New Facets of the QAP-Polytope

Pawan Aurora[a], Shashank K Mehta[a]

[a] *Indian Institute of Technology, Kanpur - 208016, India*

Abstract

The Birkhoff polytope is defined to be the convex hull of permutation matrices, P_σ $\forall \sigma \in S_n$. We define a second-order permutation matrix $P_\sigma^{[2]}$ in $\mathbb{R}^{n^2 \times n^2}$ corresponding to a permutation σ as $(P_\sigma^{[2]})_{ij,kl} = (P_\sigma)_{ij}(P_\sigma)_{kl}$. We call the convex hull of the second-order permutation matrices, the *second-order Birkhoff polytope* and denote it by $\mathcal{B}^{[2]}$. It can be seen that $\mathcal{B}^{[2]}$ is isomorphic to the QAP-polytope, the domain of optimization in *quadratic assignment problem*. In this work we revisit the polyhedral combinatorics of the QAP-polytope viewing it as $\mathcal{B}^{[2]}$. Our main contribution is the identification of an exponentially large set of new facets of this polytope. Also we present a general inequality of which all the known facets of this polytope as well as the new ones, that we present in this paper, are special instances. We also establish the existence of more facets which are yet to be identified.

Keywords: Polyhedral Combinatorics, Quadratic Assignment Problem

1. Introduction

The Birkhoff polytope is defined to be the convex hull of the permutation matrices, P_σ $\forall \sigma \in S_n$. We define a second-order permutation matrix $P_\sigma^{[2]}$ corresponding to a permutation σ as $(P_\sigma^{[2]})_{ij,kl} = (P_\sigma)_{ij}(P_\sigma)_{kl}$. We call the convex hull of the second-order permutation matrices, the *second-order Birkhoff polytope* $\mathcal{B}^{[2]}$.

Clearly, the vertices of the second order Birkhoff polytope are vertices of the unit cube, $\{0,1\}^{n^2 \times n^2}$. Such polytopes are called zero-one polytopes.

Among various definitions of the Quadratic Assignment problem (QAP), see [2], one is $min\{\sum_{ij,kl}(A_{ik}B_{jl} + D_{ij,kl})\ Y_{ij,kl} | Y \in \mathcal{B}^{[2]}\}$ [3] where A, B are input matrices and D is a diagonal matrix. This may also be stated as $min\{\langle (A \otimes B + D), Y\rangle |\ Y \in \mathcal{B}^{[2]}\}$. Thus QAP is an optimization problem over $\mathcal{B}^{[2]}$. In the literature [2] this polytope is referred to as QAP-polytope.

$\mathcal{B}^{[2]}$ is a zero-one polytope as is the Birkhoff polytope. But unlike the latter which has only n^2 facets, $\mathcal{B}^{[2]}$ has exponentially many known facets [1, 2] and exponentially many additional facets are identified in this paper.

We will identify a generic inequality such that all the previously known facets and the new facets discovered in this paper are special instances of this inequality. We will also show that $\mathcal{B}^{[2]}$ must have some facets which are not the instances of this inequality. Which implies that more facets are yet to be discovered.

Email addresses: paurora@cse.iitk.ac.in (Pawan Aurora), skmehta@cse.iitk.ac.in (Shashank K Mehta)

2. A non-linear description of $\mathcal{B}^{[2]}$

Consider the *completely positive* program CP given below. Note that the variable matrix is required to be completely positive (constraint 1a), a stronger condition compared to positive semidefiniteness. In CP Y is a $(n^2+1) \times (n^2+1)$ matrix of variables with index set $(([n] \times [n]) \cup \{w\}) \times (([n] \times [n]) \cup \{w\})$. Since Y is also positive semidefinite, there exist vectors u_{ij} for all ij and ω in $\mathbb{R}^{n^2+1}$ such that $Y_{ij,kl} = u_{ij}^T \cdot u_{kl}$ and $Y_{ij,w} = u_{ij}^T \cdot \omega$. We will refer to these vectors as the vector realization of Y.

$$\text{CP:}\quad \max \sum_{i,j \in [n]} Y_{ij,ij} \quad \text{, subject to}$$

$$Y \in \mathcal{C}^* \tag{1a}$$

$$Y_{ij,ik} = 0 \quad , 1 \le i,j,k \le n,\ j \ne k \tag{1b}$$

$$Y_{ji,ki} = 0 \quad , 1 \le i,j,k \le n,\ j \ne k \tag{1c}$$

$$Y_{\omega,\omega} = 1 \tag{1d}$$

$$Y_{ij,\omega} = Y_{ij,ij}\ , 1 \le i,j \le n \tag{1e}$$

2.1. United Vectors

Let ω be any fixed unit vector in $\mathbb{R}^n$. Then for every unit vector v, we call $u = (\omega + v)/2$ a *united vector with respect to* ω.

Observation 1. *With respect to a fixed unit vector ω,*
(i) a vector u is united if and only if $u \cdot \omega = u^2$,
(ii) if u_1 and u_2 are mutually orthogonal united vectors, then $u_1 + u_2$ is also a united vector.
(iii) let $u_1, \dots, u_k$ be a set of pairwise orthogonal united vectors. This set is maximal (i.e., no new united vector can be added to it while preserving pairwise orthogonality)

if and only if ω belongs to the subspace spanned by these vectors if and only if $\sum_i u_i = \omega$ if and only if $\sum_i u_i^2 = 1$.

Consider CP in the light of united vectors. Let Y be a solution with $Y_{ij,kl} = u_{ij}^T.u_{kl}$ for all $ijkl$. and $Y_{ij,\omega} = u_{ij}^T.\omega$. This is a $(n^2+1)\times(n^2+1)$ matrix in which last row and the last column are same as the diagonal because $u_{ij}^T.\omega = u_{ij}^2$. In our subsequent discussion we will treat it as an $n^2 \times n^2$ matrix by dropping the last row and the last column. Equations 1d and 1e imply that u_{ij} are united vectors. Equations 1b and 1c imply that $\{u_{i1},\ldots,u_{in}\}$ are orthogonal sets and so are $\{u_{1i},\ldots,u_{ni}\}$. From the Observation 1 we know that each of these sets add up to a vector of length at most 1. Hence the objective function can evaluate to at most n. Note that in arriving at the upper bound we did not make use of the fact that Y is completely positive. Hence the same bound also holds for the positive semidefinite relaxation of CP (call it SDP).

Let $\mathcal{L}$ be the feasible region of CP where the objective function attains its maximum value, n. Observe that $P_\sigma^{[2]} \in \mathcal{L}\ \forall\ \sigma \in S_n$, since these are completely positive rank-1 matrices. Clearly $\mathcal{B}^{[2]} \subseteq \mathcal{L}$. In fact the converse is also true as the following lemma (proved in Appendix A) shows.

Lemma 2. $\mathcal{L} \subseteq \mathcal{B}^{[2]}$.

