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On Convex Relaxations for Quadratically Constrained Quadratic Programming

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Abstract

We consider convex relaxations for the problem of minimizing a (possibly nonconvex) quadratic objective subject to linear and (possibly nonconvex) quadratic constraints. Let \mathcal{F} denote the feasible region for the linear constraints. We first show that replacing the quadratic objective and constraint functions with their convex lower envelopes on \mathcal{F} is dominated by an alternative methodology based on convexifying the range of the quadratic form $\begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T$ for $x \in \mathcal{F}$. We next show that the use of “ α BB” underestimators as computable estimates of convex lower envelopes is dominated by a relaxation of the convex hull of the quadratic form that imposes semidefiniteness and linear constraints on diagonal terms. Finally, we show that the use of a large class of “D.C.” underestimators is dominated by a relaxation that combines semidefiniteness with RLT constraints.

Keywords: Quadratically constrained quadratic programming, convex envelope, semidefinite programming, reformulation-linearization technique

1 Introduction

In this paper we consider a quadratically constrained quadratic programming (QCQP) problem of the form

$$\begin{aligned}
 \text{(QCQP)} \quad z^* = \min \quad & f_0(x) \\
 \text{s.t.} \quad & f_i(x) \leq d_i, \quad i = 1, \dots, q \\
 & x \geq 0, \quad Ax \leq b,
 \end{aligned}$$

where $f_i(x) = x^T Q_i x + c_i^T x$, $i = 0, 1, \dots, q$, each Q_i is an $n \times n$ symmetric matrix, and A is an $m \times n$ matrix. In the case that $Q_i \succeq 0$ for each i , QCQP is a convex programming problem that can be solved in polynomial time, but in general the problem is NP-Hard. QCQP is a fundamental problem that has been extensively studied in the global optimization literature; see for example [9, 20] and references therein.

A common approach to obtaining a lower bound for a nonconvex instance of QCQP is to somehow convexify the problem. In this paper we compare several different convexification techniques. Let $\mathcal{F} = \{x \geq 0 : Ax \leq b\}$ denote the feasible set for the linear constraints of QCQP. We assume throughout that \mathcal{F} is bounded. One methodology is to replace each function $f_i(\cdot)$ with its convex lower envelope $\hat{f}_i(\cdot)$ on \mathcal{F} . We refer to the resulting convex relaxation of QCQP as $\widehat{\text{QCQP}}$. In Section 2 we compare $\widehat{\text{QCQP}}$ with an alternative relaxation $\widetilde{\text{QCQP}}$ based on the convex set

$$\mathcal{C} = \text{Co} \left\{ \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T : x \in \mathcal{F} \right\}, \tag{1}$$

where $\text{Co}\{\cdot\}$ denotes the convex hull. We prove that $\widetilde{\text{QCQP}}$ dominates $\widehat{\text{QCQP}}$, although in general neither of these problems is computationally tractable.

In Section 3 we compare two computable relaxations that can be viewed as tractable approximations of the problems $\widehat{\text{QCQP}}$ and $\widetilde{\text{QCQP}}$. One relaxation utilizes “ α BB” underestimators [1] for the nonconvex quadratic functions of QCQP, and the other applies semidefinite and diagonal constraints that must hold for matrices in \mathcal{C} . We prove that the latter convexification dominates the former, regardless of the choice of the parameters used to define the underestimators. In Section 4 we consider a more general “D.C.” underestimation procedure suggested in [20], and a strengthened approximation of $\widetilde{\text{QCQP}}$ that

combines semidefiniteness with linear constraints from the reformulation-linearization technique (RLT). We again show that the second approach dominates the first, regardless of the parameters used to create the underestimators.

In Section 5 we consider particular instances of QCQP that were used as computational examples in [2]. The first of these are indefinite box-constrained QPs, corresponding to QCQP with $q = 0$ and $\mathcal{F} = \{x : 0 \leq x \leq e\}$. For these problems we obtain excellent computational results by further strengthening the approximation of \mathcal{C} through the addition of triangle inequalities related to the Boolean Quadric Polytope. For the second class of QCQP problems, corresponding to planar circle-packing (or equivalently point-packing) problems, we prove an interesting theoretical result that relates convex lower envelopes for reverse convex constraints to the use of RLT constraints for \mathcal{C} .

Notation We use $X \succeq 0$ to denote that a symmetric matrix X is positive semidefinite. For $n \times n$ matrices X and Y , $X \bullet Y$ denotes the matrix inner product $X \bullet Y = \sum_{i,j=1}^n X_{ij}Y_{ij}$. For an $n \times n$ matrix X , $\text{diag}(X)$ is the vector x with $x_i = X_{ii}$, $i = 1, \dots, n$, and $\text{Diag}(x)$ is the diagonal matrix with $\text{diag}(\text{Diag}(x)) = x$. We use e to denote a vector with each component equal to one.

2 Two convex relaxations for QCQP

As described in Section 1, let $\widehat{\text{QCQP}}$ denote the problem where each function $f_i(\cdot)$ in QCQP is replaced by $\hat{f}_i(\cdot)$, its convex lower envelope on \mathcal{F} . Let \hat{z} denote the solution value in $\widehat{\text{QCQP}}$. In the global optimization literature it is sometimes suggested that $\widehat{\text{QCQP}}$ is the “best possible” convex relaxation of QCQP, although \hat{z} may not be computable because the required convex lower envelopes $\hat{f}_i(\cdot)$ may be impossible to obtain.

We will compare $\widehat{\text{QCQP}}$ with an alternative convexification that is based on linearizing the problem by adding additional variables. Let X denote a symmetric $n \times n$ matrix. Then QCQP can be written

$$\begin{aligned}
 (\text{QCQP}) \quad z^* = \min \quad & Q_0 \bullet X + c_0^T x \\
 \text{s.t.} \quad & Q_i \bullet X + c_i^T x \leq d_i, \quad i = 1, \dots, q \\
 & x \geq 0, \quad Ax \leq b, \quad X = xx^T.
 \end{aligned}$$

Written in the above form, QCQP is a linear problem except for the quadratic equality constraints $X = xx^T$. A convexification of the problem can then be given in terms of the set \mathcal{C} defined in (1). Using \mathcal{C} , we obtain a convex relaxation

$$\begin{aligned} (\widetilde{\text{QCQP}}) \quad \tilde{z} = \min \quad & Q_0 \bullet X + c_0^T x \\ \text{s.t.} \quad & Q_i \bullet X + c_i^T x \leq d_i, \quad i = 1, \dots, q \\ & Y(x, X) \in \mathcal{C}, \end{aligned}$$

where

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

In this section we will demonstrate that the convex relaxation $\widehat{\text{QCQP}}$ cannot be tighter than $\widetilde{\text{QCQP}}$; in other words, it is always true that $\hat{z} \leq \tilde{z}$. To do this we will show that there is a simple relationship between the convex lower envelopes used in $\widehat{\text{QCQP}}$ and the linearized representations of the objective and constraint functions used in $\widetilde{\text{QCQP}}$.

