Binary Positive Semidefinite Matrices and Associated Integer Polytopes

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Abstract. We consider the positive semidefinite (psd) matrices with binary entries. We give a characterisation of such matrices, along with a graphical representation. We then move on to consider the associated integer polytopes. Several important and well-known integer polytopes — the cut, boolean quadric, multicut and clique partitioning polytopes — are shown to arise as projections of binary psd polytopes. Finally, we present various valid inequalities for binary psd polytopes, and show how they relate to inequalities known for the simpler polytopes mentioned. Along the way, we answer an open question in the literature on the max-cut problem, by showing that the so-called *k-gonal* inequalities define a polytope.

Key Words: polyhedral combinatorics, semidefinite programming.

1 Introduction

A real square symmetric matrix $M \in \mathbb{R}^{n\times n}$ is said to be *positive semidefinite* (psd) if and only if any of the following (equivalent) conditions hold:

- $a^T M a \geq 0$ for all $a \in \mathbb{R}^n$,
- all principal submatrices of M have non-negative determinants,
- there exists a real matrix A such that $M = AA^T$.

The set of psd matrices of order n forms a convex cone in $\mathbb{R}^{n\times n}$ (e.g., Hill & Waters [14]), and is often denoted by $\mathcal{S}^n_+$.

In this paper, we consider the *binary* psd matrices, i.e., psd matrices belonging to $\{0,1\}^{n\times n}$, and the associated family of integer polytopes, which we call *binary psd polytopes*. Although psd matrices and semidefinite programming have received much interest from the integer programming and combinatorial optimisation community (see the surveys Goemans [11] and Laurent & Rendl

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[17]), these specific matrices and polytopes appear to have received no attention. This is remarkable, because, as we will see, the binary psd matrices can be easily characterised, and they have a natural graphical interpretation. Moreover, several important and well-known integer polytopes — such as the *cut*, *boolean quadric*, *multicut* and *clique partitioning* polytopes — can in fact be viewed as nothing but faces of binary psd polytopes. In that sense, the binary psd polytopes form an important, and hitherto overlooked, family of 'master' polytopes for combinatorial optimisation.

The paper is structured as follows. In Sect. 2 we characterise the binary psd matrices and show how this leads to the graphical representation. In Sect. 3 we formally define the binary psd polytopes and show how they are related to the other polytopes mentioned. Finally, in Sect. 4 we present several classes of valid and facet-inducing linear inequalities for binary psd polytopes, and show how they imply many of the known inequalities for the simpler polytopes mentioned above. As a by-product of our analysis, we obtain (in Subsect. 4.2) a remarkably simple proof that the so-called *k-gonal* inequalities define a polytope — thus settling an open question in the literature on the max-cut problem (see Avis & Umemoto [2]).

2 Characterisation

We now give our first characterisation of the binary psd matrices. Note that the symmetric rank one binary matrices are those that can be written in the form vv^T for some binary vector $v \in \{0,1\}^n$.

Proposition 1. *A symmetric binary matrix is psd if and only if it is the sum of one or more symmetric rank one binary matrices.*

Proof. The 'if' part follows trivially from the fact that $\mathcal{S}_+^n$ is a cone. We prove the 'only if' part. Suppose that M is a binary psd matrix. Since all 2×2 principal submatrices of M must have non-negative determinant, we have that, if $M_{ii} = 0$ for some $i \in \{1, \ldots, n\}$, then $M_{ij} = M_{ji} = 0$ for $j = 1, \ldots, n$. Thus, if we let $R = \{i \in \{1, \ldots, n\} : M_{ii} = 1\}$, we have that M has zero entries outside the principal submatrix defined by the row/column indices in R. This submatrix, which must also be psd, has 1s on the main diagonal. The fact that a symmetric binary matrix with 1s on the main diagonal is psd if and only if it is the sum of symmetric rank one binary matrices is well-known and easy to prove: see, e.g., Lemma 1 of Dukanovic & Rendl [10]. □

We note in passing the following corollary:

Corollary 1. *A symmetric binary matrix is psd if and only if it is* completely positive *(i.e., if and only if it can be written as AA^T for some* non-negative *A).*

Proof. The 'if' part follows immediately from the definitions. We show the 'only if' part. Let $M \in \{0,1\}^{n \times n}$ be a binary psd matrix. If M is the zero matrix, the result is trivial. Otherwise, from Proposition 1, there exists a positive integer p and vectors $v^1, \dots, v^p \in \{0,1\}^n$ such that:

$$M = \sum_{k=1}^{p} v^k (v^k)^T.$$

If we let A be the $n \times p$ matrix whose kth column is the vector v^k, we have that $M = AA^T$. Thus, M is completely positive. □

