Semidefinite programming versus the reformulation-linearization technique for nonconvex quadratically constrained quadratic programming

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Abstract   We consider relaxations for nonconvex quadratically constrained quadratic programming (QCQP) based on semidefinite programming (SDP) and the reformulation-linearization technique (RLT). From a theoretical standpoint we show that the addition of a semidefiniteness condition removes a substantial portion of the feasible region corresponding to product terms in the RLT relaxation. On test problems we show that the use of SDP and RLT constraints together can produce bounds that are substantially better than either technique used alone. For highly symmetric problems we also consider the effect of symmetry-breaking based on tightened bounds on variables and/or order constraints.

1 Introduction

We consider a quadratically constrained quadratic programming problem of the form:

$$\text{QCQP:} \quad \begin{array}{ll} \max & x^T Q_0 x + a_0^T x \\ \text{s.t.} & x^T Q_i x + a_i^T x \le b_i, \quad i \in \mathcal{I} \\ & x^T Q_i x + a_i^T x = b_i, \quad i \in \mathcal{E} \\ & l \le x \le u, \end{array}$$

where $x \in \Re^n$ and $\mathcal{I} \cup \mathcal{E} = \{1, \dots, m\}$. We assume that $-\infty < l_i < u_i < +\infty$ for each i, and the matrices Q_i are all symmetric. If $-Q_0$ and Q_i, $i \in \mathcal{I}$ are all positive semidefinite

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and $Q_i = 0$ for $i \in \mathcal{E}$, then QCQP is a convex optimization problem. In general however QCQP is NP-hard. QCQP is a well-studied problem in the global optimization literature with many applications, frequently arising from Euclidean distance geometry. An example that has attracted considerable recent attention concerns localizing sensor networks given distance information [11].

Global optimization methods for QCQP are typically based on convex relaxations of the problem. In this paper we compare two such relaxations, based on semidefinite programming (SDP) [14] and the reformulation-linearization technique (RLT) [8]. These two relaxations are described in the next section. In Sect. 3 we analyze the effect that adding the semidefiniteness condition has on the feasible region for the three variables in the RLT relaxation corresponding to product terms induced by two original variables x_i, x_j. We show that for typical values of the original variables the semidefiniteness constraint removes a large fraction of this feasible region. In Sect. 4 we consider computational results on two different classes of test problems. For nonconvex box-constrained QPs we show that the use of SDP and RLT constraints together produces bounds that are substantially better than when either technique is used alone. We also consider SDP and RLT relaxations applied to circle-packing problems in the plane. These problems are highly symmetric, and we examine the effect of partial symmetry-breaking based on tightened bounds for subsets of variables. In Sect. 5 we consider the effect of further symmetry-breaking based on imposing additional order constraints. Computational results on these problems indicate unexpectedly regular solution values for the various relaxations, as well as an unexpected relationship between bounds from SDP relaxations and bounds from RLT relaxations with additional order constraints.

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 $X \bullet Y = \sum_{i,j=1}^{n} X_{ij} Y_{ij}$. We use e to denote a vector with each component equal to one.

2 The SDP and RLT relaxations

Relaxations of QCQP based on SDP and RLT both utilize variables X_{ij} that replace the product terms $x_i x_j$ of the original problem. The relaxations differ in the form of the constraints that are placed on these new variables. The SDP relaxation is based on the fact that since $X = xx^T$ in the actual solution of QCQP, one can obtain a relaxation of QCQP by imposing $X \succeq xx^T$ instead. The SDP relaxation of QCQP [14] may then be written

$$
\begin{aligned}
\text{SDP:} \quad \max \quad & Q_0 \bullet X + a_0^T x \\
\text{s.t.} \quad & Q_i \bullet X + a_i^T x \le b_i, && i \in \mathcal{I} \\
& Q_i \bullet X + a_i^T x = b_i, && i \in \mathcal{E} \\
& l \le x \le u, && X - xx^T \succeq 0.
\end{aligned}
$$

Moreover it is very well known that the condition $X - xx^T \succeq 0$ is equivalent to

$$
\tilde{X} := \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succeq 0, \tag{1}
$$

and therefore SDP may be alternatively written in the form

$$
\begin{aligned}
\text{SDP:} \quad \max \quad & \tilde{Q}_0 \bullet \tilde{X} \\
\text{s.t.} \quad & \tilde{Q}_i \bullet \tilde{X} \le 0, \quad i \in \mathcal{I} \\
& \tilde{Q}_i \bullet \tilde{X} = 0, \quad i \in \mathcal{E} \\
& l \le x \le u, \quad \tilde{X} \succeq 0,
\end{aligned}
$$

where

$$\tilde{Q}_i := \begin{pmatrix} -b_i & a_i^T/2 \\ a_i/2 & Q_i \end{pmatrix}.$$

When the original QCQP is a convex problem ($Q_0 \preceq 0$, $Q_i \succeq 0$ for $i \in \mathcal{I}$ and $Q_i = 0$ for $i \in \mathcal{E}$), it is straightforward to show that SDP is equivalent to QCQP. If QCQP is nonconvex, however, SDP may be unbounded even though all of the original variables have finite upper and lower bounds. This can easily be remedied by adding upper bounds to the diagonal components of X. For example, it is obvious that $X_{ii} \leq \max\{l_i^2, u_i^2\}$. Better upper bounds for X_{ii} are obtained as part of the RLT relaxation that we describe below. An approximation result based on the SDP relaxation for a special case of QCQP ($l = -e$, $u = e$, $\mathcal{I} = \emptyset$, $a_i = 0$ and Q_i diagonal for $i = 1, \ldots, m$) is given in [17].

