Valid inequalities for quadratic optimisation with domain constraints

Published Version:
Galli L., Letchford A.N. (2021). Valid inequalities for quadratic optimisation with domain constraints. DISCRETE OPTIMIZATION, 41, 1-19 [10.1016/j.disopt.2021.100661].

Availability:
This version is available at: https://hdl.handle.net/11585/983194 since: 2024-09-13

Published:
DOI: http://doi.org/10.1016/j.disopt.2021.100661

(Article begins on next page)

Valid Inequalities for Quadratic Optimisation with Domain Constraints

Laura Galli* Adam N. Letchford†

To appear in *Discrete Optimization*

Abstract

In 2013, Buchheim and Wiegele introduced a quadratic optimisation problem, in which the domain of each variable is a closed subset of the reals. This problem includes several other important problems as special cases. We study some convex sets and polyhedra associated with the problem, and derive several families of strong valid inequalities. We also present some encouraging computational results, obtained by applying our inequalities to (a) integer quadratic programs with box constraints and (b) portfolio optimisation problems with semi-continuous variables.

Keywords: mixed-integer nonlinear programming, cutting planes, global optimisation

1 Introduction

Many important problems in operational research, statistics and finance can be formulated as *mixed-integer quadratic programs* or MIQPs [3, 4, 31, 36]. An MIQP with n variables and m constraints takes the form

$$\min \left\{ x^T Q x + c^T x : \, Ax \le b, \, x \in \mathbb{R}^n_+, \, x_i \in \mathbb{Z} \, (i \in I) \right\}, \tag{1}$$

where $Q \in \mathbb{Q}^{n \times n}$, $c \in \mathbb{Q}^n$, $A \in \mathbb{Q}^{m \times n}$, $b \in \mathbb{Q}^m$ and $I \subseteq \{1, \ldots, n\}$.

When Q is *positive semidefinite* (psd), the objective function is convex. Convex MIQPs are strongly $\mathcal{NP}$-hard, but they can sometimes be solved reasonably quickly in practice [5, 14, 24]. The non-convex case, however, is still a formidable challenge [10–12, 34].

*Department of Computer Science, University of Pisa, Largo B. Pontecorvo 3, 56124 Pisa, Italy. E-mail: `laura.galli@unipi.it`

†Department of Management Science, Lancaster University, Lancaster LA1 4YW, United Kingdom. E-mail: `a.n.letchford@lancaster.ac.uk`

In 2013, Buchheim and Wiegele [8] introduced an intriguing quadratic optimisation problem. Their problem takes the form

$$\min \Big\{ x^T Q x + c^T x : \ x_i \in D_i \ (i = 1, \ldots, n) \Big\}, \tag{2}$$

where, for all i, the domain D_i is a closed subset of the reals. They point out that this problem is of interest for at least three reasons:

- When $D_i = \{0, 1\}$ for all i, the problem reduces to *quadratic unconstrained Boolean optimisation* (QUBO), which has a wealth of applications in operational research, mathematics and physics [16].
- When $D_i = [0, 1]$ for all i, we obtain *quadratic programming with box constraints* (QPB), which is a classic problem in global optimisation [9, 15, 37].
- By setting D_i to $\{0\} \cup \big[\ell_i, u_i\big]$ for some $u_i > \ell_i > 0$, we can model *semi-continuous variables*, which have applications in finance and statistics [3, 31, 36].

We will call the problem (2) *quadratic programming with domain constraints* or QPDC. We remark that there are at least three other reasons why QPDC is of interest:

- The *closest vector problem*, a key problem in cryptography and the geometry of numbers, is equivalent to the special case of QPDC in which $D_i = \mathbb{Z}$ for all i [11].
- To check if a symmetric matrix $M \in \mathbb{Q}^{n \times n}$ is *co-positive*, it suffices to minimise $x^T M x$ and set D_i to $\mathbb{R}_+$ for all i.
- Valid inequalities for QPDC can be applied to general MIQPs, especially when lower and/or upper bounds have been imposed on variables during a branch-and-bound process.

In this paper, we study some convex sets associated with QPDC. Following [19, 27], we add extra variables, representing products of pairs of original variables. We then study the closure of the convex hull of feasible solutions in this extended space. After establishing some basic properties of this convex set (extreme points, dimension and so on), we derive several families of strong valid linear inequalities. We also present some encouraging computational results, obtained by applying our inequalities to (a) integer quadratic programs with box constraints and (b) portfolio optimisation problems with semi-continuous variables.

We remark that our work consolidates and extends results in several papers: [6, 30], which were concerned with QUBO, [2, 9, 37], which dealt with QPB, and [11], which covered the cases in which $D_i \in \{\mathbb{R}, \mathbb{Z}\}$ and $D_i \in \{\mathbb{R}_+, \mathbb{Z}_+\}$.

The paper has the following structure. Section 2 reviews the literature. Section 3 defines the convex sets and establishes their basic properties. Section 4 deals with valid inequalities, and Section 5 contains the computational results. Finally, Section 6 gives some concluding remarks.

Throughout the paper, we let N denote $\{1, \ldots, n\}$. We assume without loss of generality (w.l.o.g.) that Q is symmetric and that $|D_i| \geq 2$ for $i \in N$. Given a vector $v \in \mathbb{R}^d$, we let $|v|_1$ and $|v|_2$ denote $\sum_{i=1}^d |v_i|$ and $\sum_{i=1}^d v_i^2$, respectively. We write "LP" for "linear program", "QP" for "quadratic program", "conv" for "convex hull" and "cl" for "closure". We also let $\mathcal{S}_+^n$ denote the cone of real psd matrices of order n.

We assume that the reader is familiar with the basics of polyhedral theory (see [28]). We will also use some concepts from convex analysis (see [22]). Let $S \subset \mathbb{R}^q$ be a closed convex set. A vector $r \in \mathbb{R}^q$ is a *ray* of S if, given any point $p \in S$ and any positive scalar s, the point $p + sr$ is also in S. A point in S (or ray of S) is *extreme* if it is not a convex combination of two other points in S (or rays of S). The *normal cone* of S at an extreme point p is defined as:

$$\big\{\alpha \in \mathbb{R}^q : \ \alpha^T z \leq \alpha^T p \ (z \in S)\big\}.$$

We call an extreme point a *vertex* if its normal cone is full-dimensional. A valid linear inequality for S is called *non-dominated* if it is not implied by two or more stronger valid linear inequalities. A valid inequality $\alpha^T z \leq \beta$ is non-dominated if and only if there exists an extreme point p such that α is an extreme ray of the normal cone at p. (If S is a full-dimensional polyhedron, then the non-dominated valid inequalities are those that define facets.)

2 Literature Review

In this section, we review the relevant literature. Due to space restrictions, we mention only papers of direct relevance.

2.1 0-1 quadratic programs

Glover & Woolsey [19] proposed to convert 0-1 QPs into 0-1 LPs, as follows. For $1 \leq i < j \leq n$, replace the quadratic term $x_i x_j$ with a new binary variable, say y_{ij}, and add the constraints

$$y_{ij} \geq 0, \ y_{ij} \leq x_i, \ y_{ij} \leq x_j, \ y_{ij} \geq x_i + x_j - 1. \qquad (3)$$

Adams & Sherali [1] found a simple way to generate valid inequalities in the (x, y)-space. Take any two valid linear inequalities in the x-space, say $\alpha^T x - \beta \geq 0$ and $\gamma^T x - \delta \geq 0$, and form the quadratic inequality

$\left(\alpha^T x - \beta\right)\left(\gamma^T x - \delta\right) \geq 0$. Then linearise the quadratic inequality using the y variables. This method has come to be known as the *Reformulation-Linearization Technique* or RLT [35].

Padberg [30] studied the following polytope, which he called the *Boolean quadric polytope*:

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

He showed that the constraints (3) define facets, and found some other facet-inducing inequalities, such as the following *triangle* inequalities:

$$x_i + x_j + x_k \leq y_{ij} + y_{ik} + y_{jk} + 1 \quad \big(\{i,j,k\} \subseteq N\big) \tag{4}$$

$$y_{ij} + y_{ik} \leq x_i + y_{jk} \quad \big(i \in N, \ \{j,k\} \subseteq N \setminus \{i\}\big). \tag{5}$$

(Note that i, j and k are assumed to be distinct.)