The following proposition gives an alternative characterisation of the binary psd matrices, in terms of linear inequalities:

Proposition 2. *A symmetric binary matrix $M \in \{0,1\}^{n \times n}$, with $n \geq 3$, is psd if and only if it satisfies the following inequalities:*

$$M_{ij} \leq M_{ii} \qquad (1 \leq i < j \leq n) \tag{1}$$

$$M_{ik} + M_{jk} \leq M_{kk} + M_{ij} \ (1 \leq i < j \leq n;\ k \neq i, j). \tag{2}$$

Proof. It is easy to check that the inequalities (1) and (2) are satisfied by symmetric rank one binary matrices. Proposition 1 then implies that they are satisfied by binary psd matrices (since both sets of inequalities are homogeneous). Now, suppose that a symmetric binary matrix M satisfies the inequalities (1) and (2). If $M_{ii} = 0$ for a given i, the inequalities (1) imply that $M_{ij} = M_{ji} = 0$ for all $j \neq i$. Thus, just as in the proof of Proposition 1, we can assume that M has 1s on the main diagonal. Now note that, if $M_{ik} = M_{jk} = 1$ for some indices i, j, k, then the inequalities (2) ensure that $M_{ij} = 1$. By transitivity, this implies that $\{1, \dots, n\}$ can be partitioned into subsets in such a way that, for all pairs i, j, $M_{ij} = 1$ if and only if i and j belong to the same subset. That is to say, M is the sum of one or more symmetric rank one binary matrices. By Proposition 1, M is psd. □

We will also find the following simple result useful later on (see Proposition 6 in Subsect. 3.1):

Proposition 3. *If $M \in \{0,1\}^{n \times n}$ is a binary psd matrix, and $M_{rr} = 0$ for some $1 \leq r \leq n$, then the matrix obtained from M by changing M_{rr} to 1 is also a binary psd matrix.*

Proof. If M satisfies the inequalities (1) and (2), then the modified matrix will also satisfy them. □

Finally, we point out that the binary psd matrices have a natural graphical representation. Given an $n \times n$ binary psd matrix M, we construct a subgraph of the complete graph K_n as follows. The vertex i is included in the subgraph if and only if $M_{ii} = 1$, and the edge $\{i, j\}$ is included if and only if $M_{ij} = 1$. The symmetric rank one binary matrices then correspond to *cliques* in K_n, if we define cliques in a slightly non-conventional way, so that they consist, not only of vertices, but also of the edges between them. The binary psd matrices correspond to *clique packings*, i.e., to unions of node-disjoint cliques.

3 Polytopes

In this section, we formally define the binary psd polytope and show how it is related to certain other polytopes in combinatorial optimisation.

3.1 The Binary Psd Polytope

Note that any binary psd matrix M, being symmetric, satisfies the $\binom{n}{2}$ equations $M_{ij} = M_{ji}$ for all $1 \le i < j \le n$. Therefore, if we defined the binary psd polytope in $\mathbb{R}^{n \times n}$, it would not be full-dimensional. Therefore, we decided to work in $\mathbb{R}^{\binom{n+1}{2}}$ instead.

We will need the following notation. We let $V_n = \{1, \dots, n\}$ and $E_n = \{S \subset V_n : |S| = 2\}$. We then define, for all $i \in V_n$, the binary variable x_i, which takes the value 1 if and only if $M_{ii} = 1$; and we define, for all $\{i, j\} \in E_n$, the binary variable y_{ij}, which takes the value 1 if and only if $M_{ij} = M_{ji} = 1$. We denote by $\mathcal{M}(x, y)$ the linear operator that maps a given pair $(x, y) \in \{0, 1\}^{V_n \cup E_n}$ onto the corresponding $n \times n$ symmetric matrix. Then, the *binary psd polytope* of order n is defined as:

$$\mathcal{P}_n = \text{conv}\left\{(x, y) \in \{0, 1\}^{V_n \cup E_n} : \mathcal{M}(x, y) \in \mathcal{S}^n_+\right\}.$$

Example 1. For $n = 2$, there are 5 binary psd matrices:

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

The corresponding vectors (x_1, x_2, y_{12}) are $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$, $(1, 1, 0)$ and $(1, 1, 1)$, respectively. The polytope $\mathcal{P}_2$ is described by the linear inequalities $x_1 \le 1$, $x_2 \le 1$, $y_{12} \ge 0$, $y_{12} \le x_1$ and $y_{12} \le x_2$.

Proposition 2 enables us to define $\mathcal{P}_n$ more explicitly.