The RLT relaxation of QCQP is based on using products of upper and lower bound constraints on the original variables to obtain valid linear inequality constraints on the new variables X_{ij} [8]. For two variables x_i and x_j we have constraints $x_i - l_i \geq 0$, $u_i - x_i \geq 0$, $x_j - l_j \geq 0$, $u_j - x_j \geq 0$. Multiplying each of the constraints involving x_i by a constraint involving x_j, and replacing the product term $x_i x_j$ with the new variable X_{ij}, we obtain the constraints

$$X_{ij} - l_i x_j - l_j x_i \geq -l_i l_j,$$
$$X_{ij} - u_i x_j - u_j x_i \geq -u_i u_j,$$
$$X_{ij} - l_i x_j - u_j x_i \leq -l_i u_j,$$
$$X_{ij} - l_j x_i - u_i x_j \leq -l_j u_i,$$

$i, j = 1, \ldots, n$. Note that these constraints also hold when $i = j$, in which case the last two constraints are identical. Moreover the last two constraints are identical for all i, j once the condition $X_{ij} = X_{ji}$ is imposed. The resulting relaxation of QCQP can then be written

$$
\begin{aligned}
\text{RLT:} \quad \max \quad & Q_0 \bullet X + a_0^T x \\
\text{s.t.} \quad & Q_i \bullet X + a_i^T x \leq b_i, && i \in \mathcal{I} \\
& Q_i \bullet X + a_i^T x = b_i, && i \in \mathcal{E} \\
& X - lx^T - xl^T \geq -ll^T \\
& X - ux^T - xu^T \geq -uu^T \\
& X - lx^T - xu^T \leq -lu^T \\
& l \leq x \leq u, \quad X = X^T.
\end{aligned}
$$

Using the fact that $X_{ij} = X_{ji}$, the result is an ordinary linear programming (LP) problem with $n(n+3)/2$ variables and a total of $m + n(2n+3)$ constraints. (In fact it is known that the original bound constraints $l \leq x \leq u$ are redundant and could be removed [10, Proposition 1].)

If QCQP contains linear constraints other than the simple bounds ($Q_i = 0$ for some $0 < i \leq m$), then additional constraints can be imposed on the variables X in the SDP and/or RLT relaxations. For RLT the standard methodology is to form all possible products of pairs of linear inequality constraints, including the bound constraints on the variables [10]. If $|\{i \in \mathcal{I} : Q_i = 0\}| = k$ this would add an additional $2kn + k(k+1)/2$ linear inequality constraints to the RLT relaxation. If there are linear equality constraints then it suffices to consider the constraints on X obtained by multiplying individual equality constraints by each variable x_j [8, Remark 8.1], so if $|\{i \in \mathcal{E} : Q_i = 0\}| = p$, a total of pn additional linear equality constraints would be added to the RLT relaxation. It is also possible to construct higher-order RLT relaxations corresponding to linearizations of polynomial terms of order

greater than two [8]. Such relaxations obtain tighter bounds at the expense of a larger number of variables and constraints. For linear equality constraints the standard approach in forming SDP relaxations (see for example [16, Remark 13.4.1]) is to add only the "squared" constraints

$$a_i^T x = b_i \Rightarrow a_i^T X a_i = b_i^2.$$

The treatment of linear inequality constraints in SDP relaxations is less obvious, because the constraint obtained by "squaring" a linear inequality $a_i^T x - b_i \geq 0$ is already implied by $\tilde{X} \succeq 0$. In [2] some theoretical justification is given for generating additional constraints from linear inequalities by first adding slack variables to obtain equalities and then forming the squared equality constraints.

