On Non-Convex Quadratic Programming with Box Constraints

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Abstract

Non-Convex Quadratic Programming with Box Constraints is a fundamental $\mathcal{NP}$-hard global optimisation 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, characterise 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.

Keywords: non-convex quadratic programming — global optimisation — polyhedral combinatorics — convex analysis.

1 Introduction

Non-Convex Quadratic Programming with Box Constraints (QPB) is the problem of minimising a non-convex quadratic function of a set of variables, subject to lower and upper bounds on the variables. A QPB instance with n variables takes the form:

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

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.

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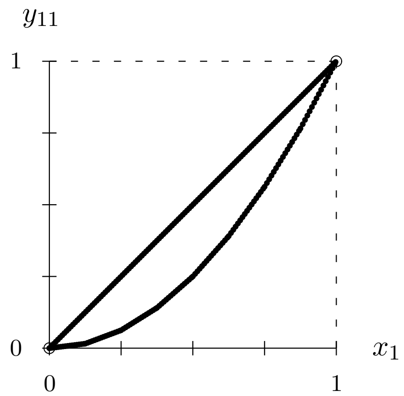

Figure 1: The convex set QPB_1.

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 $\mathcal{NP}$-hard, is regarded as a fundamental problem in global optimisation (see Horst *et al.* [14]). A survey of research on QPB up to 1997 was given by De Angelis *et al.* [7]. More recent relevant papers include Yajima & Fujie [31], Vandenbussche & Nemhauser [29, 30], Burer & Vandenbussche [6], Anstreicher [1] and Anstreicher & Burer [3].

It is common practice to linearise 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 non-convex constraints $y_{ij} = x_i x_j$ can then be approximated by either linear constraints (as in [25, 29, 30, 31]) or conic constraints (as in [1, 3, 6]).

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

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

Note that 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, 31], 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 *RLT* and *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

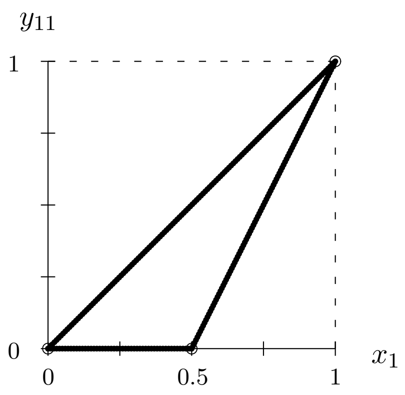

Figure 2: Region defined by RLT inequalities when $n = 1$.

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 & Wolsey [18] or Schrijver [24]) and convex analysis (see Hiriart-Urruty & 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:

$$y_{ij} \geq 0,\ y_{ij} \leq x_i,\ y_{ij} \leq x_j,\ y_{ij} \geq x_i + x_j - 1.$$

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-Linearisation Technique* of Sherali & Adams [25].

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

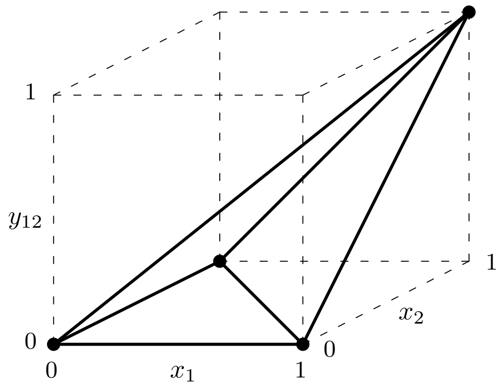

Figure 3: Region defined by RLT inequalities with $i \neq j$ when $n = 2$.

