Extended Triangle Inequalities for Nonconvex Box-Constrained Quadratic Programming

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Abstract

Let $\text{Box}_n = \{x \in \mathbb{R}^n : 0 \le x_i \le 1, \ i = 1, \ldots, n\}$, and let QPB_n denote the convex hull of $\{(1, x^T)^T(1, x^T) : x \in \text{Box}_n\}$. The quadratic programming problem $\min\{x^T Q x + q^T x : x \in \text{Box}_n\}$ where Q is not positive semidefinite (PSD), is equivalent to a linear optimization problem over QPB_n and could be efficiently solved if a tractable characterization of QPB_n was available. It is known that QPB_2 can be represented using a PSD constraint combined with constraints generated using the reformulation-linearization technique (RLT). The triangle (TRI) inequalities are also valid for QPB_3, but the PSD, RLT and TRI constraints together do not fully characterize QPB_3. In this paper we describe new valid linear inequalities for QPB_n, $n \ge 3$ based on strengthening the approximation of QPB_3 given by the PSD, RLT and TRI constraints. These new inequalities are generated in a systematic way using a known disjunctive characterization for QPB_3. We also describe a conic strengthening of the linear inequalities that incorporates second-order cone constraints. We show computationally that the new inequalities and their conic strengthenings obtain exact solutions for some nonconvex box-constrained instances that are not solved exactly using the PSD, RLT and TRI constraints.

Keywords: triangle inequalities, box-constrained quadratic programming, nonconvex quadratic programming.

Mathematics Subject Classification: 90C20, 90C26, 90C15.

1 Introduction

In this paper we are concerned with the box-constrained quadratic programming problem

$$
\begin{aligned}
\text{BoxQP}: \quad \max \quad & x^T Q x + q^T x \\
\text{s.t.} \quad & 0 \le x_i \le 1, \quad i = 1, \ldots, n.
\end{aligned}
$$

If the matrix Q is positive semidefinite (PSD) then BoxQP can be efficiently solved by a variety of methods, but in general BoxQP is an NP-hard problem that has been heavily

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studied in the global optimization literature; see for example [16] and references therein. BoxQP problems can be approached using general-purpose software such as BARON [13], or specialized methods that are tailored to the problem. Examples of the latter include the finite branching algorithm of [7], a specialization of [6] which itself is a strengthening of the finite branching algorithm of [16], and methods based on mixed-integer linear programming [3, 17].

Let $\text{Box}_n = \{x \in \mathbb{R}^n : 0 \leq x_i \leq 1,\ i = 1,\ldots,n\}$, and $\text{QPB}_n = \text{Co}\{(1, x^T)^T(1, x^T) : x \in \text{Box}_n\}$, where Co denotes the convex hull. For $x \in \mathbb{R}^n$ and a symmetric $n \times n$ matrix X, let

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

The BoxQP problem can then be rewritten in the form of a linear optimization problem

$$\text{BoxQP}: \quad \max \quad Q \bullet X + q^T x$$
$$\text{s.t.} \quad Y(x, X) \in \text{QPB}_n,$$

where $Q \bullet X$ denotes the matrix inner product equal to the trace of QX. Since the extreme points of QPB_n correspond to rank-one solutions with $X = xx^T$, and the objective is linear, there will always be an optimal solution of the latter problem for which $Q \bullet X + q^T x = x^T Q x + q^T x$, the original objective. Rewritten in this second form, the problem of solving BoxQP becomes the problem of obtaining a tractable characterization, or approximation, of QPB_n.

In the sequel we will sometimes write $(x, X) \in \text{QPB}_n$ to mean $Y(x, X) \in \text{QPB}_n$ in order to reduce notation. There are a variety of valid constraints on $Y(x, X)$ that are known for $(x, X) \in \text{QPB}_n$. Two examples are the PSD condition $Y(x, X) \succeq 0$, and the constraints obtained by applying the reformulation-linearization technique (RLT) [14], also commonly referred to as the McCormick inequalities,

$$X_{ij} \leq x_i, \quad X_{ij} \leq x_j, \quad X_{ij} \geq 0, \quad X_{ij} \geq x_i + x_j - 1, \quad 1 \leq i \leq j \leq n. \tag{1}$$

It is obvious that the PSD condition $Y(x, X) \succeq 0$ implies the diagonal constraint $X_{ii} \geq 0$, and it is easy to show that the PSD condition also implies $X_{ii} \geq 2x_i - 1$. In the sequel we will be assuming the PSD constraint $Y \succeq 0$, so we will use DIAG to refer to the diagonal constraints $X_{ii} \leq x_i,\ i = 1,\ldots,n$, and RLT to refer to the constraints in (1) for $j > i$ with the addition of the DIAG constraints.

It was shown in [2] that QPB_2 is exactly represented by the combination of the PSD and RLT constraints, which we will denote by PSD+RLT in the sequel, and that for larger n the combination of these constraints usually gives a close approximation of the optimal value, if not the exact optimal value, for test instances of BoxQP problems. It was also shown in [2] that the PSD+RLT constraints are not sufficient to exactly characterize QPB_3, but that an exact disjunctive representation for QPB_3 can be obtained by utilizing a triangulation of Box_3. Subsequently [5], extending results of [17], showed that any constraint that is valid for the Boolean quadric polytope is also valid for $(x, X) \in \text{QPB}_n$. In our setting we consider the Boolean quadric polytope to be the set $\text{BQP}_n = \text{Co}\{(1, x^T)^T(1, x^T) : x_i \in \{0, 1\}, i = 1,\ldots,n\}$. It is then clear that $\text{BQP}_n \subset \text{QPB}_n$. Note that if $(x, X) \in \text{BQP}_n$ then $X_{ii} = x_i,\ i = 1,\ldots,n$, and X is certainly a symmetric matrix. In the literature for

polyhedral methods, for example [11], the variables for BQP_n are typically taken to be x and $\{X_{ij},\ 1 \le i < j \le n\}$.

There are many known constraints that are valid for BQP_n, including the RLT constraints and the triangle inequalities (TRI)

$$
\begin{array}{rcl}
X_{ij} + X_{ik} & \le & x_i + X_{jk}, \\
X_{ij} + X_{jk} & \le & x_j + X_{ik}, \\
X_{ik} + X_{jk} & \le & x_k + X_{ij}, \\
x_i + x_j + x_k & \le & X_{ij} + X_{ik} + X_{jk} + 1
\end{array}
\tag{2}
$$

$1 \le i < j < k \le n$. It is also known [11] that BQP_3 is fully characterized by the RLT and TRI constraints. Adding the TRI constraints to PSD+RLT strengthens the approximation of QPB_3, but it is shown in [5] that the combination of these constraints, denoted PSD+RLT+TRI in the sequel, is not sufficient to fully characterize QPB_3.

The goal of this paper is to strengthen the approximation of QPB_3 that is given by the PSD+RLT+TRI relaxation. Our methodology is based on extracting information from the disjunctive representation of QPB_3 from [2] to derive additional valid constraints. This process is described in Section 2 and results in a total of 24 new valid inequalities on $(x, X) \in \text{QPB}_3$. We refer to these as ETRI1 constraints, where "ETRI" stands for "extended triangle inequality." In Section 3 we consider a strengthening of the process used in Section 2 that results in an additional 24 ETRI2 inequalities and 48 ETRI3 inequalities. In Section 4 we derive conic strengthenings of the ETRI1/2/3 inequalities that utilize second-order cone (SOC) constraints and one additional variable. In Section 5 we give computational results applying the ETRI constraints and their conic strengthenings to a variety of BoxQP instances. For $n = 3$ we show that the conic strengthening of the ETRI1 constraints obtains the exact solution value for the counterexample from [5] used to demonstrate that the PSD+RLT+TRI relaxation does not fully characterize QPB_3. We also show, based on extensive computations, that the conic strengthening of the ETRI constraints reduces the worst-case gap for a normalized objective by better than a factor of 2, compared to the PSD+RLT+TRI relaxation of QPB_3. For a set of BoxQP instances with $5 \le n \le 10$, where the PSD+RLT+TRI relaxation is not tight, we show that applying the ETRI constraints and their conic strengthenings reduces the gap and almost always obtains the true optimal solution value.