Consequence of the above observations is that $\mathcal{L} = \mathcal{B}^{[2]}$. Hence we have a non-linear description of $\mathcal{B}^{[2]}$. A similar non-linear description appears in [3]. In the rest of this paper our objective is to develop a linear description for $\mathcal{B}^{[2]}$.

3. The Affine Plane of $\mathcal{B}^{[2]}$

In this section we will develop a system of equations whose solution is the affine plane of $\mathcal{B}^{[2]}$, i.e., the affine-hull of all $P_\sigma^{[2]}$s.

3.1. A System of Equations for the Affine Plane

Consider a solution Y of CP (or SDP). If the objective function achieves its maximum value for Y, then each set $\{u_{i1},\ldots,u_{in}\}$ is a maximal orthogonal set. Similarly each set $\{u_{1i},\ldots,u_{ni}\}$ is also a maximal orthogonal set. In that case from united vector property $\sum_i u_{ij} = \sum_j u_{ij} = \omega$. We then have $1 = \omega^T\cdot\omega = \sum_i \omega^T \cdot u_{ij} = \sum_i u_{ij}^T \cdot u_{ij} = \sum_i Y_{ij,ij}$. Similarly $\sum_j Y_{ij,ij} = 1$. We also have $\sum_k Y_{ij,kl} = u_{ij}^T\cdot(\sum_k u_{kl}) = u_{ij}^T\cdot\omega = Y_{ij,ij}$. Similarly $\sum_l Y_{ij,kl} = Y_{ij,ij}$. So we have the following linear conditions:

$$Y_{ij,kl} - Y_{kl,ij} = 0 \qquad \forall i,j,k,l \tag{2a}$$

$$Y_{ij,il} = Y_{ji,li} = 0 \qquad \forall i, \forall j \neq l \tag{2b}$$

$$\sum_k Y_{ij,kl} = \sum_k Y_{ij,lk} = Y_{ij,ij} \qquad \forall i,j,l \tag{2c}$$

$$\sum_j Y_{ij,ij} = \sum_j Y_{ji,ji} = 1 \qquad \forall i \tag{2d}$$

It is easy to verify that every $P_\sigma^{[2]}$ satisfies these equations. We make a stronger claim in the following lemma (proved in Appendix B).

Lemma 3. *The only $0/1$ solutions of Equations 2a-2d are the $P_\sigma^{[2]}$s.*

The following lemma (proved in Appendix C) sums up the main result of this section.

Lemma 4. *The solution plane P of equations 2a-2d is the affine plane spanned by $P_\sigma^{[2]}$s, i.e., $P = \{\sum_\sigma \alpha_\sigma P_\sigma^{[2]} \mid \sum_\sigma \alpha_\sigma = 1\}$.*

4. Some Facets of $\mathcal{B}^{[2]}$

To develop a linear description of $\mathcal{B}^{[2]}$, we need the inequalities corresponding to its facets. The complete linear description will be these inequalities along with equations 2a-2d. In this section we will identify exponentially many new facets of $\mathcal{B}^{[2]}$, in addition to exponentially many already known facets given in [1, 2].

We will represent a facet by an inequality $f(x) \geq 0$ which defines the half space that contains the polytope and the plane $f(x) = 0$ contains the facet.

Let $\{\omega\} \cup \{u_{ij} | 1 \leq i,j \leq n\}$ represent a (united) vector realization of any point $Y \in \mathcal{B}^{[2]}$. Define a vector $A = \sum_{ij} n_{ij}u_{ij}$ for some choice of $n_{ij} \in \mathbb{Z}$ and let $\beta \in \mathbb{Z}$. Consider the following inequality.

$$(A - (\beta - 0.5)\omega)^2 \geq 0.25. \tag{3}$$

The above inequality defines the half space $\sum_{ij}(n_{ij}^2 - (2\beta-1)n_{ij})\ Y_{ij,ij} + \sum_{ij\neq kl} n_{ij}n_{kl}Y_{ij,kl} + \beta^2 - \beta \geq 0$. The united vector realization of $P_\sigma^{[2]}$ is $u_{ij} = \omega$ if $\sigma(i) = j$, else $u_{ij} = 0$. It is easy to see that every $P_\sigma^{[2]}$, hence every point of $\mathcal{B}^{[2]}$, satisfies the inequality (3).

If there exists a permutation σ such that $\sum_{(ij):\sigma(i)=j} n_{ij}$ is either equal to β or $\beta-1$, then $P_\sigma^{[2]}$ satisfies (3) with equality. In this case the plane $(A-(\beta-0.5)\omega)^2 = 0.25$ is a supporting plane of $\mathcal{B}^{[2]}$ and hence defines a face. We will show that some instances of this inequality define facets for $\mathcal{B}^{[2]}$. Later we will also show that all the facets identified in [1, 2] also belong to the same inequality.

It may be pointed out that another inequality, which can define faces, is $(A - \beta\omega)^2 \geq 0$. But no known facets correspond to this inequality.

We will discuss the following three sets of inequalities:
1. $(u_{ij} + u_{kl} - 0.5\omega)^2 \geq 0.25$,
2. $(u_{p_1q_1} + u_{p_2q_2} + u_{p_1q_2} - u_{kl} - 0.5\omega)^2 \geq 0.25$,
3. $(u_{i_1j_1} + \cdots + u_{i_mj_m} - u_{kl} - 0.5\omega)^2 \geq 0.25$, and show that each instance of each of these inequalities defines a facet of $\mathcal{B}^{[2]}$.

The following lemma gives a method to establish a facet.

Let X be a set of vectors. Then $LS(X)$ denotes the subspace spanned by the vectors of X.

Lemma 5. *Let V be the set of vertices of a polytope such that the affine plane of V does not contain the origin and $f(x) \geq 0$ be a linear inequality satisfied by all the vertices. Let $S = \{v \in V | f(v) = 0\}$ such that $V \setminus S \neq \emptyset$. And let $v_0 \in V \setminus S$ such that each vertex in V can be expressed as a linear combination of $\{v_0\} \cup S$. Then S is a facet, i.e., $f(x) \geq 0$ defines a facet.*

PROOF. Let d denote the dimension of $LS(V)$. So the dimension of the affine plane of V is $d-1$. Also $V \subset LS(\{v_0\} \cup S)$ so the dimension of $LS(S)$ is at least $d-1$. As the affine plane of S does not contain the origin, the dimension of the affine plane of S is at least $d-2$. Observe that V is not contained in $LS(S)$ since $f(x)$ is non-zero for $x \in V \setminus S$. We conclude that the dimension of the affine plane of S is exactly one less than that of the affine plane of V. □

Corollary 6. *Let $G = (V \setminus S, E)$ be a graph with the property that for each $\{u, v\} \in E$, $u - v \in LS(S)$. If G is connected, then S is a facet.*

