ON NONCONVEX QUADRATIC PROGRAMMING WITH BOX CONSTRAINTS\textsuperscript{*}

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Abstract. Nonconvex quadratic programming with box constraints is a fundamental NP-hard global optimization problem. Recently, some authors have studied a certain family of convex sets associated with this problem. We prove several fundamental results concerned with these convex sets: we determine their dimension, characterize their extreme points and vertices, show their invariance under certain affine transformations, and show that various linear inequalities induce facets. We also show that the sets are closely related to the Boolean quadric polytope, a fundamental polytope in the field of polyhedral combinatorics. Finally, we give a classification of valid inequalities and show that this yields a finite recursive procedure to check the validity of any proposed inequality.

Key words. nonconvex quadratic programming, global optimization, polyhedral combinatorics, convex analysis

AMS subject classifications. 90C20, 90C26, 90C09, 90C22, 90C25

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1. Introduction. Nonconvex quadratic programming with box constraints (QPB) is the problem of minimizing a nonconvex quadratic function of a set of variables subject to lower and upper bounds on the variables. A QPB instance with $n$ variables takes the following form:

$$\min \{ c^T x + x^T Q x : l \leq x \leq u, \ x \in \mathbb{R}^n \} ,$$

where $x$ is the vector of decision variables, $c \in \mathbb{R}^n$ is the vector of linear costs, $Q \in \mathbb{R}^{n \times n}$ is the matrix of quadratic costs, and $l \in \mathbb{R}^n$ and $u \in \mathbb{R}^n$ are the vectors of lower and upper bounds, respectively.

As usual in the literature, we assume throughout this paper that the box constraints take the simple form $x \in [0,1]^n$. Any instance not satisfying this property can be easily transformed into one that does.

QPB, which is NP-hard, is regarded as a fundamental problem in global optimization (see Horst, Pardalos, and Thoai [13]). A survey of research on QPB up to 1997 was given by De Angelis, Pardalos, and Toraldo [7]. More recent relevant papers include Yajima and Fujie [29], Vandenbussche and Nemhauser [27, 28], Burer and Vandenbussche [6], Anstreicher [1], and Anstreicher and Burer [3].

It is common practice to linearize the objective function by introducing, for $1 \leq i \leq j \leq n$, a new variable $y_{ij}$, representing the product $x_i x_j$. The nonconvex constraints $y_{ij} = x_i x_j$ can then be approximated by either linear constraints (as in [23, 27, 28, 29]) or conic constraints (as in [1, 3, 6]).

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In order to derive stronger relaxations in the \((x, y)\)-space, it is natural to study the convex hull of feasible solutions to the problem, i.e., the set
\[
QPB_n = \text{conv} \left\{ (x, y) \in [0, 1]^{n+1} : y_{ij} = x_i x_j \ (\forall 1 \leq i \leq j \leq n) \right\}.
\]
Note that \(QPB_n\), though convex, is not polyhedral even for \(n = 1\); see Figure 1. Although a few authors have studied \(QPB_n\) explicitly \([1, 3, 29]\), many fundamental questions about its structure remain unanswered. (For example, a complete linear description of \(QPB_3\) is not known \([3]\).) The goal of this paper is to understand \(QPB_n\) better.

The structure of the paper is as follows. In section 2, we review the relevant literature. In section 3, we explore some fundamental properties of \(QPB_n\): its dimension, extreme points, vertices, and affine symmetries. In section 4, we consider the so-called reformulation-linearization technique (RLT) and positive semidefinite (psd) inequalities and determine the dimension of the corresponding faces of \(QPB_n\). In section 5, we establish a connection between \(QPB_n\) and the so-called Boolean quadric polytope, a fundamental polytope in the field of polyhedral combinatorics. This yields a huge class of facet-inducing inequalities for \(QPB_n\). In section 6, we give a “classification” of valid inequalities and show that it yields a finite procedure to check the validity of any proposed inequality. We also use it to explore the structure of \(QPB_3\). Finally, concluding remarks are given in section 7.

We assume throughout that the reader is familiar with the basics of polyhedral theory (see Nemhauser and Wolsey \([17]\) or Schrijver \([22]\)) and convex analysis (see Hiriart-Urruty and Lemaréchal \([12]\)).

2. Key concepts from the literature. Some key concepts from the literature are now explained.

2.1. The RLT inequalities. It is well-known that the constraint \(y_{ij} = x_i x_j\), together with the bounds \(0 \leq x_i \leq 1\) and \(0 \leq x_j \leq 1\), imply the following four linear inequalities:
\[
y_{ij} \geq 0, \quad y_{ij} \leq x_i, \quad y_{ij} \leq x_j, \quad y_{ij} \geq x_i + x_j - 1.
\]
These inequalities remain valid when \(i = j\), in which case the second and third of them coincide. They have come to be known as RLT inequalities, because they can
be derived using the so-called reformulation-linearization technique of Sherali and Adams [23].

Replacing the constraints $y_{ij} = x_i x_j$ with the RLT inequalities, we obtain a linear programming relaxation of QPB. See Figure 2 for an illustration, again for the trivial case $n = 1$.

In Figure 3, we display the polytope defined by the RLT inequalities with $i \neq j$ for the case $n = 2$. Here, the variables $y_{11}$ and $y_{22}$ have been omitted. McCormick [16] pointed out that this polytope is equal to the following convex hull:

$$
\text{conv} \left\{ (x_1, x_2, y_{12}) \in [0, 1]^3 : y_{12} = x_1 x_2 \right\}.
$$

We will see in subsection 2.4 that this polytope is nothing but the Boolean quadric polytope for $n = 2$.

2.2. Using positive semidefiniteness. The idea of applying semidefinite programming to nonconvex quadratic programs is due to Shor [26] (see also Lovász and Schrijver [15]). The idea is as follows. We begin by defining the $n \times n$ symmetric matrix $Y = xx^T$. Note that, for any $1 \leq i \leq j \leq n$, $Y_{ij} = y_{ij}$. We also define the augmented matrix

$$
\hat{Y} := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x^T \end{pmatrix} = \begin{pmatrix} 1 & x^T \\ x & Y \end{pmatrix}.
$$
Since $\hat{Y}$ is defined as the product of a vector and its transpose, we should have $\hat{Y} \succeq 0$ in a feasible solution (i.e., $\hat{Y}$ should be positive semidefinite).

It is well-known that imposing $\hat{Y} \succeq 0$ is equivalent to imposing $Y - xx^T \succeq 0$, which in turn amounts to imposing the convex quadratic constraints $b^T Y b \geq (b^T x)^2$ for all $b \in \mathbb{R}^n$. Moreover, as first noted by Ramana [20], $\hat{Y} \succeq 0$ if and only if

$$v^T Y v + (2s)v^T x + s^2 \geq 0$$

for all vectors $v \in \mathbb{R}^n$ and scalars $s \in \mathbb{R}$. This is equivalent to imposing the following linear inequalities:

$$(1) \quad (2s)v^T x + \sum_{i=1}^{n} v_i^2 y_{ii} + 2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} + s^2 \geq 0 \quad (\forall v \in \mathbb{R}^n, s \in \mathbb{R}).$$

We will call the inequalities (1). Note that the RLT inequalities $y_{ii} \geq 0$ and $y_{ii} \geq 2x_i - 1$ are psd inequalities.