Proposition 4. *For $n \ge 3$, $\mathcal{P}_n$ is the convex hull of pairs $(x, y) \in \{0, 1\}^{V_n \cup E_n}$ satisfying the following inequalities:*

$$y_{ij} \le x_i \qquad (i \in V_n,\ j \in V_n \setminus \{i\}) \tag{3}$$

$$y_{ik} + y_{jk} \le x_k + y_{ij} \quad (\{i, j\} \in E_n,\ k \in V_n \setminus \{i, j\}). \tag{4}$$

The following result is also easy to prove:

Proposition 5. *For all positive integers n, $\mathcal{P}_n$ is full-dimensional, i.e., has dimension $\binom{n+1}{2}$. For $n \ge 3$, the following inequalities induce facets:*

- *The upper bounds $x_i \le 1$ for all $i \in V_n$.*
- *The non-negativity inequalities $y_e \ge 0$ for all $e \in E_n$.*
- *The inequalities (3) and (4).*

Finally, Proposition 3 can be used to show the following result:

Proposition 6. *Every inequality defining a facet of $\mathcal{P}_n$, apart from the upper bounds $x_i \le 1$ for all $i \in V_n$, can be written in the form $b^T y \le a^T x + c$, with $a \ge 0$ and $c \ge 0$.*

3.2 The Boolean Quadric Polytope

The *boolean quadric polytope* (Padberg [21]) of order n is defined as:

$$\mathrm{BQP}_n = \mathrm{conv}\left\{(x,y) \in \{0,1\}^{V_n \cup E_n} : y_{ij} = x_i x_j \ (\{i,j\} \in E_n)\right\}.$$

The boolean quadric polytope, sometimes called the *correlation polytope*, arises naturally in quadratic 0-1 programming, and also has many applications in statistics, probability and theoretical physics (see Deza & Laurent [9]). Moreover, the *stable set polytope* of a graph $G = (V_n, E)$ is a projection of a face of BQP_n (e.g., Padberg [21]).

Note that a pair (x,y) is an extreme point of BQP_n if and only if $\mathcal{M}(x,y)$ is a symmetric rank one binary matrix. Therefore, the boolean quadric polytope is contained in the binary psd polytope. Moreover, the fact that binary psd matrices can be decomposed into the sum of symmetric rank one binary matrices can be used to show the following result:

Proposition 7. *The boolean quadric polytope* BQP_n *and the binary psd polytope* $\mathcal{P}_n$ *have the same homogeneous facets; i.e., an inequality* $a^T x + b^T y \le 0$ *is facet-defining for* BQP_n *if and only if it is facet-defining for* $\mathcal{P}_n$.

The homogeneous facets of a polyhedron are the facets that contain the origin, so that they are also facets of the cone that is generated by the incidence vectors of all feasible solutions. In the case of BQP_n and $\mathcal{P}_n$, this cone is sometimes called the *correlation cone* (see again Deza & Laurent [9]).

In fact, the relationship between the boolean quadric and binary psd polytopes goes deeper than this.

Proposition 8. *The boolean quadric polytope* BQP_n *is a face of the binary psd polytope* $\mathcal{P}_{n+1}$.

Proof (sketch). From Proposition 5, the following $n+1$ linear inequalities induce facets of $\mathcal{P}_{n+1}$:

$$\begin{aligned} x_{n+1} &\le 1 \\ y_{i,n+1} &\le x_i \ (i \in V_n). \end{aligned}$$

So consider the face of $\mathcal{P}_{n+1}$ satisfying these inequalities at equality, and let $(x^*, y^*) \in \{0,1\}^{V_{n+1} \cup E_{n+1}}$ be a vertex of it. A consideration of the 3×3 principal submatrices involving the last row/column shows that $y^*_{ij} = x^*_i x^*_j$ for all $\{i,j\} \in E_n$. Thus, the matrix $\mathcal{M}(x^*, y^*)$ is of the form

$$\begin{pmatrix} \tilde{x} \\ 1 \end{pmatrix} \left(\tilde{x}^T \ 1\right) = \begin{pmatrix} \tilde{x}\tilde{x}^T & \tilde{x} \\ \tilde{x}^T & 1 \end{pmatrix},$$

where $\tilde{x} \in \{0,1\}^n$ is the vector obtained from x^* by dropping the last component. So, $\mathcal{M}(x^*, y^*)$ is of rank one and there is a one-to-one correspondence between the symmetric rank one binary matrices and the vertices of the face. Thus, BQP_n is nothing but the projection of the face onto $\mathbb{R}^{V_n \cup E_n}$. □

The idea underlying the construction of the matrix $\mathcal{M}(x^*, y^*)$ in the proof of Proposition 8 is due to Lovász & Schrijver [19] (see also Shor [22]), but the above polyhedral interpretation is new to our knowledge.