3 Adding SDP to RLT

In this section we examine the effect of adding the semidefiniteness condition $X \succeq xx^T$ to the RLT relaxation of QCQP. We will focus on the effect that adding semidefiniteness has on the feasible values for the product variables X_{ij}. It is well known that the RLT relaxation is invariant with respect to an invertible affine transformation of the original variables [8, Proposition 8.4], and it is easy to show that such an invariance also holds for the SDP relaxation. As a result we may assume without loss of generality that $l = 0$, $u = e$. We will consider two variables x_i, x_j, and for convenience assume that $i = 1$, $j = 2$. By interchanging and/or complementing the variables we may further assume that $0 \leq x_1 \leq x_2 \leq .5$. Under these assumptions the RLT constraints on X_{11}, X_{22} and X_{12} become

$$0 \leq X_{11} \leq x_1, \tag{2a}$$

$$0 \leq X_{22} \leq x_2, \tag{2b}$$

$$0 \leq X_{12} \leq x_1. \tag{2c}$$

Next we consider imposing the semidefiniteness condition $X - xx^T \succeq 0$. As described in the previous section this is equivalent to $\tilde{X} \succeq 0$, where $\tilde{X}$ is defined as in (1). Restricting attention to the principal submatrix of $\tilde{X}$ corresponding to x_1 and x_2, we certainly have

$$\begin{pmatrix} 1 & x_1 & x_2 \\ x_1 & X_{11} & X_{12} \\ x_2 & X_{12} & X_{22} \end{pmatrix} \succeq 0, \tag{3}$$

and it is straightforward to show that (3) is equivalent to the constraints

$$X_{11} \geq x_1^2, \tag{4a}$$

$$X_{22} \geq x_2^2, \tag{4b}$$

$$X_{12} \leq x_1 x_2 + \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)}, \tag{4c}$$

$$X_{12} \geq x_1 x_2 - \sqrt{(X_{11} - x_1^2)(X_{22} - x_2^2)}. \tag{4d}$$

Our goal is to compare, for fixed values of x_1 and x_2, the three-dimensional feasible regions for (X_{11}, X_{22}, X_{12}) corresponding to (2) before and after the addition of (4). Assuming that $x_1 > 0$, $x_2 > 0$ it is clear that adding (4) has no effect on the upper bounds for X_{ii}, $i = 1, 2$ but improves the lower bounds from $X_{ii} \geq 0$ to $X_{ii} \geq x_i^2$. (The use of these convex, nonlinear constraints to strengthen the RLT relaxation was suggested in [10].) For any values X_{ii} satisfying $x_i^2 \leq X_{ii} \leq x_i, i = 1, 2$, values of X_{12} for which (X_{11}, X_{22}, X_{12}) are feasible

in both (2) and (4) must satisfy (2c) as well as (4c) and (4d). In Fig. 1 we show the resulting feasible region as a subset of the RLT feasible region (2) for the case $x_1 = .5$, $x_2 = .5$. For these values it is clear that the bounds (4c) and (4d) dominate the original RLT bounds on X_{12} for all values of X_{11} and X_{22} that satisfy $x_i^2 \le X_{ii} \le x_i$, $i = 1, 2$. However for more general values x_1, x_2 the situation is more complex. For example, in Fig. 2 we illustrate the case of $x_1 = .1$, $x_2 = .5$. In the next theorem we characterize the three-dimensional volume of the combined SDP+RLT region for all relevant values of x_1, x_2.

Fig. 1 RLT versus SDP+RLT regions, $0 \le x \le e$, $x_1 = .5$, $x_2 = .5$
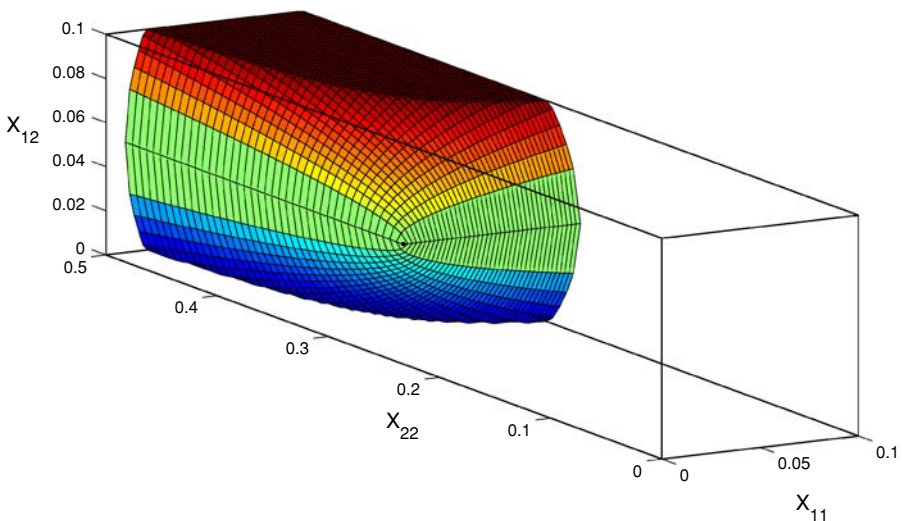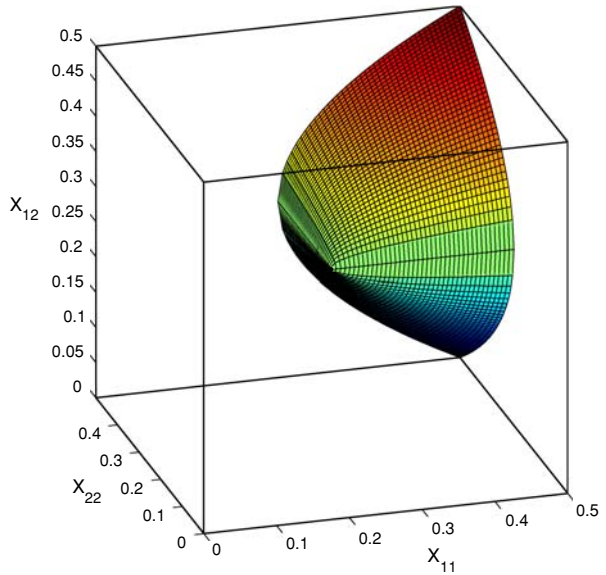
Fig. 2 RLT versus SDP+RLT regions, $0 \le x \le e$, $x_1 = .1$, $x_2 = .5$