Imposing $\hat{Y} \succeq 0$ strengthens the RLT relaxation of QPB considerably [1, 6, 24, 29]. When $n = 1$, the relaxation is exact: Figure 1 shows that $QPB_1$ is completely described by the RLT inequality $y_{11} \leq x_1$ and the convex quadratic constraint $y_{11} \geq x_1^2$. Anstreicher and Burer [3] showed that the relaxation is exact if and only if $n \leq 2$. For $n = 3$, they found the following four inequalities, which are valid for $QPB_3$ but cut off points satisfying the RLT and psd constraints:

$$(2) \quad y_{11} + y_{22} + y_{33} \leq y_{12} + y_{13} + y_{23} + 1,$$

$$(3) \quad y_{11} + y_{22} + y_{33} + y_{12} + y_{13} \leq 2x_1 + x_2 + x_3 + y_{23},$$

$$(4) \quad y_{11} + y_{22} + y_{33} + y_{12} + y_{23} \leq x_1 + 2x_2 + x_3 + y_{13},$$

$$(5) \quad y_{11} + y_{22} + y_{33} + y_{13} + y_{23} \leq x_1 + x_2 + 2x_3 + y_{12}.$$
In addition to the RLT inequalities, Padberg defined various facet-inducing inequalities for $BQP_n$, called triangle, clique, cut, and generalized cut inequalities. The triangle inequalities consist of the following inequalities for all triples $(i, j, k)$:

\begin{align}
  x_i + x_j + x_k &\leq y_{ij} + y_{ik} + y_{jk} + 1, \\
y_{ij} + y_{ik} &\leq x_i + y_{jk}.
\end{align}

We remark that the inequalities (2)–(5) are dominated by triangle inequalities.

Further valid inequalities for $BQP_n$ have been introduced, for example, by Boros and Hammer [5] and Sherali, Lee, and Adams [25]. Still more inequalities can be derived from the fact that $BQP_n$ is an affine image of the well-known cut polytope (see De Simone [8] and Deza and Laurent [10]).

Yajima and Fujie [29] proved that all of the inequalities of Padberg, along with some more general inequalities called cut-type inequalities, are valid for $QPB_n$ as well as for $BQP_n$. We extend this result significantly in section 5.

### 3. Fundamental properties of $QPB_n$. In this section, we establish some fundamental properties of $QPB_n$. Throughout the section, we denote by $S$ the set of all feasible solutions to $QPB$ in the extended $(x, y)$-space. That is,

\[ S = \left\{ (x, y) \in [0, 1]^{n+\binom{n+1}{2}} : y_{ij} = x_i x_j \ (\forall 1 \leq i \leq j \leq n) \right\}. \]

Note that $S$ contains an uncountable number of members.

#### 3.1. Dimension. We begin by determining the dimension of $QPB_n$.

**Lemma 1.** $QPB_n$ is full-dimensional (i.e., of dimension $n + \binom{n+1}{2}$).

**Proof.** Consider the following members of the set $S$:

- the origin (i.e., all variables set to zero);
- for $i = 1, \ldots, n$, the point having $x_i = y_{ii} = 1$ and all other variables zero;
- for $i = 1, \ldots, n$, the point having $x_i = \frac{1}{2}$, $y_{ii} = \frac{1}{4}$, and all other variables zero;
- for $1 \leq i < j \leq n$, the point having $x_i = x_j = 1$, $y_{ii} = y_{jj} = y_{ij} = 1$, and all other variables zero.

These $n + \binom{n+1}{2} + 1$ points are easily shown to be affinely independent.\[ \square \]

Being full-dimensional is a desirable property to have, because it means that each face of maximal dimension is defined by a unique linear inequality (up to scaling by a constant).

#### 3.2. Extreme points and vertices. Next, we recall some other terms from convex analysis. Let $K \subseteq \mathbb{R}^d$ be a full-dimensional convex set. An extreme point of $K$ is a point in $K$ that cannot be expressed as a convex combination of other points in $K$. A vector $v \in \mathbb{R}^d$ is said to be normal at an extreme point $p$ if $v^T p' \leq v^T p$ for all $p' \in K$. If there exist $d$ linearly independent normal vectors at $p$, then $p$ is called a vertex of $K$.

Laurent and Poljak [14] characterized the extreme points and vertices of the set of correlation matrices. Here, we do the same for $QPB_n$.

**Lemma 2.** The extreme points of $QPB_n$ are the members of $S$.

**Proof.** By definition, every extreme point of $QPB_n$ is a member of $S$. We show that every member of $S$ is an extreme point. Let $(\bar{x}, \bar{y})$ be an arbitrary point in $S$. Consider the QP instance that arises when the objective function is equal to $\sum_{i=1}^n (x_i^2 - 2\bar{x}_i x_i)$. Minimizing this function is equivalent to minimizing $\sum_{i=1}^n (x_i - \bar{x}_i)^2$. Therefore, $\bar{x}$ is the unique optimal solution to the given instance. Equivalently, $(\bar{x}, \bar{y})$
is the unique point in $QPB_n$ that minimizes the linear function $\sum_{i=1}^n (y_{ii} - 2\bar{x}_i)x_i$. Thus, $(\bar{x}, \bar{y})$ is an extreme point of $QPB_n$. 

Figure 1 enables one to visualize this result for the case $n = 1$: the members of $S$ form a segment of a parabola, and it is clear that every point on that parabola segment is an extreme point of $QPB_1$.

**Theorem 1.** An extreme point $(\bar{x}, \bar{y})$ of $QPB_n$ is a vertex if and only if it is binary, i.e., if and only if $\bar{x} \in \{0, 1\}^n$.

**Proof.** First we prove sufficiency. Let $(\bar{x}, \bar{y})$ be a member of $S$ that is binary. Assume without loss of generality that $\bar{x}_i = 0$ for $i = 1, \ldots, q$ and $\bar{x}_i = 1$ for $i = q + 1, \ldots, n$. Then $(\bar{x}, \bar{y})$ satisfies the following valid inequalities at equality:

- $x_i \geq 0$ for $i = 1, \ldots, q$;
- $x_i \leq 1$ for $i = q + 1, \ldots, n$;
- $y_{ij} \geq 0$ for $1 \leq i \leq q$ and $i \leq j \leq n$;
- $y_{ij} \leq 1$ for $q + 1 \leq i \leq j \leq n$.

These inequalities are linearly independent, and there are $n + (n+1)$ of them. Thus, there exist $n + (n+1)$ independent normal vectors at $(\bar{x}, \bar{y})$. So $(\bar{x}, \bar{y})$ is a vertex.

Now we prove necessity. Let $(\bar{x}, \bar{y})$ be an extreme point, and suppose that $\bar{x}_k \in (0, 1)$ for some $k$. Let $\epsilon$ be a small positive quantity. If we increase $x_k$ by $\epsilon$, we obtain a second extreme point, say, $(x^+, y^+)$, that is identical to $(\bar{x}, \bar{y})$ except that

- $x_k^+$ is increased by $\epsilon$,
- $y_{ik}^+$ is increased by $\epsilon \bar{x}_i$ for all $i \neq k$,
- $y_{kk}^+$ is increased by $2\epsilon \bar{x}_k + \epsilon^2$.

