the fact that if $Q \succeq 0$, then QPS is equivalent to the Shor relaxation

$$\begin{aligned} \mathrm{SQPS:} \quad \min \quad & Q \bullet X \\ \text{s.t.} \quad & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0 \\ & x \in \Delta. \end{aligned}$$

(Note that if $Q \not\succeq 0$ then the solution value in SQPS is $-\infty$.) By first expressing SQPS in a standard conic linear formulation $\min\{c^T u : Au = b,\ u \in K\}$, where K is a closed, convex cone, the dual of SQPS may be expressed as $\max\{b^T w : A^T w + s = c,\ s \in K^*\}$, where K^* is the polar cone of K. In the case of SQPS we have $K = K^* = \Re^n_+ \times \mathcal{S}^{(n+1)}_+$, and it is not difficult (but somewhat tedious) to show that the dual of SQPS is

$$\begin{aligned} \mathrm{DQPS:} \quad \max \quad & \mu - \sigma \\ \text{s.t.} \quad & \begin{pmatrix} \sigma & s^T \\ s & Q \end{pmatrix} \succeq 0 \\ & 2s + \mu e \leqslant 0. \end{aligned}$$

For any $Q \succeq 0$ the solution values of SQPS and DQPS are equal, and are both attained, since SQPS is equivalent to QPS and satisfies a Slater condition [8].

Now suppose that $Q = S - T$, where $S \succeq 0$, $T \succeq 0$. Then the first term in (3) can be expressed using DQPS, with S in place of Q, and the second is simply equal to $\min\{-t_{ii} \mid i = 1, \dots, n\} = \max\{-\theta \mid \theta \geqslant t_{ii},\ \ i = 1, \dots, n\}$. Combining the two terms written as maximizations, and considering S to be a variable, we arrive at the *optimal d.c. bound*

$$\begin{array}{lll} \mathrm{DQPS}_{\mathrm{DC}}: & \sup & \mu - \sigma - \theta \\ & \text{s.t.} & \begin{pmatrix} \sigma & s^T \\ s & S \end{pmatrix} \succeq 0 \\ & & 2s + \mu e \leqslant 0 \\ & & S \succeq Q, \quad \theta e \geqslant \operatorname{diag}(S - Q). \end{array}$$

The dual of $\mathrm{DQPS}_{\mathrm{DC}}$ has a surprisingly simple interpretation as a strengthening of the Shor relaxation SQPS. Again applying the duality theory of conic linear programs, it is not difficult to show that the dual of $\mathrm{DQPS}_{\mathrm{DC}}$ is

$$\begin{array}{ll} \min & Q \bullet X \\ \text{s.t.} & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0 \\ & X \preceq \operatorname{Diag}(y) \\ & x \in \Delta, \ \ y \in \Delta. \end{array}$$

Note that if (X, x, y) are feasible in this problem, then

$$1 = e^T(xx^T)e \leqslant e^T X e \leqslant e^T \operatorname{Diag}(y) e = 1, \tag{4}$$

and therefore $e^T(X - xx^T)e = e^T(\operatorname{Diag}(y) - X)e = 0$. It follows that $Xe = x$ and $Xe = y$, so $x = y$ and the dual of $\mathrm{DQPS}_{\mathrm{DC}}$ can be written in the simplified form

$$\begin{array}{lll} \mathrm{SQPS}_{\mathrm{DC}}: & \min & Q \bullet X \\ & \text{s.t.} & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0 \\ & & X \preceq \operatorname{Diag}(x) \\ & & x \in \Delta. \end{array}$$

