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The QAP-polytope and the Graph Isomorphism problem

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Abstract In this paper we propose a geometric approach to solve the Graph Isomorphism (GI in short) problem. Given two graphs G_1, G_2, the GI problem is to decide if the given graphs are isomorphic i.e., there exists an edge preserving bijection between the vertices of the two graphs. We propose an Integer Linear Program (ILP) that has a non-empty solution if and only if the given graphs are isomorphic. The convex hull of all possible solutions of the ILP has been studied in literature as the Quadratic Assignment Problem (QAP) polytope. We study the feasible region of the linear programming relaxation of the ILP and show that the given graphs are isomorphic if and only if this region intersects with the QAP-polytope. As a consequence, if the graphs are not isomorphic, the feasible region must lie entirely outside the QAP-polytope. We study the facial structure of the QAP-polytope with the intention of using the facet defining inequalities to eliminate the feasible region outside the polytope. We determine two new families of facet defining inequalities of the QAP-polytope and show that all the known facet defining inequalities are special instances of a general inequality. Further we define a partial ordering on each exponential sized family of facet defining inequalities and show that if there exists a common minimal violated inequality for all points in the feasible region outside the QAP-polytope, then we can solve the GI problem in polynomial time. We also study the general case when there are k such inequalities and give an algorithm for the GI problem that runs in time exponential in k.

Keywords Quadratic Assignment Problem · Graph Isomorphism Problem · Polyhedral Combinatorics

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1 Introduction

The graph isomorphism problem (GI) is a well-studied computational problem; listed as an open problem in [25] and [17]. Formally, given two graphs G_1 and G_2 on n vertices each, GI is a decision problem that asks if there exists a bijection $\sigma : V(G_1) \to V(G_2)$ such that $\{u,v\} \in E(G_1)$ iff $\{\sigma(u),\sigma(v)\} \in E(G_2)$. Each such bijection is called an isomorphism between G_1, G_2. Without loss of generality, we assume that the vertices in both the graphs are labeled by integers $1,\ldots,n$. Hence $V(G_1) = V(G_2) = [n]$ and each bijection is a permutation of $1,\ldots,n$. Apart from its practical applications in chemical identification [22], scene analysis [2] and construction and enumeration of combinatorial configurations [15], what makes this problem interesting is the fact that it is not known to be NP-complete [3] nor is there an algorithm known that can solve it in polynomial time. In fact, if GI were NP-complete then the "polynomial time hierarchy", a hierarchy of complexity classes between P and PSPACE, would collapse to its second level [12,38], an unlikely scenario. Moreover, the problem of counting the number of isomorphisms between the input pair of graphs is known to be polynomial-time equivalent to GI itself [32], another unlikely scenario since for all known NP-complete problems the counting version seems to be much harder. The fastest known graph isomorphism algorithm has running time $2^{O(\sqrt{n \log n})}$ [10,46,5]. A quasipolynomial time algorithm has recently been claimed [7]. However, polynomial time algorithms are known for special graph classes: trees [1,14], planar graphs [20,21], bounded genus [16,34], bounded eigenvalue multiplicity [9], bounded degree [30], graphs with excluded minors [36], bounded tree width [11], interval graphs [29,26,27], graphs with excluded topological subgraphs [18]. It may be noted here that there are certain graph classes for which the problem is as hard as the general problem (GI-complete). These include bipartite graphs, chordal graphs, rectangle intersection graphs [44], graphs of bounded degeneracy and graphs of bounded expansion. At the same time, there are softwares, the leading one called *Nauty* [33], based on heuristics that can solve the problem fairly well in practice for almost all graphs.

1.1 Related Work

All the known algorithms for GI employ one or more of three broad approaches: combinatorial, graph theoretic, and group theoretic. A polyhedral approach applies quite naturally to the graph isomorphism problem. Recently there has been a renewed interest in this approach.