Let k_1, k_2, k_3 be any three integers belonging to $[n]$. Let $\sigma_1, \ldots, \sigma_6$ be a set of permutations of S_n which have same image for each element of $[n] \setminus \{k_1, k_2, k_3\}$, i.e., $\sigma_i(z) = \sigma_j(z)$ for all $z \in [n] \setminus \{k_1, k_2, k_3\}$ for every $i, j \in \{1, \ldots, 6\}$. Let images of k_1, k_2, k_3 under $\sigma_1, \ldots, \sigma_6$ be (a, b, c), (a, c, b), (b, a, c), (b, c, a), (c, a, b), (c, b, a) respectively. Further, suppose x, y be any two elements of $[n] \setminus \{k_1, k_2, k_3\}$. Let σ'_i be transposition of σ_i on indices x and y, for each $i = 1, \ldots, 6$. That is, $\sigma'_i(z) = \sigma_i(z)$ for all $z \in [n] \setminus \{x, y\}$, $\sigma'_i(x) = \sigma_i(y)$, and $\sigma'_i(y) = \sigma_i(x)$. Let $\Sigma = \{\sigma_1, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6\}$. Following is a useful identity.

Lemma 7. *Let $\sigma_1, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6$ be a set of permutations as defined above. Then $\sum_{\sigma \in \Sigma} sign(\sigma) P^{[2]}_{\sigma} = 0$.*

In this section V will denote the set $\{P^{[2]}_{\sigma} | \sigma \in S_n\}$ and S will denote $\{P^{[2]}_{\sigma} | f(P^{[2]}_{\sigma}) = 0\}$.

Theorem 8. *The non-negativity constraint $Y_{ij,kl} \geq 0$, which is same as $(u_{ij} + u_{kl} - 0.5\omega)^2 \geq 0.25$, defines a facet of $\mathcal{B}^{[2]}$ for every i, j, k, l such that $i \neq k$ and $j \neq l$.*

PROOF. Observe that the non-negativity condition is satisfied by every $P^{[2]}_{\sigma}$. Every vertex in the set $V \setminus S$ corresponds to a permutation σ where $\sigma(i) = j$ and $\sigma(k) = l$. Consider a graph $G = (V \setminus S, E)$ where $E = \{P^{[2]}_{\sigma}, P^{[2]}_{\sigma'}\}$ where σ' is a transposition of σ. Since the set of permutations corresponding to the vertices in $V \setminus S$ is isomorphic to the group S_{n-2}, G must be a connected graph.

Let σ_1 and σ'_1 be a pair of permutations in $V \setminus S$ which are transpositions of each other at indices x, y, i.e., $\sigma_1(x) = \sigma'_1(y)$ and $\sigma_1(y) = \sigma'_1(x)$. Let $k_1 = i, k_2 = k$ and k_3 be any element other than x, y, i, k. Consider all the permutations $\sigma_2, \ldots, \sigma_6, \sigma'_2, \ldots, \sigma'_6$ as defined in the context of lemma 7. Observe that all the $P^{[2]}_{\sigma}$s corresponding to these ten permutations belong to S. Hence we can express $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1}$ in terms of vertices in S using the identity of the lemma. From corollary 6 the inequality defines a facet. □

Lemma 9. *(1) Let X be a set of permutations σ such that $\sigma(1) = 1, \ldots, \sigma(a) = a$ and $\sigma(a+1) \notin I_1, \ldots, \sigma(a+b) \notin I_b$ where I_j are subsets of $[n]$ such that $|\cup_i I_i| \leq n-a-b$. Let $G = (X, E)$ be a graph in which $\{P^{[2]}_{\sigma}, P^{[2]}_{\sigma'}\} \in E$ if σ and σ' are transpositions of each other. Then G is connected.*

(2) Let X be a set of permutations σ such that $\sigma(1) = 1, \ldots, \sigma(a) = a, \sigma(a+1) \neq x_1, \ldots, \sigma(a+b) \neq x_b$, where all x_i are distinct and greater than a and $a+b < n$. Let $G = (X, E)$ be a graph in which $\{P^{[2]}_{\sigma}, P^{[2]}_{\sigma'}\} \in E$ if σ and σ' are transpositions of each other. Then G is connected.

PROOF. (1) Let $I = \cup_i I_i$. Without loss of generality assume that $I = \{a+b+1, a+b+2, \ldots\}$. Hence the identity permutation belongs to X.

Given any permutation $\sigma_0 \in X$, we will show that there is a path from σ_0 to the identity. Starting from σ_0, suppose the current permutation σ is such that for some $i \in \{a+1, \ldots, a+b\}$, $\sigma(i) \in \{a+b+1, \ldots, n\}$. Hence there must exist a $j \in \{a+b+1, a+b+2, \ldots, n\}$ such that $\sigma(j) \in \{a+1, \ldots, a+b\}$. Performing transposition on i and j we extend the path as the new permutation is also in X. Finally we will reach a permutation in which all indices in the range $a+1, \ldots, a+b$ map to $a+1, \ldots, a+b$ and hence all indices of $a+b+1, \ldots n$ map to $a+b+1, \ldots, n$.

Next perform transpositions within indices of $a+1, \ldots, a+b$ so that finally $\sigma(i)$ maps to i for all i in this range. Note that all the permutations generated in the process belong to X. In the end we do the same for indices in the range $a+b+1, \ldots, n$.

(2) The claim is vacuously true if X is empty. So we assume that it is non-empty. By relabeling we can make sure that $x_i \neq a+i$ for all $1 \leq i \leq b$. So without loss of generality we can assume that the identity permutation belongs to X. To prove the claim we will show that starting from any arbitrary permutation $\sigma_0 \in X$ there is a path from σ_0 to the identity permutation. While tracing this path, the current permutation has $\sigma(a+i) \neq a+i$ while $\sigma(a+j) = a+j$ for all $j < i$. Let $\sigma^{-1}(a+i) = a+k$.

If $a+k > a+b$ or if $a+k \leq a+b$ & $\sigma(a+i) \neq x_k$, then perform transposition on indices $a+i$ and $a+k$ resulting into the new permutation σ' which belongs to X and is "closer" to the identity.

Now consider the case where $\sigma(a+i) = x_k$. Observe that there must be at least three indices beyond $a+i-1$. Let $a+j$ be any index greater than $a+b$. Perform transposition on indices $a+j$ and $a+k$ giving σ' and then perform transposition on $a+i$ and $a+j$. Let the new permutation be σ''. Observe that both, σ' and σ'', belong to X. So the path extends by edges $\{\sigma, \sigma'\}$ and $\{\sigma', \sigma''\}$. Further, σ'' is closer to the identity.