Notation: We use $\mathcal{S}_n$ to denote symmetric $n \times n$ matrices and $\mathcal{S}_n^+$ to denote symmetric positive semidefinite matrices. For A and B both in S_n, $A \succeq B$ denotes that $A - B \in \mathcal{S}_n^+$ and $A \bullet B$ denotes the trace inner product $A \bullet B = \text{tr}(AB)$. We use e to denote a vector of arbitrary dimension with each component equal to one and e_i to denote a vector with a 1 in the ith coordinate and all other entries equal to zero.

2 Extended triangle inequalities

In this section we derive new valid inequalities for QPB_3. The construction of these inequalities is based on a disjunctive representation for QPB_3 given in [2]. To describe this representation, let $\mathcal{T}_{ijk} \subset \text{Box}_3$ be the simplex $\{0 \le x_i \le x_j \le x_k \le 1\}$. There are 6 such simpleces corresponding to different ordering of the variables (x_1, x_2, x_3), and these 6 simpleces triangulate Box_3. For convenience we can put these orderings in lexicographic order

as $(123, 132, 213, 231, 312, 321)$, so the first ordering is 123, the fifth is 312, etc. For the pth ordering, corresponding to $x_i \leq x_j \leq x_k$, let A_p be a 3×4 matrix whose columns are the extreme points of $\mathcal{T}_{ijk}$, where the order of the columns in A_p is arbitrary. For example, a matrix A_1 corresponding to the ordering $0 \leq x_1 \leq x_2 \leq x_3 \leq 1$ is

$$A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

For each such A_p let $\bar{A}_p$ be the matrix

$$\bar{A}_p = \begin{pmatrix} e^T \\ A_p \end{pmatrix}.$$

It is then proved in [2] that

$$\mathrm{QPB}_3 = \left\{ \sum_{p=1}^{6} \bar{A}_p X_p \bar{A}_p^T : X_p \in \mathrm{DNN}_4, e^T X_p e = \lambda_p, e^T \lambda = 1 \right\}, \tag{3}$$

where DNN_4 are 4×4 matrices that are doubly nonnegative; that is, componentwise nonnegative and PSD.

The representation (3) is computable, but cannot be reduced to a system of constraints in the original variables (x, X) due to the constraints $X_p \succeq 0$, $p = 1, \ldots, 6$. However, by dropping these constraints we obtain a polyhedral set

$$\mathcal{P}_0 = \left\{ \sum_{p=1}^{6} \bar{A}_p X_p \bar{A}_p^T : X_p \geq 0, e^T X_p e = \lambda_p, e^T \lambda = 1 \right\}, \tag{4}$$

and it is certainly then the case that $\mathrm{QPB}_3 \subset \mathcal{P}_0 \cap \mathcal{S}_4^+$. Note that the set $\mathcal{P}_0$ is the convex hull of the union of 6 polyhedral sets of the form

$$\left\{ \bar{A}_p X_p \bar{A}_p^T : X_p \geq 0, e^T X_p e = 1 \right\},$$

each corresponding to an ordering of the variables $\{x_1, x_2, x_3\}$. For any one such ordering, the extreme point matrices of this set are

$$\left\{ \bar{A}_p (E_{ij} + E_{ji}) \bar{A}_p^T / 2 : 1 \leq i \leq j \leq 4 \right\}, \tag{5}$$

where E_{ij} is a 4×4 matrix with a one in the (i, j) position and zeros elsewhere. There are 10 such extreme points, 4 coming from the diagonal components $i = j$ and 6 from the off-diagonal components $i < j$. There are 9 variables associated with the matrices $Y(x, X) \in \mathrm{BQP}_3$, corresponding to (x_1, x_2, x_3), (X_{11}, X_{22}, X_{33}) and (X_{12}, X_{13}, X_{23}), so these 10 extreme points represent a simplex in $\mathbb{R}^9$. It is also possible to give the hyperplane description of this simplex. To do this, for a given matrix $\bar{A}_p$, let $M_p = \bar{A}_p^{-1}$. Then for

$$Y = \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} = \bar{A}_p X_p \bar{A}_p^T,$$

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$X_p \geq 0 \iff M_p Y M_p \geq 0$, so a hyperplane description of the simplex is given by

$$M_p Y M_p^T \geq 0, \tag{6}$$

For example, for the matrix $\bar{A}_1$ corresponding to the ordering $0 \leq x_1 \leq x_2 \leq x_3 \leq 1$,

$$M_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & -1 \end{pmatrix}.$$

The diagonal constraints from (6) are then

$$X_{11} \geq 0, \ X_{11} + X_{22} - 2X_{12} \geq 0, \ X_{22} + X_{33} - 2X_{23} \geq 0, \ 1 + X_{33} - 2x_3 \geq 0,$$

and these constraints are all implied by the condition $Y \succeq 0$. The off-diagonal constraints from (6) are

$$
\begin{aligned}
X_{12} - X_{11} &\geq 0, \ X_{13} - X_{12} \geq 0, \ x_1 - X_{13} \geq 0, \\
X_{12} + X_{23} - X_{13} - X_{22} &\geq 0, \\
x_2 - x_1 + X_{13} - X_{23} &\geq 0, \\
x_3 - x_2 + X_{23} - X_{33} &\geq 0.
\end{aligned}
$$

and by direct computation these hyperplanes are exactly the RLT constraints that can be formed from the ordering constraints $0 \leq x_1 \leq x_2 \leq x_3 \leq 1$.

We next set out to obtain a hyperplane description of the set $\mathcal{P}_0$. To do this, we took the union of the extreme points from each of the 6 sets as in (5) and then used Polymake to obtain a hyperplane description of the convex hull of this set. This resulted in a total of 72 facet-defining constraints which included all permutation equivalences, to be expected given the form of the disjunction used to construct $\mathcal{P}_0$. The 72 constraints included:

- All of the diagonal and off-diagonal RLT constraints,

- The first three of the four triangle inequalities (2),

- Nine constraints that were clearly implied by the PSD condition $Y \succeq 0$.

We next checked computationally which constraints were *not* dominated by the PSD, RLT and TRI constraints, and found that there were 24 such constraints, three of which are:

$$
\begin{aligned}
2x_1 + X_{11} - 2X_{12} - 2X_{13} + X_{23} &\geq 0, \\
2x_2 - 2X_{12} + X_{13} + X_{22} - 2X_{23} &\geq 0, \\
2x_3 + X_{12} - 2X_{13} - 2X_{23} + X_{33} &\geq 0.
\end{aligned} \tag{7}
$$

Before proceeding, we note that any linear constraint that is valid for $(x, X) \in \text{QPB}_3$ implies other valid constraints that can be constructed by combining two operations; permuting the indices of variables and switching (or complementing) variables, where switching a variable x_i refers to replacing x_i with $1 - x_i$. Switching x_i results in X_{ij} being replaced by $x_j - X_{ij}$ and similarly switching x_j results in X_{ij} being replaced by $x_i - X_{ij}$. Switching

both x_i and x_j results in X_{ij} being replaced by $X_{ij} + 1 - x_i - x_j$. The constraints in (7) are clearly equivalent under permutation of indices. Since $3 \times 8 = 24$, one might expect that the remaining 21 constraints corresponded to switching variables in these constraints, but that was not the case. However we determined that the remaining 21 constraints were all dominated by the PSD, RLT and TRI constraints combined with the constraints in (7) and their switchings, a total of 24 additional constraints. We refer to these constraints as ETRI1 constraints, for "extended triangle inequalities, type 1." For completeness we give the coefficients for all 24 of these ETRI1 constraints in the Appendix.