The Sherali-Adams hierarchy [39] gives a mechanical way to obtain progressively stronger relaxations of integer polytopes. In this method we are given an explicit description of a starting polytope P_0 in terms of a system of linear inequalities $Ax - b \geq 0$. Also, P_0 is contained in the unit cube in $\mathbb{R}^n$. We have the integer polytope, $P = conv(P_0 \cap \{0,1\}^n)$. Starting from P_0, the Sherali-Adams method constructs a hierarchy of progressively stronger linear relaxations of P, given as $P_0 \supseteq P_1 \supseteq \cdots \supseteq P_n = P$. The procedure for obtaining P_k for some $k \geq 1$, is summarized in [31].

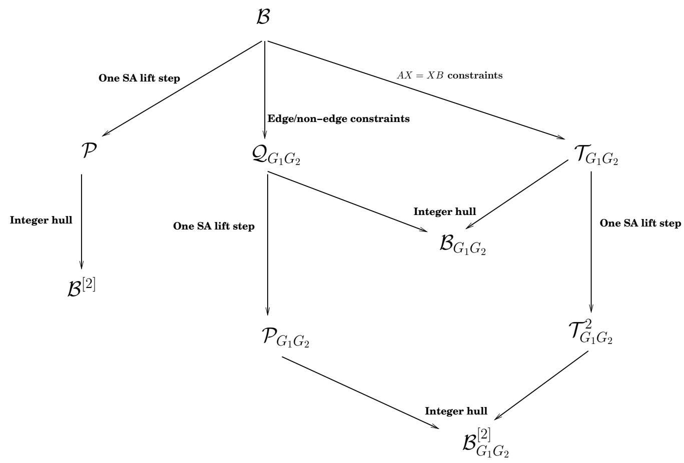

Fig. 1: Relationships between the various polytopes

In this paper we will refer to the polytopes defined below. Some of these appear in the literature related to the polyhedral approach.

Figure 1 shows the relationships between the various polytopes and also gives an idea about their origins. We will now define these formally in the order in which they appear in the figure, starting from the top.

$\mathscr{B}$: is popularly known as the Birkhoff polytope. It is the convex hull of all the permutation matrices, where a permutation matrix P_σ is a $n \times n$ $0/1$ matrix such that $(P_\sigma)_{ij} = 1$ if and only if $\sigma(i) = j$, for some permutation $\sigma \in S_n$, where S_n is the symmetric group of permutations of $[n]$. Clearly, $\mathscr{B}$ lies in $\mathbb{R}^{n\times n}$. From the Birkhoff-von Neumann theorem that every doubly-stochastic matrix can be expressed as the convex combination of permutation matrices, we have $\mathscr{B} = \{X \in [0,1]^{n\times n} | Xe = X^T e = e\}$, where e is a vector of all 1s.

$\mathscr{P}$: is the polytope that is obtained after one lift step of the Sherali-Adams (SA) lift-and-project method, starting with the polytope $\mathscr{B}$. $\mathscr{P}$ lies in the space $\mathbb{R}^{n^2\times n^2}$.

$\mathscr{Q}_{G_1G_2}$: is actually not a polytope, but simply an algebraic set. It is defined as $\{X \in [0,1]^{n\times n} |\, X_{uv}X_{pq} = 0 \text{ for all } \{u,p\} \in E_{G_1}, \{v,q\} \notin E_{G_2} \text{ or } \{u,p\} \notin E_{G_1}, \{v,q\} \in E_{G_2}, Xe = X^T e = e\}$ in [31]. Here G_1, G_2 are simple undirected graphs on n vertices each. Clearly, $\mathscr{Q}_{G_1G_2} \subseteq \mathscr{B}$.

$\mathscr{T}_{G_1G_2}$: is the standard GI polytope, also known as the Tinhofer polytope. It is defined as $\{X \in [0,1]^{n\times n} |\, AX = XB, Xe = eX = e\}$ in [43]. Here A, B are the adjacency matrices of the graphs G_1, G_2, respectively. Again, $\mathscr{T}_{G_1G_2} \subseteq \mathscr{B}$.