Theorem 1 *Suppose that $l = 0$, $u = e$, $0 < x_1 \leq x_2 \leq .5$. Then the three-dimensional volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in* (2) *is $x_1^2 x_2$, and the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in both* (2) *and* (4) *is*

$$x_1^2 x_2 (1 - x_2) - \frac{1}{9} x_1^3 \left(6x_2^2 - 6x_2 + 5 \right) + \frac{1}{3} x_1^3 \left((1 - x_2)^3 - x_2^3 \right) \ln \left(\frac{1 - x_2}{x_2} \right)$$

$$- \frac{1}{3} x_1^3 \left((1 - x_2)^3 + x_2^3 \right) \ln \left(\frac{1 - x_1}{x_1} \right).$$

Proof The volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in (2) is trivial. To compute the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in (2) and (4) it is convenient to consider the regions with $X_{12} \leq x_1 x_2$ and $X_{12} \geq x_1 x_2$ separately.

Assume that $x_i^2 \leq X_{ii} \leq x_i, i = 1, 2$. It is then easy to compute that the lower bound (4d) will dominate the lower bound $X_{12} \geq 0$ from (2c) exactly when

$$X_{22} \leq \frac{x_2^2 X_{11}}{X_{11} - x_1^2}. \tag{5}$$

Since $X_{22} \leq x_2$ by assumption, (5) certainly holds if

$$x_2 \leq \frac{x_2^2 X_{11}}{X_{11} - x_1^2},$$

which is equivalent to

$$X_{11} \leq \frac{x_1^2}{1 - x_2}. \tag{6}$$

Note moreover that since by assumption $0 < x_1 \leq .5$ and $0 < x_2 \leq .5$, we have

$$x_1 + x_2 \leq 1 \Rightarrow 1 - x_2 \geq x_1 \Rightarrow \frac{1}{1 - x_2} \leq \frac{1}{x_1} \Rightarrow \frac{x_1^2}{1 - x_2} \leq x_1,$$

so the upper bound on X_{11} in (6) cannot be greater than the original upper bound $X_{11} \leq x_1$ from (2). It follows that the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in both (2) and (4) with $X_{12} \leq x_1 x_2$ is given by

$$\int_{\frac{x_1^2}{1-x_2}}^{x_1} \int_{\frac{x_2^2 X_{11}}{X_{11}-x_1^2}}^{x_2} x_1 x_2 \, dX_{22} \, dX_{11} + \int_{\frac{x_1^2}{1-x_2}}^{x_1} \int_{x_2^2}^{\frac{x_2^2 X_{11}}{X_{11}-x_1^2}} (X_{11} - x_1^2)^{\frac{1}{2}} (X_{22} - x_2^2)^{\frac{1}{2}} \, dX_{22} \, dX_{11}$$

$$\tag{7}$$

$$+ \int_{x_1^2}^{\frac{x_1^2}{1-x_2}} \int_{x_2^2}^{x_2} (X_{11} - x_1^2)^{\frac{1}{2}} (X_{22} - x_2^2)^{\frac{1}{2}} \, dX_{22} \, dX_{11}.$$

A straightforward integration exercise shows that the volume given by (7) is equal to

$$x_1^2 x_2^2 (1 - x_1 - x_2) + \frac{4}{9} x_1^3 x_2^3 - \frac{1}{3} x_1^3 x_2^3 \ln \left(\frac{1 - x_1}{x_1} \frac{1 - x_2}{x_2} \right). \tag{8}$$

Fig. 3 Ratio of volume of SDP+RLT region to RLT region, $0 \leq x_1 \leq x_2 \leq .5$
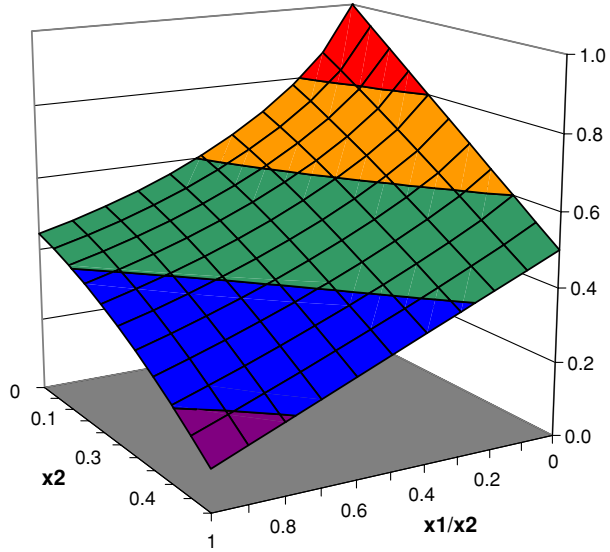
The derivation of the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in (2) and (4) with $X_{12} \geq x_1 x_2$ is similar and we omit the details. The resulting volume is