We next describe a simple derivation for the constraints in (7) that is independent of how we actually found them. For example, to derive the first constraint in (7), consider the valid constraint $x_2 x_3 \geq x_2 + x_3 - 1$. Multiplying both sides by x_1 results in the constraint $x_1(x_2 + x_3 - 1) \leq x_1 x_2 x_3 \leq x_2 x_3$, which implies the ordinary triangle inequality $X_{12} + X_{13} \leq x_1 + X_{23}$. However it is also true that $2x_1 x_2 x_3 \leq x_1^2 + (x_2 x_3)^2$, so

$$2x_1(x_2 + x_3 - 1) \leq 2x_1 x_2 x_3 \leq x_1^2 + (x_2 x_3)^2 \leq x_1^2 + x_2 x_3,$$

which implies the ETRI1 constraint $2x_1 + X_{11} - 2X_{12} - 2X_{13} + X_{23} \geq 0$.

Considering $\{(x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23}) : (x, X) \in \mathrm{QPB}_3\}$ to be a subset of $\mathbb{R}^9$, it is known [5] that this set is full-dimensional, and that faces corresponding to the RLT and TRI constraints being satisfied with equality correspond to facets of dimension 8. In the next lemma we prove that the ETRI1 constraints are tight on faces of dimension 5.

Lemma 1. *The set of* $\{x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23}\} \subset \mathbb{R}^9$ *with* $(x, X) \in \mathrm{QPB}_3$ *that also satisfy* $2x_1 + X_{11} - 2X_{12} - 2X_{13} + X_{23} = 0$ *has dimension 5.*

Proof. To characterize the dimension of the face it suffices to consider points where $X_{ij} = x_i x_j$ for all (i, j). We first consider the points used in [5] to prove that the set of feasible points is full dimensional. Of these, six satisfy the additional constraint with equality:

- The point with all variables equal to 0;

- The point having $x_2 = X_{22} = 1$ (respectively $x_3 = X_{33} = 1$) and all other variables equal to 0;

- The point having $x_2 = \frac{1}{2}$, $X_{22} = \frac{1}{4}$ (respectively $x_3 = \frac{1}{2}$, $X_{33} = \frac{1}{4}$) and all other variables equal to 0;

- The point having all variables equal to 1.

Since these 6 points are affinely independent, the face on which the constraint is tight has dimension at least 5. To show that the dimension is no higher, consider the equation $2x_1 + x_1^2 - 2x_1 x_2 - 2x_1 x_3 + x_2 x_3 = 0$ as a quadratic equation in x_1,

$$x_1^2 - 2x_1(x_2 + x_3 - 1) + x_2 x_3 = 0. \tag{8}$$

This equation has a solution if and only if $(x_2 + x_3 - 1)^2 \geq x_2 x_3$, in which case there are two possible values for x_1,

$$\begin{aligned} x_1^+ &= x_2 + x_3 - 1 + \sqrt{(x_2 + x_3 - 1)^2 - x_2 x_3}, \\ x_1^- &= x_2 + x_3 - 1 - \sqrt{(x_2 + x_3 - 1)^2 - x_2 x_3}. \end{aligned} \tag{9}$$

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Table 1: Maximum constraint violations I

Enforced Constraints	Max violation			Max normalized		
	RLT	TRI	ETRI1	RLT	TRI	ETRI1
PSD+DIAG	0.1250	0.1250	0.1250	0.1250	0.0625	0.0377
PSD+RLT	0	0.1250	0.1111	0	0.0625	0.0335
PSD+RLT+TRI	0	0	0.0625	0	0	0.0188

Assume first that $x_2+x_3 \geq 1$. Since both variables are in $[0,1]$ we have $x_2 x_3 \geq x_2 + x_3 - 1 \geq 0$, so $(x_2 + x_3 - 1)^2 \leq (x_2 x_3)^2 \leq x_2 x_3$. We must then have $x_1^+ = x_1^-$, and either $x_2 x_3 = 0$ or $x_2 x_3 = 1$. In the first case we then have either $x_2 = 0, x_3 = 1$ or $x_2 = 1, x_3 = 0$ (implying $x_1 = 0$), or $x_2 = x_3 = 1$, implying $x_1 = 1$ as well. Assume alternatively that $x_2 + x_3 < 1$. Then $x_1^- < 0$, x_1^+ cannot be strictly positive, and to have $x_1^+ = 0$ requires $x_2 x_3 = 0$, implying either $x_2 = 0$ or $x_3 = 0$. Thus all points that satisfy the constraint with equality, other than the point with all variables equal to 1, are in the face with $x_1 = X_{11} = X_{12} = X_{13} = X_{23} = 0$, the last since either $x_2 = 0$ or $x_3 = 0$. This face has dimension at most 4, so adding the point with all variables equal to one, the set of points satisfying the constraint with equality can have dimension no greater than 5. □

Geometrically, the set of $(x_1, x_2, x_3) \in \text{Box}_3$ satisfying (8) corresponds to the vertex $(0,0,0)$, the two adjacent edges with $x_1 = x_2 = 0$ and $x_1 = x_3 = 0$, and the opposite vertex $(1,1,1)$. In Box_3 there are 24 possible choices for 2 adjacent edges, corresponding exactly to the 24 ETRI1 constraints obtained from (7) and their switchings.

In addition to the dimension of the face corresponding to a constraint being tight, it is interesting to consider the maximum violation of a constraint when it is not imposed. In Table 1 we consider several cases of increasingly tight constraints that contain QPB_3, and the maximum violations of other constraints on these sets. In the first case, the DIAG constraints are added to the PSD condition in order to bound the feasible region. In addition to the unscaled maximum violations, we also consider the maximum violations for constraints scaled so that the coefficient vector for the variables $(x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23})$ is equal to one. The maximum violations are invariant to switching, but the norm of the coefficient vector may vary. For example, switching the variable x_1 in the RLT constraint $X_{12} \geq 0$ results in the RLT constraint $x_1 - X_{12} \geq 0$. Similarly, switchings of the ETRI1 constraints (7) do not all result in coefficient vectors of the same norm, and the minimum norm is $\sqrt{11}$ rather than $\sqrt{14}$ for the constraints in (7); see Table 7 in the Appendix for details. The normalized violation has a simple geometric interpretation as the Euclidean distance that a constraint hyperplane which is tight on the relaxed constraint set must be shifted to be tight on QPB_3.

Finally, note that the derivation of the ETRI1 constraints above was based on a particular triangulation of Box_3; this triangulation is based on orderings of the variables and has 6 simpleces. It is known [8] that there are six equivalence classes for triangulations of Box_3, five of which have 6 simpleces and one with only 5 simpleces. To investigate a possible dependence on the triangulation used, we repeated the derivation of constraints described above using a triangulation from each of the other 5 equivalence classes. The different triangulations have different permutation and/or switching symmetries, and the exact constraints obtained

vary with the triangulation used. However we determined that in each case, all constraints obtained using a different triangulation are implied by the PSD,RLT,TRI and ETRI1 constraints as derived above, and moreover the PSD, RLT and TRI constraints together with the constraints derived from another triangulation, with permutations and switchings, imply the ETRI1 constraints derived above. We therefore conclude that the construction of the ETRI1 constraints is independent of the triangulation used.