An immediate consequence of Proposition 8 is that valid or facet-inducing inequalities for BQP_n can be *lifted* to yield valid or facet-inducing inequalities for $\mathcal{P}_{n+1}$:

Proposition 9. *Suppose the inequality*

$$\sum_{i \in V_n} a_i x_i + \sum_{e \in E_n} b_e y_e \leq c$$

defines a facet of BQP_n*. Then there exists at least one facet-defining inequality for* $\mathcal{P}_{n+1}$ *of the form*

$$\sum_{i \in V_n} (a_i + \beta_i) x_i - \alpha x_{n+1} + \sum_{e \in E_n} b_e y_e - \sum_{i \in V_n} \beta_i y_{i,n+1} \leq c - \alpha,$$

with $\alpha \in \mathbb{R}$ *and* $\beta \in \mathbb{R}^n$*.*

3.3 The Clique Partitioning Polytope

The *clique partitioning polytope* (Grötschel & Wakabayashi [13]) of order n is defined as:

$$\text{PAR}_n = \text{conv}\left\{ y \in \{0,1\}^{E_n} : \ y_{ik} + y_{jk} \leq y_{ij} + 1 \ (\forall \{i,j\} \in E_n, \ k \in V_n \setminus \{i,j\}) \right\}.$$

When a vector $y \in \{0,1\}^{E_n}$ belongs to PAR_n, it means that there exists a partition of V_n into sets such that, for all $e \in E_n$, $y_e = 1$ if and only if both end-vertices of e are in the same set. The clique partitioning polytope has applications in statistical clustering.

It is not hard to see that a vector $y \in \{0,1\}^{E_n}$ is a vertex of PAR_n if and only if there exists a vector $x \in \{0,1\}^{V_n}$ such that $\mathcal{M}(x, y)$ is a binary psd matrix. Thus:

Proposition 10. *The clique partitioning polytope* PAR_n *is the projection of the binary psd polytope* $\mathcal{P}_n$ *onto* $\mathbb{R}^{E_n}$*.*

In fact, we can say something stronger.

Proposition 11. *The clique partitioning polytope* PAR_n *is a face of the binary psd polytope* $\mathcal{P}_n$*.*

Proof (sketch). Let $\mathbf{1}_n$ denote the vector of n ones. Using Proposition 3, we have that a vector $y \in \{0,1\}^{E_n}$ is a vertex of PAR_n if and only if $\mathcal{M}(\mathbf{1}_n, y)$ is a binary psd matrix. Now, from Proposition 5, the following n linear inequalities induce facets of $\mathcal{P}_n$:

$$x_i \leq 1 \ (i \in V_n).$$

Thus, the face of $\mathcal{P}_n$ satisfying these n inequalities at equality, projected onto $\mathbb{R}^{E_n}$, is PAR_n. □

As in the previous subsection, this implies a lifting result:

Proposition 12. *Let $b^T y \leq c$ be a facet-defining inequality for* PAR_n*. Then there exists at least one facet-defining inequality for $\mathcal{P}_n$ of the form*

$$\sum_{i \in V_n} \alpha_i x_i + b^T y \leq c + \sum_{i \in V_n} \alpha_i,$$

where $\alpha_i \leq 0$ for all $i \in V_n$.

3.4 The Cut and Multicut Polytopes

Finally, we mention connections between the above polytopes and the *cut* and *multicut* polytopes.

Given any $S \subseteq V_n$, the set of edges

$$\delta_n(S) = \{\{i,j\} \in E_n : i \in S,\ j \in V_n \setminus S\}$$

is called an *edge cutset* or simply *cut*. The *cut polytope* CUT_n is the convex hull of the incidence vectors of all cuts in K_n (Barahona & Mahjoub [3]), i.e.,

$$\mathrm{CUT}_n = \mathrm{conv}\left\{y \in \{0,1\}^{E_n} : \exists S \subset V_n : y_e = 1 \iff e \in \delta_n(S)\ (\forall \{i,j\} \in E_n)\right\}.$$

The cut polytope and the boolean quadric polytope are related via the so-called *covariance mapping* [9] which maps the boolean quadric polytope in $\mathbb{R}^{E_n \cup V_n}$ to the cut polytope in $\mathbb{R}^{E_{n+1}}$. This means that there is a one-to-one correspondence between the facets of the respective polytopes. This correspondence is the following [9, Proposition 5.2.7]:

Proposition 13. *Let $a \in \mathbb{R}^{V_n}$, $b \in \mathbb{R}^{E_n}$, $c \in \mathbb{R}^{E_{n+1}}$ be linked by*

$$\begin{cases} c_{i,n+1} = a_i + \frac{1}{2} \sum_{j \in V_n \setminus \{i\}} b_{ij} & \text{for } i \in V_n, \\ c_e \quad\ \ = -\frac{1}{2} b_e & \text{for } e \in E_n. \end{cases}$$

Given $a_0 \in \mathbb{R}$, the inequality $c^T y \leq a_0$ is valid (resp. facet-defining) for the cut polytope CUT_{n+1} *if and only if the inequality $a^T x + b^T y \leq a_0$ is valid (resp. facet-defining) for the boolean quadric polytope* BQP_n*.*

We remark that the cut polytope is also equivalent (under a simple linear mapping) to the convex hull of the psd matrices with ± 1 entries (see Goemans & Williamson [12], Laurent & Poljak [15]).