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 [17] 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 non-convex quadratic programs is due to Shor [28] (see also Lovász & Schrijver [16]). 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

$$\hat{Y} := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T = \begin{pmatrix} 1 & x^T \\ x & Y \end{pmatrix}.$$

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 [21], $\hat{Y} \succeq 0$ 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:

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

We will call these (1) *psd* inequalities. 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, 26, 31]. 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 & 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:

$$\begin{aligned} y_{11} + y_{22} + y_{33} &\leq y_{12} + y_{13} + y_{23} + 1 && (2) \\ y_{11} + y_{22} + y_{33} + y_{12} + y_{13} &\leq 2x_1 + x_2 + x_3 + y_{23} && (3) \\ y_{11} + y_{22} + y_{33} + y_{12} + y_{23} &\leq x_1 + 2x_2 + x_3 + y_{13} && (4) \\ y_{11} + y_{22} + y_{33} + y_{13} + y_{23} &\leq x_1 + x_2 + 2x_3 + y_{12}. && (5) \end{aligned}$$

2.3 QPB as a generalisation of UBQP

A folklore result, possibly due to Rosenberg [23], is that QPB includes *Unconstrained Boolean Quadratic Programming* (UBQP) as a special case. An instance of UBQP takes the form

$$\min \left\{ c^T x + x^T Q x : \ x \in \{0,1\}^n \right\},$$

where $c \in \mathbb{R}^n$ and $Q \in \mathbb{R}^{n \times n}$ as before. To reduce a UBQP instance to a QPB instance, it suffices to add the penalty term $M \sum_{i=1}^n (x_i - x_i^2)$ to the objective function, where M is a large positive integer. Note that the resulting QPB instance has a concave objective.

Another folklore result (e.g., Barahona *et al.* [4], De Simone [8], Padberg [19]) is that UBQP is equivalent to the well-known *max-cut* problem. Since the max-cut problem is $\mathcal{NP}$-hard in the strong sense (Garey *et al.* [11]), so is UBQP, and therefore so is QPB, even in the concave case.

2.4 The Boolean quadric polytope

Padberg [19] associated a family of zero-one polytopes with UBQP, which he called *Boolean quadric polytopes*. The Boolean quadric polytopes are defined as:

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

Note that, unlike in the case of QPB, there are no variables y_{ii}. (There is no need for them, since $x_i^2 = x_i$ when x_i is binary.) We remark that BQP_2 is nothing but the polytope presented in Figure 3.

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):

$$x_i + x_j + x_k \leq y_{ij} + y_{ik} + y_{jk} + 1 \tag{6}$$

$$y_{ij} + y_{ik} \leq x_i + y_{jk}. \tag{7}$$

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 & Hammer [5] and Sherali *et al.* [27]. 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 & Laurent [10]).

Yajima & Fujie [31] 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 $\mathcal{S}$ the set of all feasible solutions to QPB, in the extended (x, y)-space. That is:

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

Note that $\mathcal{S}$ 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 $\mathcal{S}$:

- 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 $K \in \mathbb{R}^d$ 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 & Poljak [15] characterised 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 $\mathcal{S}$.*

Proof. By definition, every extreme point of QPB_n is a member of $\mathcal{S}$. We show that every member of $\mathcal{S}$ is an extreme point. Let $(\bar{x}, \bar{y})$ be an arbitrary point in $\mathcal{S}$. Consider the QPB instance that arises when the objective function is equal to $\sum_{i=1}^n (x_i^2 - 2\bar{x}_i x_i)$. Minimising this function is equivalent to minimising $\sum_{i=1}^n (x_i - \bar{x}_i)^2$. 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 minimises the *linear* function $\sum_{i=1}^n (y_{ii} - 2\bar{x}_i x_i)$. Thus, $(\bar{x}, \bar{y})$ an extreme point of QPB_n. $\square$

Figure 1 enables one to visualise this result for the case $n = 1$: the members of $\mathcal{S}$ 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 $\mathcal{S}$ 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 $n+\binom{n+1}{2}$ of them. Thus there exist $n+\binom{n+1}{2}$ 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 ϵ be a small positive quantity. If we increase x_k by ϵ, we obtain a second extreme point, say (x^+,y^+), that is identical to $(\bar{x},\bar{y})$ except that:

- x_k^+ is increased by ϵ,
- 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 ϵ.