Thus the optimal d.c. bound corresponds exactly to adding the constraint $X \preceq \operatorname{Diag}(x)$ to SQPS. Note that if $x \in \Delta$ then $xx^T \preceq \operatorname{Diag}(x)$ holds (for example through an application of the Gerschgorin circle theorem), so this added constraint is certainly valid. The objective value in $\mathrm{DQPS_{DC}}$ is bounded (because $\mathrm{SQPS_{DC}}$ is feasible) and the feasible region satisfies a Slater condition, so the optimal values of $\mathrm{SQPS_{DC}}$ and $\mathrm{DQPS_{DC}}$ are equal and the value is attained in $\mathrm{SQPS_{DC}}$. However $\mathrm{SQPS_{DC}}$ does *not* satisfy a Slater condition, because $Xe = x$ implies that

$$\begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \begin{pmatrix} -1 \\ e \end{pmatrix} = 0, \tag{5}$$

for any feasible solution. Note that it is obvious that the level sets in $\mathrm{DQPS_{DC}}$ are unbounded, since $v(S+\lambda E, T+\lambda E) = v(S,T)$ for any $\lambda \geqslant 0$.

3. Comparison with a Copositive Bound

In this section we will show that the optimal d.c. bound obtained in the previous section is dominated by another known bound for QPS. Consider a second semidefinite relaxation of QPS,

$$\begin{array}{lll} \mathrm{SQPS^0_{CP}}: & \min & Q \bullet X \\ & \text{s.t.} & E \bullet X = 1 \\ & & X \in \mathcal{K}_0^*, \end{array}$$

where $\mathcal{K}_0^* = \{X \mid X \succeq 0, X \geqslant 0\}$. A problem of the form $\mathrm{SQPS^0_{CP}}$ is sometimes referred to as the ‘strengthened Shor relaxation’ of QPS. The dual of $\mathrm{SQPS^0_{CP}}$ is

$$\begin{array}{lll} \mathrm{DQPS^0_{CP}}: & \max & \lambda \\ & \text{s.t.} & Q - \lambda E \in \mathcal{K}_0, \end{array}$$

where $\mathcal{K}_0 = \{X = S + P \mid S \succeq 0, P \geqslant 0\}$. The solution values in $\mathrm{SQPS^0_{CP}}$ and $\mathrm{DQPS^0_{CP}}$ are equal, and are both attained, since the feasible region in $\mathrm{SQPS^0_{CP}}$ is compact and satisfies a Slater condition [8].

It is known that if $\mathcal{K}_0$ and $\mathcal{K}_0^*$ are replaced by the cone of symmetric copositive matrices and its dual, respectively, then $\mathrm{DQPS^0_{CP}}$ and $\mathrm{SQPS^0_{CP}}$ are equivalent to QPS [3]. Unfortunately these cones are not computationally tractable. However, it has been shown [4,9] that there is a family of cones with SDP representations $\mathcal{K}_r$, $r \geqslant 0$, so that for any given Q, $\mathrm{SQPS^r_{CP}}$ and $\mathrm{DQPS^r_{CP}}$ approximate QPS to any given accuracy when r is taken sufficiently large. (Here $\mathrm{SQPS^r_{CP}}$ and $\mathrm{DQPS^r_{CP}}$ denote problems of the form $\mathrm{SQPS^0_{CP}}$ and $\mathrm{DQPS^0_{CP}}$ but with $\mathcal{K}_0$ replaced by $\mathcal{K}_r$.) In [2] it is shown that the use of the cone $\mathcal{K}_r$ in place of $\mathcal{K}_0$ produces a lower bound $v^r = v^r_{\mathrm{CP}}$ satisfying (2).

Comparison of $\mathrm{SQPS_{DC}}$ and $\mathrm{SQPS^0_{CP}}$ will be facilitated by the following problem, which is equivalent to $\mathrm{SQPS_{DC}}$ by Lemma 1 below.

$$
\begin{aligned}
\mathrm{SQPS}'_{\mathrm{DC}}: \quad & \min && Q \bullet X \\
& \text{s.t.} && E \bullet X = 1 \\
& && Xe \geqslant 0, \quad X \preceq \mathrm{Diag}(Xe) \\
& && X \succeq 0.
\end{aligned}
$$

LEMMA 1. *(X, x) is feasible for* $\mathrm{SQPS}_{\mathrm{DC}}$ *if and only if $x = Xe$ and X is feasible for* $\mathrm{SQPS}'_{\mathrm{DC}}$.