Similarly, we can create a third extreme point, say, $(x^-, y^-)$, by decreasing $x_k$ by $\epsilon$.

Now let $(v, w)$ be a normal vector at $(\bar{x}, \bar{y})$. By definition, we must have $v^T x^+ + w^T y^+ \leq v^T \bar{x} + w^T \bar{y}$ and $v^T x^- + w^T y^- \leq v^T \bar{x} + w^T \bar{y}$, where $w^T y^+ := \sum_{1 \leq i \leq j \leq n} w_{ij} y_{ij}$, and $w^T y^-$ and $w^T \bar{y}$ are defined similarly. But this implies that the following two inequalities must hold:

$$v_k + \sum_{i \neq k} \bar{x}_i w_{ik} + (2\bar{x}_k + \epsilon) w_{kk} \leq 0,$$

$$- v_k - \sum_{i \neq k} \bar{x}_i w_{ik} - (2\bar{x}_k - \epsilon) w_{kk} \leq 0.$$

Since $\epsilon$ can approach zero arbitrarily closely, this implies that all normal vectors satisfy the equation

$$v_k + \sum_{i \neq k} \bar{x}_i w_{ik} + 2\bar{x}_k w_{kk} = 0.$$

Thus, there cannot exist $n + (n+1)/2$ linearly independent normal vectors. 

Indeed, in Figure 1 one sees that there are only two vertices, namely, the points at which $x_i \in \{0, 1\}$.

### 3.3. Invariance under permutation and switching

It is known (see, e.g., Deza and Laurent [10]) that $BQP_n$ is invariant under two transformations, called permutation and switching. Here, we adapt these concepts in a straightforward way to $QPB_n$.

**Definition 1.** (permutation). Let $\pi : \{1, \ldots, n\} \mapsto \{1, \ldots, n\}$ be an arbitrary permutation. Consider the linear transformation $\phi^\pi : \mathbb{R}^{n+\binom{n}{2}} \mapsto \mathbb{R}^{n+\binom{n}{2}}$ that

- replaces $x_i$ with $x_{\pi(i)}$ for all $i \in \{1, \ldots, n\},$
• replaces \( y_{ij} \) with \( y_{\pi(i),\pi(j)} \) for all \( 1 \leq i \leq j \leq n \).

By abuse of terminology, we call this transformation itself a permutation.

**Definition 2** (switching). For an arbitrary set \( S \subseteq \{1, \ldots, n\} \), let \( \psi^S : \mathbb{R}^{n+\binom{n+1}{2}} \rightarrow \mathbb{R}^{n+\binom{n+1}{2}} \) be the affine transformation that

- replaces \( x_i \) with \( 1-x_i \) for all \( i \in S \),
- replaces \( y_{ii} \) with \( 1-2x_i+y_{ii} \) for all \( i \in S \),
- replaces \( y_{ij} \) with \( x_i-y_{ij} \) for all \( i \in \{1, \ldots, n\} \setminus S \) and all \( j \in S \),
- replaces \( y_{ij} \) with \( 1-x_i-x_j+y_{ij} \) for all \( \{i,j\} \subseteq S \),
- leaves all other \( x_i \) and \( y_{ij} \) variables unchanged.

Applying the transformation \( \psi^S \) is called switching (on \( S \)).

It is obvious that \( QPB_n \) is invariant under permutation. (That is, for any \( n \) and any permutation \( \pi \) of \( \{1, \ldots, n\} \), we have \( \phi^\pi(QPB_n) = QPB_n \).) We now show that the same holds for switching.

**Proposition 1.** \( QPB_n \) is invariant under switching. That is, for any \( n \) and any \( S \subseteq \{1, \ldots, n\} \), \( \psi^S(QPB_n) = QPB_n \).

**Proof.** Let \( (\tilde{x}, \tilde{y}) \) be an extreme point of \( QPB_n \). From Lemma 2, we have \( \tilde{y}_{ij} = \tilde{x}_i\tilde{x}_j \) for all \( 1 \leq i \leq j \leq n \). Now let \( (\tilde{x}, \tilde{y}) = \psi^S(\tilde{x}, \tilde{y}) \). From the definition of switching, one can easily show that \( 0 \leq \tilde{x}_i \leq 1 \) for all \( i \leq n \), and that \( \tilde{y}_{ij} = \tilde{x}_i\tilde{x}_j \) for all \( 1 \leq i \leq j \leq n \). Thus, from Lemma 2, \( (\tilde{x}, \tilde{y}) \) is an extreme point of \( QPB_n \). This shows that every extreme point of \( \psi^S(QPB_n) \) is an extreme point of \( QPB_n \). A similar argument shows that every extreme point of \( QPB_n \) is an extreme point of \( \psi^S(QPB_n) \). Since \( \psi^S(QPB_n) \) and \( QPB_n \) are convex and have the same extreme points, they are equal. \( \square \)

Just as in the case of \( BQP_n \), the permutation and switching transformations enable one to convert valid linear inequalities into other valid linear inequalities that induce faces of the same dimension. For example, if we take the RLT inequality \( y_{ij} \geq 0 \) and switch on \( \{i\} \) or \( \{j\} \), we obtain the RLT inequalities \( y_{ij} \leq x_j \) and \( y_{ij} \leq x_i \), respectively. If we switch on \( \{i,j\} \), we obtain the RLT inequality \( y_{ij} \geq x_i + x_j - 1 \).

Note that the permutation transformation, unlike switching, is an isometry (that is, it preserves distances and angles). It is known that the permutations are the only isometries of \( BQP_n \) (see [10], p. 410). It is not hard to show that the same holds for \( QPB_n \).

4. On the RLT and psd inequalities. In this section, we examine the RLT and psd inequalities. In subsection 4.1 we show that most of the RLT inequalities induce facets of \( QPB_n \). In subsection 4.2 we show that the psd inequalities induce not facets but faces of high dimension. As a by-product of our analysis, we obtain an “extension” result, which is presented in subsection 4.3.

4.1. The RLT inequalities. We now show that most of the RLT inequalities induce facets of \( QPB_n \).

**Proposition 2.** The RLT inequalities of the form \( y_{ii} \leq x_i \) induce facets of \( QPB_n \), and so do all of the RLT inequalities with \( i \neq j \) (when \( n \geq 2 \)).

**Proof.** An RLT inequality of the form \( y_{ii} \leq x_i \) is satisfied at equality by all but one of the \( n + \binom{n+1}{2} + 1 \) vectors listed in the proof of Lemma 1. (Indeed, the only vector that does not satisfy it at equality is the one that has \( x_i = 1/2 \) and \( y_{ii} = 1/4 \).) The same is true for an RLT inequality of the form \( y_{ij} \geq 0 \) with \( j \neq i \). (Indeed, the only vector that does not satisfy it at equality is the one that has \( x_i = x_j = y_{ij} = 1 \).) The remaining RLT inequalities with \( j \neq i \) are switchings of this latter inequality, and therefore they too induce facets. \( \square \)
The only remaining RLT inequalities are those of the form \( y_{ij} \geq 0 \) and \( y_{ij} \geq 2x_i - 1 \). Since these RLT inequalities are also psd inequalities, we deal with them in the next subsection.