Thus the path eventually reaches the identity and its length is at most $2b$ steps. □

Theorem 10. *Inequality $Y_{p_1q_1,kl} + Y_{p_2q_2,kl} + Y_{p_1q_2,kl} \leq Y_{kl,kl} + Y_{p_1q_1,p_2q_2}$, which is same as $(u_{p_1q_1} + u_{p_2q_2} + u_{p_1q_2} - u_{kl} - 0.5\omega)^2 \geq 0.25$, defines a facet of $\mathcal{B}^{[2]}$, where p_1, p_2, k are distinct and q_1, q_2, l are also distinct and $n \geq 6$.*

Proof. The set of vertices which satisfy the inequality strictly is the union of $X_1 = \{P^{[2]}_\sigma | \sigma(p_1) = q_1, \sigma(p_2) = q_2, \sigma(k) \neq l\}$ and $X_2 = \{P^{[2]}_\sigma | \sigma(p_1) \neq q_1,\ \sigma(p_1) \neq q_2,\ \sigma(p_2) \neq q_2,\ \sigma(k) = l\}$. So $V \setminus S = X_1 \cup X_2$.

Define a graph $G = (X_1 \cup X_2, E)$ where E is the set of edges $\{P^{[2]}_\sigma, P^{[2]}_{\sigma'}\}$ where σ is a transposition of σ' and both matrices belong to $X_1 \cup X_2$. From lemma 9 the subgraphs on X_1 and X_2 are each connected. We also notice that there is no edge connecting these components. So we add a special edge $\{P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}\}$ to G making the graph connected. Let α_1 be any arbitrary member of X_1. Let $i_2 = \alpha_1^{-1}(l)$ and r be any index other than p_1, p_2, k, i_2. So α_1 maps $p_1 \to q_1, p_2 \to q_2, k \to b, i_2 \to l, r \to a$ for some a and b. Define α_2 to be the permutation which maps $p_1 \to a, p_2 \to q_1, k \to l, i_2 \to b, r \to q_2$ and in all other cases images of α_1 and α_2 coincide. Observe that $P^{[2]}_{\alpha_2} \in X_2$.

Now we will show that for each edge $\{P^{[2]}_{x'}, P^{[2]}_{y'}\}$ of the graph, $P^{[2]}_{x'} - P^{[2]}_{y'}$ belongs to $LS(S)$. We begin with the edge $\{P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}\}$. Let $\sigma_1 = \alpha_1$. Define $\sigma_2, \ldots, \sigma_6$ using $k_1 = p_1, k_2 = p_2, k_3 = r$ as described before lemma 7. Taking $x = k$ and $y = i_2$, define $\sigma'_1, \ldots, \sigma'_6$. See that $\alpha_2 = \sigma'_5$. The rest of the permutations are in S. Hence from lemma 7 $P^{[2]}_{\alpha_1} - P^{[2]}_{\alpha_2}$ can be expressed as a linear combination of vertices in S.

Next we will show that each edge in the graph on X_1 has the same property. Let $\{P^{[2]}_{\sigma_1}, P^{[2]}_{\sigma'_1}\}$ be an edge in the graph on X_1. In both permutations p_1 and p_2 map to q_1 and q_2 respectively. Define $k_1 = p_1$ and $k_2 = p_2$. There is at least one index, other than p_1, p_2, k, which has the same image in both the permutations because $n \geq 6$. Label it k_3. Consider 5 new permutations formed from σ_1 by permuting the images of k_1, k_2 and k_3. Call them $\sigma_2, \ldots, \sigma_6$. Similarly define $\sigma'_2, \ldots, \sigma'_6$ from σ'_1. Observe that in each σ_i for $i \geq 2$, k does not map to l. In addition either p_1 does not map to q_1 or p_2 does not map to q_2. Hence $P^{[2]}_{\sigma_2}, \ldots, P^{[2]}_{\sigma_6}$ belong to S. Similarly $P^{[2]}_{\sigma'_2}, \ldots, P^{[2]}_{\sigma'_6}$ also belong to S. From lemma 7, $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1} \in LS(S)$.

Now we consider the edges of X_2. Let $\{P^{[2]}_{\sigma_1}, P^{[2]}_{\sigma'_1}\}$ be one such edge. Let x, y be the indices at which σ_1 and σ'_1 differ. Consider two cases of σ_1: (1) $\sigma_1(p_1) = a, \sigma_1(p_2) = b, \sigma_1(k) = l, \sigma_1(r) = q_1, \sigma_1(s) = q_2$, (2) $\sigma_1(p_1) = a, \sigma_1(p_2) = q_1, \sigma_1(k) = l, \sigma_1(r) = q_2$.

Case (1) Subcase $|\{p_1, p_2, r, s\} \cap \{x, y\}| \leq 1$: If $p_1 \notin \{x, y\}$, then define $k_1 = k$, $k_2 = p_1$, and k_3 be any index in $\{r, s\} \setminus \{x, y\}$. Otherwise $k_1 = k, k_2 = p_2, k_3 = s$. All the permutations $\sigma_2, \ldots, \sigma_6$ and $\sigma'_2, \ldots, \sigma'_6$ as defined before lemma 7 are in S. So $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1}$ can be expressed as a linear combination of points in S using the identity.

Subcase $\{x, y\} \subset \{p_1, p_2, r, s\}$: Only three cases are possible here: $x = p_2, y = r$; $x = r, y = s$; and $x = p_1, y = p_2$, apart from exchanging the roles of x and y. In the first case let $k_1 = p_1, k_2 = s, k_3 = k$ and use lemma 7. The remaining two cases are proven differently.

In these two cases we will not show that $P^{[2]}_\sigma - P^{[2]}_{\sigma'}$ can be expressed as a linear combination of vertices in S. Instead, we will delete such edges from E and show that the reduced graph is still connected. Consider an edge $\{P^{[2]}_\sigma, P^{[2]}_{\sigma'}\}$ of the second type where σ maps: $p_1 \to a, p_2 \to b, k \to l, r \to q_1, s \to q_2, u \to v$ and σ' maps: $p_1 \to a, p_2 \to b, k \to l, r \to q_2, s \to q_1, u \to v$. Note that $n \geq 6$ so there always exists the pair u, v. Rest of the indices have the same images in the two permutations. To show that after dropping an edge of this class the graph remains connected, define two new permutations: α_1: $p_1 \to a, p_2 \to b, k \to l, r \to v, s \to q_2, u \to q_1$ and α_2: $p_1 \to a, p_2 \to b, k \to l, r \to q_2, s \to v, u \to q_1$. Other mappings are same as in σ. Observe that $\{P^{[2]}_\sigma, P^{[2]}_{\alpha_1}\}, \{P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}\}$ and $\{P^{[2]}_{\alpha_2}, P^{[2]}_{\sigma'}\}$ are edges in the reduced graph, hence there is a path from $P^{[2]}_\sigma$ to $P^{[2]}_{\sigma'}$ in it.