Proof. Let (X, x) be feasible for $\mathrm{SQPS}_{\mathrm{DC}}$. Arguments similar to (4) show that $Xe = x$ so that X is feasible for $\mathrm{SQPS}'_{\mathrm{DC}}$. On the other hand, suppose X is feasible for $\mathrm{SQPS}'_{\mathrm{DC}}$ and $x = Xe$. Clearly, $x \in \Delta$ and $X \preceq \mathrm{Diag}(x)$. Moreover, the identity

$$
\begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} = \begin{pmatrix} e^T \\ I \end{pmatrix} X(e, I)
$$

combined with $X \succeq 0$ completes the proof that (X, x) is feasible for $\mathrm{SQPS}_{\mathrm{DC}}$. □

THEOREM 1. *Let v_{DC} and v^0_{CP} denote the solution values in* $\mathrm{SQPS}_{\mathrm{DC}}$ *and* $\mathrm{SQPS}^0_{\mathrm{CP}}$*, respectively. Then $v^0_{\mathrm{CP}} \geqslant v_{\mathrm{DC}}$.*

Proof. Let X be a feasible solution in $\mathrm{SQPS}^0_{\mathrm{CP}}$. The nonnegativity of X and the Gerschgorin circle theorem imply that $Xe \geqslant 0$ and $X \preceq \mathrm{Diag}(Xe)$, which show that X is feasible for $\mathrm{SQPS}'_{\mathrm{DC}}$. Defining $x = Xe$, Lemma 1 thus implies that (X, x) is feasible for $\mathrm{SQPS}_{\mathrm{DC}}$ with the same objective value as X in $\mathrm{SQPS}^0_{\mathrm{CP}}$, which proves the theorem. □

Note that if $Q \succeq 0$, then it is obvious that $v_{\mathrm{DC}} = v_{\mathrm{QPS}}$, since $v_{\mathrm{QPS}} = v(S, T)$ for $S = Q, T = 0$. From Theorem 1 it follows that $v^0_{\mathrm{CP}} = v_{\mathrm{QPS}}$ as well. This was not obvious *a-priori* since the constraint $X \succeq xx^T$ does not appear in $\mathrm{SQPS}^0_{\mathrm{CP}}$.

It is easy to construct cases where $v_{\mathrm{DC}} < v^0_{\mathrm{CP}}$. A very simple example uses the matrix

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

For this Q it is clear that $v_{\mathrm{QPS}} = 0$, and $v^0_{\mathrm{CP}} = 0$ as well, since $\lambda = 0$ is feasible in $\mathrm{DQPS}^0_{\mathrm{CP}}$. However $v_{\mathrm{DC}} = \frac{-1}{8}$, where the optimal solution in $\mathrm{SQPS}_{\mathrm{DC}}$ is

$$
X = \frac{1}{16} \begin{pmatrix} 3 & -1 & 2 \\ -1 & 3 & 2 \\ 2 & 2 & 4 \end{pmatrix}.
$$

4. Extension to General Linear Constraints

Suppose the vectors $\{a_i\}_{i=1}^m \subset \Re^n$ define a polytope $P = \{x \in \Re^n_+ : a_i^T x = b_i, \text{i} = 1, \ldots, m\}$. Note that since P is bounded it must be that $b_i \neq 0$ for some i, and P is the convex hull of its extreme points. Suppose that the set $\{w_j\}_{j=1}^p$ is a complete listing of the extreme points of P, and let $W \in \Re^{n\times p}$ be the matrix whose j-th column is w_j.