We will let BQP_n denote the Boolean quadric polytope of order n. Many more valid inequalities have been derived for BQP_n [16]. Among them, we mention the following inequalities, due to Boros & Hammer [6]:

$$2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq \sum_{i \in N} v_i (2s + 1 - v_i) x_i - s(s+1) \qquad \big(v \in \mathbb{Z}^n, \ s \in \mathbb{Z}\big). \tag{6}$$

We will call these *BH* inequalities. Following [16], we call a BH inequality *pure* if $v \in \{0, \pm 1\}^n$. The pure BH inequalities include all of Glover, Woolsey and Padberg's inequalities, and define facets under mild conditions [16].

It is also possible to derive *semidefinite programming* (SDP) relaxations of 0-1 QPs (e.g., [23, 32]). Define the matrix $Y = xx^T$, along with 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 psd, it satisfies $b^T \hat{Y} b \geq 0$ for all $b \in \mathbb{R}^{n+1}$. This implies the following valid inequalities for BQP_n:

$$2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq \sum_{i \in N} v_i (2s - v_i) x_i - s^2 \qquad \big(v \in \mathbb{R}^n, \ s \in \mathbb{R}\big).$$

These inequalities are weaker than the BH inequalities, but the associated separation problem can be solved efficiently [16].

2.2 Non-convex quadratic programs

McCormick [27] considered non-convex QPs in which explicit bounds $0 \leq x \leq u$ are given. He proposed to construct an LP relaxation as follows. For $1 \leq i < j \leq n$, replace $x_i x_j$ with a new continuous variable, say y_{ij}, and add the linear inequalities

$$y_{ij} \geq 0, \ y_{ij} \leq u_j x_i, \ y_{ij} \leq u_i x_j, \ y_{ij} \geq u_j x_i + u_i x_j - u_i u_j. \tag{7}$$

Similarly, for $i \in N$, replace x_i^2 with y_{ii}, and add

$$y_{ii} \geq 0, \; y_{ii} \leq u_i x_i, \; y_{ii} \geq 2u_i x_i - u_i^2. \tag{8}$$

Ramana [33] applied SDP to non-convex QPs. He used the same matrix $\hat{Y}$ that we mentioned in the previous subsection. The resulting inequalities in (x, y)-space are:

$$\sum_{i \in N} v_i^2 y_{ii} + 2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq (2s) v^T x - s^2 \qquad \big(v \in \mathbb{R}^n, \, s \in \mathbb{R}\big). \tag{9}$$

We will follow [9, 18] in calling (9) *psd* inequalities.

Yajima & Fujie [37] studied the following convex set, associated with QPB:

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

They showed that some of the BH inequalities (6) are valid for it.

Burer & Letchford [9] studied Yajima & Fujie's set in more detail. They called it "QPB_n". They showed that, in fact, *any* inequality valid for BQP_n is valid also for QPB_n. They also gave conditions for psd and BH inequalities to define maximal faces of QPB_n.

2.3 More general quadratic problems

Burer & Letchford [11] considered the special case of QPDC in which $D_i \in \big\{\mathbb{R}, \mathbb{R}_+, \mathbb{Z}, \mathbb{Z}_+\big\}$ for all $i \in N$. They showed that the following inequalities are valid for all $s \in \mathbb{Z}$ and all $v \in \mathbb{Z}^n$ such that $v_i = 0$ whenever $D_i \in \big\{\mathbb{R}, \mathbb{R}_+\big\}$:

$$\sum_{i \in N} v_i^2 y_{ii} + 2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq (2s + 1) v^T x - s(s + 1). \tag{10}$$

They call these *split* inequalities. Note that they reduce to the BH inequalities (6) when all variables are binary.

In 2011, Galli *et al.* [18] considered MIQPs of the form (1). They showed the following. Let $v \in \mathbb{R}^n$ and $s, t \in \mathbb{R}$, with $s < t$, be such that every feasible solution satisfies the disjunction $\big(v^T x \leq s\big) \vee \big(v^T x \geq t\big)$. The following *gap* inequality is valid:

$$\sum_{i \in N} v_i^2 y_{ii} + 2 \sum_{1 \leq i < j \leq n} v_i v_j y_{ij} \geq (s + t) v^T x - st. \tag{11}$$

The gap inequalities are a generalisation of some inequalities that were found earlier for the so-called *cut polytope* [26]. Note that the gap inequalities reduce to split inequalities when $v \in \mathbb{Z}^n$, $s \in \mathbb{Z}$ and $t = s + 1$.

Finally, we mention that there are several other works concerned with strengthening McCormick relaxations of bounded MIQPs (e.g., [10, 12, 34, 35]). We omit details for brevity.

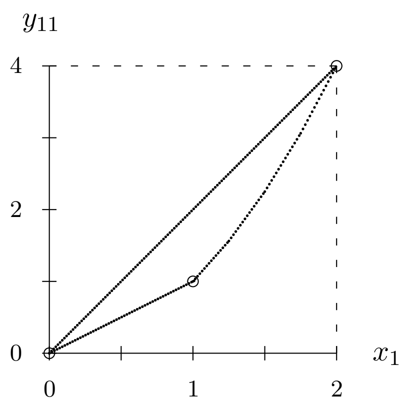

Figure 1: Convex set C when $n = 1$ and $D_1 = \{0\} \cup [1, 2]$.

3 The Convex Sets

In this section, we define the convex sets and derive some of their properties.

3.1 Preliminaries

For $1 \le i \le j \le n$, we let y_{ij} denote the product $x_i x_j$. We also identify y_{ij} and y_{ji} when convenient. We then define the sets

$$\begin{aligned} S_x &= \left\{ x \in \mathbb{R}^n : \, x_i \in D_i \ (i \in N) \right\} \\ S_{xy} &= \left\{ (x, y) \in \mathbb{R}^{n + \binom{n+1}{2}} : \, x \in S_x, \ y_{ij} = x_i x_j \ (1 \le i \le j \le n) \right\}. \end{aligned}$$

The convex set of interest in this paper is then

$$C = \text{cl conv} \left\{ S_{xy} \right\}.$$

(Of course, if the D_i are bounded, the closure operator is unnecessary.)

Figure 1 shows C for the case $n = 1$ and $D_1 = \{0\} \cup [1, 2]$. Note that, even in this simple case, C is not polyhedral, since the lower convex envelope of C, over the interval $[1, 2]$, is defined by the nonlinear inequality $y_{11} \ge x_1^2$. Yet, C has two facets, defined by the (McCormick) inequality $y_{11} \le 2x_1$ and the (gap) inequality $y_{11} \ge x_1$.

Figure 1 is instructive for another reason. Observe that the (psd) inequality $y_{11} \ge 2x_1 - 1$ is non-dominated, but it does not define a facet of C. In fact, it does not even define a maximal face. So, when C is non-polyhedral, linear inequalities that do not define maximal faces can still be of interest.

We will find the following lemma useful.

Lemma 1 *For $i \in N$, let s_i, t_i be scalars with $s_i \neq 0$. Given any pair $(x, y) \in S_{xy}$, let $x' \in \mathbb{R}^n$ be the vector obtained from x by setting x'_i to $s_i x_i + t_i$ for $i \in N$, and let $y' \in \mathbb{R}^{\binom{n+1}{2}}$ be the vector obtained by setting y'_{ij} to $x'_i x'_j$ for $1 \leq i \leq j \leq n$. Finally, let C' be the closure of the convex hull of all possible pairs (x', y'). Then C and C' are affinely congruent.*

Proof. By definition, we have

$$y'_{ij} = \big(s_i s_j\big) y_{ij} + \big(s_i t_j\big) x_i + \big(t_i s_j\big) x_j + t_i t_j \quad (1 \leq i \leq j \leq n).$$

The map from (x, y) to (x', y') is clearly affine and invertible. □

An immediate consequence of this lemma is that a complete linear description of C' yields a complete linear description of C. Accordingly, we make the following assumptions w.l.o.g. in the remainder of the paper.

- $0 \in D_i$ for all $i \in N$ (i.e., the origin belongs to S_x);
- For each $i \in N$, exactly one of the following holds: (a) x_i is neither lower-bounded nor upper-bounded (i.e., D_i has no minimum or maximum element), (b) x_i is lower-bounded but not upper-bounded (i.e., D_i has 0 as its minimum element but does not have a maximum), or (c) x_i is both lower- and upper-bounded (i.e., D_i has 0 as its minimum element and some positive constant u_i as its maximum).