$$x_1^2 (1 - x_2)^2 (x_2 - x_1) + \frac{4}{9} x_1^3 (1 - x_2)^3 - \frac{1}{3} x_1^3 (1 - x_2)^3 \ln \left(\frac{1 - x_1}{x_1} \frac{x_2}{1 - x_2} \right), \quad (9)$$

which is exactly (8) with $(1 - x_2)$ substituted for x_2 throughout. The proof is completed by combining (8) and (9). □

Theorem 1 has several interesting implications. For example, for any $0 < x_1 \leq x_2 \leq .5$ one can use the results of the theorem to compute the ratio of the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in both (2) and (4) to the volume of $\{(X_{11}, X_{22}, X_{12})\}$ feasible in (2) alone. In Fig. 3 we illustrate this fraction in terms of x_2 and the ratio x_1/x_2. The minimum fraction of $1/9$ is achieved at $x_1 = x_2 = .5$, as depicted in Fig. 1. The worst-case ratio of 1.0 corresponds to the limit as $x_2 \to 0$, $x_1/x_2 \to 0$. In Fig. 4 we illustrate $\{(X_{11}, X_{22}, X_{12})\}$ feasible in both (2) and (4) for $x_1 = .01$, $x_2 = .1$; for these values the (SDP+RLT)/RLT volume fraction is approximately .7923. It should also be noted that for any $0 < x_1 \leq x_2 \leq .5$, the point $(X_{11}, X_{22}, X_{12}) = (x_1^2, x_2^2, x_1 x_2)$ is always in the interior of the RLT feasible region, but is an extreme point of the SDP+RLT region.

In addition to comparing the volumes of the RLT and SDP+RLT feasible regions for fixed values of x_1 and x_2, Theorem 1 can be used to derive the five-dimensional volumes of the corresponding feasible regions based on the original bounds $0 \leq x_i \leq 1$, $i = 1, 2$. We give this result in the following theorem.

Theorem 2 *Suppose that $0 \leq x_i \leq 1$, $i = 1, 2$. Then the volume of $\{(x_1, x_2, X_{11}, X_{22}, X_{12})\}$ that are feasible for the RLT constraints is $1/60$, and the volume of $\{(x_1, x_2, X_{11}, X_{22}, X_{12})\}$ that are feasible for the RLT constraints and (3) is $1/240$.*
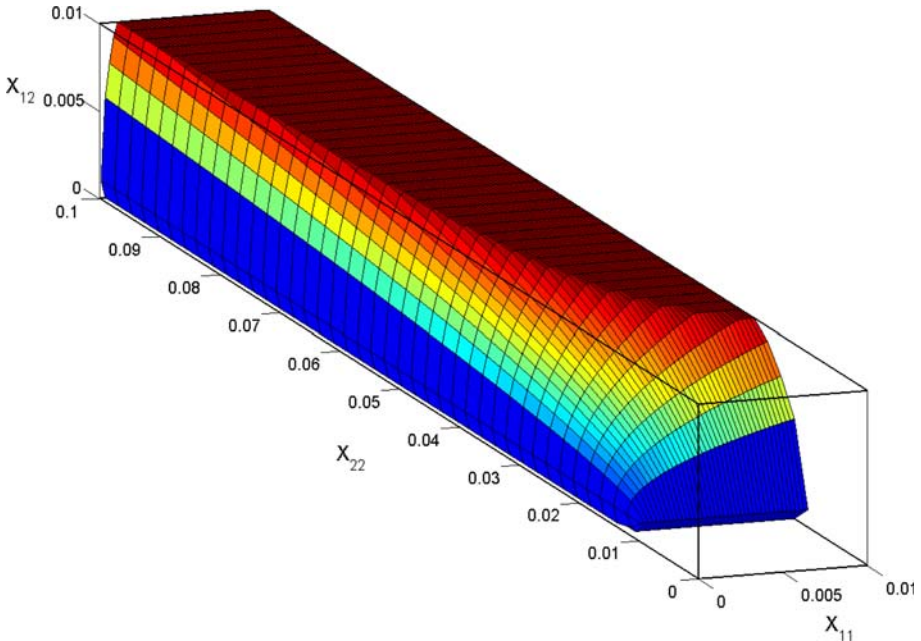
Fig. 4 RLT versus SDP+RLT regions, $0 \leq x \leq e$, $x_1 = .01$, $x_2 = .1$

