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Gap inequalities for non-convex mixed-integer quadratic programs

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ABSTRACT

Laurent and Poljak introduced a very general class of valid linear inequalities, called gap inequalities, for the max-cut problem. We show that an analogous class of inequalities can be defined for general non-convex mixed-integer quadratic programs. These inequalities dominate some inequalities arising from a natural semidefinite relaxation.

1. Introduction

A popular and very powerful approach to solving $\mathcal{NP}$-hard optimisation problems is to formulate them as integer or mixed-integer programs, and then derive strong valid linear inequalities, which can be used within cutting-plane or branch-and-cut algorithms (see, e.g., [7,8]).

Laurent and Poljak [18] introduced an intriguing class of inequalities, called *gap inequalities*, for a combinatorial optimisation problem known as the max-cut problem. They showed that the gap inequalities not only dominate some inequalities arising from the well-known semidefinite programming (SDP) relaxation of the max-cut problem, but also include many other known inequalities as special cases.

In this paper, we show that the idea underlying the gap inequalities can be adapted, in a natural way, to yield gap inequalities for non-convex *Mixed-Integer Quadratic Programs* (MIQPs). Following Laurent and Poljak, we show that these inequalities dominate some inequalities arising from a natural SDP relaxation of non-convex MIQPs. This leads us to conjecture that the generalised gap inequalities are likely to make useful cutting planes for such problems, provided that effective heuristics for generating them can be developed.

The structure of the paper is as follows. In Section 2, we review the relevant literature. In Section 3, we derive gap inequalities for unconstrained 0–1 quadratic programs. Then, in Section 4, we derive them for general non-convex MIQPs.

2. Literature review

For surveys on the max-cut problem and related problems, we refer the reader to [11,16]. Here, we present only what is needed for the sake of exposition.

A set F of edges in an undirected graph is called an *edge cutset*, or simply *cut*, if there exists a set S of vertices such that an edge is in F if and only if exactly one of its end-vertices is in S. It is known that a vector $y \in \{0,1\}^{\binom{n}{2}}$ is the incidence vector of a cut in the complete graph K_n if and only if it satisfies the following *triangle inequalities*:

$$y_{ij} + y_{ik} + y_{jk} \le 2 \quad (1 \le i < j < k \le n) \tag{1}$$

$$y_{ij} - y_{ik} - y_{jk} \le 0 \quad (1 \le i < j \le n;\ k \ne i, j). \tag{2}$$

The cut polytope, which we will denote by CUT_n, is the convex hull in $\mathbb{R}^{\binom{n}{2}}$ of such incidence vectors (Barahona & Mahjoub [3]). That is,

$$\mathrm{CUT}_n = \mathrm{conv}\left\{ y \in \{0,1\}^{\binom{n}{2}} : (1), (2) \text{ hold} \right\}.$$

This polytope has been studied in great depth; see again [11,16].

The well-known SDP relaxation of the max-cut problem (see [13,17,23]) is based on the following fact (which is easily proved). Let M be the matrix of order n with $M_{ii} = 1$ for $1 \le i \le n$ and $M_{ij} = M_{ji} = 1 - 2y_{ij}$ for all $1 \le i < j \le n$. Then M is positive semidefinite (psd).

As pointed out by Laurent and Poljak [17], M is psd if and only if y satisfies the following infinite family of linear inequalities:

$$\sum_{1 \le i < j \le n} \alpha_i \alpha_j y_{ij} \le \sigma(\alpha)^2/4 \quad (\forall \alpha \in \mathbb{R}^n), \tag{3}$$

where $\sigma(\alpha)$ denotes $\sum_{i \in V} \alpha_i$. We call the inequalities (3) *psd inequalities*.

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Observe that, if $\alpha \in \mathbb{Z}^n$ and $\sigma(\alpha)$ is odd, then the psd inequalities can be strengthened by rounding down the right-hand side to the nearest integer. These 'rounded' psd inequalities collectively dominate all of the psd inequalities [11], and have been studied in [2,11,12,20]. They include as special cases the *hypermetric* inequalities of Deza [10] and Kelly [15], the *triangle* inequalities (1)–(2), and the *odd clique* inequalities of Barahona and Mahjoub [3].