Note that these assumptions imply that $|D_i| = 2$ if and only if $D_i = \big\{0, u_i\big\}$.

3.2 Polyhedrality

The following lemma gives a necessary and sufficient condition for C to be polyhedral:

Lemma 2 *C is polyhedral if and only if $|D_i|$ is finite for all i.*

Proof. Sufficiency is obvious. Now suppose that D_i contains a closed interval. Let C' be the projection of C into a two-dimensional subspace, having x_i and y_{ii} as axes. As shown in Figure 1, the lower convex envelope of C', over the given interval, is defined by the nonlinear inequality $y_{ii} \geq x_i^2$.

Suppose instead that D_i consists of an infinite but countable number of points. Figure 2, taken from [11], shows C' for the case $D_i = \mathbb{Z}_+$. It is apparent that C' has an infinite number of facets, and therefore is not polyhedral. □

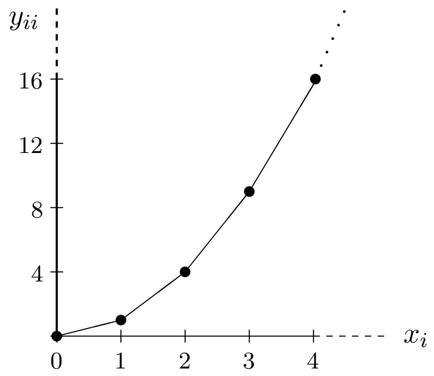

Figure 2: Projection C' when $D_i = \mathbb{Z}_+$.

3.3 Extreme points, rays and vertices

Next, we look at the extreme points, extreme rays, and vertices of C. The extreme points are easy:

Lemma 3 *A pair (x, y) is an extreme point of C if and only if $(x, y) \in S_{xy}$.*

Proof. Similar to Lemma 2 in [9]. □

The rays are more complicated. We will need the following definition.

Definition 1 *We say that a non-zero vector $v \in \mathbb{R}^n$ is "approachable" if there exists an infinite sequence of vectors $x^1, x^2, \ldots$ in S_x and an infinite sequence of positive scalars $s_1, s_2, \ldots$ such that both s_k and $\left|v - s_k x^k\right|_1$ tend to zero as k goes to infinity.*

For example, if $n = 2$ and $D_1 = D_2 = \mathbb{Z}_+$, then the vector $\left(1, \sqrt{2}\right)$ is approachable, because we can set x^k to $\left(k, \lfloor\sqrt{2}k\rfloor\right)$ and s_k to $1/k$.

Proposition 1 *Suppose that the non-zero vector $v \in \mathbb{R}^n$ is approachable. Define the vector $\hat{v} \in \mathbb{R}^{\binom{n+1}{2}}$ by setting $\hat{v}_{ij}$ to $v_i v_j$ for all i and j. Then $\left(0, \hat{v}\right)$ is an extreme ray of C, and all extreme rays of C are of this type.*

Proof. Let $\left(x^0, y^0\right)$ be the origin in $\mathbb{R}^{n+\binom{n+1}{2}}$, and let $x^1, x^2, \ldots$ and $s_1, s_2, \ldots$ be the infinite sequence associated with v. Also let $\left(x^k, y^k\right)$ be the point in S_{xy} that corresponds to x^k. Now consider the following point, which is a convex combination of $\left(x^0, y^0\right)$ and $\left(x^k, y^k\right)$:

$$\left(1 - s_k^2\right)\left(x^0, y^0\right) + s_k^2\left(x^k, y^k\right) = s_k^2\left(x^k, y^k\right).$$

This tends to $(0, \hat{v})$ as k goes to infinity. This establishes that $(0, \hat{v})$ is a ray. The fact that the ray is extreme follows easily from the fact that every matrix of the form xx^T for some $x \in \mathbb{R}^n$ is an extreme point of $\mathcal{S}_+^n$ [21].

Now, let M be a large positive real. If any point $(x, y) \in S_{xy}$ satisfies $|x_i| \geq M$ for some $i \in N$, then it also satisfies $y_{ii} \geq M^2$. Thus, in any extreme ray, at least one of the variables y_{ii} must take a positive value. In particular, y cannot be the zero vector. So we can assume that any extreme ray $(\bar{x}, \bar{y})$ has been scaled so that $|\bar{y}| = 1$.

Assume that we have such a ray. Let k be a positive integer, and let ϵ be a small positive constant. From the definition of C and the definition of extreme rays, we can find a point $(x^k, y^k) \in S_{xy}$ with norm at least 2^k such that

$$\left| (\bar{x}, \bar{y}) - \frac{(x^k, y^k)}{|(x^k, y^k)|} \right| \leq \epsilon.$$

Now observe that $|x^k| = \sqrt{|y^k|}$, and therefore $|x^k| / |(x^k, y^k)| \leq 2^{-k/2}$. Since k can be made arbitrarily large and ϵ arbitrarily small, $\bar{x}$ must be the zero vector.

Finally, define a vector $v \in \mathbb{R}^n$ by setting v_i to $\sqrt{\bar{y}_{ii}}$ for all $i \in N$. As k tends to infinity and ϵ tends to 0, $y_{ii}^k / |(x^k, y^k)|$ approaches v_i^2. This implies that $x^k / |(x^k, y^k)|$ approaches v. Thus, v is approachable and $\bar{y} = \hat{v}$. □

Finally, to characterise the vertices, we will need the following definition.

Definition 2 *For a given $i \in N$, we say that a given $s \in D_i$ is a "low-point" if there exists some $\epsilon > 0$ such that $[s - \epsilon, s] \cap D_i = \{s\}$. Similarly, we call it a "high-point" if there exists some $\epsilon > 0$ such that $[s, s + \epsilon] \cap D_i = \{s\}$. A point that is a high-point or a low-point will be called a "boundary point". A point that is both a high-point and a low-point will be called "isolated".*

For example, if $D_i = \mathbb{R}_+$, then 0 is both a low-point and a boundary point. If $D_i \subseteq \mathbb{Z}$, then every point in D_i is an isolated boundary point.

Theorem 1 *A point $(x^*, y^*) \in S_{xy}$ is a vertex of C if and only if x_i^* is a boundary point for all $i \in N$.*

Proof. Suppose the stated condition on x^* holds. From Lemma 1, we can assume w.l.o.g. that (a) x^* is the origin and (b) 0 is a low-point for all $i \in N$. Observe that, for all $i \in N$, the inequality $x_i \geq 0$ is valid and satisfied at equality by (x^*, y^*). Also, for $1 \leq i \leq j \leq n$, the inequality $y_{ii} \geq 0$ is satisfied at equality by (x^*, y^*). This gives $n + \binom{n}{2}$ tight inequalities in total, and they are linearly independent. Thus, the normal cone at (x^*, y^*) is full-dimensional. This proves sufficiency.

The proof of necessity is similar to that of Theorem 1 in [9]. □

3.4 Dimension and affine hull

The next thing to settle is the dimension and affine hull of C.

Lemma 4 *If $|D_i| = 2$ for some $i \in N$, then all points in S_{xy} and C satisfy the equation*

$$y_{ii} = u_i x_i. \tag{12}$$

Proof. Trivial. □

Proposition 2 *If $|D_i| > 2$ for all $i \in N$, then C is full-dimensional. Otherwise, a complete and non-redundant description of the affine hull of C is given by the equation (12) for all $i \in N$ with $|D_i| = 2$.*

Proof. Suppose that $|D_i| > 2$ for all $i \in N$. For each $i \in N$, let a_i and b_i be distinct members of $D_i \setminus \{0\}$. We construct a point in S_x, which we call x^0, by setting x_i to 0 for all i. For $i \in N$, we construct another point in S_x by taking x^0 and changing x_i to a_i. Next, for any pair $\{i, j\}$ with $1 \le i < j \le n$, we construct another point in S_x by taking x^0 and changing x_i and x_j to a_i and a_j, respectively. Finally, for $i \in N$, we construct still another point in S_x, which we call x^i, by taking x^0 and changing x_i to b_i. This gives a total of $1 + n + \binom{n+1}{2}$ points in S_x. One can check that the corresponding points in S_{xy} are affinely independent.