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

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

Since ϵ 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 $n+\binom{n+1}{2}$ linearly-independent normal vectors. $\square$

Indeed, in Figure 1 one sees that there are only two vertices, namely the points at which $x_1 \in \{0,1\}$.

3.3 Invariance under permutation and switching

It is known (see, e.g., Deza & 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 $\phi^\pi : \mathbb{R}^{n+\binom{n+1}{2}} \mapsto \mathbb{R}^{n+\binom{n+1}{2}}$ 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* $1 \le i \le j \le n$.

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

Definition 2 (Switching) *For an arbitrary set* $S \subset \{1, \ldots, n\}$*, let* $\psi^S : \mathbb{R}^{n+\binom{n+1}{2}} \mapsto \mathbb{R}^{n+\binom{n+1}{2}}$ *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* $\{i, j\} \subset S$*,*
- *leaves all other* x_i *and* y_{ij} *variables unchanged.*

Applying the transformation ψ^S *is called* switching *(on* S*).*

It is obvious that QPB_n is invariant under permutation. (That is, for any n and any permutation π 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* $S \subset \{1, \ldots, n\}$, $\psi^S(QPB_n) = QPB_n$.

Proof. Let $(\bar{x}, \bar{y})$ be an extreme point of QPB_n. From Lemma 2, we have $\bar{y}_{ij} = \bar{x}_i \bar{x}_j$ for all $1 \le i \le j \le n$. Now let $(\tilde{x}, \tilde{y}) = \psi^S(\bar{x}, \bar{y})$. From the definition of switching, one can easily show that $0 \le \tilde{x}_i \le 1$ for $1 \le i \le n$, and that $\tilde{y}_{ij} = \tilde{x}_i \tilde{x}_j$ for $1 \le i \le j \le n$. 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 $y_{ij} \ge 0$ and switch on $\{i\}$ or $\{j\}$, we obtain the RLT inequalities $y_{ij} \le x_j$ and $y_{ij} \le x_i$, respectively. If we switch on $\{i, j\}$, we obtain the RLT inequality $y_{ij} \ge x_i + x_j - 1$.

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 $y_{ii} \geq 0$ and $y_{ii} \geq 2x_i - 1$. 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:

$$\begin{aligned} F(v,s) &= \left\{(x,y) \in QPB_n : v^T x + s = 0\right\} \\ K(v,s) &= \left\{x \in [0,1]^n : v^T x + s = 0\right\}. \end{aligned}$$

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 non-empty 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 non-negative linear combination of the RLT inequalities of the form $y_{ij} \geq 0$. $\square$

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 $\binom{n+1}{2} - 1$.*

Proof. First we show that the dimension of $F(v,s)$ is at most $\binom{n+1}{2} - 1$. 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:

$$\sum_{j=1}^{n} v_j y_{ij} + s x_i = 0 \qquad (i = 1, \ldots, n).$$

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 $\binom{n+1}{2} - 1$. 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 ϵ be a small positive quantity. Consider the following $\binom{n+1}{2} - 1$ 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 $\binom{n+1}{2} - 1$ extreme points of QPB_n therefore lie in $F(v,s)$. They can be shown to be affinely-independent. $\square$

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 [20]), 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 non-dominated (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 non-dominated.*

This last result may seem counter-intuitive, 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 non-dominated 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 to 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 [19] called the resulting inequality the 'canonical extension' of the original inequality.

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

We will need the following lemma:

Lemma 5 *Suppose that F is a face of QPB_n whose co-dimension 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 co-dimension at least $n+1$. $\square$

With this lemma, we can prove the following theorem:

Theorem 3 *Suppose that the linear inequality*

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

induces a face of QPB_n of co-dimension k, where $1 \le k \le n$. Then it also induces a face of $QPB_{n'}$ of co-dimension k, for all $n' > n$.