The *gap* inequalities, derived by Laurent and Poljak [18], are even stronger and more general than the rounded psd inequalities. They take the form:

$$\sum_{1\le i<j\le n} \alpha_i\alpha_j y_{ij} \le \left(\sigma(\alpha)^2 - \gamma(\alpha)^2\right)/4 \quad (\forall \alpha \in \mathbb{Z}^n), \tag{4}$$

where

$$\gamma(\alpha) := \min\left\{|z^T\alpha| : z \in \{\pm 1\}^n\right\}$$

is the so-called *gap* of α. In [18], it is shown that every gap inequality defines a proper face of CUT_n, though not necessarily a facet. Equivalently, the right-hand side of (4) is best possible. On the other hand, they point out that computing $\gamma(\alpha)$ is $\mathcal{NP}$-hard, since testing whether $\gamma(\alpha) = 0$ is equivalent to the *partition problem*, proven to be $\mathcal{NP}$-complete by Karp [14].

Finally, we mention the *Boolean quadric polytope*, which was introduced by Padberg [22], in the context of unconstrained 0–1 quadratic programming. The Boolean quadric polytope of order n, which we denote by BQP_n, is defined as:

$$\text{BQP}_n = \text{conv}\left\{(x, X) \in \{0, 1\}^{n+\binom{n}{2}} : X_{ij} = x_i x_j \ (1 \le i < j \le n)\right\}.$$

(Note that the X_{ij} variables are not defined when $i = j$. There is no need, given that $x_i = x_i^2$ when x_i is binary.) It is known [4,9,22] that CUT_{n+1} can be mapped onto BQP_n using the following linear transformation, known as the *covariance mapping*:

$$x_i = y_{i,n+1} \quad (1 \le i \le n)$$
$$X_{ij} = (y_{i,n+1} + y_{j,n+1} - y_{ij})/2 \quad (1 \le i < j \le n).$$

As a result, if $a^Ty \le b$ is any valid inequality for CUT_{n+1}, the inequality

$$\sum_{i=1}^{n}\left(\sum_{j\in\{1,\dots,n+1\}\setminus\{i\}} a_{ij}\right)x_i - 2\sum_{1\le i<j\le n} a_{ij}X_{ij} \le b$$

is valid for BQP_n. We will use this fact in the next section.

3. From max-cut to unconstrained 0–1 QP

Given any vector $\alpha = (\alpha_1, \dots, \alpha_{n+1})^T \in \mathbb{R}^{n+1}$, one can form a psd inequality for CUT_{n+1}. Now, if the covariance mapping is applied to the psd inequality, one obtains a valid inequality for BQP_n that can be written in the following form:

$$\sum_{i=1}^{n} \alpha_i(\alpha_i - \sigma(\alpha))x_i + 2\sum_{1\le i<j\le n} \alpha_i\alpha_j X_{ij} + \sigma(\alpha)^2/4 \ge 0. \tag{5}$$

These valid inequalities for BQP_n were also derived by Sherali and Fraticelli [26] in a different way, using the well-known fact [21] that the matrix

$$\begin{pmatrix}1\\x\end{pmatrix}\begin{pmatrix}1\\x\end{pmatrix}^T = \begin{pmatrix}1 & x^T\\ x & xx^T\end{pmatrix}$$

is psd.

Now suppose that $\alpha \in \mathbb{Z}^{n+1}$ and $\sigma(\alpha)$ is odd. Then, one can form a rounded psd inequality for CUT_{n+1}. Applying the covariance mapping again, one finds that the right-hand side of (5) can be increased by 1/4 when α satisfies the stated conditions. We remark that, if we let $\tilde{\alpha}$ denote the truncated vector $(\alpha_1, \dots, \alpha_n)^T$, and β denote $\lfloor\sigma(\alpha)/2\rfloor$, the resulting inequalities for BQP_n can be written in the following form:

$$\sum_{i=1}^{n} \tilde{\alpha}_i(\tilde{\alpha}_i - 2\beta - 1)x_i + 2\sum_{1\le i<j\le n} \tilde{\alpha}_i\tilde{\alpha}_j X_{ij} + \beta(\beta+1) \ge 0$$
$$(\forall \tilde{\alpha} \in \mathbb{Z}^n, \beta \in \mathbb{Z}). \tag{6}$$

These valid inequalities for BQP_n were also derived by Boros and Hammer [6], again in a different way. Their proof is based on the observation that

$$(\tilde{\alpha}^Tx - \beta)(\tilde{\alpha}^Tx - \beta - 1) \ge 0$$

whenever x, $\tilde{\alpha}$ and β are integral.