Now, given any partition of V_n into sets $S_1, \ldots, S_r$, the set of edges

$$\delta_n(S_1, \ldots, S_r) = \{\{i,j\} \in E_n : i \in S_p,\ j \in S_q \text{ for some } p \neq q\}$$

is called a *multicut*. The *multicut polytope* MCUT_n is defined accordingly (e.g., Deza *et al.* [7]). It is not hard to see that the multicut polytope is nothing but the *complement* of the clique partitioning polytope: $\mathrm{MCUT}_n = \{\mathbf{1}_{E_n} - y \mid y \in \mathrm{PAR}_n\}$. As the incidence vectors in MCUT_n are just affine transformations of the incidence vectors in PAR_n, and vice versa, facets of one polytope are easily transformed to facets of the other. Suppose that the inequality $b^T y \leq b_0$ defines a facet of PAR_n (respectively MCUT_n). Substituting $1 - y_e$ for y_e for all $e \in E_n$ yields the inequality $-b^T y \leq b_0 - \sum_{e \in E_n} b_e$, which defines a facet of MCUT_n (respectively PAR_n). We refer to the mapping $y \mapsto \mathbf{1}_{E_n} - y$ between PAR_n and MCUT_n as *complementing*.

Finally, we 'complete the circle' of results by establishing a link between the cut and clique partitioning polytopes:

Proposition 14. *The cut polytope* CUT_n *and the multicut polytope* MCUT_n *have the same homogeneous facets.*

This fact was pointed out in Deza *et al.* [7].

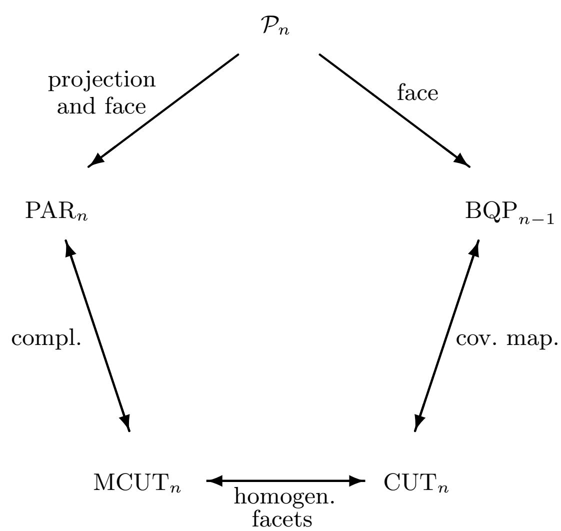

Fig. 1. A pentagon of polyhedral relations

In Fig. 1, we summarize the relationships between the five polytopes as established by Propositions 8 to 14. (Note that Proposition 7 is not displayed.) As we remarked in the introduction, the binary psd polytope is the most complex of the five polytopes under discussion. We point out however that the multicut and clique partitioning polytopes are themselves more complex than the cut and boolean quadric polytopes: the latter polytopes exhibit a high degree of symmetry, via the so-called *switching* operation, which enables one to derive all facets of CUT_n or BQP_n given a list of only the homogeneous facets (see Barahona & Mahjoub [3] and Deza & Laurent [9]). Thus, a complete description of CUT_n and BQP_{n-1} can be obtained from a complete description of MCUT_n or PAR_n, which in turn can be obtained from a complete description of the binary psd polytope $\mathcal{P}_n$.

4 Valid Inequalities

We now move on to consider some specific classes of valid inequalities for the binary psd polytope, and show how they imply existing known results for the other polytopes mentioned above.

4.1 Some Simple Results

In Proposition 5 we pointed out that the upper bounds $x_i \leq 1$, the non-negativity inequalities $y_e \geq 0$ for all $e \in E_n$, and the inequalities (3) and (4) induce facets of the binary psd polytope $\mathcal{P}_n$. All of these inequalities were shown by Padberg to induce facets of the boolean quadric polytope BQP_n. Moreover, the inequalities (4) imply, via Proposition 8, the validity of the following inequalities for BQP_n:

$$x_i + x_j \leq 1 + y_{ij} \qquad (\{i,j\} \in E_n).$$

These inequalities too were proved to induce facets of BQP_n by Padberg.