Proof. By induction, it suffices to prove that the inequality induces a face of QPB_{n+1} of co-dimension 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 co-dimension 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:

- $\tilde{x}^k_i = x^k_i$ for $k = 1, \ldots, n+1$ and $i = 1, \ldots, n$,
- $\tilde{x}^k_{n+1} = 1$ 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 $\bar{x}$ be identical to $\tilde{x}^1$, apart from the fact that $\bar{x}_{n+1} = 1/2$. The corresponding extreme point of QPB_{n+1}, say $(\bar{x}, \bar{y})$, also lies in F'. It is affinely independent of the other points mentioned, since it is the only one that does not satisfy the equation $y_{n+1,n+1} = x_{n+1}$. $\square$

5 Facets from the Boolean Quadric Polytope

As mentioned in Subsection 2.4, Yajima & Fujie [31] 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 $\mathbb{R}^{n+\binom{n}{2}}$, respectively. The following proposition states that the projection of QPB_n onto $\mathbb{R}^{n+\binom{n}{2}}$ is nothing but BQP_n:

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

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

is equal to BQP_n.

Proof. Let $(\bar{x}, \bar{y}) \in [0, 1]^{n+\binom{n}{2}}$ lie in the projection, and suppose that $\bar{x}$ is fractional, i.e., that $\bar{x}_k \in (0, 1)$ for some $1 \le k \le n$. 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 $y^0_{ij} = x^0_i x^0_j$ and $y^1_{ij} = x^1_i x^1_j$ for $1 \le i < j \le n$.) Finally, let $\lambda = \bar{x}_k$. One can check that:

$$\begin{aligned} \bar{x}_i &= \lambda x^1_i + (1 - \lambda)x^0_i \quad (i = 1, \dots, n) \\ \bar{y}_{ij} &= \lambda y^1_{ij} + (1 - \lambda)y^0_{ij} \quad (1 \le i < j \le n). \end{aligned}$$

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. □

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*

$$\sum_{i=1}^{n} \alpha_i x_i + \sum_{1 \le i < j \le n} \beta y_{ij} \le \gamma$$

is valid for BQP_n, then it is valid for QPB_n as well.

This implies the above-mentioned result of Yajima & Fujie [31].

From now on, we let $\mathrm{proj}(x, y)$ denote the linear operator that projects points in $\mathbb{R}^{n+\binom{n+1}{2}}$ onto $\mathbb{R}^{n+\binom{n}{2}}$, by simply dropping the components y_{ii} for all $1 \le i \le n$. 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 $\mathrm{proj}(F) = BQP_n$.*

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

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 $0 \le x_1 \le 1$.

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 $j \ne i$ 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 $\mathcal{S}$, and suppose that $\bar{x}_k \in (0, 1)$ for some $1 \le k \le n$. 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, $\mathrm{proj}(\bar{x}, \bar{y})$ is a convex combination of $\mathrm{proj}(x^0, y^0)$ and $\mathrm{proj}(x^1, y^1)$. 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). $\square$

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;*
- $x_i^i \in (0, 1)$ *for* $i = 1, \ldots, n$.
- $x_j^i \in \{0, 1\}$ *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 ith 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 BQP_n, say $(\bar{x}^1, \bar{y}^1), \ldots, (\bar{x}^n, \bar{y}^n)$ and $(\hat{x}^1, \hat{y}^1), \ldots, (\hat{x}^n, \hat{y}^n)$, with the following properties:*

- *each satisfies the inequality at equality;*
- $\hat{x}_j^i = \bar{x}_j^i$ *for* $i = 1, \ldots, n$ *and* $j \neq i$,
- $\bar{x}_i^i = 0$ *and* $\hat{x}_i^i = 1$ *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 & 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 & 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*

$$\sum_{i=1}^{n} v_i(v_i + 2s - 1)x_i + 2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq s(1 - s) \tag{8}$$

is valid for BQP_n.