Clearly, the same transformation can be applied to the gap inequalities. The resulting valid inequalities for BQP_n, which are valid for all $\alpha \in \mathbb{Z}^{n+1}$, can be written in the following form:

$$\sum_{i=1}^{n} \alpha_i(\alpha_i - \sigma(\alpha))x_i + 2\sum_{1\le i<j\le n} \alpha_i\alpha_j X_{ij} + \left(\sigma(\alpha)^2 - \gamma(\alpha)^2\right)/4$$
$$\ge 0. \tag{7}$$

We call these inequalities the *gap inequalities for* BQP_n. As far as we know, they have never appeared explicitly before in the literature.

From the above results on the cut polytope and the covariance mapping, it follows that the gap inequalities for BQP_n dominate the Boros–Hammer inequalities (6), which in turn dominate the inequalities (5).

The following proposition shows that gap inequalities of a specific kind dominate all others.

Proposition 1. *For a given vector $\tilde{\alpha} \in \mathbb{Z}^n$, let $S(\tilde{\alpha})$ be the set of all possible distinct values that $\tilde{\alpha}^Tx$ can take when x is binary. That is, let*

$$S(\tilde{\alpha}) = \left\{z \in \mathbb{Z} : \exists x \in \{0, 1\}^n : \tilde{\alpha}^Tx = z\right\}.$$

Let $c = |S(\tilde{\alpha})|$, and suppose that the elements of $S(\tilde{\alpha})$ have been ordered as $v_1 < v_2 < \cdots < v_c$. Then, for $k = 1, \dots, c-1$, the inequality

$$\sum_{i=1}^{n} \tilde{\alpha}_i(\tilde{\alpha}_i - v_k - v_{k+1})x_i + 2\sum_{1\le i<j\le n} \tilde{\alpha}_i\tilde{\alpha}_j X_{ij} + v_k v_{k+1} \ge 0 \tag{8}$$

is a gap inequality for BQP_n. Moreover, every gap inequality for BQP_n is either an inequality of the form (8), or dominated by such inequalities.

Proof. To see that inequality (8) is a special case of inequalities (7), set $\alpha_i = \tilde{\alpha}_i$ for $i = 1, \dots, n$, and set α_{n+1} to $v_k + v_{k+1} - \sigma(\tilde{\alpha})$. This causes $\sigma(\alpha)$ to equal $v_k + v_{k+1}$, and causes $\gamma(\alpha)$ to equal $v_{k+1} - v_k$, which in turn causes (7) to reduce to (8).

To prove dominance, it is helpful to let t denote $\tilde{\alpha}^Tx$ and let T denote

$$\sum_{i=1}^{n} \tilde{\alpha}_i^2 x_i + 2\sum_{1\le i<j\le n} \tilde{\alpha}_i\tilde{\alpha}_j X_{ij}.$$

Then, we make the following three observations:

1. The trivial bounds $0 \le x_i \le 1$ for $i = 1, \dots, n$ imply that $v_1 \le t \le v_c$.
2. The gap inequalities (7) can be written as
$$T \ge \sigma(\alpha)t - \left(\sigma(\alpha)^2 - \gamma(\alpha)^2\right)/4. \tag{9}$$
3. The special gap inequality (8) can be written as
$$T \ge (v_k + v_{k+1})t - v_k v_{k+1}. \tag{10}$$

To complete the proof, we show that the inequalities of the form (10) dominate the inequalities (9). We consider three cases:

Case 1: $\sigma(\alpha) \leq v_1 + v_2$. In this case, $\gamma(\alpha) = |\sigma(\alpha) - 2v_1|$ and inequality (9) reduces to $T \geq \sigma(\alpha)t + v_1(\sigma(\alpha) - v_1)$. This inequality is dominated by the inequality $T \geq (v_1 + v_2)t - v_1 v_2$ and the inequality $t \geq v_1$, which we have already seen to be dominated by the trivial bounds.

Case 2: $\sigma(\alpha) \geq v_{c-1} + v_c$. In this case, $\gamma(\alpha) = |\sigma(\alpha) - 2v_c|$ and inequality (9) reduces to $T \geq \sigma(\alpha)t + v_c(\sigma(\alpha) - v_c)$. This inequality is dominated by the inequality $T \geq (v_{c-1} + v_c)t - v_{c-1}v_c$ and the inequality $t \leq v_c$, which we have already seen to be dominated by the trivial bounds.