Let $\{P^{[2]}_\sigma, P^{[2]}_{\sigma'}\}$ be third type of edge. So σ maps $p_1 \to a, p_2 \to b, k \to l, r \to q_1, s \to q_2$ and σ' maps $p_1 \to b, p_2 \to a, k \to l, r \to q_1, s \to q_2$. Again to show a path from $P^{[2]}_\sigma$ to $P^{[2]}_{\sigma'}$ in the reduced graph, define α_1: $p_1 \to a, p_2 \to q_1, k \to l, r \to b, s \to q_2$ and α_2: $p_1 \to b, p_2 \to q_1, k \to l, r \to a, s \to q_2$. Other mappings are same as in σ. In case (2) we will show that $\{P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}\}$ and $\{P^{[2]}_{\alpha_2}, P^{[2]}_{\sigma'}\}$ are edges in the reduced graph. Hence $P^{[2]}_\sigma, P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}, P^{[2]}_{\sigma'}$ is a path in the reduced graph. Note that $\{P^{[2]}_\sigma, P^{[2]}_{\alpha_1}\}$ is an edge of the first type.

Case (2) Subcase $\{p_1, p_2, r = \sigma^{-1}(q_2)\} \cap \{x, y\} = \emptyset$: In this case define $k_1 = p_1, k_2 = p_2, k_3 = r$.

Subcase $|\{p_1, p_2, r = \sigma^{-1}(q_2)\} \cap \{x, y\}| = 1$: If $x = p_1$ or $y = p_1$, then $k_1 = p_2, k_2 = r, k_3 = k$. If $x = p_2$ or $y = p_2$, then $k_1 = p_1, k_2 = r, k_3 = k$. Finally if $x = r$ or $y = r$, then $k_1 = p_1, k_2 = p_2, k_3 = k$. In each case lemma 7 gives a desired linear expression in terms of points in S for $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1}$.

Subcase $\{x, y\} \subset \{p_1, p_2, r = \sigma^{-1}(q_2)\}$ does not arise because in this case every transposition leads to a permutation in S.

From Corollary 6 we conclude that S is a facet. □

Consider the following inequality where $3 \leq m \leq n-3$.

$$Y_{i_1j_1,kl} + Y_{i_2j_2,kl} + \ldots + Y_{i_mj_m,kl} \leq Y_{kl,kl} + \sum_{r \neq s} Y_{i_rj_r,i_sj_s}. \quad (4)$$

Observe that it can also be written as $(u_{i_1j_1} + \cdots + u_{i_mj_m} - u_{kl} - 0.5\omega)^2 \geq 0.25$, where $3 \leq m \leq n-3$. In the rest of this section we will show that inequality (4) also defines a facet of $\mathcal{B}^{[2]}$.

We will continue to use S to denote the set of vertices that satisfy the given inequality with equality. Let T denote the set of remaining vertices. For the system (4) the set T can be subdivided into the following classes:

1. $T_1 : k \to l, i_1 \not\to j_1, i_2 \not\to j_2, \ldots, i_m \not\to j_m$.
2. $T_2 : k \to l$ and three or more $i_r \to j_r$.
3. $T_3 : k \not\to l$ and two or more $i_r \to j_r$.

In classes T_2 and T_3 we do further subdivision. If a permutation in T_2 maps i_r to j_r for x out of m indices, then such a permutation belongs to subclass denoted by $T_{2,x}$. Similarly $T_{3,x}$ is defined. Observe that $T_2 = \cup_{x \geq 3} T_{2,x}$ and $T_3 = \cup_{x \geq 2} T_{3,x}$.

Lemma 11. *Let $m \geq 3$. The graph G_1 on T_1, with edge set $\{P^{[2]}_{\sigma'}, P^{[2]}_{\sigma''}\}$ where σ' is a transposition of σ'', is connected. Further the difference vector corresponding to each edge belongs to $LS(S)$.*

Proof. The first part of the lemma is a special case of the second part of lemma 9.

For the second part let $\{P^{[2]}_{\sigma_1}, P^{[2]}_{\sigma'_1}\}$ be an edge in G_1 where $\sigma_1(x) = \sigma'_1(y)$ and $\sigma_1(y) = \sigma'_1(x)$. As m is at least 3, there exists $r \leq m$ such that $i_r \notin \{x, y\}$ and $j_r \notin \{\sigma_1(x), \sigma_1(y)\}$. Without loss of generality assume that $r = 1$. So we have description of σ_1 and σ'_1 as follows: $\sigma_1 : k \to l, x \to \alpha, y \to \beta, i_1 \to \gamma, \delta \to j_1, \ldots$ and $\sigma'_1 : k \to l, x \to \beta, y \to \alpha, i_1 \to \gamma, \delta \to j_1, \ldots$.

Taking $k_1 = k, k_2 = i_1, k_3 = \delta$, x as x and y as y, generate permutations $\sigma_2, \ldots, \sigma_6, \sigma'_2, \ldots, \sigma'_6$ as defined before lemma 7. Vertices corresponding to each of these permutations belong to S. Hence from lemma 7, $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1} \in LS(S)$. $\square$

Corollary 12. *Given any $P^{[2]}_{\sigma*}$ in T_1, each $P^{[2]}_{\sigma}$ in T_1 belongs to $LS(\{P^{[2]}_{\sigma*}\} \cup S)$.*

Lemma 13. *Let $n \geq 5$. Then $T_{3,2} \subset LS(T_1 \cup S)$.*

Proof. Consider any arbitrary permutation, σ, with the corresponding vertex belonging to $T_{3,2}$. Let $\beta = \sigma^{-1}(l)$ and γ be any arbitrary element from $[n] \setminus \{k, i_1, i_2, \beta\}$. The description of σ is: $k \to \alpha, i_1 \to j_1, i_2 \to j_2, \beta \to l, \gamma \to \delta$ and all other maps are different from (i_p, j_p) for any p, where $\alpha \neq l$. Our goal is to show that $P^{[2]}_{\sigma} \in LS(T_1 \cup S)$. Consider two cases.

Case: $(\beta, \alpha) \neq (i_p, j_p)$ for any p. Take $\sigma_1 = \sigma, k_1 = i_1, k_2 = i_2, k_3 = \gamma, x = k, y = \beta$. All the vertices corresponding to permutations $\sigma_2, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6$ generated with these parameters belong to $S \cup T_1$. From lemma 7 $P^{[2]}_{\sigma_1} \in LS(T_1 \cup S)$.