The inequalities (8) do not always induce facets of BQP_n, but they do under certain conditions (see De Simone [9] and Deza & 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 [19], and the inequalities introduced in Sherali *et al.* [27], which were called *cut-type* inequalities by Yajima & Fujie [31]. 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 & Fujie [31] 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 BQP_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 $(\bar{x}^1, \bar{y}^1), \ldots, (\bar{x}^n, \bar{y}^n)$ and $(\hat{x}^1, \hat{y}^1), \ldots, (\hat{x}^n, \hat{y}^n)$, with the properties described in Corollary 2. For any given $1 \leq i \leq n$, we have three possible cases:

- $v^T \bar{x}^i = v^T \hat{x}^i \in \{0, 1\}$, in which case $v_i = 0$
- $v^T \bar{x}^i = 0$ and $v^T \hat{x}^i = 1$, in which case $v_i = 1$
- $v^T \bar{x}^i = 1$ and $v^T \hat{x}^i = 0$, 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. $\square$

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 $Q_{\alpha,\beta}(x, y) \le \gamma$ be any valid linear inequality for QPB_n, where $\alpha \in \mathbb{R}^n$, $\beta \in \mathbb{R}^{n+\binom{n+1}{2}}$, $\gamma \in \mathbb{R}$, and

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

Also, define the corresponding quadratic form

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

Let us call a valid linear inequality $Q(\alpha, \beta) \le \gamma$ '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 characterise the inequalities of these three different types. Then, in Subsection 6.4, we use these characterisations 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 non-redundant concave inequalities are, essentially, the psd inequalities:

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

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

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 β). Likewise,

$$Q_{\alpha,\beta}(x, y) = \alpha^T x + B \bullet Y,$$

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

$$\begin{aligned} Q_{\alpha,\beta}(x, y) &= \alpha^T x + B \bullet Y \\ &= \alpha^T x + B \bullet (Y - x x^T) + x^T B x \\ &\leq \alpha^T x + x^T B x \\ &= q_{\alpha,\beta}(x), \end{aligned}$$

where the inequality follows from $B \preceq 0$ and $Y - x x^T \succeq 0$. 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 non-redundant 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 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:*

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

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 γ because $Q_{\alpha,\beta}(x, y) \leq \gamma$ is valid for QPB_n by assumption. So:

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

which shows that the inequality

$$\sum_{i=1}^{n}(\alpha_i + \beta_{ii})x_i + \sum_{i<j}\beta_{ij}y_{ij} \le \gamma \tag{9}$$

is valid for BQP_n.

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

$$\begin{aligned}
Q_{\alpha,\beta}(x,y) &= \sum_{i=1}^{n}\alpha_i x_i + \sum_{i\le j}\beta_{ij}y_{ij} \\
&= \sum_{i=1}^{n}\alpha_i x_i + \sum_{i<j}\beta_{ij}y_{ij} + \sum_{i=1}^{n}\beta_{ii}(x_i - x_i + y_{ii}) \\
&\le \sum_{i=1}^{n}\alpha_i x_i + \sum_{i<j}\beta_{ij}y_{ij} + \sum_{i=1}^{n}\beta_{ii}x_i \\
&= \sum_{i=1}^{n}(\alpha_i + \beta_{ii})x_i + \sum_{i<j}\beta_{ij}y_{ij} \\
&\le \gamma,
\end{aligned}$$

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 $Q_{\alpha,\beta}(x, y) \le \gamma$ is valid for QPB_n amounts to checking that $q_{\alpha,\beta}(x)$ does not exceed γ 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

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

where $\bar{x} \in \mathbb{R}^{n-1}$. One can think of $q^{i,\delta}_{\alpha,\beta}(\bar{x})$ as $q_{\alpha,\beta}(x)$ with the value δ 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 $Q^{i,\delta}_{\alpha,\beta}(\bar{x}, \bar{y})$ 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 $Q_{\alpha,\beta}(x,y) \le \gamma$, with $q_{\alpha,\beta}(x)$ indefinite, is valid for QPB_n if and only if the inequality*

$$Q^{i,\delta}_{\alpha,\beta}(\bar{x},\bar{y}) \le \gamma - \alpha_i\delta - \beta_{ii}\delta^2 \tag{10}$$

is valid for QPB_{n-1} for all $i = 1,\dots,n$ and $\delta \in \{0,1\}$.