Now suppose that $|D_i| = 2$ for some $i \in N$. We can set a_i to u_i, but then b_i does not exist. As a result, we can construct all of the above-mentioned points in S_x, apart from x^i. Thus, the dimension of C drops by one for each such index i. □

4 Valid Inequalities and Facets

In this section, we consider various valid inequalities for C. Subsections 4.1 to 4.3 deal with McCormick, psd and gap inequalities, respectively. Subsections 4.4 and 4.5 give two different procedures for converting valid inequalities for the Boolean quadric polytope into valid inequalities for C.

4.1 McCormick Inequalities

First, we consider the McCormick inequalities (7), (8). The results in this subsection generalise the results in Subsection 4.1 of [9].

The following three propositions deal with the inequalities (7).

Proposition 3 *Suppose that x_i and x_j are lower-bounded, so that the McCormick inequality $y_{ij} \ge 0$ is valid for C. This inequality defines a facet.*

Proof. Let F be the face of C defined by the inequality. Observe that a point $(x,y) \in S_{xy}$ lies in F if and only if at least one of x_i and x_j is 0. One can check that all but one of the members of S_{xy} in the proof of Proposition 2 meet this condition. □

Proposition 4 *Suppose that x_i is lower-bounded and x_j is upper-bounded, so that the McCormick inequality $y_{ij} \leq u_j x_i$ is valid for C. This inequality defines a facet.*

Proof. We apply Lemma 1, setting x'_j to $u_j - x_j$, and setting x'_k to x_k for $k \in N \setminus \{j\}$. Note that $y'_{ij} = x_i(u_j - x_j) = u_j x_i - y_{ij}$. Thus, the inequality $y_{ij} \leq u_j x_i$, which is valid for C, maps to the inequality $y'_{ij} \geq 0$, which is valid for C'. The result then follows from Proposition 3. □

Proposition 5 *Suppose that x_i and x_j are both upper-bounded, so that the McCormick inequality $y_{ij} \geq u_j x_i + u_i x_j - u_i u_j$ is valid for C. This inequality defines a facet.*

Proof. We apply Lemma 1, setting x'_i to $u_i - x_i$, x'_j to $u_j - x_j$, and x'_k to x_k for $k \in N \setminus \{i,j\}$. Note that $y'_{ij} = \big(u_i - x_i\big)\big(u_j - x_j\big) = y_{ij} - u_j x_i - u_i x_j + u_i u_j$. Thus, the inequality $y_{ij} \geq u_j x_i + u_i x_j - u_i u_j$, which is valid for C, maps to the inequality $y'_{ij} \geq 0$, which is valid for C'. The result then again follows from Proposition 3. □

Next, we consider one of the inequalities in (8).

Proposition 6 *Suppose that x_i is upper-bounded, so that the McCormick inequality $y_{ii} \leq u_i x_i$ is valid for C. If $|D_i| > 2$, the inequality defines a facet of C. If $|D_i| = 2$, it does not define a proper face.*

Proof. The proof that the inequality defines a facet when $|D_i| > 2$ is similar to the proof of Proposition 2, the main difference being that we use u_i in place of a_i when constructing the members of S_x. If $|D_i| = 2$, then all points in C satisfy the McCormick inequality at equality (as already shown in Lemma 4). □

The remaining McCormick inequalities (i.e., those of the form $y_{ii} \geq 0$ and $y_{ii} \geq 2u_i x_i - u_i^2$) are dealt with in the next subsection. To end the current subsection, we mention one more result.

Proposition 7 *Suppose that x_i is lower-bounded, so that the inequality $x_i \geq 0$ is valid for C. If x_j is upper-bounded for some $j \in N \setminus \{i\}$, the inequality is dominated by McCormick inequalities. The same is true if $|D_i| > 2$ and x_i is upper-bounded. In all other cases, the inequality defines a facet.*

Proof. If x_j is upper-bounded for some $j \in N \setminus \{i\}$, then the inequality is dominated by the McCormick inequalities $y_{ij} \geq 0$ and $y_{ij} \leq u_j x_i$. If $|D_i| > 2$ and x_i is upper-bounded, then the inequality is dominated by the McCormick inequalities $y_{ii} \geq 0$ and $y_{ii} \leq u_i x_i$.

Now suppose that none of the x variables are upper-bounded. Let F be the face of C defined by the inequality $x_i \geq 0$. Most of the points in S_{xy} mentioned in the proof of Proposition 2 lie on F, but there are $n+1$ points that do not. So we have $\dim(C) - n$ affinely independent points on F. To complete the proof, we need n additional points or rays. By Proposition 1, we can obtain a ray for each $j \in N$, by setting all variables to zero, apart from y_{ij}, which is set to 1. One can check that these n rays, plus the $\dim(C) - n$ points already mentioned, are affinely independent.

A similar proof works when $|D_i| = 2$ and x_j is not upper-bounded for all $j \in N \setminus \{i\}$. The only difference is that the dimension of C drops by one, and we therefore do not need to use a ray with $y_{ii} = 1$. □

4.2 Psd inequalities

Next, we consider Ramana's psd inequalities (9). The results in this subsection generalise some of the results in Subsection 4.2 of [9].

We start with a simple observation.

Lemma 5 *The McCormick inequalities $y_{ii} \geq 0$ and $y_{ii} \geq 2u_i x_i - u_i^2$ are psd inequalities.*

Proof. The first is obtained by setting v_i to 1, s to 0, and v_j to 0 for all $j \in N \setminus \{i\}$. The second is obtained by changing s to u_i. □

Next, we show that psd inequalities almost never define facets.

Proposition 8 *If $n > 1$ or $|D_1| > 2$, then none of the psd inequalities (9) define facets of C. If $n = 1$ and $|D_1| = 2$, then the only facet-defining inequalities are the ones mentioned in Lemma 5 (with i set to 1).*

Proof. Let F be the face of C defined by a given psd inequality. Note that the psd inequality can be derived by linearising the quadratic inequality $\left(v^T x - s\right)^2 \geq 0$. Thus, all points in F satisfy the equation $v^T x = s$. This implies that all points in F also satisfy the (quadratic) equation $\left(v^T x - s\right) x_i = 0$ for all $i \in N$. Linearising these quadratic equations (as in the RLT) yields n additional linear equations that are all satisfied by F. This immediately shows that F cannot be a facet when C is full-dimensional.

Now suppose that C is not full-dimensional, but $n > 1$. At least one of the n RLT equations involves a variable y_{ij} with $i \neq j$. Such an equation is not a linear combination of the equations (12). Thus, F cannot be a facet in this case either. The case $n = 1$ and $|D_1| = 2$ is trivial. □

To make further progress, we need to define some more convex sets. Recall the definition of $\hat{Y}$ from Subsection 2.1, and let $\hat{Y}_{00}$ denote the top-left entry in $\hat{Y}$. Define:

$$\hat{\mathcal{S}} = \text{conv}\left\{\hat{Y} \in \mathcal{S}_+^{n+1} : \hat{Y}_{00} = 1\right\}$$
$$\hat{C} = \text{cl conv}\left\{\hat{Y} \in \mathcal{S}_+^{n+1} : \hat{Y} = \begin{pmatrix}1\\x\end{pmatrix}\begin{pmatrix}1\\x\end{pmatrix}^T \text{ for some } x \in S_x\right\}.$$

Note that $\hat{\mathcal{S}}$ has dimension $\binom{n+1}{2} + n$. Moreover, each psd inequality is non-dominated and defines a maximal face of $\hat{\mathcal{S}}$ of dimension $\binom{n+1}{2} - 1$. (These facts follow from analogous results on the psd cone; see, e.g., [21].) As for $\hat{C}$, it is clearly affinely congruent to C, since $y_{ij} = \hat{Y}_{ij} = \hat{Y}_{ji}$ for $1 \le i \le j \le n$. Moreover, $\hat{C} \subseteq \hat{\mathcal{S}}$, and therefore its dimension is at most $\binom{n+1}{2} + n$.

We can now present another result concerned with psd inequalities.