Case 3: $v_{k-1} + v_k \leq \sigma(\alpha) < v_k + v_{k+1}$ for some $1 < k < c$. In this case, $\gamma(\alpha) = |\sigma(\alpha) - 2v_k|$ and inequality (9) reduces to $T \geq \sigma(\alpha)t + v_k(\sigma(\alpha) - v_k)$. This inequality is dominated by the inequalities $T \geq (v_{k-1} + v_k)t - v_{k-1}v_k$ and $T \geq (v_k + v_{k+1})t - v_k v_{k+1}$. □

We remark that the set $S(\tilde{\alpha})$ defined in Proposition 1 can be easily computed in pseudo-polynomial time, or, more specifically, in $\mathcal{O}\left(n \sum_{i=1}^n |\tilde{\alpha}_i|\right)$ time, using a slightly modified form of Bellman's dynamic programming algorithm for the subset-sum problem [5]. We also remark that one can form an analog of Proposition 1 for the cut polytope, via the covariance mapping. We omit details for brevity.

Although we believe Proposition 1 to be of interest in its own right, our main reason for presenting it is that the 'special' gap inequalities (8) can be adapted in a natural way to the case of general non-convex MIQPs. This is the topic of the next section.

4. An extension to non-convex MIQP

A *Mixed-Integer Quadratic Program* (MIQP) is an optimisation problem of the form:

$$\min\left\{x^T Q x + c^T x : Ax \leq b, x_i \in \mathbb{Z}_+(i \in I), x_i \in \mathbb{R}_+(i \in C)\right\},$$

where x is the vector of decision variables, Q is the matrix of quadratic cost terms, c is the vector of linear profit terms, $Ax \leq b$ is a system of linear inequalities, I is the set of integer-constrained variables, and C is the set of continuous variables. We let n denote $|I \cup C|$.

When the objective function is non-convex (i.e., when Q is not psd), even solving the continuous relaxation of an MIQP is $\mathcal{NP}$-hard. In that case, it is common practice (e.g., [1,24–26]) to introduce additional variables X_{ij} for $1 \leq i \leq j \leq n$, representing the products $x_i x_j$. (Note that, unlike in the 0–1 case, we now need to define these variables also when $i = j$.) These variables can be viewed as being arranged in a symmetric matrix $\hat{X} = xx^T$. The MIQP can now be reformulated as:

$$\min\{Q \bullet \hat{X} + c^T x : Ax \leq b, x_i \in \mathbb{Z}_+(i \in I), \quad x_i \in \mathbb{R}_+(i \in C), \hat{X} = xx^T\},$$

where $Q \bullet \hat{X} = \text{tr}(Q\hat{X})$ denotes the trace inner product (sometimes called the Frobenius inner product) of Q and $\hat{X}$. The advantage of this reformulation is that all of the non-linearity and non-convexity is now encapsulated in the equation $\hat{X} = xx^T$. This equation can be approximated using linear or conic constraints (see again [1,24–26]).

It is quite easy to extend the results in the previous section to the case of non-convex MIQP. First, observe that the matrix

$$\begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T = \begin{pmatrix} 1 & x^T \\ x & \hat{X} \end{pmatrix}$$

remains psd, regardless of whether variables are continuous, binary or integer-constrained. From this, it follows that

$$\begin{pmatrix} \beta \\ \alpha \end{pmatrix}^T \begin{pmatrix} 1 & x^T \\ x & \hat{X} \end{pmatrix} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} \geq 0 \quad (\forall \alpha \in \mathbb{R}^n, \beta \in \mathbb{R}),$$

or, equivalently,

$$(2\beta)\alpha^T x + \sum_{i=1}^n \alpha_i^2 X_{ii} + 2 \sum_{1 \leq i < j \leq n} \alpha_i \alpha_j X_{ij} + \beta^2 \geq 0 \quad (\forall \alpha \in \mathbb{R}^n, \beta \in \mathbb{R}). \tag{11}$$

These inequalities can be viewed as a natural generalisation of the psd inequalities (5). (To see this, just set β to $-\sigma(\alpha)/2$ and then recall that $x_i = X_{ii}$ when x_i is binary.) In fact, they appeared in the unpublished Ph.D. thesis of Ramana [24].