4.2. The psd inequalities. Next, we will determine the dimension of the faces of \( QPB_n \) induced by the psd inequalities (1). We will find the following (trivial) lemma useful.

Lemma 3. An extreme point \((x, y)\) of \( QPB_n \) satisfies a psd inequality (1) at equality if and only if it satisfies the equation \( v^T x + s = 0 \).

We will also find it helpful to let \( F(v, s) \) denote the face of \( QPB_n \) induced by the psd inequality and \( K(v, s) \) denote the set of associated \( x \) vectors. That is,

\[
F(v, s) = \{(x, y) \in QPB_n : v^T x + s = 0\}, \\
K(v, s) = \{x \in [0,1]^n : v^T x + s = 0\}.
\]

It turns out that the dimension of \( K(v, s) \) plays a key role.

Lemma 4. If the dimension of \( K(v, s) \) is less than \( n-1 \), then the psd inequality (1) is dominated by the RLT inequalities.

Proof. If the dimension of \( K(v, s) \) is \( -1 \) (i.e., \( K(v, s) = \emptyset \)), the psd inequality does not even induce a nonempty face, and the result is trivial. So suppose that the dimension is between 0 and \( n-2 \). In this case, since the equation \( v^T x + s = 0 \) defines an affine subspace of dimension \( n-1 \), \( K(v, s) \) must be contained in the boundary of \([0,1]^n\) and hence induces a face of the hypercube that is not a facet. By switching, we can assume that the face contains the origin. This implies that \( s = 0 \) and \( v \in \mathbb{R}_+^n \cup \mathbb{R}_-^n \).

(Indeed, if \( v \) contained a mixture of positive and negative entries, then \( K(s, v) \) would have dimension \( n-1 \), a contradiction.) The psd inequality is then easily shown to be a nonnegative linear combination of the RLT inequalities of the form \( y_{ij} \geq 0 \).

When the dimension of \( K(v, s) \) is \( n-1 \), on the other hand, the psd inequality induces a face of high dimension.

Theorem 2. If \( K(v, s) \) has dimension \( n-1 \), then \( F(v, s) \) has dimension \( \left(\binom{n+1}{2}\right) - 1 \).

Proof. First we show that the dimension of \( F(v, s) \) is at most \( \left(\binom{n+1}{2}\right) - 1 \). From Lemma 3, all extreme points of \( F(v, s) \) satisfy the equation \( v^T x + s = 0 \). Multiplying this equation by each variable in turn and then using the identities \( y_{ij} = x_i x_j \), we obtain \( n \) additional equations of the form

\[
\sum_{j=1}^n v_j y_{ij} + sx_i = 0 \quad (i = 1, \ldots, n).
\]

These \( n+1 \) equations are easily shown to be linearly independent. The upper bound on the dimension then follows from Lemma 1.

Now we show that the dimension of \( F(v, s) \) is at least \( \left(\binom{n+1}{2}\right) - 1 \). Let \( x^* \) be an arbitrary point lying in the relative interior of \( K(v, s) \). Let \( v^1, \ldots, v^{n-1} \in \mathbb{R}^n \) be a set of vectors that are orthogonal to each other and to \( v \). Finally, let \( \epsilon \) be a small positive quantity. Consider the following \( \left(\binom{n+1}{2}\right) - 1 \) vectors in \([0,1]^n\):

- \( x^* \),
- \( x^* + \epsilon v^r \) for \( r = 1, \ldots, n-1 \),
- \( x^* + 2\epsilon v^r \) for \( r = 1, \ldots, n-1 \),
- \( x^* + \epsilon (v^r + v^s) \) for \( 1 \leq r < s \leq n-1 \).

All of these vectors lie in \( K(v, s) \). The corresponding \( \left(\binom{n+1}{2}\right) - 1 \) extreme points of \( QPB_n \) therefore lie in \( F(v, s) \). They can be shown to be affinely independent.
Now note that when the dimension of $K(v, s)$ is $n - 1$, we have two possibilities: either $K(v, s)$ contains an interior point of the unit hypercube (i.e., there exists some $x^* \in (0, 1)^n$ such that $v^T x^* + s = 0$), or $K(v, s)$ is a facet of the unit hypercube. In the latter case, the psd inequality is nothing but an RLT inequality of the form $y_{ii} \geq 0$ or $y_{ii} \geq 2x_i - 1$. Thus, those particular RLT inequalities do not induce facets of $QPB_n$.

Using known results on the positive semidefinite cone (see, e.g., Pataki [19]), one can also show the following. We omit the proofs for brevity.

**Proposition 3.** If $K(v, s)$ contains an interior point of the hypercube, then $F(v, s)$ is a maximal face of $QPB_n$ (i.e., it is not contained in any other face). Moreover, the psd inequality is nondominated (i.e., it is not a convex combination of other valid inequalities).

**Proposition 4.** If $K(v, s)$ is a facet of the hypercube (i.e., if the psd inequality is an RLT inequality), then $F(v, s)$ is contained in the facet induced by an RLT inequality of the form $y_{ii} \leq x_i$. Yet, the psd inequality is still nondominated.

This last result may seem counterintuitive but is also apparent in Figure 1 for $n = 1$. Specifically, taking $(v, s) = (1, 0)$, we have $K(v, s) = \{0\}$ and $F(v, s) = \{(0, 0)\}$, and the associated psd inequality is the RLT constraint $y_{11} \geq 0$. The facet induced by $y_{11} \leq x_1$ is $\{(x, y) \in [0, 1]^2 : x = y\}$, which contains $F(v, s)$. However, $y_{11} \geq 0$ is still nondominated because it cannot be written as the convex combination of other valid (linear) inequalities.

### 4.3. Canonical extension.

Our analysis of the psd inequalities led us to derive an additional result that we describe in this subsection. Our starting point is the fact that if the linear inequality

$$\sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \leq i \leq j \leq n} \beta_{ij} y_{ij} \leq \gamma$$

is valid for $QPB_n$, then it is also valid for $QPB_{n'}$ for any $n' > n$. That is to say, given any valid inequality for $QPB_n$, we can construct a valid inequality for $QPB_{n'}$ simply by introducing zero coefficients for the additional variables. Padberg [18] called the resulting inequality the “canonical extension” of the original inequality.

To explain our result, we will find it helpful to use the term codimension: a face of $QPB_n$ has codimension $k$ if it has dimension $n + \binom{n+1}{2} + 1 - k$. (Thus, the codimension of a facet is 1, and the codimension of a psd inequality is at least $n + 1$.) Our result essentially states that the codimension of the canonical extension of an inequality is identical to the codimension of the original inequality.

We will need the following lemma.

**Lemma 5.** Suppose that $F$ is a face of $QPB_n$ whose codimension is no more than $n$. Then $F$ contains $n + 1$ extreme points, say, $(x^k, y^k)$ for $k = 1, \ldots, n + 1$ such that the vectors $x^1, \ldots, x^{n+1}$ are affinely independent in $\mathbb{R}^n$.

**Proof.** If this were not so, then the face would satisfy an equation of the form $v^T x = s$. The face would then be contained in the face induced by a psd inequality, and therefore have codimension at least $n + 1$.  

With this lemma, we can prove the following theorem.