In a similar way, Propositions 5 and 11 show that the inequalities $y_e \geq 0$ for all $e \in E_n$, and the inequalities

$$y_{ik} + y_{jk} \leq 1 + y_{ij} \qquad (\{i,j\} \in E_n,\, k \in V_n \setminus \{i,j\}),$$

are valid for the clique partitioning polytope PAR_n. These inequalities were proved to induce facets of PAR_n by Grötschel and Wakabayashi [13].

4.2 Hypermetric Correlation Inequalities

If we apply the first definition of psd-ness given in the introduction to the matrix $\mathcal{M}(x,y)$, we see that the following inequalities are valid for $\mathcal{P}_n$:

$$\sum_{i \in V_n} a_i^2 x_i + 2 \sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \geq 0 \qquad (\forall a \in \mathbb{R}^n). \tag{5}$$

It follows from known results on the cut and correlation cones, however, that these inequalities do not define facets of $\mathcal{P}_n$. Indeed, the following *hypermetric* inequalities are well-known to be valid for the cut cone (see Deza & Laurent [9]):

$$\sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \leq 0 \qquad (\forall a \in \mathbb{Z}^n : \sum_{i=1}^{n} a_i = 1). \tag{6}$$

Under the covariance mapping, they correspond to the following inequalities, which are valid for the correlation cone:

$$\sum_{i \in V_n} a_i(a_i - 1) x_i + 2 \sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \geq 0 \qquad (\forall a \in \mathbb{Z}^n). \tag{7}$$

We will follow Deza & Grishukhin [5] in calling them *hypermetric correlation* inequalities. Note that the hypermetric correlation inequalities, being homogeneous, are valid for BQP_n. Then, by Proposition 7, they are valid for $\mathcal{P}_n$ as well. They are easily shown to dominate the inequalities (5).

The hypermetric and hypermetric correlation inequalities have been studied in depth by Deza and colleagues (e.g., [4–6, 8, 9]). Conditions under which the hypermetric inequalities induce facets of the cut cone are surveyed in [9]. Via the covariance mapping, one can derive analogous conditions under which the hypermetric correlation inequalities induce facets of the correlation cone, and therefore of BQP_n. By Proposition 7, they induce facets of $\mathcal{P}_n$ under the same conditions.

Note that the non-negativity inequalities $y_e \geq 0$ for all $e \in E_n$, and the inequalities (3) and (4), are hypermetric correlation inequalities.

An important result, which will be of relevance in what follows, is that the hypermetric inequalities define a polyhedral cone [6]. That is, although the inequalities (6) are infinite in number, there exists a finite subset of them that dominates all the others. Via the covariance mapping, the hypermetric correlation inequalities also define a polyhedral cone.

Now, we consider the implications of moving 'clockwise' in Fig. 1. The hypermetric correlation inequalities (7) imply, via Proposition 8, the validity of the following inequalities for BQP_n:

$$\sum_{i \in V_n} a_i(2b + a_i - 1)x_i + 2 \sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \geq b(1 - b) \qquad (\forall a \in \mathbb{Z}^n,\, b \in \mathbb{Z}). \quad (8)$$

These inequalities, which include the hypermetric correlation inequalities as a special case, are also well-known in the literature [9]. Most of the inequalities shown by Padberg [21] to induce facets of BQP_n — such as the *clique* and *cut* inequalities — are in fact special cases of the inequalities (8).

Under the covariance mapping, the inequalities (8) correspond to the following inequalities for CUT_n:

$$\sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \leq \lfloor \sigma(a)^2/4 \rfloor \qquad (\forall a \in \mathbb{Z}^n : \sigma(a) \text{ odd}), \quad (9)$$

where $\sigma(a) = \sum_{i \in V_n} a_i$. These inequalities, which include the hypermetric inequalities as a special case, are sometimes called *k-gonal* inequalities (see Deza & Laurent [9], Avis & Umemoto [2]). They induce facets of CUT_n if and only if they can be obtained from facet-inducing hypermetric inequalities via the switching operation.

We now present several new results. (Detailed proofs will be given in the full version of the paper.) The first two results show that the separation problems for the inequalities (8) and (9) can be reduced to the separation problems for the inequalities (7) and (6), respectively. They can be proved either directly or by using Proposition 8 and the covariance mapping.