3   More extended triangle inequalities

The derivation of the ETRI1 inequalities in the previous section was based on dropping the constraints that $X_p \succeq 0$ in the disjunctive representation (3), resulting in the set $\mathcal{P}_0$ (4). In this we consider a strengthening of this procedure based on adding constraints on the X_p matrices from (3). Clearly any constraint of the form $a^T X_p a \geq 0$ is valid, since we are relaxing the condition that $X_p \succeq 0$. Our choice of constraints to add is based on the form of the extreme point matrices in (5). As described below (5), 4 of these matrices correspond to diagonal components $i = j$, each resulting in a matrix of the form $\bar{A}_p E_{ii} \bar{A}_p^T$ which is PSD. The remaining 6 matrices, corresponding to $i < j$, result in matrices of the form $\bar{A}_p (E_{ij} + E_{ji}) \bar{A}_p^T / 2$, each of which has one positive and one negative eigenvalue, where the latter is due to an eigenvalue of -1, with an eigenvector of the form $e_i - e_j$, from the matrix $(E_{ij} + E_{ji})$. Our idea is to add constraints to X_p which cut off these extreme points by using the eigenvectors corresponding to negative eigenvalues. To this end, let

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

The rows of U can then be used to generate valid constraints that are violated by the 6 extreme points from (5) with $i < j$. For each $1 \leq p \leq 6$, the result is then a polyhedral set of the form

$$
\left\{ \bar{A}_p X_p \bar{A}_p^T : X_p \geq 0, e^T X_p e = 1, \ u_i^T X_p u_i \geq 0, i = 1, \ldots, 6 \right\}, \tag{10}
$$

where u_i^T denotes the ith row of U. Taking the convex combination of the resulting six sets results in a new polyhedral set $\mathcal{P}_1 \subset \mathcal{P}_0$,

$$
\mathcal{P}_1 = \left\{ \sum_{p=1}^{6} \bar{A}_p X_p \bar{A}_p^T : X_p \geq 0, e^T X_p e = \lambda_p, e^T \lambda = 1, u_i^T X_p u_i \geq 0, \ i = 1, \ldots, 6 \right\}. \tag{11}
$$

To obtain an explicit hyperplane description of $\mathcal{P}_1$ we used a procedure similar to what was done in the previous section for $\mathcal{P}_0$. To start, it is not difficult to show that for each p, the extreme point matrices from (10) are of the form $A_p X A_p$, where X is one of the following 4×4 matrices:

- $X = E_{ii}$, $1 \leq i \leq 4$,

- $X = E_{ii}/2 + (E_{ij} + E_{ji})/4$, $1 \leq i \neq j \leq 4$,

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- $X = E_{ii}/3 + (E_{ij} + E_{ji} + E_{ik} + E_{ki})/6$, $1 \leq i \neq j < k \neq i \leq 4$,

- $X = (e_i e^T + e e_i^T)/8$, $1 \leq i \leq 4$.

There are a total of 32 such extreme matrices for each p. We then used Polymake to obtain a hyperplane description of the convex hull of the union of these sets of extreme matrices. The result of the above procedure was a system of 3723 inequality constraints. We then checked numerically to see which of these constraints were dominated by the PSD, RLT, TRI and ETRI1 constraints together. The result was a set of 330 non-dominated constraints, including the following 9 constraints:

$$
\begin{aligned}
4x_1 + 4X_{11} - 4X_{12} - 4X_{13} + X_{23} &\geq 0 \\
4x_2 - 4X_{12} + X_{13} + 4X_{22} - 4X_{23} &\geq 0 \\
4x_3 + X_{12} - 4X_{13} - 4X_{23} + 4X_{33} &\geq 0
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
4x_1 + 4X_{11} - 8X_{12} - 4X_{13} + X_{22} + 3X_{23} &\geq 0 \\
4x_1 + 4X_{11} - 4X_{12} - 8X_{13} + 3X_{23} + X_{33} &\geq 0 \\
4x_2 + X_{11} - 8X_{12} + 3X_{13} + 4X_{22} - 4X_{23} &\geq 0 \\
4x_2 - 4X_{12} + 3X_{13} + 4X_{22} - 8X_{23} + X_{33} &\geq 0 \\
4x_3 + X_{11} + 3X_{12} - 8X_{13} - 4X_{23} + 4X_{33} &\geq 0 \\
4x_3 + 3X_{12} - 4X_{13} + X_{22} - 8X_{23} + 4X_{33} &\geq 0
\end{aligned}
\tag{13}
$$

We refer to the constraints in (12) and their switchings (a total of 24 constraints) as ETRI2 constraints, and the constraints in (13) and their switchings (a total of 48 constraints) as ETRI3 constraints. Finally, we determined that all of the remaining constraints were dominated by the PSD, RLT, TRI, ETRI1, ETRI2 and ETRI3 constraints together. For completeness we give the coefficients for all of the ETRI2 and ETRI3 constraints in the Appendix.

We next demonstrate the validity of the ETRI2 and ETRI3 constraints independently of how they were derived, as we did for the ETRI1 constraints in the previous section. Multiplying the constraint $x_2 x_3 \geq x_2 + x_3 - 1$ by $4x_1$, we obtain the valid constraint $4x_1 x_2 + 4x_1 x_3 - 4x_1 \leq 4x_1 x_2 x_3$. But $(2x_1 - x_2 x_3)^2 = 4x_1^2 - 4x_1 x_2 x_3 + (x_2 x_3)^2 \geq 0$, implying $4x_1 x_2 x_3 \leq 4x_1^2 + (x_2 x_3)^2 \leq 4x_1^2 + x_2 x_3$. Combining these facts we obtain $4X_{12} + 4X_{13} - 4x_1 \leq 4X_{11} + X_{23}$, which is the first constraint in (12). To derive the first constraint in (13), we add $4x_1 x_2$ to both sides of $4x_1 x_2 + 4x_1 x_3 - 4x_1 \leq 4x_1 x_2 x_3$, resulting in $8x_1 x_2 + 4x_1 x_3 - 4x_1 \leq 4x_1 x_2 x_3 + 4x_1 x_2$. Then $(2x_1 - x_2(1 + x_3))^2 = 4x_1^2 - 4x_1 x_2(1 + x_3) + x_2^2(1 + x_3)^2 \geq 0$ implies that $4x_1 x_2 x_3 + 4x_1 x_2 = 4x_1 x_2 (1 + x_3) \leq 4x_1^2 + x_2^2(1 + x_3)^2 = 4x_1^2 + x_2^2 + 2x_2^2 x_3 + x_2^2 x_3^2 \leq 4x_1^2 + x_2^2 + 3x_2 x_3$, and combining these facts we obtain the constraint $8X_{12} + 4X_{13} - 4x_1 \leq 4X_{11} + X_{22} + 3X_{23}$.

Next we consider the dimensions of the faces of QPB_3 corresponding to the ETRI2 or ETRI3 constraints being tight.

Lemma 2. *The set of $\{x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23}\} \subset \mathbb{R}^9$ with $(x, X) \in \text{QPB}_3$ that also satisfy $4x_1 + 4X_{11} - 4X_{12} - 4X_{13} + X_{23} = 0$ has dimension 5.*

Proof. The proof is very similar to the proof of Lemma 1. We first give 6 affinely independent points where $X_{ij} = x_i x_j$ for all (i, j) that satisfy the constraint with equality. These points are identical to the six points used in the proof of Lemma 1, except that the point with all variables equal to one is replaced by the point with $x_1 = X_{12} = X_{13} = \frac{1}{2}$, $X_{11} = \frac{1}{4}$, $x_2 = x_3 = X_{22} = X_{33} = 1$. Since these 6 points are affinely independent, the face on which the constraint is tight has dimension at least 5. To show that the dimension is no greater than 5, we consider $4x_1 + 4x_1^2 - 4x_1 x_2 - 4x_1 x_3 + x_2 x_3 = 0$ to be a quadratic equation in x_1. The solutions of this equation are then exactly the values of x_1^+ and x_1^- in (9) multiplied by one-half. The remainder of the proof is identical to that of Lemma 1, except that the solution with $x_2 = x_3 = 1$ has $x_1 = \frac{1}{2}$ rather than $x_1 = 1$. $\qquad\square$

Lemma 3. *The set of $\{x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23}\} \subset \mathbb{R}^9$ with $(x, X) \in \mathrm{QPB}_3$ that also satisfy $4x_1 + 4X_{11} - 8X_{12} - 4X_{13} + X_{22} + 3X_{23} = 0$ has dimension 4.*

Proof. The proof is similar to the proof of Lemma 1, but proving the upper bound for the dimension is more complex. To begin, we give 5 affinely independent points where $X_{ij} = x_i x_j$ for all (i, j) that satisfy the constraint with equality:

- the point with all variables equal to 0;

- the point having $x_3 = X_{33} = 1$ and all other variables equal to 0;

- the point having $x_3 = \frac{1}{2}$, $X_{33} = \frac{1}{4}$ and all other variables equal to 0;

- the point having $x_1 = \frac{1}{2}$, $X_{11} = \frac{1}{4}$, $x_2 = X_{22} = 1$, $X_{12} = \frac{1}{2}$ and all other variables equal to 0;

- the point with all variables equal to 1.