Proof From Theorem 1, the volume of $\{(x_1, x_2, X_{11}, X_{22}, X_{12})\}$ feasible for the RLT constraints, with $0 \leq x_1 \leq x_2 \leq .5$, is

$$\int_0^{\frac{1}{2}} \int_0^{x_2} x_1^2 x_2 \, dx_1 dx_2,$$

which is easily computed to be 1/480. To find the corresponding volume of $\{(x_1, x_2, X_{11}, X_{22}, X_{12})\}$ that also satisfy (3) requires computing

$$\int_0^{\frac{1}{2}} \int_0^{x_2} v(x_1, x_2) \, dx_1 dx_2,$$

where $v(x_1, x_2)$ is the three-dimensional volume given in Theorem 1. Using Maple™ 11 this integral evaluates to equal 1/1920. Moreover the region $0 \leq x_1 \leq x_2 \leq .5$ represents 1/8 of the original feasible region $0 \leq x_i \leq 1$, $i = 1, 2$, and volumes are invariant with respect to the transformations (exchanging and/or complementing variables) needed to map any other (x_1, x_2) onto this region.   □

The result of Theorem 2 is remarkably simple: adding the semidefiniteness condition (3) to the RLT relaxation removes exactly 75% of the feasible region determined by two of the original variables. It must be noted, however, that in general there is no simple relationship between the volumes of different relaxations and the quality of bounds obtained using them. Moreover Theorem 2 applies to only two of the n variables in QCQP. The following result,

proved in [1], shows that no further improvement is possible for a convex relaxation of the terms corresponding to two of the original variables.

Theorem 3 ([1]) *For $n = 2$ and $0 \leq x \leq e$, the set of $\tilde{X} \succeq 0$ such that (x, X) are feasible for the RLT constraints is equal to the convex hull of $\{ \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T : 0 \leq x \leq e \}$.*

4 Computational results

In this section we compare bounds obtained using the SDP, RLT and SDP+RLT relaxations on two different classes of test problems. All problems were solved on a 2.8 GHz Pentium 4 PC with 2 Gb of RAM, using the Matlab-based SeDuMi solver [12] with a feasibility/optimality tolerance of 1E-8. To begin we consider indefinite box-constrained QPs, corresponding to the case $\mathcal{E} = \mathcal{I} = \emptyset$ in QCQP. Box-constrained QPs have a number of applications and have been well-studied in the global optimization literature; see for example [4] and references therein. In Table 1 we compare the bounds, and relative gaps between bounds and the optimal value, for a group of test problems from [15]. These problems all have $n = 30$, $0 \leq x \leq e$, and were solved to optimality using a finite branch-and-bound method based on polyhedral bounds in [15]. (An extension of this method that uses semidefinite relaxations is given in [3].) In Table 1, PS is the value of the polyhedral bound at the root problem, and BARON is the root bound obtained by the BARON global optimization package [7] after tightening based on range reduction (Vandenbussche, private communication, 2005). The columns RLT and SDP correspond to values obtained by the relaxations RLT and SDP of Sect. 2, and SDP+RLT corresponds to the problem with both sets of constraints imposed. (The SDP relaxation also includes the upper bounds on diagonal components $X_{ii} \leq x_i$.)

Examining Table 1, we conclude that on these problems the bounds from RLT, BARON and PS are similar, while those from SDP have gaps that are an order of magnitude smaller and those from SDP+RLT are an order of magnitude smaller again. It is also notable that the bounds from RLT and BARON are quite close, as one would expect since BARON is based on the reformulation-linearization technique. (The fact that the BARON bounds are always somewhat better is consistent with the fact that they are being reported after tightening based on range reduction.) In terms of computational cost, each RLT or SDP bound for these problems required approximately 1 second of computation, but each SDP+RLT bound required over 200 seconds of computation. It is well known that "mixed" SDP/LP problems involving large numbers of inequality constraints are computionally challenging, and reducing the work to solve such problems is an area of ongoing algorithmic research. An alternative approach taken in [9] is to add linear constraints implied by $\tilde{X} \succeq 0$ to the RLT relaxation in an effort to obtain stronger bounds without incurring the computational cost of solving the SDP+RLT problem directly. Computational results in [9] show that this approach can produce significantly tighter root bounds and substantially reduce the total computational time in a branch-and-bound algorithm compared to using RLT relaxations alone. In [5] a similar approach is proposed that adds second-order cone constraints to RLT; these are stronger than the linear constraints used in [9] but computationally still easier to handle than the full SDP+RLT problem.