Theorem 1. *For $x \in \mathcal{F}$, let $f(x) = x^T Q x + c^T x$, and let $\hat{f}(\cdot)$ be the convex lower envelope of $f(\cdot)$ on \mathcal{F} . Then $\hat{f}(x) = \min\{Q \bullet X + c^T x : Y(x, X) \in \mathcal{C}\}$.*

Proof. For $x \in \mathcal{F}$, let $g(x) = \min\{Q \bullet X + c^T x : Y(x, X) \in \mathcal{C}\}$. Our goal is to show that $\hat{f}(x) = g(x)$. To do this we first show that $g(\cdot)$ is a convex function with $g(x) \leq f(x)$, $x \in \mathcal{F}$, implying that $g(x) \leq \hat{f}(x)$.

Assume that for $i \in \{1, 2\}$, $x^i \in \mathcal{F}$ and $g(x^i) = Q \bullet X^i + c^T x^i$, where $Y(x^i, X^i) \in \mathcal{C}$. For $0 \leq \lambda \leq 1$, let

$$x(\lambda) = \lambda x^1 + (1 - \lambda)x^2, \quad X(\lambda) = \lambda X^1 + (1 - \lambda)X^2.$$

Then $Y(x(\lambda), X(\lambda)) = \lambda Y(x^1, X^1) + (1 - \lambda)Y(x^2, X^2) \in \mathcal{C}$, since \mathcal{C} is convex. It follows that

$$g(x(\lambda)) \leq Q \bullet X(\lambda) + c^T x(\lambda) = \lambda g(x^1) + (1 - \lambda)g(x^2),$$

proving that $g(\cdot)$ is convex on \mathcal{F} . The fact that $g(x) \leq f(x)$ follows immediately from $Y(x, xx^T) \in \mathcal{C}$ and $Q \bullet xx^T + c^T x = f(x)$.

It remains to show that $\hat{f}(x) \leq g(x)$. Assume that $g(x) = Q \bullet X + c^T x$, where $Y(x, X) \in \mathcal{C}$. From the definition of \mathcal{C} , there exist x^i , $x^i \in \mathcal{F}$, and $\lambda_i \geq 0$, $i = 1, \dots, k$, $\sum_{i=1}^k \lambda_i = 1$ such

that

$$\sum_{i=1}^k \lambda_i x^i = x, \quad \sum_{i=1}^k \lambda_i x^i (x^i)^T = X.$$

It follows that

$$\begin{aligned} g(x) &= Q \bullet X + c^T x \\ &= Q \bullet \left(\sum_{i=1}^k \lambda_i x^i (x^i)^T \right) + c^T \left(\sum_{i=1}^k \lambda_i x^i \right) \\ &= \sum_{i=1}^k \lambda_i f(x^i). \end{aligned}$$

But $\hat{f}(\cdot)$ is convex on \mathcal{F} , and $\hat{f}(x) \leq f(x)$ for all $x \in \mathcal{F}$, so

$$\hat{f}(x) = \hat{f} \left(\sum_{i=1}^k \lambda_i x^i \right) \leq \sum_{i=1}^k \lambda_i \hat{f}(x^i) \leq \sum_{i=1}^k \lambda_i f(x^i) = g(x).$$

□

The claimed relationship between $\widetilde{\text{QCQP}}$ and $\widehat{\text{QCQP}}$ is an immediate consequence of Theorem 1. In particular, using Theorem 1, $\widehat{\text{QCQP}}$ could be rewritten in the form

$$\begin{aligned} (\widehat{\text{QCQP}}) \quad \hat{z} &= \min Q_0 X_0 + c^T x \\ \text{s.t.} \quad & Q_i \bullet X_i + c_i^T x \leq d_i, \quad i = 1, \dots, q \\ & Y(x, X_i) \in \mathcal{C}, \quad i = 0, 1, \dots, q, \end{aligned}$$

so that $\widetilde{\text{QCQP}}$ corresponds to $\widehat{\text{QCQP}}$ with the added constraints $X_0 = X_1 = \dots = X_q$.

Corollary 1. *Let \hat{z} and \tilde{z} denote the solution values in the convex relaxations $\widehat{\text{QCQP}}$ and $\widetilde{\text{QCQP}}$, respectively. Then $\hat{z} \leq \tilde{z}$.*

Corollary 1 indicates that the approach to convexifying QCQP taken in $\widetilde{\text{QCQP}}$ has theoretical advantages over the underestimation methodology used in $\widehat{\text{QCQP}}$. However, it is important to recognize that both of these approaches have practical limitations. In particular, both the problem of computing an exact convex lower envelope $\hat{f}(\cdot)$ for a quadratic function $f(\cdot)$, and the problem of characterizing \mathcal{C} , are intractable. It is, however, known

that \mathcal{C} can be exactly represented using the cone of completely positive matrices. To describe this representation it is convenient to define

$$Y^+(x, X) = \begin{pmatrix} 1 & x^T & s(x)^T \\ x & X & Z(x, X) \\ s(x) & Z(x, X)^T & S(x, X) \end{pmatrix}, \quad (2)$$

where

$$\begin{aligned} s(x) &= b - Ax, \\ S(x, X) &= bb^T - Axb^T - bx^T A^T + AXA^T, \\ Z(x, X) &= xb^T - XA^T. \end{aligned}$$

The matrices $S(x, X)$ and $Z(x, X)$ relax $s(x)s(x)^T$ and $xs(x)^T$, respectively. It can then be shown [5] that

$$\mathcal{C} = \{Y(x, X) : Y^+(x, X) \in \mathcal{CP}_{m+n+1}\},$$

where \mathcal{CP}_k is the cone of $k \times k$ completely positive matrices (that is, matrices that can be written in the form VV^T where V is a nonnegative $k \times p$ matrix). Unfortunately, for $k \geq 5$ there is no known complete description for \mathcal{CP}_k .