Case: $(\beta, \alpha) = (i_3, j_3)$. In this case $\sigma : k \to j_3, i_1 \to j_1, i_2 \to j_2, i_3 \to l, \gamma \to \delta$. Take $\sigma_1 = \sigma, k_1 = k, k_2 = i_1, k_3 = i_2, x = i_3, y = \gamma$. Then we see that $P^{[2]}_{\sigma_1}$ and $P^{[2]}_{\sigma'_1}$ both belong to $T_{3,2}$ and the vertices corresponding to the remaining ten permutations belong to S. So $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1} \in LS(S)$. Now from the first case $P^{[2]}_{\sigma'_1}$ belongs to $LS(T_1 \cup S)$. Therefore $P^{[2]}_{\sigma_1}$ also belongs to $LS(T_1 \cup S)$. $\square$

Lemma 14. *Let $n \geq 5$. Then $T_{2,3} \subset LS(T_1 \cup S)$.*

Proof. Let $P^{[2]}_{\sigma}$ be an arbitrary element of $T_{2,3}$. We will express $P^{[2]}_{\sigma}$ as a linear combination of some members of $T_{3,2} \cup S$. The rest will follow from lemma 13.

Without loss of generality assume that the given permutation σ in $T_{2,3}$ maps $k \to l, i_1 \to j_1, i_2 \to j_2, i_3 \to j_3$. Also let σ map $\alpha \to \beta$ for some $\alpha \notin \{k, i_1, i_2, i_3\}$. Now generate the permutations $\sigma_2, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6$ with parameters $\sigma_1 = \sigma, k_1 = i_2, k_2 = i_3, k_3 = \alpha, x = k, y = i_1$. See that $P^{[2]}_{\sigma'_1} \in T_{3,2}$ and the remaining ten permutations belongs to S. So $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1} \in LS(S)$. From lemma 13, $P^{[2]}_{\sigma} \in LS(S \cup T_1)$. $\square$

Lemma 15. *Let $n \geq 6$. Given any $P^{[2]}_{\sigma}$ in $T_{2,r}$ (resp. $T_{3,r}$) with $r > 3$ (resp. $r > 2$), it can be expressed as a linear combination of elements of $T_1 \cup S$.*

Proof. Let $P^{[2]}_{\sigma_1} \in T_{3,r}$ with $r \geq 3$. Assume that σ_1 maps $\alpha \to l, k \to \gamma, i_1 \to j_1, i_2 \to j_2, i_3 \to j_3, \ldots, i_r \to j_r$. If $r = 3$, then consider the parameters $x = i_3, y = \alpha, k_1 = i_1, k_2 = i_2, k_3 = \beta \notin \{i_1, i_2, i_3, k, \alpha\}$. Otherwise let $x = i_4, y = \alpha, k_1 = i_1, k_2 = i_2, k_3 = i_3$. Generate $\sigma_2, \ldots, \sigma_6, \sigma'_1, \ldots, \sigma'_6$. Corresponding vertices either belong to S or to $\cup_{2 \leq x < r} T_{3,x}$. So using induction on r and the result of lemma 13 as the base case, lemma 7 gives that $P^{[2]}_{\sigma_1} \in LS(T_1 \cup S)$.

Similar argument shows that $T_{2,r}$ vertices also belong to $LS(T_1 \cup S)$. $\square$

Corollary 16. *If $n \geq 6$, then $T_2 \cup T_3 \subset LS(T_1 \cup S)$.*

Proof. Follows from the previous three lemmas. $\square$

Theorem 17. *If $n \geq 6$, then inequality (4) defines a facet of $\mathcal{B}^{[2]}$.*

Proof. From corollaries 12 and 16 every vertex in T can be expressed as a linear combination of a fixed vertex in T and the vertices of S. Now the result follows from lemma 5. $\square$

Together $\frac{n^2(n-1)^2}{2} + \sum_{i=2}^{n-3} \frac{n^2(n-1)^2 \cdots (n-i)^2}{i!}$ facets of the polytope are defined by theorems 8,10,17.

4.1. Previously Known Facets of $\mathcal{B}^{[2]}$

Let P_1, P_2 be disjoint subsets of $[n]$. Similarly Q_1, Q_2 are also disjoint subsets of $[n]$. Then the 4-box inequality discussed in [1, 2] is $(-\sum_{i \in P_1, j \in Q_1} u_{ij} - \sum_{i \in P_2, j \in Q_2} u_{ij} + \sum_{i \in P_1, j \in Q_2} u_{ij} + \sum_{i \in P_2, j \in Q_1} u_{ij} - (\beta - 0.5)\omega)^2 \geq 0.25$. The 1-box inequality is equivalent to $(\sum_{i \in P_1, j \in Q_2} u_{ij} - (\beta - 0.5)\omega)^2 \geq 0.25$ and is obtained by setting $P_2 = Q_1 = \emptyset$ in the 4-box inequality, whereas the 2-box inequality corresponds to $(-\sum_{i \in P_2, j \in Q_2} u_{ij} + \sum_{i \in P_1, j \in Q_2} u_{ij} - (\beta - 0.5)\omega)^2 \geq 0.25$ and is obtained by setting $Q_1 = \emptyset$ in the 4-box inequality. All the facets listed in [1, 2] are special instances of either the 1-box or the 2-box inequality.

5. Insufficiency of inequality (3)

We will show that even after including every facet given by the inequality (3) in the SDP relaxation of CP, the resulting feasible region remains larger than $\mathcal{B}^{[2]}$. Hence there exist facets of $\mathcal{B}^{[2]}$ which are yet to be discovered. In the following we will replace the inequality (3) with the equivalent $\sum_{ijkl} x_{ij}x_{kl}\ Y_{ij,kl}\ -(2z-1)\sum_{ij} x_{ij}Y_{ij,ij}$ $+z^2 - z \geq 0$. Further let $\mathcal{F}$ denote the feasible region of SDP where the objective function attains its maximum value, n.

Lemma 18. *Let P_σ denote the row-major vectorization of the corresponding permutation matrix. Following statements are equivalent.*

1. Region of $\mathcal{F}$, satisfying conditions $\sum_{ijkl} x_{ij}x_{kl}\ Y_{ij,kl}$ $-(2z-1)\sum_{ij} x_{ij}Y_{ij,ij}$ $+z^2 - z \geq 0$ for all $x_{ij}, z \in \mathbb{Z}$ is exactly equal to $\mathcal{B}^{[2]}$.

2. Given any set of permutations I such that $\{P_\sigma^{[2]} | \sigma \in I\}$ is L.I. Then $\sum_{\sigma\in I} \alpha_\sigma((P_\sigma^T \cdot x)^2 - (2z-1)(P_\sigma^T \cdot x)) + z^2 - z \geq 0$ for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$ if and only if $\alpha_\sigma \geq 0\ \forall\ \sigma \in I$ and $\sum_{\sigma\in I} \alpha_\sigma = 1$.

Proof. Let Y be a point in the feasible region of the SDP. We know from lemma 4 that Y is in the affine hull of $P_\sigma^{[2]}$s. So there exist α_σ such that $Y = \sum_\sigma \alpha_\sigma P_\sigma^{[2]}$ where $\sum_\sigma \alpha_\sigma = 1$ and $\{P_\sigma^{[2]} | \alpha_\sigma \neq 0\}$ is linearly independent.