Proposition 9 *Suppose that C is full-dimensional (and therefore $|D_i| > 2$ for all i.) Let $v \in \mathbb{R}^n$ and $s \in \mathbb{R}$ be given. Let $\hat{N} = \{i \in N : v_i \neq 0\}$. Suppose there exists a point $x^* \in S_x$ and constants t_i, t'_i for all $i \in \hat{N}$ such that (a) $v^T x^* = s$, (b) $t_i < x^*_i < t'_i$ for all $i \in \hat{N}$, and (c) $[t_i, t'_i] \subseteq D_i$ for all $i \in \hat{N}$. Then the psd inequality (9) is non-dominated, and it defines a maximal face of C. The dimension of this face is $\binom{n+1}{2} - 1$.*

Proof. Assume w.l.o.g. that $\hat{N} = \{1, \ldots, k\}$. Let F be the face of C defined by the psd inequality, and let (x^*, y^*) be the member of S_{xy} that corresponds to x^*. Condition (a) ensures that $(x^*, y^*) \in F$. Conditions (b) and (c) ensure that the intersection of the hyperplane $v^T x = s$ with S_x has dimension at least $k - 1$. In particular, there exist $k - 1$ linearly independent vectors, say $x^1, \ldots, x^{k-1}$, such that, for $h = 1, \ldots, k-1$, we have (i) $v^T x^h = 0$ and (ii) $x^h_i = 0$ for all $i \in N \setminus \hat{N}$.

Now observe that there exists a small quantity $\epsilon > 0$ such that the point $x^* + \epsilon(x^h + x^{h'})$ lies in S_x for $1 \le h \le h' \le k$. This implies of course that $x^* + \epsilon x^h$ also lies in S_x for all h. In this way, we obtain an additional $k + \binom{k}{2}$ affinely independent points in S_{xy} that lie on F.

Next, for $h = 1, \ldots, k$ and $i = k+1, \ldots, n$, we create another point in S_x by taking $x^* + \epsilon x^h$ and changing the value of x_i to another value in D_i. This gives another $k(n-k)$ affinely independent points in S_{xy} that lie on F.

Next, using the same approach as in the proof of Proposition 2, we can create $(n-k) + \binom{n-k+1}{2}$ additional affinely independent points in S_{xy} that lie on F, by adjusting the values of $x_{k+1}, \ldots, x_n$. This gives $\binom{n+1}{2}$ points in total, which shows that the dimension of F is at least $\binom{n+1}{2} - 1$.

Now, F is contained in the face of $\hat{\mathcal{S}}$ defined by the psd inequality. This latter face is maximal and has dimension $\binom{n+1}{2} - 1$. Thus, F must also be maximal and have the same dimension. Finally, to show that F is non-dominated, it suffices to show that the normal cone of C at (x^*, y^*) has the same dimension as the normal cone of $\hat{\mathcal{S}}$ at the corresponding point Y^*. We omit details for brevity. □

Together with Lemma 5, this yields the following corollaries.

Corollary 1 *Suppose that C is full-dimensional. The McCormick inequality $y_{ii} \geq 0$ defines a maximal face of C if and only if 0 is not a boundary point of D_i. It is non-dominated if and only if 0 is not isolated in D_i.*

Proof. The fact that the inequality defines a maximal face when 0 is not a boundary point follows from Proposition 9. The same proposition shows that the inequality is non-dominated when 0 is not a boundary point.

Now suppose that 0 is a high-point, and let ϵ be the smallest positive member of D_i. The inequality $y_{ii} \geq \epsilon x_i$ is valid for C, and it defines a face that strictly contains the face defined by the McCormick inequality. A similar argument applies if 0 is a low-point.

Next, suppose that 0 is isolated. Let ϵ_1 be the smallest positive member of D_i, and let ϵ_2 be the largest negative member. The (gap) inequalities $y_{ii} \geq \epsilon_1 x_i$ and $y_{ii} \geq -\epsilon_2 x_i$ are valid for C, and they dominate the McCormick inequality.

To complete the proof, one must show that the McCormick inequality is non-dominated when 0 is a non-isolated boundary point. This too can be shown via a consideration of normal cones. We omit details, for brevity. □

Corollary 2 *Suppose that C is full-dimensional. The McCormick inequality $y_{ii} \geq 2u_i x_i - u_i^2$ never defines a maximal face of C. It is non-dominated if and only if u_i is not isolated in D_i.*

Proof. Similar to the previous proof. □

We leave as an open question the problem of finding a necessary and sufficient condition for a psd inequality to define a maximal face of C. We do the same with the problem of finding a necessary and sufficient condition for a psd inequality to be non-dominated. (Recall from Subsection 3.1 that a psd inequality can be non-dominated even when it does not define a maximal face of C.)

We end this subsection by mentioning that the separation problem for the psd inequalities can be solved in polynomial time. This follows from the fact that membership of the psd cone can be checked in polynomial time [20].

4.3 Gap inequalities

Next, we briefly turn our attention to the gap inequalities (11). A difficulty with gap inequalities is that, even when $D_i = \{0, 1\}$ for all i, it is $\mathcal{NP}$-hard to check whether a given gap inequality is valid [25]. Moreover, nobody has yet found a necessary and sufficient condition for a gap inequality (or even a BH inequality) to define a facet of BQP_n [16, 26].

For these reasons, we content ourselves with presenting and analysing a very simple family of gap inequalities. Let us say that the open interval $(s,t) \subset \mathbb{R}$ is an "i-gap" if (a) s is a high-point, (b) t is a low-point, and (c) $[s,t] \cap D_i = \{s,t\}$. We have the following proposition.

Proposition 10 *If $|D_i| > 2$ and (s,t) is an i-gap, then the "simple" gap inequality*

$$y_{ii} \geq (s+t)x_i - st \tag{13}$$

defines a facet of C.

Proof. To see that (13) is indeed a gap inequality, just note that the disjunction $\big(x_i \leq s\big) \vee \big(x_i \geq t\big)$ is valid. The facet proof is similar to the proof of Proposition 2, the main difference being that we use s and t in place of 0 and a_i, respectively, when constructing the members of S_x. □

It turns out that the separation problem for the simple gap inequalities can be solved efficiently, under a very mild assumption on the domains D_i. A more precise statement is given in the following definition and proposition.

Definition 3 *The domain D_i is said to be "well-behaved" if there exists a polynomial-time algorithm for the following problem: given some $r \in \mathbb{R}$, check whether $r \in D_i$ and, if not, output an i-gap that contains r.*

Proposition 11 *For a given $i \in N$, let C'_i denote the projection of C into a two-dimensional subspace, having x_i and y_{ii} as axes. If D_i is well-behaved, then the separation problem for C'_i can be solved in polynomial time.*

Proof. Let (x^*, y^*) be the point to be separated. If x_i is lower-bounded and $x^*_i < 0$, the trivial inequality $x_i \geq 0$ is violated. Similarly, if x_i is upper-bounded and $x^*_i > u_i$, the trivial inequality $x_i \leq u_i$ is violated. If x_i is both lower- and upper-bounded, and $y^*_{ii} > u_i x^*_i$, the McCormick inequality $y_{ii} \leq u_i x_i$ is violated.

Now suppose that none of the above cases apply. We run the algorithm to find out whether $x^*_i \in D_i$. If it is, we check the psd inequality $y_{ii} \geq (2x^*_i)x_i - (x^*_i)^2$ for violation. If not, x^*_i must lie in an i-gap (s,t). In that case, we check the simple gap inequality (13) for violation. □

4.4 Stretched BQP Inequalities

In this subsection, we present a simple procedure for converting valid inequalities for BQP_n into valid inequalities for C. The starting point is the following lemma.

Lemma 6 *Let $M \subseteq N$ be the set of indices of variables that are both lower- and upper-bounded, and suppose that $m = |M| \geq 2$. If the inequality*

$$\sum_{i \in M} \alpha_i x_i + \sum_{\{i,j\} \subseteq M} \beta_{ij} y_{ij} \geq \gamma \tag{14}$$

is valid for BQP_m, then the "stretched" inequality

$$\sum_{i \in M} \frac{\alpha_i}{u_i} x_i + \sum_{\{i,j\} \subseteq M} \frac{\beta_{ij}}{u_i u_j} y_{ij} \geq \gamma \tag{15}$$

is valid for C.

Proof. By assumption, we have $D_i \subseteq [0, u_i]$ for all $i \in M$. In other words, $x_i/u_i \in [0,1]$ for all $i \in M$. Thus, the projection of C into the subspace defined by the indices in M is contained in an affine image of QPB_m. Moreover, it was shown in [9] that any inequality that is valid for BQP_m is valid also for QPB_m. □

Although the above lemma may appear trivial, it yields a huge new class of facet-defining inequalities for C.