We close this section with an example that illustrates that the distinction between QCQP and $\widehat{\text{QCQP}}$ is already sharp for $m = n = q = 1$. Consider the problem

$$\begin{aligned} \min \quad & x_1^2 \\ \text{s.t.} \quad & x_1^2 \geq \frac{1}{2} \\ & 0 \leq x_1 \leq 1. \end{aligned}$$

Written in the form of QCQP, the constraint $x_1^2 \geq \frac{1}{2}$ is $-x_1^2 \leq -\frac{1}{2}$, and the convex lower envelope of $-x_1^2$ on $[0, 1]$ is $-x_1$. The relaxation $\widehat{\text{QCQP}}$ is then

$$\begin{aligned} \min \quad & x_1^2 \\ \text{s.t.} \quad & -x_1 \leq -\frac{1}{2} \\ & 0 \leq x_1 \leq 1, \end{aligned}$$

with solution value $\hat{z} = \frac{1}{4}$. The solution value for $\widetilde{\text{QCQP}}$ is $\tilde{z} = z^* = \frac{1}{2}$. The set \mathcal{C} is depicted in Figure 1. Note that for $x_1 = \frac{1}{2}$, $Y(x_1, x_{11}) \in \mathcal{C}$ for $x_{11} \in [\frac{1}{4}, \frac{1}{2}]$. The solution of $\widehat{\text{QCQP}}$

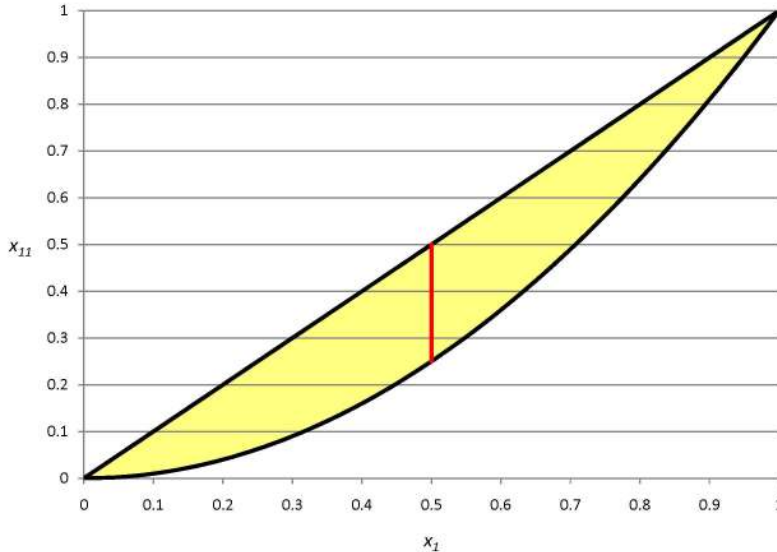


Figure 1: Set \mathcal{C} for example

then corresponds to using $x_1 = \frac{1}{2}$ along with $x_{11} = \frac{1}{4}$ for the objective, and $x_{11} = \frac{1}{2}$ for the single nonlinear constraint.

3 Two computable relaxations

As mentioned above, in general both $\widetilde{\text{QCQP}}$ and $\widehat{\text{QCQP}}$ are intractable problems due to the complexity of computing a convex lower envelope $\hat{f}(\cdot)$, or the convex hull \mathcal{C} . In this section we consider the important special case where \mathcal{F} is the box $0 \leq x \leq e$, and describe two further relaxations that are computable approximations of $\widetilde{\text{QCQP}}$ and $\widehat{\text{QCQP}}$.

For a quadratic function $f(x) = x^T Q x + c^T x$ defined on $\mathcal{F} = \{x : 0 \leq x \leq e\}$, the well-known “ α BB” underestimator [1] is

$$f_\alpha(x) = x^T (Q + \text{Diag}(\alpha)) x + (c - \alpha)^T x,$$

where $\alpha \in \mathfrak{R}_+^n$ is chosen so that $Q + \text{Diag}(\alpha) \succeq 0$. It is worthwhile to note that although here we restrict our attention to the convexification of quadratic functions, the α BB underestimator applies to more general nonlinear functions. The same convexification procedure for the quadratic case has appeared numerous times elsewhere in the literature; see for example [4, 12].

Since $f_\alpha(\cdot)$ is convex, it is immediate that $f_\alpha(x) \leq \hat{f}(x)$, $0 \leq x \leq e$. A further relaxation of $\widehat{\text{QCQP}}$ is then given by the problem

$$\begin{aligned} (\text{QCQP}_{\alpha\text{BB}}) \quad z_{\alpha\text{BB}} = \quad & \min \quad x^T(Q_0 + \text{Diag}(\alpha_0))x + (c_0 - \alpha_0)^T x \\ \text{s.t.} \quad & x^T(Q_i + \text{Diag}(\alpha_i))x + (c_i - \alpha_i)^T x \leq d_i, \quad i = 1, \dots, q \\ & 0 \leq x \leq e, \end{aligned}$$

where each α_i is chosen so that $Q_i + \text{Diag}(\alpha_i) \succeq 0$.

For the case of $\mathcal{F} = \{x : 0 \leq x \leq e\}$, there are a variety of known constraints that are valid for $Y(x, X) \in \mathcal{C}$. These include:

1. The constraints from the Reformulation-Linearization Technique (RLT) [14],

$$\begin{aligned} x_{ij} &\geq 0, \\ x_{ij} &\geq x_i + x_j - 1, \\ x_{ij} &\leq x_i, \\ x_{ij} &\leq x_j. \end{aligned}$$

2. The semidefinite programming (SDP) constraint $Y(x, X) \succeq 0$ [17].
3. Constraints on the off-diagonal components of $Y(x, X)$ coming from the Boolean Quadric Polytope (BQP) [6, 19]; for example, the triangle inequalities for $i \neq j \neq k$,

$$\begin{aligned} x_i + x_j + x_k &\leq x_{ij} + x_{ik} + x_{jk} + 1, \\ x_{ij} + x_{ik} &\leq x_i + x_{jk}, \\ x_{ij} + x_{jk} &\leq x_j + x_{ik}, \\ x_{ik} + x_{jk} &\leq x_k + x_{ij}. \end{aligned}$$

The relationship between the SDP and RLT constraints is discussed in [2]. In fact for $n = 2$, the SDP and RLT constraints together give a full characterization of \mathcal{C} [3]. For $n = 3$ the triangle inequalities and RLT constraints fully characterize the BQP, but these constraints combined with the SDP constraint do *not* give a complete characterization of \mathcal{C} [6]. For $n = 3$, an “extended-variable” description of \mathcal{C} obtained via a triangulation of the 3-cube is given in [3].

We will compare $\text{QCQP}_{\alpha\text{BB}}$ with an approximation of $\widehat{\text{QCQP}}$ that imposes some of the above constraints on \mathcal{C} . In particular, we will apply the semidefiniteness condition $Y(x, X) \succeq 0$ together with the diagonal RLT constraints $\text{diag}(X) \leq x$. Note that these conditions together imply the original bound constraints $0 \leq x \leq e$. The resulting relaxation is

$$\begin{aligned} (\text{QCQP}_{\text{SDP}}) \quad z_{\text{SDP}} = \quad & \min \quad Q_0 \bullet X + c_0^T x \\ \text{s.t.} \quad & Q_i \bullet X + c_i^T x \leq d_i, \quad i = 1, \dots, q \\ & Y(x, X) \succeq 0, \quad \text{diag}(X) \leq x. \end{aligned}$$

The following theorem shows that there is a simple relationship between the convexifications used to construct $\text{QCQP}_{\alpha\text{BB}}$ and QCQP_{SDP} .