Our second set of test problems are based on circle packing in the plane: for a given $n \geq 2$ find the maximum radius of n non-overlapping cicrles that all lie in the unit box $0 \leq x_i \leq 1$, $0 \leq y_i \leq 1$, $i = 1, \ldots, n$. This geometric problem has been extensively studied in the global optimization literature [6,13]. Via a well-known transformation the problem is equivalent to the "point packing" problem

Table 1 Comparison of bounds for indefinite box-constrained QP problems

Problem instance	Optimal value	Bound value					Relative gap to optimal value (%)				
		RLT	BARON	PS	SDP	SDP+RLT	RLT	BARON	PS	SDP	SDP+RLT
30-60-1	706.00	1454.75	1430.20	1405.25	768.12	714.67	106.06	102.58	99.04	8.80	1.23
30-60-2	1377.17	1699.50	1668.51	1637.00	1426.94	1377.17	23.41	21.15	18.87	3.61	0.00
30-60-3	1293.50	2047.00	2006.83	1966.00	1370.13	1298.21	58.25	55.15	51.99	5.92	0.36
30-70-1	654.00	1569.00	1547.43	1525.50	746.43	674.00	139.91	136.61	133.26	14.13	3.06
30-70-2	1313.00	1940.25	1888.67	1836.25	1375.07	1313.00	47.77	43.84	39.85	4.73	0.00
30-70-3	1657.40	2302.75	2251.55	2199.50	1719.77	1657.55	38.94	35.85	32.71	3.76	0.01
30-80-1	952.73	2107.50	2072.29	2036.50	1050.76	965.25	121.21	117.51	113.75	10.29	1.31
30-80-2	1597.00	2178.25	2158.29	2138.00	1622.81	1597.00	36.40	35.15	33.88	1.62	0.00
30-80-3	1809.78	2403.50	2376.47	2349.00	1836.79	1809.78	32.81	31.31	29.79	1.49	0.00
30-90-1	1296.50	2423.50	2385.44	2346.75	1348.48	1296.50	86.93	83.99	81.01	4.01	0.00
30-90-2	1466.84	2667.00	2623.11	2578.50	1527.87	1466.84	81.82	78.83	75.79	4.16	0.00
30-90-3	1494.00	2538.25	2499.69	2460.50	1516.81	1494.00	69.90	67.32	64.69	1.53	0.00
30-100-1	1227.13	2602.00	2541.99	2481.00	1285.74	1227.13	112.04	107.15	102.18	4.78	0.00
30-100-2	1260.50	2729.25	2699.12	2668.50	1365.32	1261.08	116.52	114.13	111.70	8.32	0.05
30-100-3	1511.05	2751.75	2704.14	2655.75	1611.11	1513.08	82.11	78.96	75.76	6.62	0.13
Average							76.94	73.97	70.95	5.58	0.41

PP: max θ

s.t. $(x_i - x_j)^2 + (y_i - y_j)^2 \geq \theta, \quad 1 \leq i < j \leq n$

$0 \leq x \leq e, \quad 0 \leq y \leq e.$

Regarding problem PP, note that

- 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 $\sqrt{\theta}/[2(1 + \sqrt{\theta})]$.
- The problem formulation involves no terms of the form $x_i y_j$. As a result, the RLT and SDP relaxations can be based on matrices X and Y relaxing xx^T and yy^T, respectively.
- Let $n_x = \lceil n/2 \rceil, n_y = \lceil n_x/2 \rceil$. By symmetry one can assume $.5 \leq x_i \leq 1, i = 1, \ldots, n_x$ and $.5 \leq y_i \leq 1, i = 1, \ldots, n_y$. We will use SYM to refer to any problem formulation that uses these more restricted bounds.

We have solved various relaxations of PP for $2 \leq n \leq 50$. The solution values for these relaxations have an unexpectedly simple structure described in Conjecture 4, below. We present these results as a conjecture since we have obtained the solution values only up to $n \leq 50$, and all values are approximate (but high precision) estimates of the true optimal values obtained by a numerical solver.

Conjecture 4 *For $n \geq 2$ consider the RLT and SDP relaxations of PP, where the SDP relaxation also imposes the diagonal upper bounds $X_{ii} \leq x_i, Y_{ii} \leq y_i, i = 1, \ldots, n$. 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 addition, the effect of adding the more restricted SYM bounds is very similar for both the RLT and SDP relaxations: the solution value is reduced approximately by a factor of 4. In Fig. 5 we illustrate the various bounds described in Conjecture 4 for $2 \leq n \leq 30$. (The SDP+SYM+ORD relaxation is described in the next section.) Figure 5 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 [6], available from http://packomania.com. It is worth noting that while these problems have some similarity with the sensor network problems considered in [11], the SDP relaxations for PP do not appear to be nearly as tight as those for the sensor problems. We believe that there are at least two reasons for this difference. First, the PP problem has a high degree of symmetry which is problematic for any bound based on convex optimization. Second, the distance information in the sensor network problems, especially distance information involving fixed anchor points, provides many additional constraints on components of $\tilde{X}$ that considerably tighten the SDP relaxation.