$\mathscr{B}_{G_1G_2}$: is the convex hull of those permutation matrices P_σ that correspond to the isomorphisms (given by σ) between G_1, G_2. It can be shown that a permutation matrix P_σ belongs to $\mathscr{Q}_{G_1G_2}$ if and only if σ is an isomorphism between G_1, G_2. Same is true for $\mathscr{T}_{G_1G_2}$, i.e., a permutation matrix P_σ belongs to $\mathscr{T}_{G_1G_2}$ if and only if σ is an isomorphism between G_1, G_2. Hence, $\mathscr{B}_{G_1G_2} \subseteq \mathscr{Q}_{G_1G_2}$. Also, $\mathscr{B}_{G_1G_2} \subseteq \mathscr{T}_{G_1G_2}$.

Moreover, $\mathscr{B}_{G_1G_2}$ is the convex hull of the integer points in $\mathscr{Q}_{G_1G_2}$. Similarly, $\mathscr{B}_{G_1G_2}$ is the convex hull of the integer points in $\mathscr{T}_{G_1G_2}$.

$\mathscr{B}^{[2]}$: is the convex hull of the integer points in $\mathscr{P}$. Each integer point in $\mathscr{P}$ is a $n^2 \times n^2$ symmetric $0/1$ matrix, $P_\sigma^{[2]}$, that we call the second-order permutation matrix since there is a one-to-one correspondence between these matrices and the permutation matrices, given as $P_\sigma^{[2]}(ij,kl) = P_\sigma(i,j)P_\sigma(k,l)$. In the literature $\mathscr{B}^{[2]}$ appears as the Quadratic Assignment Problem (QAP)-polytope [24].

$\mathscr{P}_{G_1G_2}$: is the polytope in $\mathbb{R}^{n^2\times n^2}$ that is obtained after one lift step of SA, starting with $\mathscr{Q}_{G_1G_2}$. Polytope $\mathscr{P}$ is same as $\mathscr{P}_{G_1G_2}$ with G_1, G_2 as either empty or complete graphs. Hence, polytope $\mathscr{P}$ can be referred to as the superset of $\mathscr{P}_{G_1G_2}$ for all G_1, G_2.

$\mathscr{T}^2_{G_1G_2}$: is the polytope in $\mathbb{R}^{n^2\times n^2}$ that is obtained after one lift step of SA, starting with $\mathscr{T}_{G_1G_2}$. It can be shown that $\mathscr{T}^2_{G_1G_2} \subseteq \mathscr{P}_{G_1G_2}$. It follows from [31, Lemma 3.2] for the case of $k = 2$.

$\mathscr{B}^{[2]}_{G_1G_2}$: is the convex hull of those vertices of $\mathscr{B}^{[2]}$ that correspond to isomorphisms between G_1, G_2. It can be shown that a second-order permutation matrix $P_\sigma^{[2]}$ belongs to $\mathscr{P}_{G_1G_2}$ if and only if σ is an isomorphism between G_1, G_2. Same is true for $\mathscr{T}^2_{G_1G_2}$, i.e., a second-order permutation matrix $P_\sigma^{[2]}$ belongs to $\mathscr{T}^2_{G_1G_2}$ if and only if σ is an isomorphism between G_1, G_2. Hence, $\mathscr{B}^{[2]}_{G_1G_2} \subseteq \mathscr{P}_{G_1G_2}$. Also, $\mathscr{B}^{[2]}_{G_1G_2} \subseteq \mathscr{T}^2_{G_1G_2}$. Moreover, $\mathscr{B}^{[2]}_{G_1G_2}$ is the convex hull of the integer points in $\mathscr{P}_{G_1G_2}$. Similarly, $\mathscr{B}^{[2]}_{G_1G_2}$ is the convex hull of the integer points in $\mathscr{T}^2_{G_1G_2}$.

Atserias and Maneva in [4] show that if a popular heuristic known as the k-dimensional Weisfeiler and Lehman (k-WL in short) [45] distinguishes G_1, G_2 then the k^{th} level of the Sherali-Adams relaxation [39] (henceforth referred to as k-SA), starting with $\mathscr{T}_{G_1G_2}$, has no solution, or $\mathscr{T}^k_{G_1G_2} = \emptyset$. Also, in the same paper they show that if k-SA has no solution, then $(k+1)$-WL distinguishes G_1, G_2. Later Grohe and Otto in their paper [19] prove the existence of graph pairs G_1, G_2 such that k-WL does not distinguish G_1, G_2 (k-WL has a solution) and k-SA has no solution (able to distinguish). They also show the existence of graph pairs G_1, G_2 such that k-SA has a solution and $(k+1)$-WL distinguishes G_1, G_2. These results establish that the distinguishing power of k-SA is sandwiched between those of k-WL and $(k+1)$-WL.