Since these 5 points are affinely independent, the face on which the constraint is tight has dimension at least 4. To show that the dimension is no greater than 4, we consider $4x_1 + 4x_1^2 - 8x_1 x_2 - 4x_1 x_3 + x_2^2 + 3x_2 x_3 = 0$ to be a quadratic equation in x_1. The possible roots of this quadratic are then

$$
\begin{aligned}
x_1^+ &= \frac{1}{2}\left((2x_2 + x_3 - 1) + \sqrt{(2x_2 + x_3 - 1)^2 - x_2(x_2 + 3x_3)}\right), \\
x_1^- &= \frac{1}{2}\left((2x_2 + x_3 - 1) - \sqrt{(2x_2 + x_3 - 1)^2 - x_2(x_2 + 3x_3)}\right).
\end{aligned}
$$

If $2x_2 + x_3 < 1$ then $x_1^- < 0$, and the only solutions with $x_1^+ \geq 0$ have $x_2 = 0$, $x_3 \in [0, 1]$ and $x_1^+ = 0$. Assume alternatively that $2x_2 + x_3 \geq 1$. The discriminant in the expressions for x_2^+ and x_2^- can be written as $3x_2^2 + x_2(x_3 - 4) + (1 - x_3)^2$, which we regard as a quadratic in x_2. This quadratic has roots

$$
\begin{aligned}
x_2^+ &= \frac{1}{6}\left((4 - x_3) + \sqrt{4 + 16x_3 - 11x_3^2}\right), \\
x_2^- &= \frac{1}{6}\left((4 - x_3) - \sqrt{4 + 16x_3 - 11x_3^2}\right),
\end{aligned}
$$

and it is easy to verify that $4 + 16x_3 - 11x_3^2 \geq 0$ and also that $x_2^- \geq 0$ for any $x_3 \in [0, 1]$. To have $x_2 \geq 0$ we then require either $0 \leq x_2 \leq x_2^-$ or $x_2^+ \leq x_2 \leq 1$.

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Table 2: Maximum constraint violations II

Enforced Constraints	Max violation		Max normalized	
	ETRI2	ETRI3	ETRI2	ETRI3
PSD+DIAG	0.3333	0.3333	0.0471	0.0311
PSD+RLT	0.1111	0.2038	0.0157	0.0190
PSD+RLT+TRI	0.1005	0.1005	0.0142	0.0094
PSD+RLT+TRI+ETRI1	0.0856	0.0856	0.0121	0.0080

Recall that we are assuming that $2x_2 + x_3 \geq 1$. Then $x_2 \leq x_2^-$ implies that $2x_2^- \geq 1 - x_3$, which is equivalent to $15x_3^2 - 12x_3 - 3 \geq 0$. For $x_3 \in [0, 1]$ this condition is satisfied only for $x_3 = 1$, resulting in $x_2 = x_2^- = 0$ and $x_1 = 0$. Other than this solution, we can then assume that $x_2^+ \leq x_2 \leq 1$. However it is straightforward to show that $x_2^+ \leq 1$ is equivalent to $x_3 - x_3^2 \leq 0$, which holds for only $x_3 = 0$ or $x_3 = 1$. For $x_3 = 0$, $x_2 = 1$ we have $x_1^+ = x_1^- = \frac{1}{2}$, and for $x_3 = 1$, $x_2 = 1$ we have $x_1^+ = 1$, $x_1^- = -1$. We have thus shown that the only solutions of $4x_1 + 4X_{11} - 8X_{12} - 4X_{13} + X_{22} + 3X_{23} = 0$ with all variables in $[0, 1]$ and $X_{ij} = x_i x_j$ for all (i, j) are the following:

- points of the form $\{x_1 = x_2 = X_{11} = X_{22} = X_{12} = X_{13} = X_{23} = 0, x_3 \in [0, 1], X_{33} = x_3^2\}$, a set of dimension 2 including the origin;

- the point having $x_1 = \frac{1}{2}$, $X_{11} = \frac{1}{4}$, $x_2 = X_{22} = 1$, $X_{12} = \frac{1}{2}$ and all other variables equal to 0;

- the point with all variables equal to 1.

$\square$

In Table 2 we consider the maximum possible violations of the ETRI2 and ETRI3 constraints when different sets of constraints are imposed. Similar to the presentation in Table 1, we give both the maximum violations for the constraints as given in (12) and (13), and the maximum violations when considering these constraints and their switchings normalized to have coefficient vectors of norm one. The minimum norm for the vector of coefficients in a switching of the ETRI2 constraints is $\sqrt{50}$, as opposed to $\sqrt{65}$ for the constraints in (12) while the minimum norm for the vector of coefficients in a switching of the ETRI3 constraints is $\sqrt{115}$, as opposed to $\sqrt{122}$ for the constraints in (13); see Tables 8 and 9 in the Appendix for details.

4 Conic strengthening

In this section we describe a conic strengthening of the ETRI constraints derived in the previous two sections. The conic strengthening is motivated by the argument used to demonstrate validity of the ETRI1 constraints in section 2, which is based on the valid constraint $x_1 x_2 + x_3 - 1 \leq x_1 x_2 x_3$ combined with the fact that $2x_1 x_2 x_3 \leq x_1^2 + (x_2 x_3)^2$. To strengthen the resulting constraint we introduce one additional variable z, which will take the place of

the trilinear term $x_1x_2x_3$. In the global optimization literature, valid constraints on the variable z are usually projected down to the set of variables (x_1, x_2, x_3, z). Retaining the variables X_{12}, X_{13}, X_{23}, it can be shown [15] that the convex hull of $\{(x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3) : x \in \text{Box}_3\}$ is given by $(x_1, x_2, x_3, X_{12}, X_{13}, X_{23}, z)$ that satisfy the following system of linear constraints:

$$
\begin{aligned}
z \;\geq\; 0, \; z \;&\leq\; X_{12}, \; z \;\leq\; X_{13}, \; z \;\leq\; X_{23} \\
X_{12} + X_{13} \;&\leq\; x_1 + z, \; X_{12} + X_{23} \;\leq\; x_2 + z, \; X_{13} + X_{23} \;\leq\; x_3 + z, \qquad (14) \\
x_1 + x_2 + x_3 + z \;&\leq\; X_{12} + X_{13} + X_{23} + 1
\end{aligned}
$$

The constraints in (14) can be viewed as extensions of the ordinary RLT and TRI constraints on $(x_1, x_2, x_3, X_{12}, X_{13}, X_{23})$. Note that the constraints in (14) do not involve the diagonal variables X_{11}, X_{22}, X_{33}. However, since z is a proxy for $x_1x_2x_3$, where $x \in \text{Box}_3$, and $(x_2x_3)^2 \leq x_2x_3$, the following constraints are also valid:

$$
z^2 \leq X_{11}X_{23}, \quad z^2 \leq X_{22}X_{13}, \quad z^2 \leq X_{33}X_{12}. \qquad (15)
$$

The constraints in (15) are rotated second-order-cone (SOC) constraints that can be imposed in addition to the constraints from (14). These SOC constraints can also be imposed on switchings of variables, where switchings of variables are applied to z in the obvious way; for example, switching x_1 results in a switched value for z of $(1 - x_1)x_2x_3 = x_2x_3 - x_1x_2x_3 = X_{23} - z$.