Proposition 12 *Let M and m be as in Lemma 6. If (14) is a pure BH inequality that defines a facet of BQP_m, then the inequality (15) defines a facet of C.*

Proof. Let F, F' and F'' be the faces of BQP_m, QPB_m and C, respectively, defined by the pure BH inequality. If F is a facet of BQP_m, then it contains $\binom{m+1}{2}$ affinely independent points. Each of these points can be converted into a point in F' simply by setting y_{ii} to x_i for all $i \in M$, or converted into a point in F'' by setting x_i to some value in D_i for all $i \in N \setminus M$.

Now, it is shown in Subsection 5.2 of [9] that, for each $i \in M$, at least one of the given points in F' has the property that, if we change the value of x_i to an arbitrary fractional value, we obtain an additional affinely independent point in F'. Thus, if $|D_i| \geq 3$ for any $i \in M$, we can create an additional affinely independent point in F''. □

We remark that the Glover–Woolsey inequalities (3) are pure BH inequalities, and an application of Proposition 12 to them yields the McCormick inequalities (7). As a more interesting example, consider a QPDC instance with $D_i = D_j = D_k = \{0, 1, 2\}$ for some $\{i, j, k\} \subseteq N$. Taking Padberg's triangle inequality (4) and applying Proposition 12 shows that the following "stretched triangle" inequality defines a facet of C:

$$(x_1 + x_2 + x_3)/2 \leq \big(y_{ij} + y_{ik} + y_{jk}\big)/4 + 1.$$

One can check that this inequality is not a McCormick, psd or gap inequality.

4.5 Internal BQP inequalities

Perhaps surprisingly, there exists a completely different way to convert valid inequalities for BQP_n into valid inequalities for C. We call the resulting inequalities "internal", because they involve a consideration of the "interior" of the D_i (unlike the inequalities in the previous subsection, which looked at the D_i from the "exterior".) The results in this subsection generalise some of the results in Subsection 5.3 of [11].

Our starting point is the following proposition.

Proposition 13 *Let M be a subset of N, with $m = |M| \geq 2$. Suppose that the following hold for each $i \in M$: (a) the interval $(0,1)$ is an i-gap, and (b) $|D_i|$ is finite. Suppose also that the inequality*

$$\sum_{i \in M} \alpha_i x_i + \sum_{\{i,j\} \subseteq M} \beta_{ij} y_{ij} \geq \gamma \tag{16}$$

defines a facet of BQP_m. Then there exists at least one vector $\delta \in \mathbb{R}^m_+$ such that the inequality

$$\sum_{i \in M} \alpha_i x_i + \sum_{\{i,j\} \subseteq M} \beta_{ij} y_{ij} + \sum_{i \in M} \delta_i \big(y_{ii} - x_i\big) \geq \gamma \tag{17}$$

defines a facet of C.

Proof. Since $(0,1)$ is an i-gap for all $i \in M$, the simple gap inequality $y_{ii} \geq x_i$ is valid for each $i \in M$. Let F be the face of C defined by these simple gap inequalities, and note that a pair $(x,y) \in S_{xy}$ lies on F if and only if $x_i \in \{0,1\}$ for all $i \in M$.

Now, let F' be the facet of BQP_m defined by (16). Given that F' is a facet, it must have $\binom{m+1}{2}$ affinely independent extreme points. Each of these points can be converted into an extreme point of F simply by setting x_i to an arbitrary value in D_i, for $i \in N \setminus M$, and determining the values of the y variables accordingly. Then, using the same argument as in the proof of Proposition 2, one can easily construct enough additional affinely independent extreme points of F to show that the inequality (17) defines a facet of F.

Finally, since F is a face of C, and $|D_i|$ is finite for all $i \in M$, there exists some $\delta \in \mathbb{R}^m_+$ such that the inequality (17) is valid for C. To ensure that (17) defines a facet, it suffices to compute δ via sequential lifting [29]. □

To make this proposition more clear, we give an example.

Example 1: Suppose that $D_i = D_j = \{0, 1, \ldots, u\}$, where $u > 1$ is an integer. The Glover–Woolsey inequality $x_i - y_{ij} \geq 0$ defines a facet of BQP_2, but it is not valid for C. If we set δ_i and δ_j to $1/2$, we obtain

$$x_i - y_{ij} + \frac{1}{2}\big(y_{ii} - x_i\big) + \frac{1}{2}\big(y_{jj} - x_j\big) \geq 0,$$

or, equivalently,

$$y_{ii} + y_{jj} - 2y_{ij} \geq -x_i + x_j.$$

This is a special case of the split inequality (10), obtained when $v_i = 1$, $v_j = -1$ and $s = -1$. It therefore defines a facet of C.

If we set δ_i to 0 and δ_j to $u/2$ instead, we obtain:

$$x_i - y_{ij} + \frac{u}{2}\big(y_{jj} - x_j\big) \geq 0.$$

One can check that this inequality also defines a facet of C. □

If $|D_i|$ is not finite for all $i \in M$, the inequalities (17), may or may not define facets of C. This is shown in the following example.

Example 2: Suppose that $D_i = \{0\} \cup [1, u_i]$ for all $i \in M$, where $u_i > 1$. The Glover–Woolsey inequality $x_i - y_{ij} \geq 0$ is not valid for C. If we set δ_i to 0 and δ_j to u_i, we obtain:

$$x_i - y_{ij} + u_i y_{jj} - u_i x_j \geq 0. \tag{18}$$

One can check that this inequality is both valid for C and non-dominated. However, it does not define a facet, because all points in S_{xy} satisfying it at equality also satisfy the equation $y_{jj} = x_j$.

The Glover-Woolsey inequality $y_{ij} - x_i - x_j \geq -1$ is not valid for C either. If we set δ_i and δ_j to 1, we obtain:

$$y_{ii} + y_{jj} + y_{ij} - 2x_i - 2x_j \geq -1. \tag{19}$$

One can check that this inequality is also valid and non-dominated. It does not define a facet of C either, because all points in S_{xy} satisfying it at equality also satisfy the equations $y_{ii} = x_i$ and $y_{jj} = x_j$.

Finally, the Glover–Woolsey inequality $y_{ij} \geq 0$ is already valid for C, so we can set δ_i and δ_j to 0. We already showed that the inequality is facet-defining (Proposition 3). □

Observe that Proposition 13 applies only when $(0, 1)$ is an i-gap for all $i \in M$. This is rather restrictive. Fortunately, one can use Lemma 1 to obtain a much more general result. Suppose that $\big(s_i, t_i\big)$ is an i-gap. Let us define a new variable, say x'_i, using the identity $x'_i = (x_i - s_i)/(t_i - s_i)$. The interval $(0, 1)$ is an i-gap for x'_i. Doing this for all $i \in M$, we can map each i-gap to $(0, 1)$. We can then generate "internal" BQP inequalities in the (x', y')-space, and use Lemma 1 to convert them into valid inequalities for C. Instead of going into details, we give an example.

Example 1 (cont.): Let us define $x'_i = x_i - s$, where s is an integer with $1 \leq s < u$. Also let $x'_j = x_j$ and $y'_{ij} = x'_i x'_j$. The domain of x'_i is

$\{-s, \ldots, u-s\}$. The Glover–Woolsey inequality $y'_{ij} \geq 0$ is not valid for C. If we set δ_i and δ_j to 1/2, we obtain the inequality

$$y'_{ij} + \frac{1}{2}\big(y'_{ii} - x'_i\big) + \frac{1}{2}\big(y'_{jj} - x'_j\big) \geq 0,$$

or, equivalently,

$$y'_{ii} + y'_{jj} + 2y'_{ij} \geq x'_i + x'_j.$$

This is a split inequality in the (x', y')-space. Mapping it back to (x, y)-space using Lemma 1, we obtain the following valid inequality for C:

$$y_{ii} + y_{jj} + 2y_{ij} \geq (2s+1)(x_i + x_j) - s(s+1). \tag{20}$$

This is also a split inequality. It defines a facet of C for $s = 1, \ldots, u-1$.