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

In addition, Proposition 10 provides a finite recursive procedure to check the validity for QPB_n of any given indefinite inequality $Q_{\alpha,\beta}(x,y) \le \gamma$: one simply checks that each of the $2n$ inequalities of the form (10) is valid for QPB_{n-1}. 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 $n \ge 2$, let $\mathcal{V}$ be the collection of all (α,β,γ) such that $q_{\alpha,\beta}(x)$ is indefinite and $Q^{i,\delta}_{\alpha,\beta}(\bar{x},\bar{y}) \le \gamma - \alpha_i\delta - \beta_{ii}\delta^2$ is valid for QPB_{n-1} for all $i = 1,\dots,n$ and $\delta \in \{0,1\}$. Then QPB_n equals*

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

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-Burer [3]). In particular, for $n = 2$, $\text{proj}(x,y) \in BQP_n$ and $y_{ii} \le x_i$ constitute precisely the RLT constraints, while the constraints for $(\alpha,\beta,\gamma) \in \mathcal{V}$ are redundant. Perhaps it is possible to simplify the description for larger n.

6.4 More on QPB_3

Consider the following convex set:

$$\mathcal{Q}_n := \left\{ (x,y) \in [0,1]^{n+\binom{n+1}{2}} : \begin{array}{c} y_{ii} \le x_i \; (1 \le i \le n) \\ \hat{Y} \succeq 0 \\ \text{proj}(x,y) \in BQP_n \end{array} \right\}. \tag{11}$$

From the results given so far, $\mathcal{Q}_n$ contains QPB_n. Moreover, one would expect $\mathcal{Q}_n$ to be a 'tight' approximation to QPB_n. Indeed:

- $\mathcal{Q}_n$ 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 & Burer [3] mentioned in Subsection 2.2.) In particular, it satisfies all RLT inequalities.

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

- $\mathcal{Q}_n$ satisfies all non-redundant 'concave' and 'convex' valid inequalities for QPB_n (as shown in Subsections 6.1 and 6.2).

Moreover, $\mathcal{Q}_3$ gives an even tighter approximation to QPB_3 than the one studied in Anstreicher & Burer [3]. (This is so since the inequalities (2)–(5) are dominated by the triangle inequalities of Padberg [19].)

A natural question to ask at this point is whether $QPB_3 = \mathcal{Q}_3$. In fact, it turns out that QPB_3 is strictly contained in $\mathcal{Q}_3$. To show this, we use the recursive procedure for checking validity discussed before Corollary 3.

Define:

$$\begin{aligned}
&\alpha = (\alpha_1, \alpha_2, \alpha_3) = (3, 1, 0)\\
&\beta = (\beta_{11}, \beta_{12}, \beta_{22}, \beta_{13}, \beta_{23}, \beta_{33}) = (-2.25, -6, 0, -6, -1, 1)\\
&\gamma = 1.
\end{aligned}$$

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

$$\max \left\{ Q_{\alpha,\beta}(x, y) : (x, y) \in \mathcal{Q}_3 \right\}.$$

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

$$\begin{aligned}
&x = (x_1, x_2, x_3) = \tfrac{1}{3}(1, 1, 1)\\
&y = (y_{11}, y_{12}, y_{22}, y_{13}, y_{23}, y_{33}) = \tfrac{1}{9}(2, 0, 3, 0, 1, 3)
\end{aligned}$$

is feasible with objective value $19/18 > 1$. It follows that $Q_{\alpha,\beta}(x, y) \leq \gamma$ is *not* valid for $\mathcal{Q}_3$, which proves that QPB_3 is strictly contained in $\mathcal{Q}_3$.

7 Concluding Remarks

Given the fact that QPB is a fundamental and much-studied problem in global optimisation, 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? And, 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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