Lemma 4. *The constraints* (14) *together with the constraints* (15) *and their switchings imply all of the ETRI1 and ETRI2 constraints.*

Proof. It suffices to show that the SOC constraint $z^2 \leq X_{11}X_{23}$ together with the constraints in (14) imply the ETRI1 constraint $2x_1 + X_{11} - 2X_{12} - 2X_{13} + X_{23} \geq 0$ and the ETRI2 constraint $4x_1 + 4X_{11} - 4X_{12} - 4X_{13} + X_{23} \geq 0$. From (14) we have $X_{12} + X_{13} - x_1 \leq z$, and $z^2 \leq X_{11}X_{23}$ implies that $z \leq (X_{11} + X_{23})/2$ from the arithmetic-geometric mean inequality. Combining these two facts we obtain $2X_{12} + 2X_{13} - 2x_1 \leq X_{11} + X_{23}$, which is exactly the required ETRI1 constraint. The same SOC constraint, written as $4z^2 \leq 4X_{11}X_{23}$, also implies that $2z \leq (4X_{11} + X_{23})/2$, or $4z \leq 4X_{11} + X_{23}$. Combining that inequality with $X_{12} + X_{13} - x_1 \leq z$ results in $4X_{12} + 4X_{13} - 4x_1 \leq 4X_{11} + X_{23}$, which is exactly the required ETRI2 constraint. $\qquad \square$

Although the constraints from (14) and (15) with their switchings imply the ETR1 and ETRI2 constraints, it turns out that these strengthened constraints have no effect on the maximum violation for the ETRI3 constraints, which remains 0.0856 as reported in Table 2. We next show that it is also possible to give a conic strengthening of the ETRI3 constraints. This strengthening is based on the fact that the rank-one matrix

$$
\begin{pmatrix}
1 & x_1 & x_2 + x_2x_3 \\
x_1 & x_1^2 & x_1x_2 + x_1x_2x_3 \\
x_2 + x_2x_3 & x_1x_2 + x_1x_2x_3 & x_2^2 + 2x_2^2x_3 + x_2^2x_3^2
\end{pmatrix}
$$

is PSD, which together with $x_2^2x_3^2 \leq x_2^2x_3 \leq x_2x_3$ implies the valid rotated SOC constraint

$$
(X_{12} + z)^2 \leq X_{11}(X_{22} + 3X_{23}). \qquad (16)
$$

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Lemma 5. *The constraints* (14) *together with the SOC constraints obtained from* (16) *by permuting indices and switching variables imply all of the ETRI3 constraints.*

Proof. It suffices to show that the constraints (14) together with (16) imply the ETRI3 constraint $4x_1 + 4X_{11} - 8X_{12} - 4X_{13} + X_{22} + 3X_{23} \geq 0$. From (14) we have $4X_{12} + 4X_{13} - 4x_1 \leq 4z$, and adding $4X_{12}$ to both sides obtains the inequality $8X_{12} + 4X_{13} - 4x_1 \leq 4X_{12} + 4z$. From (16) we have $4(X_{12} + z)^2 \leq 4X_{11}(X_{22} + 3X_{23})$, which implies that $2(X_{12} + z) \leq (4X_{11} + X_{22} + 3X_{23})/2$ from the arithmetic-geometric mean inequality. Combining these facts, we obtain $8X_{12} + 4X_{13} - 4x_1 \leq 4X_{11} + X_{22} + 3X_{23}$, which is exactly the required ETRI3 inequality. $\qquad\square$

5 Computational results

In this section we report a variety of different computational results obtained when implementing the constraints described in Sections 2, 3 and 4. We will begin with results for problems over QPB_3, and then consider instances over QPB_n for $n > 3$. All problems in this section were solved using the Mosek or SeDuMi interior-point solvers running under Matlab or Julia.

The following example from Burer and Letchford [5] shows that the PSD, RLT and TRI conditions together are not sufficient to characterize QPB_3.

$$\text{BL} : \max \left\{ x^T Q x + q^T x : x \in \text{Box}_3 \right\},$$

where

$$Q = \begin{pmatrix} -2.25 & -3 & -3 \\ -3 & 0 & -0.5 \\ -3 & -0.5 & 1 \end{pmatrix}, \quad q = \begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix}.$$

In particular, the exact solution value for the BL problem is 1.0, but the value using the relaxation of QPB_3 that imposes the PSD, RLT and TRI constraints is approximately 1.09291.

In Table 3 we give the values obtained by solving the BL problem over increasingly tight relaxations of QPB_3. The first row in the table corresponds to the PSD+RLT+TRI relaxation, and subsequent rows are labeled by the constraints in addition to PSD+RLT+TRI. For example, adding the ETRI1/2/3 constraints to the PSD+RLT+TRI relaxation reduces the gap to the true solution value from 0.09291 to 0.05882. In the last case, "SOC" refers to the constraints obtained from (15) by switching variables as well as from (16) by permuting indices and switching variable, and in this case the original RLT and TRI constraints are replaced by the extended system (14). The resulting SOC strengthening of the ETRI constraints obtains the exact solution value 1.0, and in fact this value is attained by adding only one constraint which is a switching of one of the constraints (15). To our knowledge, this is the first time that the BL problem has been solved exactly without the use of spatial branching, dynamically generated cutting planes [10], or an extended-variable formulation such as the exact disjunctive formulation or the formulation from a hierarchy of cones $\mathcal{K}_n^r$ that better approximate the copositive or completely positive cone for $r > 0$ [12, 9].

Although adding the SOC constraints to the PSD+RLT+TRI relaxation obtains the true optimal value for the BL problem, the solution does not immediately provide a feasible x with $x^T Q x + q^T x = 1$. The reason for this is that the BL problem has multiple optimal

Table 3: Objective values for Burer-Letchford problem

Enforced Constraints	Objective value
PSD+RLT+TRI	1.09291
+ETRI1	1.06613
+ETRI1/2/3	1.05882
+SOC	1.00000

solutions, and in this case an interior-point solver such as Mosek or SeDuMi will not converge to a rank-one solution. This deficiency can be overcome by an additional step that imposes a constraint $Q \bullet X + q^T x = 1$ and re-solves the problem with a random objective, which then generates a rank-one solution having $x^T Q x + q^T x = 1$.

For the BL example, the vector of objective coefficients for the variables $(x_1, x_2, x_3, X_{11}, X_{22}, X_{33}, X_{12}, X_{13}, X_{23})$ is $(3, 1, 0, -2.25, 0, 1, -6, -6, -1)$, and the norm of this coefficient vector is approximately 9.4373. If the coefficient vector is normalized to have norm 1, then the gap of 0.09291 for the original problem corresponds to a gap of 0.009845 for the normalized objective. We next consider the largest possible gap for a normalized objective when minimized over a system of constraints compared to the exact minimum over QPB_3, where the latter can be computed using the disjunctive representation. Maximizing this difference is a non-convex problem, but it can be approximated by repeatedly generating random coefficients. A coefficient vector that tentatively maximizes the difference can also be potentially improved by making smaller perturbations to it. We performed extensive computations in an effort to find normalized coefficients that approximately maximize the gap for different relaxations of QPB_3. The results of these computations are reported in Table 4. For the PSD+DIAG constraint set the maximum gap appears to be achieved for an objective corresponding to the normalized sum of 2 RLT constraints, for example $X_{12} + X_{13}$, and for the PSD+RLT constraint set the maximum appears to be achieved for objective coefficients corresponding to a normalized triangle inequality TRI. For the PSD+RLT+TRI relaxation, the maximum gap appears to be achieved by normalizing an ETRI1 inequality with coefficient vector of norm $\sqrt{11}$, as in Table 1. However, when the ETRI1 constraints are added to the PSD+RLT+TRI relaxation the maximum normalized gap does not correspond to an ETRI2 or ETRI3 constraint, as can be seen by comparing the maximum value of 0.0135 in Table 4 to the max normalized values in the last row of Table 2. As in Table 3, the rows below PSD+RLT+TRI are labeled using the constraints that are added to the PSD+RLT+TRI relaxation. As reported in the table, these computations indicate that the use of the SOC tightenings of the ETRI constraints reduce the maximum gap for a normalized objective by better than a factor of 2 compared to the PSD+RLT+TRI relaxation.