Malkin in a recent paper [31] basically confirms the results described above. Further, he shows that k lift-and-project steps of SA starting with $\mathscr{Q}_{G_1G_2}$ is the geometric analogue of the k-WL algorithm. Finally, he proves the relationship $\mathscr{Q}^{k+1}_{G_1G_2} \subseteq \mathscr{T}^k_{G_1G_2} \subseteq \mathscr{Q}^k_{G_1G_2}$ which is the same as that established by Atserias and Maneva in [4].

From the above we can conclude that there is a strong relationship between the existing polyhedral and combinatorial approaches to GI. Also, for every k there exist non-isomorphic 3-regular graphs G_k, H_k of size $O(k)$ that are not distinguished by k-WL [13]. Hence, we see the limitations of the polyhedral approach.

Recently, O'Donnell, Wright, Wu, and Zhou [35] and Codenotti, Schoenbeck, and Snook [40] studied the Lasserre hierarchy [28] of semi-definite relaxations of the integer linear program for GI. They proved that the family of 3-regular graphs mentioned above cannot be distinguished even by $o(n)$ levels of the Lasserre hierarchy.

1.2 Our Contributions

In the previous section we observed that the lift-and-project methods are not good enough to solve the Graph Isomorphism problem for general graphs, at least when we start with the polytope that corresponds to a natural formulation of the problem. All the attempts so far have been in showing that a constant number of rounds will not suffice to obtain the integer hull of the starting polytope. However, there has been no attempt to study an intermediate polytope that is obtained after a constant number of rounds. It is possible that an intermediate polytope, though not equal to the integer hull, has some interesting properties that can allow the problem to be solved efficiently, at least in some special situations. This applies to not just the Graph Isomorphism problem but also to other problems where only hardness results are known. In this paper we look closely at the polytopes, $\mathscr{P}, \mathscr{B}^{[2]}$, and observe some interesting aspects of their geometry that can be exploited to obtain a procedure for solving GI. However, several aspects of the geometry still remain unknown and in the future it would be useful to have a better understanding of them.

In this paper we show that a given pair of graphs G_1, G_2 are isomorphic if and only if $\mathscr{P}_{G_1G_2}$ contains at least one point from $\mathscr{B}^{[2]}$. Hence, for non-isomorphic graphs, $\mathscr{P}_{G_1G_2}$, if non-empty, must be confined to $\mathscr{P} \setminus \mathscr{B}^{[2]}$. Moreover, we show that the polytopes $\mathscr{P}$ and $\mathscr{B}^{[2]}$ have the same dimension and each facet plane of $\mathscr{P}$ defines a facet of $\mathscr{B}^{[2]}$. $\mathscr{B}^{[2]}$ has other facets as well. Clearly, the region $\mathscr{P} \setminus \mathscr{B}^{[2]}$ is defined by these other facets of $\mathscr{B}^{[2]}$.

We study the facial structure of $\mathscr{B}^{[2]}$. This polytope is also studied in the literature of Quadratic Assignment Problem (QAP) [24], where exponentially many facets of this polytope are identified. In this work we identify exponentially many additional facets of $\mathscr{B}^{[2]}$. Further, we define a partial ordering on each of the known families of facets.

We observe that the polytope $\mathscr{P}_{G_1G_2}$ is the disjoint union of $\mathscr{B}_{G_1G_2}$ and the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$. So the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ must violate the inequalities associated with one or more facets of $\mathscr{B}^{[2]}$. We call an inequality X a *minimal violated inequality* for a point p in the feasible region, if X is violated by p but any inequality less than X in the partial ordering, is not violated by p. We show that if there exists a single X for all p in the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$, then a simple search algorithm can solve the graph isomorphism problem in polynomial time. We also study the general case when more than one minimal violated inequalities are required to separate $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ from $\mathscr{B}^{[2]}$. We present an algorithm for GI that runs in $O(n^k)$ time where k is a minimal number of minimal violated inequalities that separate $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ from $\mathscr{B}^{[2]}$.