Proposition 15. *Given a vector* $(x^*, y^*) \in [0,1]^{V_n \cup E_n}$*, let* $(x', y') \in [0,1]^{V_{n+1} \cup E_{n+1}}$ *be defined as follows. Let* $x'_i = x^*_i$ *for* $i \in V_n$*, but let* $x'_{n+1} = 1$*. Let* $y'_e = y^*_e$ *for* $e \in E_n$*, but let* $y'_{i,n+1} = x^*_i$ *for* $i \in V_n$*. Then* (x^*, y^*) *satisfies all inequalities (8) if and only if* (x', y') *satisfies all hypermetric correlation inequalities (7).*

Proposition 16. *Given a vector* $y^* \in [0,1]^{E_n}$*, let* $y' \in [0,1]^{E_{n+1}}$ *be defined as follows. Let* $y'_e = y^*_e$ *for* $e \in E_n$*, but let* $y'_{i,n+1} = 1 - y^*_{i,n}$ *for* $i \in V_{n-1}$*, and let* $y'_{n,n+1} = 1$*. Then* y^* *satisfies all* k*-gonal inequalities (9) if and only if* y' *satisfies all hypermetric inequalities (6).*

Unfortunately, the complexity of separation for the hypermetric inequalities is unknown (see Avis [1]). Nevertheless, the above two results have interesting polyhedral implications:

Proposition 17. *Consider the intersection of the hypermetric correlation cone in* $\mathbb{R}^{V_{n+1} \cup E_{n+1}}$ *with the affine space defined by the equations* $y_{i,n+1} = x_i$ *for all* $i \in V_n$ *and the equation* $x_{n+1} = 1$*. If we project it onto* $\mathbb{R}^{V_n \cup E_n}$*, we obtain the convex set defined by the inequalities (8).*

Proposition 18. *Consider the intersection of the hypermetric cone in* $\mathbb{R}^{E_{n+1}}$ *with the affine space defined by the equations* $y_{i,n} + y_{i,n+1} = 1$ *for* $i \in V_{n-1}$ *and the equation* $y_{n,n+1} = 1$*. If we project it onto* $\mathbb{R}^{E_n}$*, we obtain the convex set defined by the* k*-gonal inequalities (9).*

Proposition 18 implies the following result, which answers in the affirmative a question raised by Avis & Umemoto [2]:

Proposition 19. *The* k*-gonal inequalities (9) define a polytope.*

Proof. The hypermetric cone is polyhedral. The intersection of a polyhedral cone with an affine subspace is also polyhedral, and so is its projection onto any subspace. The result then follows from Proposition 18. □

For similar reasons, the inequalities (8) also define a polytope.

To close this subsection, we consider moving 'anticlockwise' in Fig. 1. The inequalities (7) imply, via Proposition 11, the validity of the following inequalities for PAR_n:

$$\sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \geq \frac{1}{2} \sum_{i \in V_n} a_i (1 - a_i) \qquad (\forall a \in \mathbb{Z}^n), \tag{10}$$

and the following inequalities for MCUT_n:

$$\sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \leq \sigma(a)(\sigma(a) - 1)/2 \qquad (\forall a \in \mathbb{Z}^n).$$

The validity of these inequalities for MCUT_n, and the fact that they induce facets under certain conditions, was also observed by Deza & Laurent [9] (p. 465). We remark that, when a_i is binary for all vertices apart from one, the inequalities (10) reduce to the so-called *weighted* (s,T)*-inequalities* of Oosten *et al.* [20], shown to induce facets under certain conditions.

4.3 Gap Inequalities

We now present a class of valid inequalities that dominate the hypermetric correlation inequalities (7).

Proposition 20. *The following inequalities are valid for $\mathcal{P}_n$:*

$$\sum_{i \in V_n} a_i(a_i - a_{\min})x_i + 2 \sum_{\{i,j\} \in E_n} a_i a_j y_{ij} \geq 0 \qquad (\forall a \in \mathbb{Z}^n), \tag{11}$$

where

$$a_{\min} = \min\left\{a^T x : a^T x > 0,\, x \in \{0,1\}^n\right\}.$$

Proof. From the definition of $a_{\min}$, we have that, for any $x \in \{0,1\}^n$, either $a^T x \leq 0$ or $a^T x \geq a_{\min}$. In either case, we have $a^T x(a^T x - a_{\min}) \geq 0$. Thus, when $\mathcal{M}(x,y)$ is a symmetric rank one binary matrix, we have $a^T \mathcal{M}(x,y)a - a_{\min}a^T x \geq 0$. This establishes the validity of the inequalities (11) for BQP_n. By Proposition 7, they are also valid for $\mathcal{P}_n$. □

These strengthened inequalities can be shown to imply (via Proposition 8 and the covariance mapping) the validity of the so-called *gap* inequalities for CUT_n (Laurent & Poljak [16]). They also imply some new inequalities for BQP_n, PAR_n and MCUT_n. Details will be given in the full version of the paper.