One can also derive a natural analog of the Boros–Hammer inequalities (6). For any $\alpha \in \mathbb{Z}^n$ such that $\alpha_i = 0$ for all $i \in C$, and any $\beta \in \mathbb{Z}$, any feasible solution of the MIQP satisfies the inequality

$$(\alpha^T x + \beta)(\alpha^T x + \beta + 1) \geq 0,$$

which leads to the valid inequalities

$$(2\beta + 1)\alpha^T x + \sum_{i=1}^n \alpha_i^2 X_{ii} + 2 \sum_{1 \leq i < j \leq n} \alpha_i \alpha_j X_{ij} + \beta(\beta + 1) \geq 0. \tag{12}$$

These inequalities were previously presented in [19], but only for the case $C = \emptyset$.

Next, we derive an analog of the gap inequalities for non-convex MIQP. Rather than generalising inequalities (7), we generalise inequalities (8) instead, which as we have seen are the strongest gap inequalities for BQP_n. This is done in the following proposition.

Proposition 2. *For a given vector $\alpha \in \mathbb{Z}^n$ and a given MIQP, let $S(\alpha)$ be the set of all possible values that $\alpha^T x$ can take in a feasible solution to the given MIQP. That is, let*

$$S(\alpha) = \left\{z \in \mathbb{R} : \exists x \in \mathbb{Z}^I \times \mathbb{R}^C : Ax \leq b, \alpha^T x = z\right\},$$

and suppose that the set $S(\alpha)$ is disconnected (or, equivalently, non-convex). Moreover, let s and s' be any two 'consecutive' members of $S(\alpha)$. That is, let s and s' be any two real numbers such that the intersection of the closed interval $[s, s'] \subset \mathbb{R}$ with $S(\alpha)$ is simply $\{s, s'\}$. Then, the inequality

$$\sum_{i=1}^n \alpha_i^2 X_{ii} + 2 \sum_{1 \leq i < j \leq n} \alpha_i \alpha_j X_{ij} - (s + s') \sum_{i=1}^n \alpha_i x_i + ss' \geq 0 \tag{13}$$

is satisfied by all feasible solutions (x, X) to the MIQP.

Proof. From the definition of $S(\alpha)$ and the stated property of s and s', it follows that any vector x that is feasible for the MIQP must satisfy the following disjunction:

$$(\alpha^T x \leq s) \vee (\alpha^T x \geq s').$$

Equivalently, we have

$$(\alpha^T x - s)(\alpha^T x - s') = (\alpha^T x)^2 - (s + s')\alpha^T x + ss' \geq 0.$$

The result then follows from the identities $X_{ij} = x_i x_j$ for $1 \leq i \leq j \leq n$. □

It is easy to show that the generalised gap inequalities (13) both generalise and dominate inequalities (12), and that inequalities (12) in turn dominate all inequalities of the form (11) for which $\alpha_i = 0$ for all $i \in C$. On the other hand, when $\alpha_i \neq 0$ for some $i \in C$, it is possible for an inequality of the form (11) to be non-dominated.

Unfortunately, in the case of MIQP, computing the set $S(\alpha)$ is a hard problem. Indeed, just finding the minimum element in $S(\alpha)$ amounts to solving the mixed-integer linear program

$$\min\left\{\alpha^T x : Ax \leq b, \; x_i \in \mathbb{Z}_+ \; (i \in I), x_i \in \mathbb{R}_+ \; (i \in C)\right\},$$

which is $\mathcal{NP}$-hard in the strong sense. One way around this problem would be to compute an 'outer approximation' to $S(\alpha)$, i.e., a non-trivial subset of $\mathbb{R}$ that contains $S(\alpha)$. The corresponding inequalities would remain valid, but would in general be weaker than inequalities (13).

To use inequalities (13) in a cutting-plane algorithm, one would need a heuristic for computing suitable vectors α, along with a heuristic for computing useful outer approximations to $S(\alpha)$. We leave the devising of such heuristics, along with their incorporation into a branch-and-cut algorithm for non-convex MIQPs, to future research. Another interesting topic for research would be to identify necessary and/or sufficient conditions for gap inequalities to define facets of the convex hull of feasible solutions. We remark that this question is open even for the case of max-cut [18].

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