We believe that one of the contributions of this paper is to provide a geometric characterization of the hard instances of the graph isomorphism problem. Clearly, these are the cases when a large number of facet defining inequalities of $\mathscr{B}^{[2]}$ are required to separate $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ from $\mathscr{B}^{[2]}$.

1.3 Organization

The rest of this paper is organized as follows. In Section 2 we present our integer programming formulation of the graph isomorphism problem and in Section 3 we study its linear programming relaxation. Later in Section 3, we study the feasible region of the linear program and introduce the two polytopes, $\mathscr{P}$ and $\mathscr{B}^{[2]}$, and the special relationship that they share. In Section 4 we study the facial structure of polytope $\mathscr{B}^{[2]}$ and present an exponential set of its facets. In Section 5 we show that there exists a partial ordering on the facet planes described in Section 4 and that this ordering extends to some planes that support lower dimensional faces of $\mathscr{B}^{[2]}$. In Section 6 we show that if there exists a single *minimal violated inequality* for all points in the feasible region of our LP that lie outside the polytope $\mathscr{B}^{[2]}$, then a simple search algorithm solves the GI problem in polynomial time. In the following section, Section 7, we discuss the general case when there are k such inequalities and present an algorithm for the GI problem that runs in time exponential in k. We present the results of some limited experimentation in Section 8. We conclude in Section 9 where we summarize our contributions and present some open problems that provide avenues for further research.

2 Integer Linear Program for GI

Consider the following ILP where A, B are the adjacency matrices of G_1, G_2, respectively.

IP-GI: Find a point Y

subject to

$$Y_{ij,kl} - Y_{kl,ij} = 0\ , \qquad \forall\ i,j,k,l \qquad (1a)$$

$$Y_{ij,il} = Y_{ji,li} = 0\ , \qquad \forall\ i, \forall\ j \neq l \qquad (1b)$$

$$\sum_k Y_{ij,kl} = \sum_k Y_{ij,lk} = Y_{ij,ij}\ , \qquad \forall\ i,j,l \qquad (1c)$$

$$\sum_j Y_{ij,ij} = \sum_j Y_{ji,ji} = 1\ , \qquad \forall\ i \qquad (1d)$$

$$\sum_p A_{kp} \cdot Y_{pl,pl} = \sum_p Y_{kp,kp} \cdot B_{pl}\ , \qquad \forall\ k,l \qquad (1e)$$

$$\sum_p A_{kp} \cdot Y_{ij,pl} = \sum_p Y_{ij,kp} \cdot B_{pl}\ , \qquad \forall\ i,j,k,l \qquad (1f)$$

$$Y_{ij,kl} \in \{0,1\}\ , \qquad \forall\ i,j,k,l$$

Define a second-order permutation matrix $P^{[2]}_\sigma$ corresponding to a permutation σ as $(P^{[2]}_\sigma)_{ij,kl} = (P_\sigma)_{ij}(P_\sigma)_{kl}$, where P_σ is the permutation matrix corresponding to σ.

Lemma 1 *The only* $0/1$ *solutions of equations (1a)-(1d) are* $P^{[2]}_\sigma$*s.*

Proof Let Y be a $0/1$ solution of the system of linear equations given by (1a)-(1d). Note that equations (1d) 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 $Y_{ij,ij} = (P_\sigma)_{ij}\ \forall i,j$.