4.4 Inequalities Related to Cycles and Paths

We have discovered several classes of facet-inducing inequalities of $\mathcal{P}_n$ that are related to cycles and paths in K_n. We mention two such classes here. The first class we consider is of interest because the inequalities are inhomogeneous and involve only the y variables. Let $C \subset E_n$ be the edge set of a simple cycle of odd length at least 5, and let $\bar{C}$ be the set of 2-chords of C. The *2-chorded odd cycle inequality*

$$\sum_{e \in C} y_e - \sum_{e \in \bar{C}} y_e \leq (|C| - 1)/2 \tag{12}$$

is shown in Grötschel & Wakabayashi [13] to be facet-inducing for the clique partitioning polytope PAR_n. This inequality can be lifted, according to Proposition 12, so that we can establish the following.

Proposition 21. *The 2-chorded odd cycle inequalities (12) induce facets of $\mathcal{P}_n$.*

The existence of such inhomogeneous facet-inducing inequalities for $\mathcal{P}_n$ implies that $\mathcal{P}_n$ is strictly contained in the intersection of the correlation cone and the unit hypercube. We have found some other interesting inhomogeneous facet-inducing inequalities for $\mathcal{P}_n$, which will be mentioned in the full version of the paper.

Next, however, we consider the class of 2-chorded path inequalities. Let $P = \{e = \{i, i+1\} : i = 1, \ldots, k-1\}$ be the edge set of a path of length $k - 1 \geq 2$ and let $\bar{P} = \{e = \{i, i+2\} : i = 1, \ldots, k-2\}$ be the set of 2-chords of P. Denote by $I^- = \{i \in V_n(P) : (i \bmod 2) = 1\}$ and $I^+ = \{i \in V_n(P) : (i \bmod 2) = 0\}$ the odd and even endnodes of the edges in P, respectively. Let $Z \subseteq V_n \setminus V_n(P)$ be nonempty and define $R = \delta_n(I^+, Z)$ and $\bar{R} = \delta_n(I^-, Z)$. The following 2-chorded path inequality

$$\sum_{e \in P \cup R} y_e - \sum_{e \in \bar{P} \cup \bar{R}} y_e - \left\lfloor \frac{k+2}{4} \right\rfloor \sum_{\{i,j\} \subseteq Z} y_{ij} \le |I^+|$$

is shown in [23] to define a facet of PAR_n under mild conditions. The fact that we allow for $|Z| \ge 1$ provides a generalization of the 2-chorded path inequality that was originally introduced in [13]. In the original inequality it is assumed that $|Z| = 1$, and that inequality only induces a facet of PAR_n when the path has even length $k - 1$. We note that a similar generalization of the inequality is considered in [20], where the variables y_{ij} with $\{i, j\} \subseteq Z$ have -1 coefficients. That inequality is mistakenly claimed to be valid for PAR_n.

When the above inequality is lifted according to Proposition 12 we obtain

$$-\sum_{i \in I^+} x_i + \sum_{e \in P \cup R} y_e - \sum_{e \in \bar{P} \cup \bar{R}} y_e - \left\lfloor \frac{k+2}{4} \right\rfloor \sum_{\{i,j\} \subseteq Z} y_{ij} \le 0. \tag{13}$$

We have the following result.

Proposition 22. *The inequality (13) induces a facet of $\mathcal{P}_n$ if either i) $|Z| \ge 2$ or ii) $|Z| = 1$ and $(|P| \bmod 2) = 0$.*

Note that these inequalities are homogeneous, and therefore induce facets of the correlation cone as well.

4.5 Lifting Facets of the Clique Partitioning Polytope

Finally, we would like to mention that sometimes we are able to obtain new facets of the clique partitioning polytope PAR_{n+1} of order $n+1$ from known facets of PAR_n via the other polytopes considered here. This involves the following steps.

Suppose that $b^T y \le b_0$ is an inequality that induces a facet of PAR_n. This inequality can be lifted (Proposition 12) to a facet-inducing inequality $-\alpha^T x + b^T y \le b_0 - \alpha^T \mathbf{1}_n$ for $\mathcal{P}_n$, where $\alpha \in \mathbb{R}^n_+$. Whenever this lifted inequality for the binary psd polytope $\mathcal{P}_n$ is homogeneous, i.e., $\alpha^T \mathbf{1}_n = b_0$, it also induces a facet of the boolean quadric polytope BQP_n (Proposition 7). The inequality $c^T y \le 0$ obtained via the covariance mapping (Proposition 13) defines a facet of the cut and multicut polytopes CUT_{n+1} and MCUT_{n+1} (Proposition 14). Then, by complementing this latter inequality, we obtain a facet-inducing inequality $c^T y \ge \sum_{e \in E_{n+1}} c_e$ for PAR_{n+1}.

Examples of new facets of PAR_{n+1} obtained in this manner will be given in the full version of the paper.

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