**Theorem 3.** Suppose that the linear inequality

$$\sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \leq i \leq j \leq n} \beta_{ij} y_{ij} \leq \gamma$$

is valid for $QPB_n$, then it is also valid for $QPB_{n'}$ for any $n' > n$. That is to say, given any valid inequality for $QPB_n$, we can construct a valid inequality for $QPB_{n'}$ simply by introducing zero coefficients for the additional variables. Padberg [18] called the resulting inequality the “canonical extension” of the original inequality.
induces a face of $QPB_n$ of codimension $k$, where $1 \leq k \leq n$. Then it also induces a face of $QPB_n$ of codimension $k$ for all $n' > n$.

Proof. By induction, it suffices to prove that the inequality induces a face of $QPB_{n+1}$ of codimension $k$. Let $F$ be the original face of $QPB_n$, and let $F'$ be the face of $QPB_{n+1}$ induced by the inequality. Since $F$ has codimension $k$, it contains $n + \binom{n+1}{2} + 1 - k$ affinely independent extreme points of $QPB_n$. Each of these can be converted into an extreme point of $QPB_{n+1}$ by setting $x_{n+1} = 0$ and $y_{i,n+1} = 0$ for $i = 1, \ldots, n + 1$. In this way, one obtains $n + \binom{n+1}{2} + 1 - k$ affinely independent extreme points of $QPB_{n+1}$ that lie in $F'$. To complete the proof, we need another $n + 2$ such points.

Let $x^1, \ldots, x^{n+1} \in \mathbb{R}^n$ be the vectors mentioned in Lemma 5. We construct $n + 1$ modified vectors in $\mathbb{R}^{n+1}$, say, $\tilde{x}^1, \ldots, \tilde{x}^{n+1}$, by setting

- $\tilde{x}_i^k = x_i^k$ for $k = 1, \ldots, n + 1$ and $i = 1, \ldots, n$,
- $\tilde{x}_{n+1}^k = 1$ for $k = 1, \ldots, n + 1$.

Now note that, for $k = 1, \ldots, n + 1$, we can construct an extreme point $(\tilde{x}^k, \tilde{y}^k)$ of $QPB_{n+1}$ that lies in $F'$. These $n + 1$ extreme points, together with the original $n + \binom{n+1}{2} + 1 - k$ ones, are easily shown to be affinely independent.

Finally, we construct one more extreme point of $QPB_{n+1}$ as follows. Let $\tilde{x}$ be identical to $\tilde{x}^1$, apart from the fact that $\tilde{x}_{n+1} = 1/2$. The corresponding extreme point of $QPB_{n+1}$, say, $(\tilde{x}, \tilde{y})$, also lies in $F'$. It is affinely independent of the other points mentioned, since it is the only one that does not satisfy $y_{n+1,n+1} = x_{n+1}$.

5. Facets from the Boolean quadric polytope. As mentioned in subsection 2.4, Yajima and Fujie [29] proved that certain valid inequalities for $BQP_n$ are valid also for $QPB_n$. In this section, we extend this result in several ways.

5.1. $BQP_n$ as a projection of $QPB_n$. Recall that $QPB_n$ and $BQP_n$ “live” in $\mathbb{R}^{n+\binom{n+1}{2}}$ and $\mathbb{R}^{n+\binom{n+1}{2}}$, respectively. The following proposition states that the projection of $QPB_n$ onto $\mathbb{R}^{n+\binom{n+1}{2}}$ is nothing but $BQP_n$.

PROPOSITION 5. The projection of $QPB_n$ onto $\mathbb{R}^{n+\binom{n+1}{2}}$, i.e., the set

$$\text{conv}\left\{(x, y) \in [0, 1]^{n+\binom{n+1}{2}} : y_{ij} = x_i x_j \ (1 \leq i < j \leq n)\right\},$$

is equal to $BQP_n$.

Proof. Let $(\bar{x}, \bar{y}) \in [0, 1]^{n+\binom{n+1}{2}}$ lie in the projection, and suppose that $\bar{x}$ is fractional, i.e., that $\bar{x}_k \in (0, 1)$ for some $1 \leq k \leq n$. Let $x^0$ and $x^1$ be the vectors obtained from $\bar{x}$ by changing $x_k$ to 0 or 1, respectively, and let $(x^0, y^0)$ and $(x^1, y^1)$ be the corresponding points in the projection. (That is, let $y_{ij}^0 = x_i^0 x_j^0$ and $y_{ij}^1 = x_i^1 x_j^1$ for $1 \leq i < j \leq n$.) Finally, let $\lambda = \bar{x}_k$. One can check that

$$\bar{x}_i = \lambda x_i^1 + (1 - \lambda) x_i^0 \ (i = 1, \ldots, n),$$

$$\bar{y}_{ij} = \lambda y_{ij}^1 + (1 - \lambda) y_{ij}^0 \ (1 \leq i < j \leq n).$$

Thus, $(\bar{x}, \bar{y})$ is a convex combination of other points in the projection and therefore cannot be an extreme point of the projection. Therefore, all extreme points of the projection are binary, and the projection is nothing but $BQP_n$. $\square$

Proposition 5 implies that if one faces an instance of QPB in which the main diagonal of the quadratic cost matrix $Q$ is zero, then one can assume that the variables are binary (and therefore solve an instance of UBQP). For our purposes, the following consequence is more important.
COROLLARY 1. If the linear inequality

\[ \sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \leq i < j \leq n} \beta_{ij} y_{ij} \leq \gamma \]

is valid for \( BQP_n \), then it is valid for \( QPB_n \) as well.

This implies the above-mentioned result of Yajima and Fujie [29].

From now on, we let \( \text{proj}(x, y) \) denote the linear operator that projects points in \( \mathbb{R}^{n+\binom{n+1}{2}} \) onto \( \mathbb{R}^{n+2} \) by simply dropping the components \( y_{ii} \) for all \( 1 \leq i \leq n \). The following proposition shows that there is another link between \( QPB_n \) and \( BQP_n \).

PROPOSITION 6. Let \( F \) be the face of \( QPB_n \) defined by the equations \( y_{ii} = x_i \) for all \( i \). Then \( \text{proj}(F) = BQP_n \).

Proof. The only members of \( S \) that satisfy \( y_{ii} = x_i \) for all \( i \) are the binary ones. Thus, the extreme points of \( F \) are the binary members of \( S \). Since \( \text{proj}(F) \) is the convex hull of the projections of these binary members, it is equal to \( BQP_n \).

Thus, \( BQP_n \) is simultaneously a projection of \( QPB_n \) and a projection of a face of \( QPB_n \). This fact too can be seen clearly in Figure 1: whether we project the whole of \( QPB_1 \) or just the face \( F \) onto \( \mathbb{R} \), we still obtain the line segment defined by \( 0 \leq x_1 \leq 1 \).

5.2. Which \( BQP \) facets yield \( QPB \) facets? Corollary 1 has established that an inequality, which is valid for \( BQP_n \), may be extended to a valid inequality for \( QPB_n \) by simply introducing zero coefficients for the additional variables. Even though these two inequalities act in different spaces, we think of them—and for convenience refer to them—as the same inequality. We ask the reader to keep this terminology in mind for the proper interpretation of Lemma 6 and Theorem 4 below.

The RLT inequalities with \( j \neq i \) are examples of inequalities that induce facets of both \( BQP_n \) and \( QPB_n \). In this subsection, we give a necessary and sufficient condition for an inequality to have this property. We will need the following lemma.