We next consider results on problems with $n > 3$. Like the original TRI constraints, for $n > 3$ the ETRI constraints immediately extend to any triple of indices $1 \leq i < j < k \leq n$. The same is true for the SOC tightenings described in Section 4, with the added consideration that any such triple requires an additional variable z_{ijk} in place of the variable z used in Section 4. When solving a problem with $n > 3$, we add RLT, TRI and ETRI constraints in several "rounds," limiting the number of violated constraints on each round before re-solving the problem. This strategy prevents the addition of an excessive and ultimately unnecessary

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Table 4: Maximum gaps over relaxations

Enforced Constraints	Max gap (normalized)	Remark
PSD+DIAG	0.1768	Sum of 2 RLT
PSD+RLT	0.0625	TRI
PSD+RLT+TRI	0.0188	ETRI1
+ETRI1	0.0135	
+ETRI1/2/3	0.0111	
+SOC	0.0086	

number of constraints. We use a similar strategy when incorporating SOC constraints, and in that case add additional variables z_{ijk} and the corresponding linear constraints (14) only as needed to enforce violated SOC conditions.

A test set of 54 BoxQP instances first used in [16] has been used in several subsequent papers [1, 3, 7] to compare the performance of different methods. These problems have dimensions from 20 to 60 and were generated with varying degrees of sparsity for Q and q. It was shown in [1] that the PSD+RLT+TRI relaxation is tight for all but one of these 54 problems. We first considered adding the ETRI and SOC constraints on that one problem (instance 50-050-1), but obtained no improvement in the bound. We next generated additional instances with similar dimensions using the same methodology employed in [16]. As expected, the PSD+RLT+TRI relaxation was tight on a high proportion of these problems and obtained a rank-one solution with objective value equal to the relaxation bound. For the occasional instance where this did not occur, we obtained no improvements using the ETRI constraints or their SOC tightenings. This was disappointing but not completely unexpected given the rarity of instances with any gap and the fact that these problems have a substantial space of off-diagonal variables. As shown in [5], any constraint that is valid for the Boolean Quadric Polytope (BQP) is also valid for the variables x and $\{X_{ij} : j > i\}$. Such valid constraints include the RLT and TRI constraints, but for $n > 3$ there are large families of additional valid constraints for the BQP [4, 11].

We next considered generating problems similar to those from [16], but with smaller n. For $5 \leq n \leq 10$, and problems of the form $\max\{x^T Q x + q^T x : x \in \text{Box}_n\}$, we generated Q and q as follows. For a given density parameter d between 0 and 100, each q_i and Q_{ij}, $i < j$ is an integer randomly distributed on [-50,50] with probability $d\%$ and is otherwise zero, and $Q_{ji} = Q_{ij}$. As was the case for larger problems, the PSD+RLT+TRI relaxation was tight for a high proportion of instances generated in this way. However, for instances where the PSD+RLT+TRI relaxation was not tight, the ETRI constraints and their SOC strengthenings almost always improved the bound. In Table 5 we give results for 12 such problem instances[1]. The instances are labeled using the same scheme (n-d-#) as in [16]. In the table, P+R+T corresponds to the PSD+RLT+TRI relaxation, and the other columns correspond to additional constraints. For each relaxation we give both the relaxation value, an upper bound on the optimal value, and the feasible objective value $x^T Q x + q^T x$ from the solution (x, X), a lower bound on the optimal value. In Table 6 we give the gaps between

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[1]Data for the problems in Table 5 is available from the authors.

Table 5: Objective values on problems with $n > 3$

Instance	OPT	Relaxation objective value				Feasible objective value			
		P+R+T	+ETRI1	+ETRI1/2/3	+SOC	P+R+T	+ETRI1	+ETRI1/2/3	+SOC
05-050-1	0.0061	0.2122	0.0090	0.0090	0.0090	-7.7721	-1.1640	-1.1353	-1.1598
06-070-1	1.0000	1.0607	1.0050	1.0050	1.0000	-6.3672	-5.7869	-5.7870	1.0000
06-080-1	0.0000	0.0356	0.0000			-3.2871	0.0000		
07-060-1	5.0000	5.1521	5.0784	5.0784	5.0000	-7.9104	-6.6276	-6.6276	5.0000
08-075-1	130.3906	130.6563	130.4851	130.4794	130.3906	94.2010	97.7381	96.9528	130.3906
08-075-2	49.0000	49.1094	49.0354	49.0000		32.9629	38.0247	49.0000	
08-080-1	39.7189	40.0934	39.7189			21.1042	39.7189		
08-085-1	80.0000	80.2355	80.0000			27.2094	80.0000		
09-070-1	8.0788	8.6110	8.3477	8.0788		-9.6524	-10.6659	8.0788	
09-080-1	163.0347	163.3233	163.2550	163.2550	163.0347	144.3430	145.0280	145.0280	163.0347
10-070-1	289.0000	289.3192	289.0000			247.8940	289.0000		
10-075-1	159.2132	160.0067	159.9102	159.8997	159.2132	118.2380	118.9980	119.8370	159.2132

the relaxation value and optimal value, and relaxation value and feasible value, for the same problems.

Table 6: Objective gaps on problems with $n > 3$

Instance	OPT	Relaxation value to optimal value				Relaxation value to feasible value			
		P+R+T	+ETRI1	+ETRI1/2/3	+SOC	P+R+T	+ETRI1	+ETRI1/2/3	+SOC
05-050-1	0.0061	0.2061	0.0029	0.0029	0.0029	7.9843	1.1730	1.1442	1.1688
06-070-1	1.0000	0.0607	0.0050	0.0050	0.0000	7.4278	6.7919	6.7920	0.0000
06-080-1	0.0000	0.0356	0.0000			3.3227	0.0000		
07-060-1	5.0000	0.1521	0.0784	0.0784	0.0000	13.0625	11.7060	11.7060	0.0000
08-075-1	130.3906	0.2656	0.0945	0.0887	0.0000	36.4553	32.7470	33.5266	0.0000
08-075-2	49.0000	0.1094	0.0354	0.0000		16.1465	11.0107	0.0000	
08-080-1	39.7189	0.3745	0.0000			18.9892	0.0000		
08-085-1	80.0000	0.2355	0.0000			53.0261	0.0000		
09-070-1	8.0788	0.5322	0.2689	0.0000		18.2633	19.0136	0.0000	
09-080-1	163.0347	0.2886	0.2202	0.2202	0.0000	18.9803	18.2270	18.2270	0.0000
10-070-1	289.0000	0.3192	0.0000			41.4252	0.0000		
10-075-1	159.2132	0.7935	0.6970	0.6865	0.0000	41.7687	40.9122	40.0627	0.0000

For these 12 problems, the ETRI1 constraints obtain the optimal value on 4 instances, the ETRI1/2/3 constraints obtain the optimal value on 2 instances, and the SOC strengthenings of the ETRI1/2/3 constraints obtain the optimal value on 5 instances. For the remaining instance (05-50-01), adding the ETRI1 constraints obtains a substantial reduction in the relaxation bound, but the ETRI2/3 constraints and SOC strengthenings give no further improvement. The true optimal value for this instance was computed using Gurobi. For the 11 problems where the gap was closed to zero, in 10 instances the relaxed problem had a rank-one solution that provided a feasible x with $x^T Q x + q^T x$ equal to the bound value. In the remaining case (07-060-1) the solution is not rank-one due to the presence of multiple optimal solutions, and an optimal x can be generated using the same technique described for the BL problem earlier in the section. It is worthwhile to note that although the gaps between the PSD+RLT+TRI relaxation value and the optimal value for the problems in Table 5 are already quite small, the gaps to the feasible solution from the PSD+RLT+TRI relaxation are much larger. In addition, the feasible values may worsen as the relaxation is tightened, as can be seen in several cases. Other methods such as local search could be used in an attempt to improve these feasible values, but we did not investigate this possibility. Finally, although the potential number of ETRI and SOC constraints is quite large ($11,520$

ETRI constraints for $n = 10$), the number of ETRI or SOC constraints used in the solutions of the problems in Table 5 was very small. For problems solved to optimality using ETRI constraints, the number or ETRI constraints used was never more than 15, and for problems solved to optimality using SOC constraints, the number of SOC constraints used was at most 6.