One may extend the results of the previous sections to consider optimal d.c. bounds for the problem

$$\begin{aligned} \text{QPP}: \quad \min \quad & x^T Q x \\ \text{s.t.} \quad & x \in P. \end{aligned}$$

Note that QPS corresponds to $m = 1$, $a_1 = e$. In the current context, however, there are two natural choices for d.c. bounds. The first option is to start by describing P as the convex hull of its extreme points and then apply the results obtained for QPS. In particular, QPP is clearly equivalent to

$$\begin{aligned} \min \quad & z^T (W^T Q W) z \\ \text{s.t.} \quad & z \in \Delta_p, \end{aligned}$$

where Δ_p is the standard simplex in $\Re^p$. The optimal d.c. bound is thus calculated as

$$\begin{aligned} \text{SQPP}_{\text{DC1}}: \quad \min \quad & W^T Q W \bullet Z \\ \text{s.t.} \quad & z z^T \preceq Z \preceq \text{Diag}(z) \\ & z \in \Delta_p. \end{aligned}$$

The second option is to apply the procedures of Section 2 to QPP directly, that is, to construct an optimal lower bound of the form

$$v(S, T) = \min_{x\in P} x^T S x + \min_{x \in P} -x^T T x$$

based on writing $Q = S - T$ for $S \succeq 0$, $T \succeq 0$. Employing the Shor relaxation, the first portion of this bound can be calculated as

$$\begin{aligned} \max \quad & b^T \mu - \sigma \\ \text{s.t.} \quad & \begin{pmatrix} \sigma & s^T \\ s & S \end{pmatrix} \succeq 0 \\ & 2s + A^T \mu \leqslant 0. \end{aligned}$$

Moreover, using the extreme points of P, the second portion can be expressed as $\max\{-\theta \mid \theta \geqslant T \bullet w_j w_j^T,\ \ j = 1, \ldots, p\}$. By optimizing jointly over S and T, we thus obtain a bound

$$\begin{aligned} \max \quad & b^T\mu - \sigma - \theta \\ \text{s.t.} \quad & \begin{pmatrix} \sigma & s^T \\ s & S \end{pmatrix} \succeq 0 \\ & 2s + A^T\mu \leqslant 0 \\ & S \succeq Q, \qquad \theta \geqslant (S - Q) \bullet w_j w_j^T, \quad j = 1, \ldots, p. \end{aligned}$$

Taking the dual, this optimized bound can be written

$$\begin{aligned} \text{SQPP}_{\text{DC2}}: \quad \min \quad & Q \bullet X \\ \text{s.t.} \quad & xx^T \preceq X \preceq W \operatorname{Diag}(y) W^T \\ & x \in P, \ \ y \in \Delta_p. \end{aligned}$$

Note that in the case of QPS, for which $P = \Delta$ and $W = I$, the construction here matches that of SQPS_{DC} in Section 2.

In order to establish the relationship between SQPP_{DC1} and SQPP_{DC2} it is helpful to define a third problem,

$$\begin{aligned} \text{SQPP}'_{\text{DC2}}: \quad \min \quad & W^T Q W \bullet Z \\ \text{s.t.} \quad & W z z^T W^T \preceq W Z W^T \preceq W \operatorname{Diag}(z) W^T \\ & z \in \Delta_p. \end{aligned}$$

THEOREM 2. *Let* v_{DC1}, v_{DC2} *and* v'_{DC2} *denote the solution values in* SQPP_{DC1}, SQPP_{DC2} *and* $\text{SQPP}'_{\text{DC2}}$, *respectively. Then* $v_{\text{DC1}} \geqslant v'_{\text{DC2}} = v_{\text{DC2}}$.

Proof. It is obvious that $v_{\text{DC1}} \geqslant v'_{\text{DC2}}$, so to prove the lemma we must show that $v'_{\text{DC2}} = v_{\text{DC2}}$. We first claim $v'_{\text{DC2}} \geqslant v_{\text{DC2}}$. Let (Z, z) be feasible for $\text{SQPP}'_{\text{DC2}}$, and define $(X, x, y) = (WZW^T, Wz, z)$. Clearly $x \in P$ and $y \in \Delta_p$. Moreover, we have

$$W z z^T W \preceq W Z W^T \preceq W \operatorname{Diag}(z) W^T \implies xx^T \preceq X \preceq W \operatorname{Diag}(y) W^T,$$

which shows that (X, x, y) is feasible for SQPP_{DC2}. The claim follows by noting that $Q \bullet X = (W^T Q W) \bullet Z$.