Theorem 2. *For $0 \leq x \leq e$, let $f_\alpha(x) = x^T(Q + \text{Diag}(\alpha))x + (c - \alpha)^T x$, where $\alpha \geq 0$ and $Q + \text{Diag}(\alpha) \succeq 0$. Assume that $Y(x, X) \succeq 0$, $\text{diag}(X) \leq x$. Then $f_\alpha(x) \leq Q \bullet X + c^T x$.*

Proof. Let $Q(\alpha) = Q + \text{Diag}(\alpha)$. Since $Q(\alpha) \succeq 0$,

$$\begin{aligned} f_\alpha(x) &= (c - \alpha)^T x + \min\{Q(\alpha) \bullet X : X \succeq xx^T\} \\ &= (c - \alpha)^T x + \min\{Q(\alpha) \bullet X : Y(x, X) \succeq 0, \text{diag}(X) \leq x\}, \end{aligned}$$

the last because $\text{diag}(X) \leq x$ holds automatically for $X = xx^T$, $0 \leq x \leq e$. But then $Y(x, X) \succeq 0$ and $\text{diag}(X) \leq x$ imply that

$$\begin{aligned} f_\alpha(x) &\leq Q(\alpha) \bullet X + (c - \alpha)^T x \\ &= Q \bullet X + c^T x + \alpha^T(\text{diag}(X) - x) \\ &\leq Q \bullet X + c^T x. \end{aligned}$$

□

The following immediate corollary of Theorem 2 confirms a relationship between $\text{QCQP}_{\alpha\text{BB}}$ and QCQP_{SDP} first conjectured by Jeff Linderoth (private communication).

Corollary 2. *Let $z_{\alpha\text{BB}}$ and z_{SDP} denote the solution values in the convex relaxations $\text{QCQP}_{\alpha\text{BB}}$ and QCQP_{SDP} , respectively. Then $z_{\alpha\text{BB}} \leq z_{\text{SDP}}$.*

Note that the example at the end of Section 2 has $\mathcal{F} = \{x_1 : 0 \leq x_1 \leq 1\}$, $q = 1$. For this problem $(\alpha_1 - 1)x_1^2$ is convex for $\alpha_1 \geq 1$. Using $\alpha_1 = 1$, the problem $\text{QCQP}_{\alpha\text{BB}}$ is identical to $\widehat{\text{QCQP}}$ and has solution value $z_{\alpha\text{BB}} = \hat{z} = \frac{1}{4}$. The problem QCQP_{SDP} is identical to $\widetilde{\text{QCQP}}$, and has solution value $z_{\text{SDP}} = z^* = \frac{1}{2}$.

4 Two stronger relaxations

In this section we consider a convexification procedure for QCQP suggested in [20] that generalizes the α BB procedure described in the previous section. Consider a quadratic function $f(x) = x^T Q x + c^T x$, and let $v_j \in \mathbb{R}^n$, $j = 1, \dots, k$. Let $\mathcal{F} = \{x \geq 0 : Ax \leq b\}$, and assume that for $x \in \mathcal{F}$ we have $l_j \leq v_j^T x \leq u_j$. It follows that for $x \in \mathcal{F}$, $(v_j^T x - l_j)(v_j^T x - u_j) \leq 0$, or $(v_j^T x)^2 - (l_j + u_j)v_j^T x + l_j u_j \leq 0$. For $\alpha \in \mathbb{R}_+^k$, define

$$\begin{aligned} Q(\alpha) &= Q + \sum_{j=1}^k \alpha_j v_j v_j^T, \\ c(\alpha) &= c - \sum_{j=1}^k \alpha_j (l_j + u_j) v_j, \\ p(\alpha) &= \sum_{j=1}^k \alpha_j l_j u_j, \end{aligned}$$

and let $f_\alpha(x) = x^T Q(\alpha)x + c(\alpha)^T x + p(\alpha)$. Then if $Q(\alpha) \succeq 0$, $f_\alpha(\cdot)$ is a convex underestimator for $f(\cdot)$ on \mathcal{F} . In [20], functions of the form $f_\alpha(\cdot)$ are referred to as ‘‘D.C.’’ underestimators, and are applied to convexify the objective in QCQP problems with linear and convex quadratic constraints. Note that the α BB underestimator on $0 \leq x \leq e$ from the previous section corresponds to the case of $v_j = e_j$, $l_j = 0$, $u_j = 1$, $j = 1, \dots, n$. Additional possibilities for v_j suggested in [20] include eigenvectors corresponding to negative eigenvalues of Q , and transposed rows of the constraint matrix A . Using underestimators of the form $f_\alpha(\cdot)$, we obtain a convex relaxation

$$\begin{aligned} (\text{QCQP}_{\text{DC}}) \quad z_{\text{DC}} = \min \quad & x^T Q_0(\alpha_0)x + c_0(\alpha_0)^T x + k(\alpha_0) \\ \text{s.t.} \quad & x^T Q_i(\alpha_i)x + c_i(\alpha_i)^T x + k(\alpha_i) \leq d_i, \quad i = 1, \dots, q \\ & x \geq 0, Ax \leq b, \end{aligned}$$

where each $\alpha_i \in \mathbb{R}_+^k$ is chosen so that $Q_i(\alpha_i) \succeq 0$.

We will compare QCQP_{DC} to a relaxation of QCQP that combines the semidefiniteness condition $Y(x, X) \succeq 0$ with the RLT constraints on (x, X) that can be obtained from the original linear constraints $x \geq 0$, $Ax \leq b$. The RLT constraints can be described very succinctly using the the matrix $Y^+(x, X)$ from (2); in fact it is easy to see that these

constraints correspond exactly to $X \succeq 0$, $S(x, X) \succeq 0$, $Z(x, X) \succeq 0$. It follows that the RLT constraints and the condition that $Y(x, X) \succeq 0$ together are equivalent to $Y^+(x, X)$ being a doubly nonnegative (DNN) matrix. We therefore define the relaxation

$$\begin{aligned} (\text{QCQP}_{\text{DNN}}) \quad z_{\text{DNN}} = \min \quad & Q_0 \bullet X + c_0^T x \\ \text{s.t.} \quad & Q_i \bullet X + c_i^T x \leq d_i, \quad i = 1, \dots, q \\ & Y^+(x, X) \in \mathcal{DNN}_{m+n+1}, \end{aligned}$$

where \mathcal{DNN}_k is the cone of $k \times k$ doubly nonnegative matrices. Note that the relaxation QCQP_{DNN} is entirely determined by the data from the original problem QCQP ; in particular, QCQP_{DNN} does not involve the vectors v_j and bounds (l_j, u_j) used to construct the convexifications in QCQP_{DC} .