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

Theorem 1 *Graphs G_1, G_2 are isomorphic iff IP-GI has a feasible solution.*

Proof From Lemma 1, any feasible solution of IP-GI must be a $P_\sigma^{[2]}$ that satisfies equations (1e) and (1f). Substituting $P_\sigma^{[2]}$ in equation (1e) we have $\sum_p A_{kp} \cdot (P_\sigma^{[2]})_{pl,pl} = \sum_p (P_\sigma^{[2]})_{kp,kp} \cdot B_{pl}$ which reduces to $\sum_p A_{kp} \cdot (P_\sigma)_{pl} = \sum_p (P_\sigma)_{kp} \cdot B_{pl}$ or $AP_\sigma = P_\sigma B$, which implies that σ is an isomorphism between G_1, G_2 or G_1, G_2 are isomorphic. A similar reduction can be shown for equation (1f). For the other direction, let σ give an isomorphism between the graphs G_1, G_2. Then the corresponding $P_\sigma^{[2]}$ must be a feasible solution of IP-GI. □

Corollary 1 *$Y = P_\sigma^{[2]}$ is a solution of IP-GI iff σ is an isomorphism between G_1, G_2.*

3 Linear Programming Relaxation

Since it is NP-hard to solve IP-GI, we study its Linear Programming (LP) relaxation, where the variable $Y_{ij,kl}$ is allowed to take values between 0 and 1.

$$
\begin{aligned}
\text{LP-GI:}\quad & \text{Find a point} \quad Y \\
& \text{subject to} \quad (1a)\text{-}(1f) && \text{(2a)} \\
& \qquad\qquad\quad Y_{ij,kl} \geq 0 \ ,\ \forall\, i,j,k,l && \text{(2b)}
\end{aligned}
$$

Note that the condition $Y_{ij,kl} \leq 1$ is redundant here due to the constraints given by equation (1d).

3.1 Feasible Region of LP-GI

Let the feasible region of LP-GI be denoted as $\mathscr{P}_{G_1G_2}$. Note that $\mathscr{P}_{G_1G_2}$ is same as $\hat{\mathscr{Q}}^2_{G_1G_2}$ as defined in [31]. In [31], the author refers to $\mathscr{Q}^k_{G_1G_2}$ as the k-th Sherali-Adams relaxation [39] of $\mathscr{Q}_{G_1G_2}$ (defined in section 1.1) and $\hat{\mathscr{Q}}^k_{G_1G_2}$ as the lifted polytope in $\mathbb{R}^{n^k \times n^k}$ given via an extended formulation, whose projection in $\mathbb{R}^{n\times n}$ is the polytope $\mathscr{Q}^k_{G_1G_2}$.

Define $\mathscr{B}^{[2]}_{G_1G_2}$ as the integer hull (convex hull of integer points) of $\mathscr{P}_{G_1G_2}$, i.e., $\mathscr{B}^{[2]}_{G_1G_2} = conv(P_\sigma^{[2]} | \sigma$ is an isomorphism between $G_1, G_2)$. Note that from Lemma 1 and Corollary 1, $P_\sigma^{[2]}$ corresponding to those σ that give an isomorphism between G_1, G_2, are the only integer (0/1) points in $\mathscr{P}_{G_1G_2}$.

Consider $\mathscr{P}_{G_1G_2}$ when $G_1 = G_2 = (V, \emptyset)$ or $G_1 = G_2 = K_n$. Note that this is equivalent to dropping the graph conditions given by equations (1e) and (1f) and hence from Lemma 1, $\mathscr{P}_{G_1G_2}$ now contains all $P_\sigma^{[2]}$. Let this region be denoted as $\mathscr{P}$. Similarly, define polytope $\mathscr{B}^{[2]}$ as $\mathscr{B}^{[2]}_{G_1G_2}$ when $G_1 = G_2 = (V, \emptyset)$ or $G_1 = G_2 = K_n$. Clearly, $\mathscr{B}^{[2]}$ corresponds to the integer hull of $\mathscr{P}$ or $\mathscr{B}^{[2]} = conv(P_\sigma^{[2]} | \sigma \in S_n)$, where S_n is the symmetric group. $\mathscr{B}^{[2]}$ appears in the literature [24] as the Quadratic Assignment Problem (QAP)-polytope. Clearly, $\mathscr{B}^{[2]}$ is contained in $\mathscr{P}$. In the following section we will prove a stronger statement that in fact $\mathscr{B}^{[2]}$ is full-dimensional in $\mathscr{P}$.