Consider arbitrary $x \in \mathbb{Z}^{n^2}$ and $z \in \mathbb{Z}$. So $\sum_{ijkl} x_{ij}x_{kl}$ $Y_{ij,kl}\ -(2z-1)\sum_{ij} x_{ij}Y_{ij,ij}\ +z^2 - z = \sum_\sigma \alpha_\sigma \sum_{ijkl} x_{ij}x_{kl}$ $P_\sigma^{[2]}(ij,kl)\ -(2z-1)\sum_\sigma \alpha_\sigma \sum_{ij} x_{ij}\ P_\sigma^{[2]}(ij,ij)\ +z^2 - z =$ $\sum_\sigma \alpha_\sigma \sum_{ijkl} x_{ij}x_{kl}(P_\sigma)_{ij}(P_\sigma)_{kl}\ -(2z-1)\sum_\sigma \alpha_\sigma \sum_{ij} x_{ij}$ $(P_\sigma)_{ij}\ +z^2 - z = \sum_\sigma \alpha_\sigma (P_\sigma^T \cdot x)^2\ -(2z-1)\sum_\sigma \alpha_\sigma (P_\sigma^T \cdot x)$ $+z^2 - z$.

Besides, $Y \in \mathcal{B}^{[2]}$ if and only if $\alpha_\sigma \geq 0\ \forall\ \sigma$. $\square$

We first prove a useful lemma. In the following let $P_\sigma^T \cdot x + z = \sum_{i=1}^n x_{i,\sigma(i)} + z$ be denoted by y_σ.

Lemma 19. *$\sum_\sigma \alpha_\sigma(y_\sigma^2 - y_\sigma) = 0$ for all $x \in \mathbb{Z}^{n^2}$, $z \in \mathbb{Z}$ if and only if $\sum_\sigma \alpha_\sigma y_\sigma^2 = 0$ for all $x \in \mathbb{Z}^{n^2}$, $z \in \mathbb{Z}$.*

Proof. (If) Let $S(x,z) = \sum_\sigma \alpha_\sigma y_\sigma^2$. We have $S(x,z) = 0$ for all $x \in \mathbb{Z}^{n^2}$ and $z \in \mathbb{Z}$. Let a be any arbitrary point in $\mathbb{Z}^{n^2}$. Fix some i,j. Define a' as $a'_{i'j'} = a_{i'j'}$ if $i' \neq i$ or $j' \neq j$ and $a'_{ij} = a_{ij} + 1$. So $S(a',b) = S(a,b) + \sum_{\sigma:\sigma(i)=j} \alpha_\sigma(2y_\sigma(a,b) + 1)$. Define a'' in the similar way as a' is defined, except here $a''_{ij} = a_{ij} - 1$. Then we get $S(a'',b) = S(a,b) - \sum_{\sigma:\sigma(i)=j} \alpha_\sigma(2y_\sigma(a,b) - 1)$. So $(S(a',b) - S(a'',b))/2 = \sum_{\sigma:\sigma(i)=j} \alpha_\sigma y_\sigma(a,b)$. Setting $S(a',b) = S(a'',b) = 0$ we have $\sum_{\sigma:\sigma(i)=j} \alpha_\sigma y_\sigma(a,b) = 0$. So $\sum_\sigma \alpha_\sigma y_\sigma(a,b) = \sum_j \sum_{\sigma:\sigma(i)=j} \alpha_\sigma y_\sigma(a,b) = 0$. As a is arbitrarily chosen we have $\sum_\sigma \alpha_\sigma y_\sigma = 0$ for all $x \in \mathbb{Z}^{n^2}$ and all $z \in \mathbb{Z}$.

(Only if) This part is trivial because $S(x,z) = 0.5($ $T(x,z) + T(-x,-z))$ where $T(x,z) = \sum_\sigma \alpha_\sigma\ (y_\sigma^2 - y_\sigma)$. $\square$

Let p_σ be the (n^2+1)-dimensional vector in which the first n^2 entries are the vectorized P_σ and the last entry is 1. Define $\tilde{P}_\sigma^{[2]} = p_\sigma . p_\sigma^T$.

Lemma 20. *$\{P_\sigma^{[2]} | \sigma \in I\}$ is linearly independent if and only if $\{y_\sigma^2 - y_\sigma | \sigma \in I\}$ is linearly independent.*

Proof. The $n^2 \times n^2$ matrix $P_\sigma^{[2]}$ is a principal submatrix of $\tilde{P}_\sigma^{[2]}$. The last row and the last column of $\tilde{P}_\sigma^{[2]}$ is the same as its diagonal. Hence $\{P_\sigma^{[2]} | \sigma \in I\}$ is linearly independent if and only if $\{\tilde{P}_\sigma^{[2]} | \sigma \in I\}$ is linearly independent.

$\sum_{\sigma\in I} \alpha_\sigma \tilde{P}_\sigma^{[2]} = 0$ if and only if $\sum_{\sigma\in I} \alpha_\sigma q^T \tilde{P}_\sigma^{[2]} q =$ $0\ \forall q \in \mathbb{Q}^{n^2+1}$, where first n^2 components of q is x and the last component is z. It can be rewritten as $\sum_{\sigma\in I} \alpha_\sigma(P_\sigma^T \cdot$ $x + z)^2 = 0\ \forall x \in \mathbb{Q}^{n^2}, \forall z \in \mathbb{Q}$. Writing in terms of y_σ, the above statement is equivalent to $\sum_{\sigma\in I} \alpha_\sigma y_\sigma^2 =$ $0\ \forall x \in \mathbb{Q}^{n^2}\ \forall z \in \mathbb{Q}$. From lemma 19, this is equivalent to $\sum_{\sigma\in I} \alpha_\sigma(y_\sigma^2 - y_\sigma) = 0\ \forall x \in \mathbb{Q}^{n^2}, \forall z \in \mathbb{Q}$. $\square$

Consider the polynomial ring $A = \mathbb{Q}[\{x_{ij} | 1 \leq i,j \leq n\} \cup \{z\}]$. The subspace of A generated by $\{x_{ij} | 1 \leq i,j \leq n\} \cup \{z\} \cup \{x_{ij}x_{kl} | 1 \leq i,j,k,l \leq n\} \cup \{zx_{ij} | 1 \leq i,j \leq n\}$ is the direct sum of components of degree 1 and 2. Its dimension is $d = 1 + (n^2+1) + (n^4+n^2)/2$. For $n \geq 6$, $d \leq n!$. So the set $\{y_\sigma^2 - y_\sigma | \sigma \in S_n\}$ is linearly dependent for all $n \geq 6$.