5 Symmetry-breaking using order constraints

The results in Conjecture 4 show that the more restricted bounds based on symmetry have a substantial effect on both the SDP and RLT relaxations of PP. In this section we consider

Fig. 5 Bounds on distance from relaxations of PP
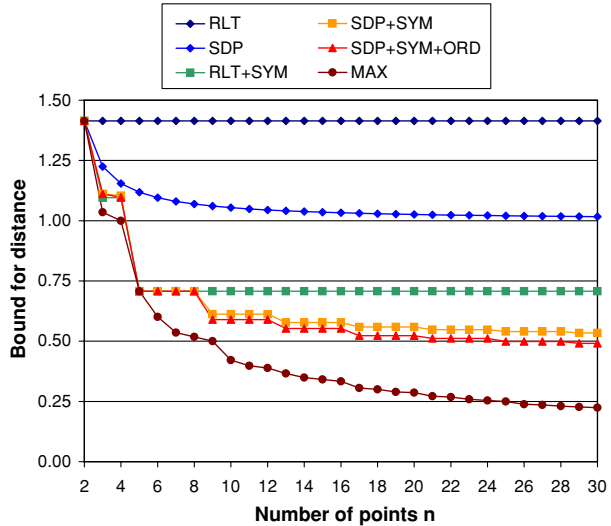
a more elaborate symmetry-breaking strategy based on orderings of variables. In particular, for the variables x and y in PP one could certainly assume that

$$x_i \geq x_{i+1}, \qquad i = 1, \ldots, n-1. \tag{10}$$

Simply adding (10) to the SDP or RLT relaxations would have no effect, since (10) can be satisfied by re-ordering the variables in any solution. However (10) can be used to generate additional linear constraints on the variables (x, X). As described in Sect. 2, the usual approach in forming RLT relaxations is to generate constraints based on all pairs of linear inequalities, including the original bound constraints on the variables. In the case of (10) this would result in an additional $O(n^2)$ constraints, which would be computationally very costly if semidefiniteness of $\tilde{X}$ is also imposed. To reduce the computational burden we will generate a total of $O(n)$ constraints by using (10) for a given i together with only the bound constraints on x_i and x_{i+1}. It is straightforward to show that the resulting constraints have the form

$$X_{ii} - X_{i,i+1} + l_i x_{i+1} - l_i x_i \geq 0,$$
$$X_{ii} - X_{i,i+1} + u_i x_{i+1} - u_i x_i \leq 0,$$
$$X_{i+1,i+1} - X_{i,i+1} + u_{i+1} x_i - u_{i+1} x_{i+1} \geq 0,$$
$$X_{i+1,i+1} - X_{i,i+1} + l_{i+1} x_i - l_{i+1} x_{i+1} \leq 0,$$

$i = 1, \ldots, n-1$. We will use ORD to denote any relaxation that imposes these additional constraints. Note that if the more restricted SYM ranges are imposed then the constraint (10) is not valid for $i = n_y$, but can still be imposed for all other i. In this case we simply omit the constraints on (x, X) corresponding to $i = n_y$.

We have solved a variety of relaxations of PP using the additional ORD constraints, for $2 \leq n \leq 50$. The unexpectedly regular behavior of the RLT and SDP relaxations with and without the SYM restrictions, described in Conjecture 4, becomes even more remarkable when the ORD constraints are added. These findings are given in Conjecture 5 below. As with Conjecture 4 we describe our results as a conjecture since they have only been observed

up to $n \leq 50$, and correspond to high-precision estimates of the true optimal values of the problems obtained by a numerical solver.

Conjecture 5 *For $n \geq 2$ consider the RLT and SDP relaxations of PP, where the SDP relaxation also imposes the diagonal upper bounds $X_{ii} \leq x_i$, $Y_{ii} \leq y_i$, $i = 1, \ldots, n$. Then:*

1. *The optimal value for the RLT+ORD relaxation is equal to that of the SDP relaxation.*
2. *For $n \geq 5$ the optimal value for the RLT+SYM+ORD relaxation is equal to that of the SDP+SYM relaxation.*
3. *For $n \geq 9$ the optimal value for the SDP+SYM+ORD relaxation is strictly less than the optimal value of the RLT+SYM+ORD relaxation.*

Loosely speaking, Conjecture 5 says that adding the ORD constraints to RLT, with or without the tightened SYM bounds, has exactly the same effect as using SDP instead. However the bounds computed by adding the ORD constraints to RLT are cheaper to compute than those based on SDP. For example, for $n = 50$ the time required to compute the RLT + SYM + ORD bound was about 36 seconds, compared to 54 seconds for SDP+SYM. The last part of Conjecture 5 indicates that for $n \geq 9$ the best bounds are obtained using SDP + SYM + ORD. However from Fig. 5 it is clear that the difference between the solution values for the RLT + SYM + ORD and SDP + SYM + ORD relaxations is relatively small, and the SDP +SYM + ORD bound is substantially more expensive to compute (for $n = 50$ the SDP + SYM + ORD bound required over 100 seconds to compute). In conclusion, for these problems a substantial amount of the bound improvement of SDP compared to RLT can be obtained relatively cheaply by appropriate tightenings of RLT based on problem symmetry. It is interesting to note that these tightenings of RLT are *not* based on trying to approximate the semidefinitess of $\tilde{X}$ using additional linear or convex quadratic constraints, as in [5] and [9].

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