In order to compare QCQP_{DC} and QCQP_{DNN} we require a generalization of Theorem 2 that applies to the convexification $f_\alpha(\cdot)$ used in this section. This result naturally involves the RLT constraints

$$v_j^T X v_j - (l_j + u_j)^T x \leq -l_j u_j, \quad j = 1, \dots, k. \quad (3)$$

that are obtained from $l_j \leq v_j^T x \leq u_j$, $j = 1, \dots, k$.

Theorem 3. *For $x \in \mathcal{F}$, let $f_\alpha(x) = x^T Q(\alpha)x + c(\alpha)^T x + p(\alpha)$, where $\alpha \geq 0$ and $Q(\alpha) \succeq 0$. Assume that $Y(x, X) \succeq 0$ and (x, X) satisfy (3). Then $f_\alpha(x) \leq Q \bullet X + c^T x$.*

Proof. The proof is similar to that of Theorem 2. Since $Q(\alpha) \succeq 0$,

$$\begin{aligned} f_\alpha(x) &= c(\alpha)^T x + p(\alpha) + \min\{Q(\alpha) \bullet X : X \succeq xx^T\} \\ &= c(\alpha)^T x + p(\alpha) + \min\{Q(\alpha) \bullet X : Y(x, X) \succeq 0, (x, X) \text{ satisfy (3)}\}, \end{aligned}$$

the last because (3) are satisfied for any $X = xx^T$, $x \in \mathcal{F}$. But then if $Y(x, X) \succeq 0$ and (x, X) satisfy (3),

$$\begin{aligned} f_\alpha(x) &\leq p(\alpha) + Q(\alpha) \bullet X + c(\alpha)^T x \\ &\leq p(\alpha) + Q \bullet X + c^T x - p(\alpha) \\ &= Q \bullet X + c^T x, \end{aligned}$$

where the second inequality uses (3). □

Theorem 4. Let z_{DC} and z_{DNN} denote the solution values in the convex relaxations QCQP_{DC} and QCQP_{DNN} , respectively. Then $z_{\text{DC}} \leq z_{\text{DNN}}$.

Proof. Consider the convex relaxation

$$\begin{aligned} z_V = \quad & \min \quad Q_0 \bullet X + c_0^T x \\ \text{s.t.} \quad & Q_i \bullet X + c_i^T x \leq d_i, \quad i = 1, \dots, q \\ & v_j^T X v_j - (l_j + u_j)^T x \leq -l_j u_j, \quad j = 1, \dots, k \\ & x \geq 0, \quad Ax \leq b, \quad Y(x, X) \succeq 0. \end{aligned}$$

By Theorem 3 we immediately have $z_{\text{DC}} \leq z_V$. However, the constraints $l_j \leq v_j^T x \leq u_j$ are implied by the original constraints $x \geq 0$, $Ax \leq b$, and therefore by [14, Proposition 8.2], the constraints (3) are implied by the RLT constraints $X \geq 0$, $S(x, X) \geq 0$, $Z(x, X) \geq 0$. It follows that $z_V \leq z_{\text{DNN}}$. \square

In [20] it is shown that if all of the quadratic constraints of QCQP are convex, then for a given set of $\{v_j\}_{j=1}^k$ the problem of choosing the vector α_0 that gives the best value of z_{DC} can be formulated as a semidefinite programming problem. Theorem 4 states that *regardless* of the vectors $\{v_j\}_{j=1}^k$ and $\{\alpha_i\}_{i=0}^q$ used to construct the convexifications in QCQP_{DC} , the resulting lower bound z_{DC} cannot be better than the bound z_{DNN} obtained from QCQP_{DNN} when the upper and lower bounds l and u correspond to the feasible set for the linear constraints \mathcal{F} . However, in the presence of convex quadratic constraints, better values of l_j and/or u_j can be obtained by minimizing or maximizing $v_j^T x$ over the set \mathcal{S} corresponding to the feasible region for the linear and convex quadratic constraints, as suggested in [20], and in this case Theorem 4 would no longer apply. Of course obtaining such improved bounds could entail substantial auxiliary computation. A different approach for utilizing convex quadratic constraints to obtain improved RLT bounds based on the second-order cone representation of the constraints is suggested in [7, Section 2.3].

5 Applications

In this section we describe applications of the convexifications described above to two particular classes of QCQP problems considered in [2]. The first application is to box-constrained

indefinite QP problems of the form

$$\begin{aligned} \text{(QP)} \quad z^* = \quad & \min \quad x^T Q_0 x + c_0^T x \\ & \text{s.t.} \quad 0 \leq x \leq e, \end{aligned}$$

corresponding to the general QCQP problem of Section 1 with $q = 0$ and $\mathcal{F} = \{x : 0 \leq x \leq e\}$. Let \hat{z} and \tilde{z} be solution values for the corresponding problems $\widehat{\text{QCQP}}$ and $\widetilde{\text{QCQP}}$ described in Section 2. It is then obvious from the definition of \mathcal{C} that $\tilde{z} = z^*$, and $\hat{z} = \tilde{z}$ follows immediately from Theorem 1, so a full description of either the convex lower envelope $\hat{f}_0(\cdot)$ or the convex hull \mathcal{C} would provide an exact solution of QPB. Several valid classes of constraints for \mathcal{C} for the case that $\mathcal{F} = \{x : 0 \leq x \leq e\}$ were described in Section 3. The relaxation QCQP_{SDP} , corresponding to imposing the semidefiniteness condition $Y(x, X) \succeq 0$ along with the diagonal RLT constraints $\text{diag}(X) \leq x$, was computationally evaluated on a set of 15 QPB test problems with $n = 30$ in [2]. The results of [2] show that the bound z_{SDP} on these problems is much better than a bound based on imposing the RLT constraints on $Y(x, X)$, and the bound z_{DNN} based on imposing both semidefiniteness and the RLT constraints is much better still. (For the 15 problems considered, using semidefiniteness and the RLT constraints together closed the gap to zero, up to numerical tolerances, on 8 problems and left an average gap of 0.88% on the remaining 7 problems.)