To prove the reverse inequality, let (X, x, y) be feasible for SQPP_{DC2}. First, pre- and post-multiplying the inequality $xx^T \preceq X \preceq W \operatorname{Diag}(y) W^T$ by a_i^T and a_i, we see that

$$\begin{aligned} & (a_i^T x)^2 \leqslant a_i^T X a_i \leqslant (W^T a_i)^T \operatorname{Diag}(y)(W^T a_i) \\ & \qquad \implies b_i^2 \leqslant a_i^T X a_i \leqslant (b_i e)^T \operatorname{Diag}(y)(b_i e) = b_i^2, \end{aligned}$$

which implies $a_i^T X a_i = b_i^2$. So a_i is in the null space of both $X - xx^T$ and $W \operatorname{Diag}(y) W^T - X$. For $b_i \neq 0$ (which must hold for at least one i) it follows that $x = Wy$. Defining $z = y$, we thus have

$$Wzz^TW \preceq X \preceq W\,\mathrm{Diag}(z)W^T.$$

It remains to show that $\exists Z,\ X = WZW^T$. Let $v \in \mathrm{Null}(W^T) \subset \Re^n$. Then the above matrix inequality shows that $v^TXv = 0$, which implies $v \in \mathrm{Null}(X)$. With $Q\,\mathrm{Diag}(\lambda)Q^T$ a spectral decomposition of X, we let Q_+ denote the submatrix of Q consisting of only those columns which correspond to positive eigenvectors, and let Q_0 denote the submatrix corresponding to zero eigenvectors. It thus follows that $\mathrm{Null}(W^T) \subseteq \mathrm{Range}(Q_0)$, which in turn implies $\mathrm{Range}(Q_+) \subseteq \mathrm{Range}(W)$. Therefore, each positive eigenvector q_i of X can be expressed as Wu_i for some $u_i \in \Re^p$. Hence, $X = WZW^T$, where we define $Z = \sum_{i:\lambda_i>0} \lambda_i u_i u_i^T$.

Clearly (Z, z) is feasible for $\mathrm{SQPP}'_{\mathrm{DC2}}$. The inequality $v'_{\mathrm{DC2}} \leqslant v_{\mathrm{DC2}}$ now follows by noting $(W^TQW) \bullet Z = Q \bullet X$. □

Note that since $\mathrm{SQPP_{DC1}}$ and $\mathrm{SQPP_{DC2}}$ involve the matrix W, and in general $p \gg n$, both of these problems are in general computationally intractible. In special cases where p is not too large, Theorem 2 indicates that $\mathrm{SQPP_{DC1}}$ is preferable. In the case of QPS, $W = I$ and $v_{\mathrm{DC1}} = v_{\mathrm{DC2}}$.

There is also more than one approach to constructing an extension of the copositive bound for QPP. By considering P to be the convex hull of its extreme points, we have the following copositive relaxation:

$$\begin{array}{lll} \mathrm{SQPP}^0_{\mathrm{CP1}}: & \min & W^TQW \bullet Z \\ & \text{s.t.} & E \bullet Z = 1 \\ & & Z \in \mathcal{K}_0^* \subset \mathcal{S}_+^p. \end{array}$$

However, one may also relax QPP directly to

$$\begin{array}{lll} \mathrm{SQPP}^0_{\mathrm{CP2}}: & \min & Q \bullet X \\ & \text{s.t.} & a_ia_i^T \bullet X = b_i^2, \quad i = 1, \dots, m \\ & & X \in \mathcal{K}_0^* \subset \mathcal{S}_+^n. \end{array}$$

By Theorems 2 and 1, $\mathrm{SQPP}^0_{\mathrm{CP1}}$ yields a stronger bound than $\mathrm{SQPP_{DC1}}$ or $\mathrm{SQPP_{DC2}}$. Moreover, it is not difficult to show that $\mathrm{SQPP}^0_{\mathrm{CP1}}$ is stronger than $\mathrm{SQPP}^0_{\mathrm{CP2}}$. However, since $\mathrm{SQPP}^0_{\mathrm{CP2}}$ does *not* utilize the $n \times p$ matrix W this relaxation will in general be more tractable than the alternatives considered in this section.