If we set δ_i to $u/2$ and δ_j to 0 instead, we obtain the following valid inequality in (x', y')-space:

$$y'_{ij} + (u/2)\big(y'_{ii} - x'_i\big) \geq 0.$$

Mapping it back to (x, y)-space, we obtain the following valid inequality for C:

$$uy_{ii} + 2y_{ij} \geq u(2s+1)x_i + 2sx_j - us(s+1). \tag{21}$$

One can check that it defines a facet of C for $s = 1, \ldots, u-1$. □

5 Computational Experiments

In this section, we present the results of some computational experiments. Subsection 5.1 deals with integer quadratic programs with box constraints (IQPB), whereas 5.2 deals with portfolio optimisation problems with semi-continuous variables.

The experiments were conducted on a 1.80 GHz Intel Core i7-8550U with 16Gb RAM, under a 64 bit Linux operating system (Ubuntu 18.04 LTS). We used `CPLEX` (v. 12.10) to solve all LPs and MIQPs.

5.1 IQPB

First, we consider IQPBs of the form

$$\min\big\{c^T x + x^T Q x : \; x \in \{0, \ldots, u\}^n\big\},$$

where u is a positive integer. We remark that this problem is strongly $\mathcal{NP}$-hard even when $u = 1$ (since it is equivalent to the max-cut problem in that case).

For the objective function, we consider three different cases: convex, concave and indefinite. To generate the convex instances, we pick a random point $x^* \in (0, u)^n$ and a random matrix $M \in \mathbb{Z}^{n \times n}$ with entries in

$\{-10, \ldots, 10\}$. We then minimise $||M(x - x^*)||_2^2$. This corresponds to setting Q to $M^T M$ and c to $-2Qx^*$. The concave instances are similar, except that we replace Q with $-Q$ and c with $-c$. The indefinite instances are obtained by picking two random points x^1, x^2 and two random matrices M^1, M^2, and minimising $||M^1(x - x^1)||_2^2 - ||M^2(x - x^2)||_2^2$.

For each of the three cases, and for $u \in \{1, \ldots, 7\}$, we created five random instances. This makes $3 \times 7 \times 5 = 105$ instances in total. We set n to a relatively small value of 25, to ensure that we could compute optimal solutions for all instances.

We began by solving the instances to proven optimality, using the MIQP solver of CPLEX. This solver is based on branch-and-reduce. After that, we solved the classical LP relaxation of each instance, which consists of minimising

$$c^T x + \sum_{i \in N} q_{ii} y_{ii} + 2 \sum_{1 \le i < j \le n} q_{ij} y_{ij}$$

subject to the McCormick constraints (7) and (8). We used the dual simplex solver of CPLEX for this purpose. We then recorded the optimal value and LP lower bound for each instance.

After that, we experimented with adding the following four families of inequalities, either alone or in combination:

- The "stretched" version of the triangle inequalities (4) and (5). They can be written as $u(x_i + x_j + x_k) \le y_{ij} + y_{ik} + y_{jk} + u^2$ and $y_{ij} + y_{ik} \le ux_i + y_{jk}$, respectively.
- Simple gap inequalities, which take the form $y_{ii} \ge (2s+1)x_i - s(s+1)$ for $i \in N$ and $s = 0, \ldots, u-1$. (These are also split inequalities.)
- "Two-index split" inequalities, which come in two types. The first is of the form (20) for $1 \le i < j \le n$ and $s = 0, \ldots, 2u-1$. The second is of the form

  $$y_{ii} + y_{jj} - 2y_{ij} \ge (2s+1)(x_i - x_j) - s(s+1)$$

  for $1 \le i < j \le n$ and $s \in \{-u, \ldots, u-1\}$.
- "Lifted internal Glover-Woolsey" inequalities, which also come in two types. The first is of the form (21) and the second is of the form

  $$uy_{ii} - 2y_{ij} \ge u(2s-1)x_i - 2sx_j - us(s-1).$$

  Both types are valid for all $i \in N$, $j \in N \setminus \{i\}$ and $s = 1, \ldots, u-1$.

We remark that the instances under consideration were small enough to make it possible to insert all of the inequalities into the LP. Thus, there was no need for any separation algorithms.

Case	u	ST	SG	2IS	LI	All
	1	54.0	43.7	43.7	—	87.6
	2	55.3	22.4	44.8	36.3	81.2
	3	55.5	25.0	44.9	31.1	79.6
conv	4	55.6	22.5	45.0	30.7	79.9
	5	55.6	23.4	45.0	28.0	79.8
	6	55.6	22.5	45.1	27.7	79.6
	7	55.7	23.0	45.1	26.4	79.7
	1	100	0.00	0.00	—	100
	2	100	0.00	0.00	0.00	100
	3	100	0.00	0.00	0.00	100
conc	4	100	0.00	0.00	0.00	100
	5	100	0.00	0.00	0.00	100
	6	100	0.00	0.00	0.00	100
	7	100	0.00	0.00	0.00	100
	1	79.4	5.56	5.56	—	80.0
	2	79.5	2.78	5.57	5.28	80.0
	3	79.5	3.10	5.58	4.14	80.0
indef	4	79.5	2.79	5.57	3.99	80.0
	5	79.5	2.90	5.58	3.62	80.0
	6	79.5	2.79	5.57	3.55	80.0
	7	79.5	2.85	5.58	3.37	80.0

Table 1: IQPB: average percentage gap closed by various inequalities.

For each instance and each family of valid inequalities, we computed the percentage of the integrality gap that is closed by the given inequalities. Table 1 shows the results. Here, "conv", "conc" and "indef" stand for convex, concave and indefinite, respectively. Also, "ST", "SG", "2IS" and "LI" stand for stretched triangle, simple gap, two-index split and lifted internal inequalities, respectively. Each figure is the average over five random instances. All results are shown to 3 significant figures. The dashed lines in the LI column appear because our lifted internal inequalities are not defined when $u = 1$.)

We were surprised to find that, for the concave instances, the stretched triangle inequalities close the gap completely. Moreover, the same inequalities are very useful also in the convex and indefinite cases. The simple gap, 2-index split inequalities and lifted internal inequalities, on the other hand, are useful only in the convex case. Indeed, in the convex case, the four families of inequalities appear to work very well in combination.

5.2 Portfolio optimisation

Although our approach is intended mainly for non-convex problems, we also applied it to a convex problem, for interest. We chose a portfolio optimisation problem with semi-continuous variables (see, e.g., [13, 17, 31]). The problem takes the form

$$\begin{aligned}
\min \quad & x^T Q x \\
\text{s.t.} \quad & \textstyle\sum_i^n x_i = 1 && (22) \\
& \mu^T x \geq \rho && (23) \\
& x_i \in \{0\} \cup [\ell_i, u_i] \quad (1 \leq i \leq n),
\end{aligned}$$

where $\mu \in \mathbb{Q}^n$ is the vector of expected returns, $\rho \in \mathbb{Q}_+$ is the minimum desired expected return, $Q \in \mathcal{S}_+^n$ is the matrix of covariances of returns, and ℓ_i and u_i are minimum and maximum buy-in thresholds, respectively.

We use the instances in Frangioni and Gentile [17]. There are 10 random instances with $n = 200$ and 10 with $n = 300$.

The most natural initial LP relaxation consists of minimising

$$\sum_{i \in N} q_{ii} y_{ii} + 2 \sum_{1 \leq i < j \leq n} q_{ij} y_{ij}$$

subject to the constraints (22) and (23), together with the McCormick constraints.

Some simple valid equations and inequalities can be derived using the RLT. In particular, multiplying (22) by each variable in turn, we obtain $\sum_{i \in N} y_{ik} = x_k$ for $k \in N$. Also, multiplying (23) by x_k and $1 - x_k$, we obtain:

$$\begin{aligned}
\textstyle\sum_{i \in N} \mu_i y_{ik} &\geq \rho x_k && (k \in N) \\
\mu^T x - \textstyle\sum_{i \in N} \mu_i y_{ik} &\geq \rho(1 - x_k) && (k \in N).
\end{aligned}$$

We then considered the following five additional families of inequalities:

- The “stretched” version of the triangle inequalities (4) and (5), as before.
- The simple gap inequalities $y_{ii} \geq \ell_i x_i$ for $i \in N$.
- The psd inequalities $y_{ii} \geq 2\ell_i x_i - \ell_i^2$ for $i \in N$.
- Inequalities obtained by “stretching” the lifted internal inequalities (18) and (19). The first take the form

$$y_{ij} - \left(\frac{u_i}{\ell_j}\right) y_{jj} \leq \ell_j x_i - u_i x_j.$$

n	RLT	ST	SG	psd	LI1	LI2	All
200	0.515	0.00	91.7	0.00	76.3	0.00	96.1
300	0.370	0.00	93.3	0.00	72.7	0.00	97.2

Table 2: Portfolio optimisation: average percentage gap closed by various inequalities.