Let J be a minimal set of permutations such that $\{y_\sigma^2 - y_\sigma | \sigma \in J\}$ is linearly dependent. So there exist α_σ such that $\sum_{\sigma\in J} \alpha_\sigma(y_\sigma^2 - y_\sigma) = 0$. Since no set of two $P_\sigma^{[2]}$ is L.D., the same holds for any pair of $y_\sigma^2 - y_\sigma$. Hence at least three coefficients are non-zero. Assume that $\alpha_{\sigma_1}, \alpha_{\sigma_2}, \alpha_{\sigma_3}$ are non-zero. Let the sign of the first two be same. We may assume that α_{σ_1} and α_{σ_2} are negative. If not, then invert the sign of every coefficient. Note that $(-\alpha_{\sigma_1})(y_{\sigma_1}^2 - y_{\sigma_1})$ is non-negative for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$. So $\sum_{\sigma\in J} \alpha_\sigma(y_\sigma^2 - y_\sigma) +$ $(-\alpha_{\sigma_1})(y_{\sigma_1}^2 - y_{\sigma_1})$ is non-negative for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$. This simplifies to $\sum_{\sigma\in J\setminus\{\sigma_1\}} \alpha_\sigma(y_\sigma^2 - y_\sigma)$ which is non-negative for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$ and $\{y_\sigma^2 - y_\sigma | \sigma \in J \setminus \{\sigma_1\}\}$ is L.I. But α_{σ_2} is negative. Hence we have established that the second statement of lemma 18 does not hold.

Theorem 21. *Region of $\mathcal{F}$ satisfying conditions (3), properly contains $\mathcal{B}^{[2]}$.*

Corollary 22. *There exists at least one facet of $\mathcal{B}^{[2]}$ which is not an instance of (3).*

[1] Michael Jünger and Volker Kaibel. Box-inequalities for quadratic assignment polytopes. In *Mathematical Programming*, pages 175–197, 1997.

[2] Volker Kaibel. *Polyhedral Combinatorics of the Quadratic Assignment Problem.* PhD thesis, Faculty of Mathematics and Natural Sciences, University of Cologne, Germany, 1997.

[3] Janez Povh and Franz Rendl. Copositive and semidefinite relaxations of the quadratic assignment problem. *Discrete Optimization*, 6(3):231 – 241, 2009.

Appendix A. Proof of Lemma 2

Proof. Consider a non-negative vector realization $\{u_{ij}| i,j \in [n]\} \cup \{\omega\}$ for a point $Y \in \mathcal{L}$. Let W denote an $n \times n$ matrix with (i,j)-th entry being u_{ij}. Conditions 1b and 1c ensure that vectors in any row or any column of W are pairwise orthogonal. Since objective function attains value n, from Observation 1 vectors of each row/column form a maximal set of pairwise orthogonal united vectors. Also from the same observation each row and each column adds up to ω. Assume that the vector realization is in an N-dimensional space. Consider the r-th component of the matrix, i.e., the matrix formed by the r-th component of each vector. Let us denote it by D_r. Each element of D_r is non-negative and each row and each column adds up to ω_r, the r-th component of ω. Hence D_r is ω_r times a doubly-stochastic matrix. But the vectors of the same row (resp. column) are orthogonal so exactly one entry is non-zero in each row (resp. column) if $\omega_r > 0$. So $D_r = \omega_r P_{\sigma_r}$ for some permutation σ_r. We can express W by $\sum_r \omega_r P_{\sigma_r} e_r$ where e_r denotes the unit vector along the r-th axis. $Y_{ij,kl}$ is the inner product of the vectors u_{ij} and u_{kl} which is $(\sum_r \omega_r (P_{\sigma_r})_{ij} e_r) \cdot (\sum_s \omega_s (P_{\sigma_s})_{kl} e_s) = \sum_r \omega_r^2 (P_{\sigma_r})_{ij}.(P_{\sigma_r})_{kl} = \sum_r \omega_r^2 (P_{\sigma_r}^{[2]})_{ij,kl}$. Thus $Y = \sum_r \omega_r^2 P_{\sigma_r}^{[2]}$. Since $\sum_r \omega_r^2 = \omega^2 = 1$, Y is a convex combination of some of the $P_\sigma^{[2]}$s. $\square$

Appendix B. Proof of Lemma 3

Proof. Let Y be a 0/1 solution of the system of linear equations 2a-2d. Note that equations 2d and the non-negativity of the entries ensure that the diagonal of the solution is a vectorized doubly stochastic matrix. As the solution is a 0/1 matrix, the diagonal must be a vectorized permutation matrix, say P_σ. Then $Y_{ij,ij} = (P_\sigma)_{ij}$.

Equations 2c imply that $Y_{ij,kl} = 1$ if and only if $Y_{ij,ij} = 1$ and $Y_{kl,kl} = 1$. Equivalently, $Y_{ij,kl} = Y_{ij,ij}.Y_{kl,kl} = (P_\sigma)_{ij}.(P_\sigma)_{kl} = (P_\sigma^{[2]})_{ij,kl}$.

Equations 2a and 2b describe the remaining entries. $\square$

Appendix C. Proof of Lemma 4

Proof. We will first show that the dimension of the solution plane is no more than $n!/(2(n-4)!) + (n-1)^2 + 1$.

Split matrix Y into n^2 non-overlapping sub-matrices of size $n \times n$ which will be called *blocks*. The n blocks that contain the diagonal entries of Y will be called *diagonal blocks*. Note that $Y_{ij,kl}$ is the jl-th entry of the ik-th block.

From the equation 2b, the off-diagonal entries of the diagonal blocks are zero. Assume that the first $n-1$ diagonal entries of the first $n-1$ diagonal blocks are given. Then all diagonal entries can be determined using equations 2d.

Consider any off diagonal block in the region above the main diagonal, other than the right most (n-th) block of that row. Note that the first entry of such a block will be $Y_{r1,s1}$ where $r < s < n$. From the equation 2b we see that its diagonal entries are zero. The sum of the entries of any row of this block is same as the main diagonal entry of that row in Y, see equation 2c. Same holds for the columns from symmetry condition 2a. Hence by fixing all but one off-diagonal entries of the first principal sub-matrix of the block of size $(n-1)\times(n-1)$, we can fill in all the remaining entries. An exception to above is the second-last block of the $(n-2)$-th block-row (with first entry $Y_{(n-2)1,(n-1)1}$). Here only the upper diagonal entries of the first principal sub-matrix of size $(n-1)\times(n-1)$ are sufficient to determine all the remaining entries of that block. From equation 2c all the entries of the right most blocks can be determined. Lower diagonal entries of Y are determined by symmetry. Hence we see that the number of free variables is no more than $(n-1)^2 + ((n-1)(n-2)-1)(2+\cdots+(n-2)) + (n-1)(n-2)/2 = n!/(2(n-4)!) + (n-1)^2 + 1$.

In [2] it is shown that the dimension of $\mathcal{B}^{[2]}$ polytope is $\frac{n!}{2(n-4)!} + (n-1)^2 + 1$. This claim along with the result of the previous paragraph leads to the conclusion that equations 2a-2d define the affine plane spanned by the $P_\sigma^{[2]}$s. $\square$