Acknowlegements

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Appendix

In the tables below we give coefficients for the ETRI1 constraints (7) and their switchings, the ETRI2 constraints (12) and their switchings and the ETRI3 constraints (13) and their switchings. In each row the coefficients $c = (c_1, c_2, c_3)$ and $C = (C_{11}, C_{22}, C_{33}, C_{12}, C_{13}, C_{23})$ and constant b correspond to a constraint given in the form

$$\sum_{i=1}^{3} c_i x_i + \sum_{i=1}^{3} \sum_{j \geq i} C_{ij} X_{ij} + b \geq 0.$$

Each group of 8 constraints corresponds to one of the constraints from (7), (12) or (13) followed by switchings of that constraint.

Table 7: Coefficients for ETRI1 constraints

x_1	x_2	x_3	X_{11}	X_{22}	X_{33}	X_{12}	X_{13}	X_{23}	b
2	0	0	1	0	0	-2	-2	1	0
0	1	0	1	0	0	-2	2	-1	0
0	0	1	1	0	0	2	-2	-1	0
-2	-1	-1	1	0	0	2	2	1	1
-4	-2	-2	1	0	0	2	2	1	3
-2	-1	2	1	0	0	2	-2	-1	1
-2	2	-1	1	0	0	-2	2	-1	1
0	1	1	1	0	0	-2	-2	1	0
0	2	0	0	1	0	-2	1	-2	0
1	0	0	0	1	0	-2	-1	2	0
-2	-4	-2	0	1	0	2	1	2	3
-1	-2	2	0	1	0	2	-1	-2	1
0	0	1	0	1	0	2	-1	-2	0
-1	-2	-1	0	1	0	2	1	2	1
2	-2	-1	0	1	0	-2	-1	2	1
1	0	1	0	1	0	-2	1	-2	0
0	0	2	0	0	1	1	-2	-2	0
-2	-2	-4	0	0	1	1	2	2	3
1	0	0	0	0	1	-1	-2	2	0
-1	2	-2	0	0	1	-1	2	-2	1
0	1	0	0	0	1	-1	2	-2	0
2	-1	-2	0	0	1	-1	-2	2	1
-1	-1	-2	0	0	1	1	2	2	1
1	1	0	0	0	1	1	-2	-2	0

Table 8: Coefficients for ETRI2 constraints

x_1	x_2	x_3	X_{11}	X_{22}	X_{33}	X_{12}	X_{13}	X_{23}	b
4	0	0	4	0	0	-4	-4	1	0
0	1	0	4	0	0	-4	4	-1	0
0	0	1	4	0	0	4	-4	-1	0
-4	-1	-1	4	0	0	4	4	1	1
-12	-4	-4	4	0	0	4	4	1	8
-8	-3	4	4	0	0	4	-4	-1	4
-8	4	-3	4	0	0	-4	4	-1	4
-4	3	3	4	0	0	-4	-4	1	1
0	4	0	0	4	0	-4	1	-4	0
1	0	0	0	4	0	-4	-1	4	0
-4	-12	-4	0	4	0	4	1	4	8
-3	-8	4	0	4	0	4	-1	-4	4
0	0	1	0	4	0	4	-1	-4	0
-1	-4	-1	0	4	0	4	1	4	1
4	-8	-3	0	4	0	-4	-1	4	4
3	-4	3	0	4	0	-4	1	-4	1
0	0	4	0	0	4	1	-4	-4	0
-4	-4	-12	0	0	4	1	4	4	8
1	0	0	0	0	4	-1	-4	4	0
-3	4	-8	0	0	4	-1	4	-4	4
0	1	0	0	0	4	-1	4	-4	0
4	-3	-8	0	0	4	-1	-4	4	4
-1	-1	-4	0	0	4	1	4	4	1
3	3	-4	0	0	4	1	-4	-4	1

Table 9: Coefficients for ETRI3 constraints

x_1	x_2	x_3	X_{11}	X_{22}	X_{33}	X_{12}	X_{13}	X_{23}	b
4	0	0	4	1	0	-8	-4	3	0
0	3	0	4	1	0	-8	4	-3	0
-4	-2	3	4	1	0	8	-4	-3	1
-8	-5	-3	4	1	0	8	4	3	4
-12	-8	-4	4	1	0	8	4	3	8
-8	-5	4	4	1	0	8	-4	-3	4
-4	6	-1	4	1	0	-8	4	-3	1
0	3	1	4	1	0	-8	-4	3	0
4	0	0	4	0	1	-4	-8	3	0
-4	3	-2	4	0	1	-4	8	-3	1
0	0	3	4	0	1	4	-8	-3	0
-8	-3	-5	4	0	1	4	8	3	4
-12	-4	-8	4	0	1	4	8	3	8
-4	-1	6	4	0	1	4	-8	-3	1
-8	4	-5	4	0	1	-4	8	-3	4
0	1	3	4	0	1	-4	-8	3	0
0	4	0	1	4	0	-8	3	-4	0
3	0	0	1	4	0	-8	-3	4	0
-8	-12	-4	1	4	0	8	3	4	8
-5	-8	4	1	4	0	8	-3	-4	4
-2	-4	3	1	4	0	8	-3	-4	1
-5	-8	-3	1	4	0	8	3	4	4
6	-4	-1	1	4	0	-8	-3	4	1
3	0	1	1	4	0	-8	3	-4	0
0	4	0	0	4	1	-4	3	-8	0
3	-4	-2	0	4	1	-4	-3	8	1
-4	-12	-8	0	4	1	4	3	8	8
-1	-4	6	0	4	1	4	-3	-8	1
0	0	3	0	4	1	4	-3	-8	0
-3	-8	-5	0	4	1	4	3	8	4
4	-8	-5	0	4	1	-4	-3	8	4
1	0	3	0	4	1	-4	3	-8	0
0	0	4	1	0	4	3	-8	-4	0
-8	-4	-12	1	0	4	3	8	4	8
3	0	0	1	0	4	-3	-8	4	0
-5	4	-8	1	0	4	-3	8	-4	4
-2	3	-4	1	0	4	-3	8	-4	1
6	-1	-4	1	0	4	-3	-8	4	1
-5	-3	-8	1	0	4	3	8	4	4
3	1	0	1	0	4	3	-8	-4	0
0	0	4	0	1	4	3	-4	-8	0
-4	-8	-12	0	1	4	3	4	8	8
3	-2	-4	0	1	4	-3	-4	8	1
-1	6	-4	0	1	4	-3	4	-8	1
0	3	0	0	1	4	-3	4	-8	0
4	-5	-8	0	1	4	-3	-4	8	4
-3	-5	-8	0	1	4	3	4	8	4
1	3	0	0	1	4	3	-4	-8	0