The QPB test problems used in [2] are from a larger set of 54 problems with $n = 20, 30, 40, 50$ and 60 that were solved using the finite branch-and-bound algorithm of [8]; 50 of these problems were previously solved using the finite branch-and-bound algorithm of [18]. (The computational results in [18] omit the problems 50-050-1/2/3, and the problem 40-100-3 was unsolved.) In Table 1 we report the results of applying several increasingly tight approximations of \mathcal{C} on the full set of 54 problems. The column labeled “SDP” gives the gap to optimality for the bound z_{SDP} , and the column labeled “SDP+RLT” gives the gap for the bound z_{DNN} that imposes both semidefiniteness and the RLT constraints on $Y(x, X)$. For 29 of the 54 problems, the SDP+RLT bound is exact up to the numerical tolerances used by the SeDuMi solver [15]; for these problems the solution matrix $Y(x, X)$ is numerically rank-one. For the remaining 25 problems we consider adding triangle inequalities coming from the Boolean Quadric Polytope [6, 19]. For 24 of these 25 problems, adding triangle inequalities closes the gap to zero up to numerical tolerances; a positive gap remains for

Table 1: Comparison of bounds for indefinite QPB

Problem	Optimum	Cuts Added		Relative Gaps to Optimum		
		RLT	TRI	SDP	SDP+RLT	SDP+RLT+TRI
20-100-1	706.50	197	55	4.655%	0.002%	0.000%
20-100-2	856.50	184	172	5.102%	0.171%	0.000%
20-100-3	772.00	168		1.750%	0.000%	
30-060-1	706.00	371	777	8.799%	1.229%	0.000%
30-060-2	1377.17	381		3.614%	0.000%	
30-060-3	1293.50	394	288	5.924%	0.368%	0.000%
30-070-1	654.00	369	784	14.133%	3.058%	0.000%
30-070-2	1313.00	449		4.727%	0.000%	
30-070-3	1657.40	452	442	3.763%	0.010%	0.000%
30-080-1	952.73	365	718	10.290%	1.315%	0.000%
30-080-2	1597.00	376		1.616%	0.000%	
30-080-3	1809.78	317		1.492%	0.000%	
30-090-1	1296.50	370		4.009%	0.000%	
30-090-2	1466.84	344		4.160%	0.000%	
30-090-3	1494.00	420		1.527%	0.000%	
30-100-1	1227.13	356		4.777%	0.000%	
30-100-2	1260.50	427	465	8.316%	0.048%	0.000%
30-100-3	1511.05	377	265	6.622%	0.139%	0.000%
40-030-1	839.50	656		4.419%	0.000%	
40-030-2	1429.00	889		4.747%	0.000%	
40-030-3	1086.00	705		6.494%	0.000%	
40-040-1	837.00	710	1966	14.228%	3.117%	0.000%
40-040-2	1428.00	600		1.718%	0.000%	
40-040-3	1173.50	745	1427	8.209%	0.626%	0.000%
40-050-1	1154.50	797	1608	10.592%	0.515%	0.000%
40-050-2	1430.98	788	961	6.047%	0.354%	0.000%
40-050-3	1653.63	680		5.665%	0.000%	
40-060-1	1322.67	696	1722	12.043%	2.287%	0.000%
40-060-2	2004.23	739		4.758%	0.000%	
40-060-3	2454.50	701		2.207%	0.000%	
40-070-1	1605.00	584		3.675%	0.000%	
40-070-2	1867.50	650		3.418%	0.000%	
40-070-3	2436.50	828		3.538%	0.000%	
40-080-1	1838.50	615		5.312%	0.000%	
40-080-2	1952.50	639		3.094%	0.000%	
40-080-3	2545.50	755	742	3.647%	0.015%	0.000%
40-090-1	2135.50	763		5.948%	0.000%	
40-090-2	2113.00	731	336	7.376%	0.035%	0.000%
40-090-3	2535.00	598		2.338%	0.000%	
40-100-1	2476.38	673		3.265%	0.000%	
40-100-2	2102.50	707	1251	5.428%	0.184%	0.000%
40-100-3	1866.07	664	1732	9.176%	2.257%	0.000%
50-030-1	1324.50	903		4.877%	0.000%	
50-030-2	1668.00	831	233	5.257%	0.200%	0.000%
50-030-3	1453.61	830	180	7.715%	0.087%	0.000%
50-040-1	1411.00	1017		5.103%	0.000%	
50-040-2	1745.76	868	509	7.766%	0.212%	0.000%
50-040-3	2094.50	1081		3.938%	0.000%	
50-050-1	1198.41	723	1531	18.304%	8.664%	0.144%
50-050-2	1776.00	867	667	9.377%	0.765%	0.000%
50-050-3	2106.10	937	933	7.689%	0.752%	0.000%
60-020-1	1212.00	1199		7.048%	0.000%	
60-020-2	1925.50	1319		4.418%	0.000%	
60-020-3	1483.00	1040	735	8.200%	0.543%	0.000%
Average				5.969%	0.499%	

only one problem (50-050-1, with a gap of 0.144%). In the “Cuts Added” columns we report the number of RLT cuts required for problems solved to optimality using only added RLT constraints, or the number of RLT cuts and triangle (TRI) inequalities added for problems that could not be solved using RLT cuts alone. In both cases, violated constraints were added in several “rounds” with a decreasing infeasibility tolerance to avoid adding a large number of redundant inequalities, which would substantially degrade the performance of the solver.

The results reported in Table 1 suggest that on QPB problems of these dimensions, the approach based on approximating \mathcal{C} is highly competitive with other methodologies. The solution process for individual problems in [18] required the solution of up to approximately 28,000 linear programs, with a total of up to approximately 500,000 cuts generated. The SDP relaxations used in [8] substantially reduce the amount of enumeration compared to the algorithm of [18], but still required up to 10^4 CPU seconds on a 2.7 GHz Linux-based computer to solve individual problems. Results for the general-purpose global optimization solver BARON [13] on these problems were also reported in [18]. Of the 51 problems considered, BARON was unable to solve 21 problems within 4000 CPU seconds on a 1.8 GHz Linux-based computer, and the problems that were solved required approximately 20 times more computation than that required using the algorithm of [18] running on a slower machine. Good results using a methodology similar to that applied here for indefinite QPB problems of similar dimensions were previously reported in [19]. (Yajima and Fujie [19] consider additional valid inequalities for the BQP beyond the triangle inequalities, but only approximate the semidefiniteness condition $Y(x, X) \succeq 0$ by adding linear inequalities.)