LEMMA 6. Suppose we are given an inequality that induces a face of \( BQP_n \). Moreover, let \( (\bar{x}, \bar{y}) \) be a member of \( S \), and suppose that \( \bar{x}_k \in (0, 1) \) for some \( 1 \leq k \leq n \). Let \( (x^0, y^0) \) and \( (x^1, y^1) \) be defined as in Proposition 5. Then \( (\bar{x}, \bar{y}) \) satisfies the inequality at equality if and only if \( (x^0, y^0) \) and \( (x^1, y^1) \) do.

Proof. As in the proof of Proposition 5, \( \text{proj}(\bar{x}, \bar{y}) \) is a convex combination of \( \text{proj}(x^0, y^0) \) and \( \text{proj}(x^1, y^1) \). Thus, the slack of the inequality at \( (\bar{x}, \bar{y}) \) is a convex combination of the slacks of the inequality at \( (x^0, y^0) \) and \( (x^1, y^1) \).

We then have the following result.

THEOREM 4. Suppose an inequality induces a facet of \( BQP_n \). A necessary and sufficient condition for it to also induce a facet of \( QPB_n \) is the existence of \( n \) extreme points of \( QPB_n \), say, \( (x^1, y^1), \ldots, (x^n, y^n) \), such that

- each satisfies the inequality at equality;
- \( x^i_1 \in (0, 1) \) for \( i = 1, \ldots, n \);
- \( x^0_j \in \{0, 1\} \) for \( i = 1, \ldots, n \) and \( j \neq i \).

Proof. First we prove necessity. For any \( i \in \{1, \ldots, n\} \), there must exist an extreme point of \( QPB_n \) that lies on the face and such that \( x_i \) is fractional. (If this were not so, then all extreme points of \( QPB_n \) lying on the face would satisfy the RLT inequality \( y_{ii} \leq x_i \) with equality.) Now, by a repeated application of Lemma 6 with \( k \neq i \), we can convert the \( i \)th such point into the desired point \( (x^i, y^i) \).

Next, we prove sufficiency. Since the inequality induces a facet of \( BQP_n \), there exist \( n + \binom{n}{2} \) affinely independent binary extreme points of \( QPB_n \) lying on the face.
For the inequality to induce a facet of $QPB_n$, one needs an additional $n$ affinely independent extreme points. To see that $(x^1, y^1), \ldots, (x^n, y^n)$ are the desired points, note that, for any $i$, the point $(x^i, y^i)$ is the only point in the collection that does not satisfy the equation $y_{ii} = x_i$. □

It is possible to express the condition in Theorem 4 entirely in terms of $BQP_n$.

**Corollary 2.** Suppose an inequality induces a facet of $BQP_n$. A necessary and sufficient condition for it to also induce a facet of $QPB_n$ is that there exist 2n vertices of $QPB_n$, say, $(\tilde{x}^1, \tilde{y}^1), \ldots, (\tilde{x}^n, \tilde{y}^n)$ and $(\tilde{x}^1, y^1), \ldots, (\tilde{x}^n, y^n)$, with the following properties:

- each satisfies the inequality at equality;
- $\tilde{x}^j_\ell = \tilde{x}_\ell^j$ for $i = 1, \ldots, n$ and $j \neq i$;
- $\tilde{x}^i_\ell = 0$ and $\tilde{x}^i_\ell = 1$ for $i = 1, \ldots, n$.

**Proof.** To create the desired vertices of $BQP_n$, it suffices to take the $n$ extreme points of $QPB_n$ described in Theorem 4, decompose each of them into two binary extreme points of $QPB_n$ as in Lemma 6, and then project the resulting 2n extreme points onto $\mathbb{R}^{n+\binom{n}{2}}$. □

**5.3. A huge class of facets.** To illustrate the ideas given in the previous subsection, we now consider a well-known class of valid inequalities for $BQP_n$, due to Boros and Hammer [5], and derive a surprisingly simple necessary and sufficient condition for them to induce facets of $QPB_n$. The class of inequalities concerned is given in the following proposition.

**Proposition 7** (Boros and Hammer [5]). For any $v \in \mathbb{Z}^n$ and $s \in \mathbb{Z}$, all extreme points of $BQP_n$ satisfy $(v^T x + s)(v^T x + s - 1) \geq 0$. Thus, the inequality

\[
\sum_{i=1}^{n} v_i (v_i + 2s - 1)x_i + 2 \sum_{1 \leq i < j \leq n} v_iv_jy_{ij} \geq s(1 - s)
\]

is valid for $QPB_n$.

The inequalities (8) do not always induce facets of $BQP_n$, but they do under certain conditions (see De Simone [9] and Deza and Laurent [10]). Moreover, they include a variety of facet-inducing inequalities for $BQP_n$ as special cases. This includes the triangle, clique, cut, and generalized cut inequalities of Padberg [18] and the inequalities introduced in Sherali, Lee, and Adams [25], which were called cut-type inequalities by Yajima and Fujie [29]. The cut-type inequalities are the special case obtained when $v \in \{0, \pm 1\}^n$ and induce facets under mild conditions.

As mentioned in subsection 2.4, Yajima and Fujie [29] proved that the cut-type inequalities are valid for $QPB_n$. We now give a much stronger result.

**Theorem 5.** Suppose that an inequality of the form (8) induces a facet of $QPB_n$. It induces a facet of $QPB_n$ as well if and only if $v \in \{0, \pm 1\}^n$, i.e., if and only if it is a cut-type inequality.

**Proof.** It follows from the derivation of the inequality (8) that a vertex of $BQP_n$ satisfies it at equality if and only if it satisfies $v^T x + s \in \{0, 1\}$. Suppose that the inequality induces a facet of both $BQP_n$ and $QPB_n$. Then there exist 2n extreme points of $BQP_n$, say, $(\tilde{x}^1, \tilde{y}^1), \ldots, (\tilde{x}^n, \tilde{y}^n)$ and $(\tilde{x}^1, y^1), \ldots, (\tilde{x}^n, y^n)$, with the properties described in Corollary 2. For any given $1 \leq i \leq n$, we have three possible cases:

- $v^T \tilde{x}_i = v^T \tilde{x}_i \in \{0, 1\}$, in which case $v_i = 0$;
- $v^T \tilde{x}_i = 0$ and $v^T \tilde{x}_i = 1$, in which case $v_i = 1$;
- $v^T \tilde{x}_i = 1$ and $v^T \tilde{x}_i = 0$, in which case $v_i = -1$.

Thus, $v \in \{0, \pm 1\}^n$, and the inequality is a cut-type inequality.
Similarly, when \( v \in \{0, \pm 1\}^n \), it is easy to construct the \( 2n \) vertices of \( BQP_n \) required by Corollary 2. Thus, if a cut-type inequality induces a facet of \( BQP_n \), it also induces a facet of \( QPB_n \). □

We know of other inequalities that induce facets of both \( BQP_n \) and \( QPB_n \), along with other inequalities that induce facets of \( BQP_n \) but not of \( QPB_n \). We do not go into details for the sake of brevity.