5. Bounding the Stability Number of a Graph

In this section we consider in more detail the application of QPS to determining the size of the maximum stable set in a graph. Let G be a graph with vertex set $\{1, 2, \dots, n\}$, edge set $\mathcal{E}$ and adjacency matrix A. It is well known that if $Q = I + A$, then $v_{\mathrm{QPS}} = 1/\alpha(G)$, where $\alpha(G)$ is the size of the maximum stable set [6]. Thus a lower bound on v_{QPS} provides an upper bound on the stability number. It is also known that for such problems $1/v^0_{\mathrm{CP}} = \vartheta'$, where ϑ' is Schrijver's strengthening of the Lovasz ϑ number [4]. The relationship between ϑ and ϑ' is well known, and that between v_{DC} and v^0_{CP} is described in Section 3, amounting to the following corollary of Theorem 2.

COROLLARY 1. *Let G be a graph with vertex set $\{1, 2, \ldots, n\}$, edge set $\mathcal{E}$ and adjacency matrix A. Then $\vartheta' \leqslant 1/v_{\mathrm{DC}}$, where $Q = I + A$.*

The relationship between ϑ and v_{DC} is less clear, despite the fact that there are a variety of equivalent formulations of ϑ [5]. In this section we give a formulation of ϑ via a lower bound on QPS that facilitates a comparison with v_{DC}.

We use $X_{\mathcal{E}} = 0$ (respectively $X_{\mathcal{E}} \geqslant 0$) to denote that $X_{ij} = 0$ (respectively $X_{ij} \geq 0$) for all $(i, j) \in \mathcal{E}$. The Lovasz ϑ number can be defined via the SDP

$$\begin{aligned} \vartheta = \max \quad & E \bullet X \\ \text{s.t.} \quad & \mathrm{tr}(X) = 1 \\ & X_{\mathcal{E}} = 0, \ \ X \succeq 0, \end{aligned}$$

while Schrijver's ϑ' is given by the problem

$$\begin{aligned} \vartheta' = \max \quad & E \bullet X \\ \text{s.t.} \quad & \mathrm{tr}(X) = 1 \\ & A \bullet X = 0 \\ & X \geqslant 0, \ \ X \succeq 0. \end{aligned}$$

It is clear from the above formulations that ϑ' is a strengthening of ϑ obtained by replacing $X_{\mathcal{E}} = 0$ with $A \bullet X = 0$ and $X \geqslant 0$. It is well known that

$$\alpha(G) \leqslant \vartheta' \leqslant \vartheta \leqslant \chi(\bar{G}),$$

where $\chi(\bar{G})$ is the coloring number of the complement of G.

In [4] the relationship $1/v^0_{\mathrm{CP}} = \vartheta'$ is established by first showing that

$$\begin{aligned} \vartheta' = \max \quad & E \bullet X \\ \text{s.t.} \quad & (I + A) \bullet X = 1 \\ & X \in \mathcal{K}_0^*, \end{aligned}$$

which corresponds to simply replacing the two equality constraints in the original formulation for ϑ' with their sum. Swapping objective and constraint then yields an instance of $\mathrm{SQPS}^0_{\mathrm{CP}}$, with $Q = I + A$, whose optimal value is $1/\vartheta'$. Let $\mathcal{K}^*_{\mathcal{E}} = \{X \mid X_{\mathcal{E}} \geqslant 0,\ X \succeq 0\}$ and define

$$\begin{aligned} v_{\mathcal{E}} = \min \quad & Q \bullet X \\ \text{s.t.} \quad & E \bullet X = 1 \\ & X \in \mathcal{K}^*_{\mathcal{E}}. \end{aligned}$$

Noting that ϑ may be reformulated as

$$\begin{aligned} \vartheta = \max \quad & E \bullet X \\ \text{s.t.} \quad & \mathrm{tr}(X) = 1 \\ & A \bullet X = 0 \\ & X_{\mathcal{E}} \geqslant 0,\ \ X \succeq 0, \end{aligned}$$

the exact same argument as in [4] implies the following theorem.