The second example of QCQP that we consider is a circle-packing problem in the plane: for a given $n \geq 2$, find the maximum radius of n non-overlapping circles that all lie in the unit box $0 \leq x_i \leq 1, 0 \leq y_i \leq 1, i = 1, \dots, n$. This geometric problem has been extensively studied in the global optimization literature [10, 16]. Via a well-known transformation the problem is equivalent to the “point packing” problem

$$\begin{aligned}
 \text{PP :} \quad & \max \quad \theta \\
 & \text{s.t.} \quad (x_i - x_j)^2 + (y_i - y_j)^2 \geq \theta, \quad 1 \leq i < j \leq n \\
 & \quad \quad 0 \leq x \leq e, \quad 0 \leq y \leq e.
 \end{aligned}$$

Obviously PP corresponds to an instance of QCQP with a linear objective and constraints of the form $f_{ij}(x, y, \theta) \leq 0$, where

$$f_{ij}(x, y, \theta) = -(x_i - x_j)^2 - (y_i - y_j)^2 + \theta, \quad 1 \leq i < j \leq n.$$

Note that these are all “reverse convex” constraints; i.e. each $f_{ij}(\cdot, \cdot, \cdot)$ is a concave quadratic function. The variable θ represents the minimum squared distance separating n points in the unit square; the corresponding radius for n circles that can be packed into the unit square is $\sqrt{\theta}/[2(1 + \sqrt{\theta})]$.

In [2], bounds for the solution value of PP were computed using several combinations of semidefiniteness and RLT constraints. Note that since PP involves no terms of the form $x_i y_j$, all SDP and RLT constraints can be based on matrices X and Y relaxing xx^T and yy^T , respectively. In addition, it is clear that by symmetry one can assume that $.5 \leq x_i \leq 1$, $i = 1, \dots, n_x$ and $.5 \leq y_i \leq 1$, $i = 1, \dots, n_y$ where $n_x = \lceil n/2 \rceil$ and $n_y = \lfloor n_x/2 \rfloor$. We use “SYM” to refer to any problem formulation that uses these more restricted bounds. (Section 5 of [2] considers more elaborate symmetry-breaking using order constraints, but we omit discussion of this topic here.) The computational results obtained in [2] using the SDP, RLT and SYM conditions are summarized in Conjecture 1. (As in Section 3, the SDP relaxation includes the diagonal constraints $\text{diag}(X) \leq x$ and $\text{diag}(Y) \leq y$.) As described in [2], these findings are stated as a conjecture since the solution values given were numerically obtained for instances of size $n \leq 50$.

Conjecture 1. [2] *For $n \geq 2$ consider the RLT and SDP relaxations of PP. Then:*

1. *The optimal value for the RLT relaxation is 2.*
2. *The optimal value for the SDP relaxation is $1 + \frac{1}{n-1}$ and adding the RLT constraints does not change this value.*
3. *For $n \geq 5$ the optimal value for the RLT+SYM relaxation is $\frac{1}{2}$.*
4. *For $n \geq 5$ the optimal value for the SDP+SYM relaxation is $\frac{1}{4} \left(1 + \frac{1}{\lfloor (n-1)/4 \rfloor} \right)$.*

Note that the RLT bound of 2.0 is “worst possible” in that this is the maximum squared distance between two points in the unit square. In Figure 2 we illustrate the various bounds

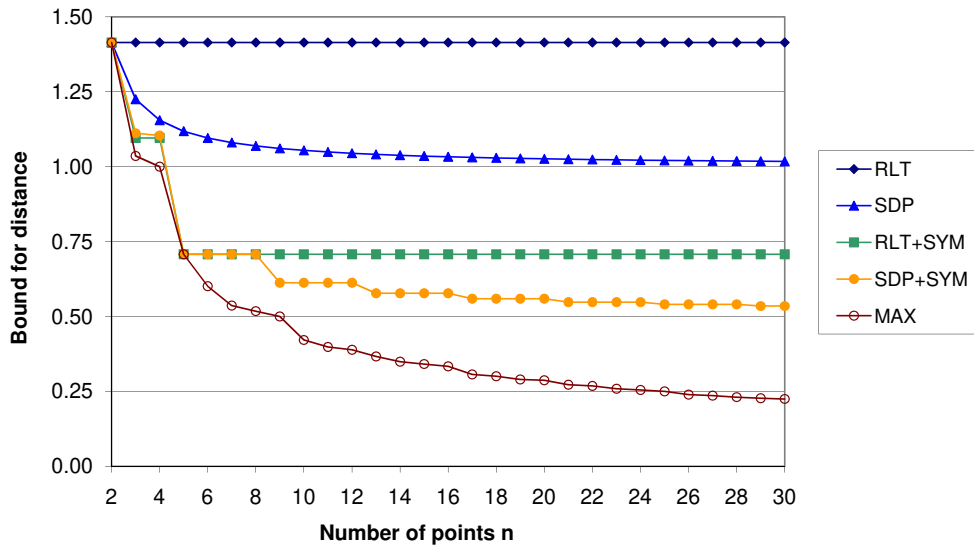


Figure 2: Bounds on distance from relaxations of PP

described in Conjecture 1 for $2 \leq n \leq 30$. (Figure 2 gives the square roots of the solution values for the various relaxations, corresponding to bounds on the minimum distance between two points.) The “MAX” values correspond to high-precision estimates for the exact optimal values of PP obtained by verified computing techniques [10].

Our interest here is to demonstrate a relationship between the bounds described in Conjecture 1 and bounds that correspond to replacing the quadratic constraints $f_{ij}(x, y, \theta) \leq 0$ with their convex lower envelopes. To do this we will utilize a specialization of Theorem 1 that applies when $\mathcal{F} = \{x : 0 \leq x \leq e\}$ and $f(\cdot)$ is concave.

Following the notation of [6], let \mathcal{BQP}_n denote the Boolean Quadric Polytope [11]

$$\mathcal{BQP}_n = \text{Co}\{(x, \{y_{ij}\}_{1 \leq i < j \leq n}) : x \in \{0, 1\}^n, y_{ij} = x_i x_j, 1 \leq i < j \leq n\}.$$

The definition of \mathcal{BQP}_n avoids duplication of variables due to the symmetry of xx^T and the fact that $\text{diag}(xx^T) = x$ for binary x . For $x \in \mathfrak{R}^n$, $X \in \mathfrak{R}^{n \times n}$ it is then convenient to define the projection operator

$$\text{proj}(x, X) = (x, \{x_{ij}\}_{1 \leq i < j \leq n})$$

that deletes the components of X on and below the diagonal. Finally, define the convex set

$$\mathcal{B}_n = \{(x, X) : \text{proj}(x, X) \in \mathcal{BQP}_n, 0 \leq \text{diag}(X) \leq x\}.$$

We remark that the lower bounds $0 \leq \text{diag}(X)$ are not actually required in the sequel, but we prefer to include them so as to make \mathcal{B}_n bounded.