6. A classification of valid inequalities for \( QPB_n \).

Let \( Q_{\alpha, \beta}(x, y) \leq \gamma \) be any valid linear inequality for \( QPB_n \), where \( \alpha \in \mathbb{R}^n \), \( \beta \in \mathbb{R}^{n+1} \), \( \gamma \in \mathbb{R} \), and

\[
Q_{\alpha, \beta}(x, y) := \sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \leq i \leq j \leq n} \beta_{ij} y_{ij}.
\]

Also, define the corresponding quadratic form

\[
q_{\alpha, \beta}(x) := \sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \leq i \leq j \leq n} \beta_{ij} x_i x_j.
\]

Let us call a valid linear inequality \( Q_{\alpha, \beta}(x, y) \leq \gamma \) “concave,” “convex,” or “indefinite” according to whether the quadratic form \( q_{\alpha, \beta}(x) \) is concave, convex, or indefinite, respectively. In the following three subsections, we characterize the inequalities of these three different types. Then, in subsection 6.4, we use these characterizations to shed light on the structure of \( QPB_3 \).

In a couple of places, we will use the following (easy) lemma.

**Lemma 7.** The maximum value of \( Q_{\alpha, \beta}(x, y) \) over \( QPB_n \) equals the maximum value of \( q_{\alpha, \beta}(x) \) over \([0, 1]^n\).

6.1. The concave case. First we deal with the concave case. The following proposition shows that the only nonredundant concave inequalities are, essentially, the psd inequalities.

**Proposition 8.** Suppose that \( Q_{\alpha, \beta}(x, y) \leq \gamma \) is valid for \( QPB_n \) and that \( q_{\alpha, \beta}(x) \) is concave. Then \( Q_{\alpha, \beta}(x, y) \leq \gamma \) is valid for the following convex set:

\[
\{(x, y) \in [0, 1]^n \times \mathbb{R}^{\binom{n+1}{2}} : \hat{Y} \succeq 0\},
\]

where \( \hat{Y} \) is defined as in subsection 2.2.

**Proof.** Let \((x, y)\) with associated \( \hat{Y} \) be arbitrary in the above convex set. Because \( q_{\alpha, \beta}(x) \) is concave, it can be expressed as

\[
q_{\alpha, \beta}(x) = \alpha^T x + x^T B x,
\]

with symmetric, negative semidefinite matrix \( B \) (defined easily in terms of \( \beta \)). Likewise,

\[
Q_{\alpha, \beta}(x, y) = \alpha^T x + B \cdot Y,
\]

where \( B \cdot Y := \sum_{i,j=1}^{n} B_{ij} Y_{ij} \). Note that \( x^T B x = B \cdot xx^T \) also. Thus,

\[
Q_{\alpha, \beta}(x, y) = \alpha^T x + B \cdot Y
\]

\[
= \alpha^T x + B \cdot (Y - xx^T) + x^T B x
\]

\[
\leq \alpha^T x + x^T B x
\]

\[
= q_{\alpha, \beta}(x),
\]
where the inequality follows from $B \preceq 0$ and $Y - xx^T \succeq 0$. Now, by Lemma 7, the validity of $Q_{\alpha, \beta}(x, y) \leq \gamma$ for $QPB_n$ ensures that $q_{\alpha, \beta}(x) \leq \gamma$ for any $x \in [0, 1]^n$. This proves the result. 

6.2. The convex case. Now we move on to the convex case. The following proposition shows that the only nonredundant convex inequalities are the inequalities that come from $BQP_n$, together with certain RLT constraints. (This result was conjectured to us by Anstreicher [2].)

Proposition 9. Suppose that the inequality $Q_{\alpha, \beta}(x, y) \leq \gamma$ is valid for $QPB_n$ and that $q_{\alpha, \beta}(x)$ is convex. Then $Q_{\alpha, \beta}(x, y) \leq \gamma$ is valid for the following polytope:

$$\{(x, y) : \text{proj}(x, y) \in BQP_n, y_{ii} \leq x_i (1 \leq i \leq n)\}.$$

Proof. Because $q_{\alpha, \beta}(x)$ is convex, it attains its maximum over $[0, 1]^n$ at $\{0, 1\}^n$, i.e., at one of the $2^n$ extreme points. This maximum is less than or equal to $\gamma$ because $Q_{\alpha, \beta}(x, y) \leq \gamma$ is valid for $QPB_n$ by assumption. So

$$\gamma \geq \max_{x \in \{0, 1\}^n} \left( \sum_{i=1}^{n} \alpha_i x_i + \sum_{i \leq j} \beta_{ij} x_i x_j \right)$$

$$= \max_{x \in \{0, 1\}^n} \left( \sum_{i=1}^{n} (\alpha_i + \beta_{ii}) x_i + \sum_{i<j} \beta_{ij} x_i x_j \right),$$

which shows that the inequality

$$\sum_{i=1}^{n} (\alpha_i + \beta_{ii}) x_i + \sum_{i<j} \beta_{ij} y_{ij} \leq \gamma$$

is valid for $BQP_n$.

Now let $(x, y)$ be such that $\text{proj}(x, y) \in BQP_n$ with $y_{ii} \leq x_i$ for all $i$, and note that $\beta_{ii} \geq 0$ for all $i$ because $q_{\alpha, \beta}(x)$ is convex. We wish to show that $Q_{\alpha, \beta}(x, y) \leq \gamma$:

$$Q_{\alpha, \beta}(x, y) = \sum_{i=1}^{n} \alpha_i x_i + \sum_{i \leq j} \beta_{ij} y_{ij}$$

$$= \sum_{i=1}^{n} \alpha_i x_i + \sum_{i<j} \beta_{ij} y_{ij} + \sum_{i=1}^{n} \beta_{ii}(x_i - x_i + y_{ii})$$

$$\leq \sum_{i=1}^{n} \alpha_i x_i + \sum_{i<j} \beta_{ij} y_{ij} + \sum_{i=1}^{n} \beta_{ii} x_i$$

$$= \sum_{i=1}^{n} (\alpha_i + \beta_{ii}) x_i + \sum_{i<j} \beta_{ij} y_{ij}$$

$$\leq \gamma,$$

where the final inequality follows by the validity of (9) for $BQP_n$. 

6.3. The indefinite case. Finally, we consider the indefinite case. We will need the following standard result.
LEMMA 8. Suppose \( q_{\alpha,\beta}(x) \) is indefinite. Then its maximum over \([0,1]^n\) is necessarily obtained on the boundary.

Thus, checking whether \( Q_{\alpha,\beta}(x,y) \leq \gamma \) is valid for \( QPB_n \) amounts to checking that \( q_{\alpha,\beta}(x) \) does not exceed \( \gamma \) on each of the \( 2n \) facets of \([0,1]^n\).