THEOREM 3. *Let G be a graph with vertex set $\{1, 2, \ldots, n\}$, edge set $\mathcal{E}$ and adjacency matrix A. Then $\vartheta = 1/v_{\mathcal{E}}$, where $Q = I + A$.*

Using Lemma 1 and Theorem 3 we can give a clear comparison between the bounds $\vartheta = 1/v_{\mathcal{E}}$, $\vartheta' = 1/v^0_{\mathrm{CP}}$, and $1/v_{\mathrm{DC}}$ on the stability number. All three arise from optimization problems of the form

$$\begin{aligned} \min \quad & Q \bullet X \\ \text{s.t.} \quad & E \bullet X = 1 \\ & X \succeq 0, \end{aligned}$$

with additional constraints that vary for the three bounds. The added constraints corresponding to each of the three bounds are as follows.

$$\begin{aligned} \vartheta \ = 1/v_{\mathcal{E}}: &\quad X_{\mathcal{E}} \geqslant 0, \\ \vartheta' = 1/v^0_{\mathrm{CP}}: &\quad X \geqslant 0, \\ 1/v_{\mathrm{DC}}: &\quad Xe \geqslant 0, \quad X \preceq \mathrm{Diag}(Xe). \end{aligned}$$

Note that for v_{DC} we are using the alternative formulation $\mathrm{SQPS}'_{\mathrm{DC}}$ described in Section 3. We have been unable to find an instance G where $v_{\mathrm{DC}} > v_{\mathcal{E}}$, but we are also unable to prove that $v_{\mathrm{DC}} \leqslant v_{\mathcal{E}}$.

6. Computational Results

In order to computationally compare v_{DC} with other bounds for QPS we considered a set of test problems used in [2]. The first two, problems 5.1 and 5.2, arise in estimating the maximum stable set on the graphs corresponding to the pentagon and the complement of the icosahedron, respectively. The next two problems, 5.3 and 5.4, arise from applications in population genetics and portfolio optimization, respectively. See [2] for more details and references. In Table 1 we give the values of several bounds for these four problems. The bounds v^0_{CP} and v^1_{CP} are the SDP bounds for $r=0$ and $r=1$, and v^1_{LP} is the LP bound for $r=1$, all from [2]. Opt denotes the optimal solution value. All figures are rounded to 4 digits after the decimal point. Some caution is required in computing v_{DC} due to the fact that all feasible solutions of SQPS_{DC} are singular (5). We obtained values of v_{DC} using the self-dual SDP code SeDuMi [11], which remains stable on problems of this type. (Alternatively one could use the reformulation SQPS'_{DC} described in Section 3.)

We know that in all cases $v_{DC} \leqslant v^0_{CP} \leqslant v^1_{CP}$ and $v^1_{LP} \leqslant v^1_{CP}$ must hold. For the problems considered in Table 1 it is interesting to note that $v^1_{LP} < v_{DC}$ throughout, and $v_{DC} < v^0_{CP}$ except on problem 5.4. It is also worth noting that the Lovasz ϑ number gives the same bound on problems 5.1 and 5.2 as $\vartheta' = 1/v^0_{CP}$.