Theorem 5. *Let $\mathcal{F} = \{x : 0 \leq x \leq e\}$. For $x \in \mathcal{F}$, let $f(x) = x^T Q x + c^T x$, where $\text{diag}(Q) \leq 0$, and let $\hat{f}(\cdot)$ be the convex lower envelope of $f(\cdot)$ on \mathcal{F} . Then $\hat{f}(x) = \min\{Q \bullet X + c^T x : (x, X) \in \mathcal{B}_n\}$.*

Proof. The proof is similar to that of Theorem 1, but since several steps require modifications we include the details. For $x \in \mathcal{F}$, let $g(x) = \min\{Q \bullet X + c^T x : (x, X) \in \mathcal{B}_n\}$. Our goal is to show that $\hat{f}(x) = g(x)$. To do this we first show that $g(\cdot)$ is a convex function with $g(x) \leq f(x)$, $x \in \mathcal{F}$, implying that $g(x) \leq \hat{f}(x)$.

Assume that for $i \in \{1, 2\}$, $x^i \in \mathcal{F}$ and $g(x^i) = Q \bullet X^i + c^T x^i$, where $(x^i, X^i) \in \mathcal{B}_n$. For $0 \leq \lambda \leq 1$, let

$$x(\lambda) = \lambda x^1 + (1 - \lambda)x^2, \quad X(\lambda) = \lambda X^1 + (1 - \lambda)X^2.$$

Then $(x(\lambda), X(\lambda)) \in \mathcal{B}_n$, since \mathcal{B}_n is convex. It follows that

$$g(x(\lambda)) \leq Q \bullet X(\lambda) + c^T x(\lambda) = \lambda g(x^1) + (1 - \lambda)g(x^2),$$

proving that $g(\cdot)$ is convex on \mathcal{F} . It is shown in [6, Proposition 5] that if $x \in \mathcal{F}$, then $\text{proj}(x, xx^T) \in \mathcal{BQP}_n$, and $0 \leq \text{diag}(xx^T) \leq x$ for $x \in \mathcal{F}$. It follows that $(x, xx^T) \in \mathcal{B}_n$ for any $x \in \mathcal{F}$, and therefore $g(x) \leq Q \bullet xx^T + c^T x = f(x)$.

It remains to show that $\hat{f}(x) \leq g(x)$. Assume that $g(x) = Q \bullet X + c^T x$, where $(x, X) \in \mathcal{B}_n$. From the definition of \mathcal{B}_n , there exist $x^i \in \{0, 1\}^n$, and $\lambda_i \geq 0$, $i = 1, \dots, k$, $\sum_{i=1}^k \lambda_i = 1$ such that

$$\text{proj} \left(\sum_{i=1}^k \lambda_i x^i, \sum_{i=1}^k \lambda_i x^i (x^i)^T \right) = \text{proj}(x, X).$$

Define

$$\bar{X} = \sum_{i=1}^k \lambda_i x^i (x^i)^T.$$

From the definition of \mathcal{B}_n we then have

$$\begin{aligned} X_{ij} &= \bar{X}_{ij}, & i &\neq j \\ 0 \leq X_{ii} &\leq \bar{X}_{ii} = x_i, & i &= 1, \dots, n. \end{aligned}$$

Therefore

$$\begin{aligned}
g(x) &= Q \bullet X + c^T x \\
&= Q \bullet \bar{X} + c^T x + \sum_{i=1}^n q_{ii}(X_{ii} - x_i) \\
&\geq Q \bullet \bar{X} + c^T x \\
&= \sum_{i=1}^k \lambda_i f(x^i).
\end{aligned}$$

But $\hat{f}(\cdot)$ is convex on \mathcal{F} , and $\hat{f}(x) \leq f(x)$ for all $x \in \mathcal{F}$, so

$$\hat{f}(x) = \hat{f}\left(\sum_{i=1}^k \lambda_i x^i\right) \leq \sum_{i=1}^k \lambda_i \hat{f}(x^i) \leq \sum_{i=1}^k \lambda_i f(x^i) \leq g(x).$$

□

See [6, Proposition 9] for a result closely related to Theorem 5. Using Theorem 5 we can prove an interesting relationship between bounds for PP obtained using convex lower envelopes of the constraints versus bounds obtained using RLT constraints on (x, X) and (y, Y) . Slightly abusing notation, we can write the constraint functions for PP in the form

$$f_{ij}(x, y, \theta) = f_{ij}(x) + f_{ij}(y) + \theta,$$

where $f_{ij}(x) = -(x_i - x_j)^2$, and therefore the convex lower envelope can be written in the form

$$\hat{f}_{ij}(x, y, \theta) = \hat{f}_{ij}(x) + \hat{f}_{ij}(y) + \theta.$$

Theorem 6. *For $\mathcal{F} = \{(x, y) : 0 \leq x \leq e, 0 \leq y \leq e\}$, let \hat{z} be the solution value for the relaxation of PP obtained by replacing the constraint functions with their convex lower envelopes on \mathcal{F} , and let z_{RLT} be the solution value for the relaxation that imposes the RLT constraints on (x, X) and (y, Y) . Then $\hat{z} \geq z_{\text{RLT}}$. Moreover this relationship continues to hold if \mathcal{F} is replaced by the tighter SYM bounds.*

Proof. By Theorem 5,

$$f_{ij}(x) = \min\{2x_{ij} - x_{ii} - x_{jj} : ((x_i, x_j), X_{[i,j]}) \in \mathcal{B}_2\},$$

where $X_{[i,j]}$ is the principal submatrix of X corresponding to row and column indices i and j . However, \mathcal{BQP}_2 is completely characterized by the RLT inequalities on x_{ij} [11], and the

additional constraints $0 \leq x_{ii} \leq x_i$, $0 \leq x_{jj} \leq x_j$ of \mathcal{B}_2 are RLT constraints on the diagonal elements of X . The result immediately follows. When applying the tighter SYM bounds, we can apply an affine transformation to the variables to re-write the problem in terms of transformed variables (x', y') with $0 \leq x' \leq e$, $0 \leq y' \leq e$, and use the fact that the convex lower envelopes and RLT constraints [14, Proposition 8.4] are both invariant with respect to affine transformations of the variables. \square

Since the RLT constraints on (x, X) and (y, Y) are already sufficient to characterize the convex lower envelopes of the quadratic constraints in PP, it would be natural to speculate that adding the semidefiniteness conditions $X \succeq xx^T$ and $Y \succeq yy^T$ would have no effect on bounds for the solution value. The values given in Conjecture 1 show that this is not the case. Note, however, that each convex lower envelope $\hat{f}_{ij}(x)$ requires only values of the variables $X_{[i,j]}$, and the semidefiniteness condition $Y(x, X) \succeq 0$ is stronger than the condition that all principal submatrices of $Y(x, X)$ corresponding to two variables are semidefinite.

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