To formalize ideas, for all \( i = 1, \ldots, n \) and each \( \delta \in \{0,1\} \), define the quadratic function

\[
q_{\alpha,\beta}^{i,\delta}(\bar{x}) := q_{\alpha,\beta}(\bar{x}_1, \ldots, \bar{x}_{i-1}, \delta, \bar{x}_i, \ldots, \bar{x}_{n-1}),
\]

where \( \bar{x} \in \mathbb{R}^{n-1} \). One can think of \( q_{\alpha,\beta}^{i,\delta}(\bar{x}) \) as \( q_{\alpha,\beta}(x) \) with the value \( \delta \) substituted for \( x_i \), and so one can work out an explicit representation in terms of linear \( (\bar{x}_i) \), quadratic \( (\bar{x}_i \bar{x}_j) \), and constant terms (although we do not provide the full representation here). Note that the constant term is \( \alpha_i \delta + \beta_{ii} \delta^2 \). We also define \( Q_{\alpha,\beta}^{i,\delta}(\bar{x}, \bar{y}) \) to be the linear function arising from the above explicit representation—without constant term—when \( \bar{x}_i \bar{x}_j \) is linearized by \( \bar{y}_{ij} \). The following result now follows directly from these constructions.

PROPOSITION 10. The inequality \( Q_{\alpha,\beta}(x,y) \leq \gamma \), with \( q_{\alpha,\beta}(x) \) indefinite, is valid for \( QPB_n \) if and only if the inequality

\[
(10) \quad Q_{\alpha,\beta}^{i,\delta}(\bar{x}, \bar{y}) \leq \gamma - \alpha_i \delta - \beta_{ii} \delta^2
\]

is valid for \( QPB_{n-1} \) for all \( i = 1, \ldots, n \) and \( \delta \in \{0,1\} \).

Proof. By Lemma 7, \( Q_{\alpha,\beta}(x,y) \leq \gamma \) is valid for \( QPB_n \) if and only if \( q_{\alpha,\beta}(x) \leq \gamma \) for all \( x \in [0,1]^n \). By Lemma 8, this occurs if and only if \( q_{\alpha,\beta}^{i,\delta}(\bar{x}) \leq \gamma - \alpha_i \delta - \beta_{ii} \delta^2 \) for all \( \bar{x} \in [0,1]^{n-1} \) and for each \( i \) and \( \delta \), which in turn occurs only under the stated condition.

In addition, Proposition 10 provides a finite recursive procedure to check the validity for \( QPB_n \) of any given indefinite inequality \( Q_{\alpha,\beta}(x,y) \leq \gamma \): one simply checks that each of the \( 2n \) inequalities of the form (10) is valid for \( QPB_n \). The recursion is well defined because the validity of any inequality for \( QPB_1 \) can be easily checked.

Propositions 8–10 also give rise to a semi-infinite description of \( QPB_n \).

COROLLARY 3. For \( n \geq 2 \), let \( V \) be the collection of all \( (\alpha, \beta, \gamma) \) such that \( q_{\alpha,\beta}(x) \) is indefinite and \( Q_{\alpha,\beta}^{i,\delta}(\bar{x}, \bar{y}) \leq \gamma - \alpha_i \delta - \beta_{ii} \delta^2 \) is valid for \( QPB_{n-1} \) for all \( i = 1, \ldots, n \) and \( \delta \in \{0,1\} \). Then \( QPB_n \) equals

\[
\left\{ (x,y) \in [0,1]^{n+\binom{n+1}{2}} : \begin{array}{c} y_{ii} \leq x_i \ (1 \leq i \leq n), \\ \hat{Y} \succeq 0, \ \proj(x,y) \in BQP_n, \\ Q_{\alpha,\beta}(x,y) \leq \gamma \forall (\alpha, \beta, \gamma) \in V \end{array} \right\}.
\]

The semi-infinite nature of this description certainly makes it difficult to work with directly, but it is interesting that the description reduces to a finite one when \( n = 2 \) (Anstreicher and Burer [3]). In particular, for \( n = 2 \), \( \proj(x,y) \in BQP_n \) and \( y_{ii} \leq x_i \) constitute precisely the RLT constraints, while the constraints for \( (\alpha, \beta, \gamma) \in V \) are redundant. Perhaps it is possible to simplify the description for larger \( n \).

6.4. More on \( QPB_3 \). Consider the following convex set:

\[
(11) \quad Q_n := \left\{ (x,y) \in [0,1]^{n+\binom{n+1}{2}} : \begin{array}{c} y_{ii} \leq x_i \ (1 \leq i \leq n), \\ \hat{Y} \succeq 0, \\ \proj(x,y) \in BQP_n \end{array} \right\}.
\]
From the results given so far, $Q_n$ contains $QPB_n$. Moreover, one would expect $Q_n$ to be a “tight” approximation to $QPB_n$. Indeed, then the following hold:

- $Q_n$ satisfies all valid inequalities for $QPB_n$ that involve at most two indices, i.e., all inequalities of the form

$$\alpha_i x_i + \alpha_j x_j + \beta_{ii} y_{ii} + \beta_{ij} y_{ij} + \beta_{jj} y_{jj} \leq \gamma.$$  

(This follows from the result of Anstreicher and Burer [3] mentioned in subsection 2.2.) In particular, it satisfies all RLT inequalities.

- $Q_n$ satisfies all valid inequalities for $QPB_n$ that have zero coefficients for the variables $y_{ii}$. (This follows from Proposition 5.)

- $Q_n$ satisfies all nonredundant “concave” and “convex” valid inequalities for $QPB_n$ (as shown in subsections 6.1 and 6.2).

Moreover, $Q_3$ gives an even tighter approximation to $QPB_3$ than the one studied in Anstreicher and Burer [3]. (This is so since the inequalities (2)–(5) are dominated by the triangle inequalities of Padberg [18].)

A natural question to ask at this point is whether $QPB_3 = Q_3$. In fact, it turns out that $QPB_3$ is strictly contained in $Q_3$. To show this, we use the recursive procedure for checking validity discussed before Corollary 3.

Define

$$\alpha = (\alpha_1, \alpha_2, \alpha_3) = (3, 1, 0),$$

$$\beta = (\beta_{11}, \beta_{12}, \beta_{22}, \beta_{13}, \beta_{23}, \beta_{33}) = (-2.25, -6, 0, -6, -1, 1),$$

$$\gamma = 1.$$  

Using the recursive procedure, one can show that $Q_{\alpha,\beta}(x, y) \leq \gamma$ is valid for $QPB_3$. We next consider the maximization

$$\max \{Q_{\alpha,\beta}(x, y) : (x, y) \in Q_3\}.$$  

Using the fact that $BQP_3$ is completely described by RLT and triangle inequalities, one can easily verify that the fractional point

$$x = (x_1, x_2, x_3) = \frac{1}{3} (1, 1, 1),$$

$$y = (y_{11}, y_{12}, y_{22}, y_{13}, y_{23}, y_{33}) = \frac{1}{3} (2, 0, 3, 0, 1, 3)$$

is feasible with objective value $19/18 > 1$. (Note that the optimal objective value is approximately 1.0929.) It follows that $Q_{\alpha,\beta}(x, y) \leq \gamma$ is not valid for $Q_3$, which proves that $QPB_3$ is strictly contained in $Q_3$.

7. Concluding remarks. Given the fact that QPB is a fundamental and much-studied problem in global optimization, it is surprising that many of its basic properties were not established before now. We have addressed this gap in the literature, using the tools of polyhedral theory and convex analysis.

There are some interesting topics for future research. For example, can one find an explicit description of $QPB_3$ in terms of linear inequalities? In addition, if an inequality induces a facet of $BQP_n$ but not of $QPB_n$, can it be strengthened in some way so that it induces a facet of $QPB_n$? Finally, the algorithmic implications of our results should be investigated.

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REFERENCES