In addition to problems 5.1–5.4, [2] considers 20 problems based on estimating the maximum stable set for random graphs on 12 vertices constructed so as to have a maximum stable set of size 6. In [2] it is reported that for all 20 instances the QPS problem resulted in a bound v^1_{LP} of zero, and a value of v^1_{CP} equal to the true optimum ($v_{QPS} = \frac{1}{6}$). We constructed 20 similar instances and obtained positive values for v_{DC} in all cases. The resulting bounds on the max stable set were however quite poor; greater than 12 in all but one case. (We have found other instances of random graphs where $v_{DC} < 0$.) We also found that the Lovasz ϑ number gave the exact value $\vartheta = \alpha(G) = 6$ for all 20 instances, so that no improvement was possible from the more complex bounds v^0_{CP} and v^1_{CP}.

In addition to the quality of the various bounds it is interesting to consider the relative computational effort of obtaining them. Although each of

Table 1. Comparison of bounds for instances of QPS

Problem [2]	n	v^1_{LP}	v_{DC}	v^0_{CP}	v^1_{CP}	Opt
5.1	5	0.3333	0.3528	0.4472	0.5000	0.5000
5.2	12	0.0000	0.0243	0.3090	0.3090	0.3333
5.3	5	−21.0000	−17.0096	−16.3333	−16.3333	−16.3333
5.4	5	0.3015	0.4839	0.4839	0.4839	0.4839

the problems mentioned above took just a few seconds to solve by SeDuMi, the problems tested are not large-scale as would be encountered in applications. The discussion in the following paragraph is particularly relevant when solving relaxations of large-scale instances of QPS.

SeDuMi requires the conversion of $\mathrm{SQPS}_{\mathrm{DC}}$ and $\mathrm{SQPS}^0_{\mathrm{CP}}$ to a standard self-dual conic form, in which each variable is constrained to be in at most one cone. For any variable in the original form of the problem that is in two or more cones simultaneously, the conversion to standard form is achieved by introducing auxiliary variables, which are then themselves constrained to be in a single cone, as well as equality constraints linking the original and auxiliary variables. For example, in the case of $\mathrm{SQPS}^0_{\mathrm{CP}}$, which has $X \succeq 0$ and $X \geqslant 0$, we introduce $Y \geqslant 0$ and set $X = Y$. After the conversion, it is not difficult to see that $\mathrm{SQPS}_{\mathrm{DC}}$ corresponds to optimization over the cone $\mathcal{S}^{n+1}_+ \times \mathcal{S}^n_+ \times \Re^n_+$ with $n(n+1)/2 + n + 2$ equality constraints, while $\mathrm{SQPS}^0_{\mathrm{CP}}$ is over the cone $\mathcal{S}^n_+ \times \Re^{n(n+1)/2}_+$ with $n(n+1)/2 + 1$ equality constraints. From a theoretical standpoint, $\mathrm{SQPS}_{\mathrm{DC}}$ is simpler to solve using an interior-point algorithm since it has a barrier parameter that is $O(n)$, as opposed to $O(n^2)$ for $\mathrm{SQPS}^0_{\mathrm{CP}}$ [8]. In practice, however, it is well known that the number of iterations required by interior-point algorithms is almost independent of the barrier parameter. From a computational perspective, the work in each iteration for either problem is dominated by the time needed to form and factor the Schur complement matrix for calculating the Newton direction, which can be seen to be proportional to the cube of the number of equality constraints. This work is of the same order for $\mathrm{SQPS}_{\mathrm{DC}}$ and $\mathrm{SQPS}^0_{\mathrm{CP}}$. In particular, neither problem appears to have an inherent structure – for example, a sparse Schur complement matrix – that would allow faster calculation of the Newton direction. Hence, one would expect similar computational effort for solving both problems in practice.

In the specific case of calculating a bound on the stability number of a graph, it is also worth mentioning that the optimization problem that defines $v_{\mathcal{E}}$ is over the cone $\mathcal{S}^n_+ \times \Re^{|\mathcal{E}|}_+$ with $|\mathcal{E}| + 1$ constraints. This problem is computationally cheaper than both $\mathrm{SQPS}_{\mathrm{DC}}$ and $\mathrm{SQPS}^0_{\mathrm{CP}}$, especially when the underlying graph is sparse.

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