The second take the form

$$\left(\frac{\ell_j}{\ell_i}\right) y_{ii} + \left(\frac{\ell_i}{\ell_j}\right) y_{jj} + y_{ij} \geq 2\ell_j x_i + 2\ell_i x_j - \ell_i \ell_j.$$

We call these "LI1" and "LI2", respectively.

Table 2 shows the results. Each figure is the average over the ten instances of the given size. We were very surprised to see that the RLT constraints close only a tiny fraction of the gap. Also, the stretched triangle, psd and "LI2" constraints close no gap at all. On the other hand, the simple gap and "LI1" inequalities perform extremely well, both alone and in combination.

6 Conclusion

We believe that Buchheim and Wiegele [8] have introduced an important and interesting family of non-convex quadratic optimisation problems, which we have called QPDC. In this paper, we have studied the associated convex sets, deriving several families of strong valid linear inequalities, and presented some encouraging computational results. As mentioned in the introduction, our work consolidates and extends results in [2, 6, 9, 11, 30, 37].

There are several interesting possible topics for future research. The first is to devise effective (exact or heuristic) separation algorithms for various families of inequalities (see [7] for the separation of split inequalities). A second is to incorporate our inequalities into an exact algorithm for QPDCs, or even general MIQPs (using the fact that variable domains are restricted when branching takes place). A third is to find ways to exploit *sparsity* in the quadratic cost matrix Q. Indeed, if $Q_{ij} = 0$, then we can in principle omit the variable y_{ij} from the formulation, which may enable instances to be solved more quickly. However, omitting variables corresponds to projecting the convex sets into a subspace, and this is unlikely to be easy in general. (Of course, we can use the inequalities in this paper whenever the y variables with a non-zero coefficient are present.)

References

[1] W.P. Adams & H.D. Sherali (1986) A tight linearization and an algorithm for zero-one quadratic programming problems. *Mgmt. Sci.*, 32, 1274–1290.

[2] K.M. Anstreicher & S. Burer (2010) Computable representations for convex hulls of low-dimensional quadratic forms. *Math. Program.*, 124, 33–43.

[3] D. Bienstock (1996) Computational study of a family of mixed-integer quadratic programming problems. *Math. Program.*, 74, 121–140.

[4] A. Billionnet, S. Elloumi & A. Lambert (2012) Extending the QCR method to general mixed-integer programs. *Math. Program.*, 131, 381–401.

[5] P. Bonami, M. Kilinç & J. Linderoth (2012) Algorithms and software for convex mixed integer nonlinear programs. In: J. Lee & S. Leyffer (eds.), *Mixed Integer Nonlinear Programming*, pp. 1–40. New York: Springer.

[6] E. Boros & P.L. Hammer (1993) Cut-polytopes, Boolean quadric polytopes and nonnegative quadratic pseudo-Boolean functions. *Math. Oper. Res.*, 18, 245–253.

[7] C. Buchheim & E. Traversi (2015) On the separation of split inequalities for non-convex quadratic integer programming. *Discr. Optim.*, 15, 1–14.

[8] C. Buchheim & A. Wiegele (2013) Semidefinite relaxations for non-convex quadratic mixed-integer programming. *Math. Program.*, 141, 435–452.

[9] S. Burer & A.N. Letchford (2009) On non-convex quadratic programming with box constraints. *SIAM J. Optim.*, 20, 1073–1089.

[10] S. Burer & A.N. Letchford (2012) Non-convex mixed-integer nonlinear programming: a survey. *Surveys in Oper. Res. & Mgmt. Sci.*, 17, 97–106.

[11] S. Burer & A.N. Letchford (2014) Unbounded convex sets for non-convex mixed-integer quadratic programming. *Math. Program.*, 143, 231–256.

[12] S. Burer & A. Saxena (2012) The MILP road to MIQCP. In: J. Lee & S. Leyffer (eds.), *Mixed Integer Nonlinear Programming*, pp. 373–405. New York: Springer.

[13] T.J. Chang, N. Meade, J.E. Beasley & Y.M. Sharaiha (2000. Heuristics for cardinality constrained portfolio optimisation. *Comput. Oper. Res.*, 27, 1271–1302.

[14] C. D'Ambrosio & A. Lodi (2013) Mixed integer nonlinear programming tools: an updated practical overview. *Ann. Oper. Res.*, 204, 301–320.

[15] P. De Angelis, P.M. Pardalos & G. Toraldo (1997) Quadratic programming with box constraints. In I. Bomze *et al.* (eds.) *Developments in Global Optimization*, pp. 73–93. Dordrecht: Kluwer.

[16] M.M. Deza & M. Laurent (1997) *Geometry of Cuts and Metrics.* Berlin: Springer.

[17] A. Frangioni & C. Gentile (2006) Perspective cuts for a class of convex 0–1 mixed integer programs. *Math. Program.*, 106, 225–236.

[18] L. Galli, K. Kaparis & A.N. Letchford (2011) Gap inequalities for non-convex mixed-integer quadratic programs. *Oper. Res. Lett.*, 39, 297–300.

[19] F. Glover & E. Woolsey (1974) Converting the 0-1 polynomial program to a 0-1 linear program. *Oper. Res.*, 22, 180–182.

[20] M. Grötschel, L. Lovász & A. Schrijver (1981) The ellipsoid method and its consequences in combinatorial optimization. *Combinatorica*, 1, 169–197.

[21] R.D. Hill & S.R. Waters (1987) On the cone of positive semidefinite matrices. *Lin. Alg. Appl.*, 90, 81–88.

[22] J.B. Hiriart-Urruty & C. Lemaréchal (2004) *Fundamentals of Convex Analysis.* Berlin: Springer.

[23] F. Körner & C. Richter (1982) Zur effektiven Lösung von Booleschen, quadratischen Optimierungsproblemen. *Numer. Math.*, 40, 99–109.

[24] J. Kronqvist, D.E. Bernal, A. Lundell & I.E. Grossmann (2019) A review and comparison of solvers for convex MINLP. *Optim. & Engin.*, 20, 397–455.

[25] M. Laurent & S. Poljak (1995) On a positive semidefinite relaxation of the cut polytope. *Lin. Alg. Appl.*, 223, 439–461.

[26] M. Laurent & S. Poljak (1996) Gap inequalities for the cut polytope. *SIAM J. Math. Anal.*, 17, 530–547.

[27] G.P. McCormick (1976) Computability of global solutions to factorable nonconvex programs. Part I: convex underestimating problems. *Math. Program.*, 10, 147–175.

[28] G.L. Nemhauser & L.A. Wolsey (1988) *Integer and Combinatorial Optimization.* New York: Wiley.

[29] M.W. Padberg (1975) A note on zero-one programming. *Oper. Res.*, 23, 833–837.

[30] M.W. Padberg (1989) The boolean quadric polytope: some characteristics, facets and relatives. *Math. Program.*, 45, 139–172.

[31] A.F. Perold (1984) Large-scale portfolio optimization. *Mgmt. Sci.*, 30, 1143–1160.

[32] S. Poljak, F. Rendl & H. Wolkowicz (1995) A recipe for semidefinite relaxation for (0,1)-quadratic programming. *J. Global Optim.*, 7, 51–73.

[33] M. Ramana (1993) *An Algorithmic Analysis of Multiquadratic and Semidefinite Programming Problems.* Ph.D. thesis, Johns Hopkins University, Baltimore, MD.

[34] A. Saxena, P. Bonami & J. Lee (2010) Convex relaxations of non-convex mixed integer quadratically constrained programs: extended formulations. *Math. Program.*, 124, 383–411.

[35] H.D. Sherali & W.P. Adams (1998) *A Reformulation-Linearization Technique for Solving Discrete and Continuous Nonconvex Problems.* Dordrecht: Kluwer.

[36] X. Sun, X. Zheng & D. Li (2013) Recent advances in mathematical programming with semi-continuous variables and cardinality constraint. *J. Oper. Res. Soc. China*, 1, 55–77.

[37] Y. Yajima & T. Fujie (1998) A polyhedral approach for nonconvex quadratic programming problems with box constraints. *J. Glob. Optim.*, 13, 151–170.