3.2 Affine Plane of $\mathscr{B}^{[2]}$

Any translated subspace of $\mathbb{R}^n$ is called an affine plane or just plane. Formally, if S is an arbitrary subspace and u is an arbitrary non-zero vector, then $X = \{x + u | x \in S\}$ is a plane. Dimension of X is defined as the dimension of S. If X is of dimension $n-1$, then it is called a hyper-plane.

Affine span of a point set S, $Aff(S)$, is the smallest plane containing that set. Let p_0 be a fixed point in S. So $Aff(S) = \{p_0 + \sum_{p \in S} \alpha_p (p - p_0) | \alpha_p \in \mathbb{R}\}$. The dimension of S refers to the dimension of $Aff(S)$. $Aff(S)$ can also stated as $\{\sum_{p \in S} \alpha_p p | \sum_p \alpha_p = 1, \alpha_p \in \mathbb{R}\}$. Note that the dimension of a polytope defined by its set of vertices S, is also the dimension of $Aff(S)$.

Lemma 2 *The set of all feasible solutions to the system of equations (1a)-(1d), P, is the affine span of the* $P_\sigma^{[2]}$*s, i.e.,* $P = \{\sum_\sigma \alpha_\sigma P_\sigma^{[2]} | \sum_\sigma \alpha_\sigma = 1\}$.

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

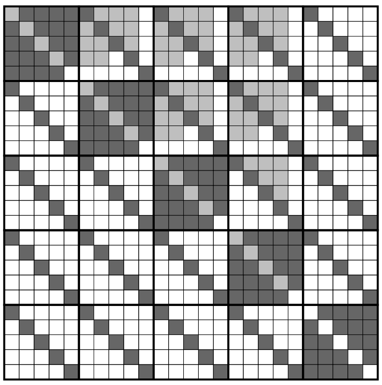

Fig. 2: A toy example for $n = 5$ showing the $n^2 = 25$ blocks each of size 5×5. The dark shaded cells are set to 0 in (1b). Knowledge of the entries in the light shaded cells is sufficient to determine the remaining entries in the unshaded cells with the help of (1a)-(1d). Note that the number of light shaded cells is equal to $5!/(2(1!)) + 4^2 + 1 = 77$.

Split the matrix Y into n^2 non-overlapping sub-matrices of size $n \times n$ each as shown in Fig. 2. We call these sub-matrices as *blocks*. The n blocks that contain the diagonal entries of Y are called the diagonal blocks. Note that $Y_{ij,kl}$ is the jl-th entry of the ik-th block. From the equation (1b), the off-diagonal entries of the diagonal blocks are zero and the diagonal entries of the off-diagonal blocks are also zero. Assume that the first $n-1$ diagonal entries of the first $n-1$ diagonal blocks are given. Then all the remaining diagonal entries can be determined using equations (1d). Therefore there are at most $(n-1)^2$ independent entries in the diagonal blocks.

Consider any off-diagonal block with first entry given by $Y_{r1,s1}$ where $r \le n-3, r < s < n$. The sum of the entries in any row of this block is same as the main diagonal entry of that row in Y, see equation (1c). Same holds for the columns from symmetry condition (1a). 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.

From equation (1c) all the entries in the right most blocks $1n,\dots,(n-3)n$ can be determined. Lower triangular entries of Y are determined by symmetry. At this stage we have only three blocks viz., $(n-2)(n-1)$, $(n-2)n$ and $(n-1)n$ above the main diagonal and their symmetric blocks below the main diagonal, whose entries remain to be determined.

Consider the first principal $(n-1)\times(n-1)$ sub-matrix of the $(n-2)(n-1)$-th block. Let's say we are given the entries in the upper triangular portion of this sub-matrix. We will show that this is sufficient to determine the remaining entries in matrix Y. Clearly the entry $Y_{(n-2)1,(n-1)n}$ can be determined from equation (1c). Now using equation (1c) we can determine all the entries in the first row of the $(n-2)n$-th block. So we know the entries in the first column of the $n(n-2)$-th block from symmetry. Again using condition (1c) we can determine the entries in the first column of the $n(n-1)$-th block. That leads to the determination of entries in the first column of the $(n-2)(n-1)$-th block using conditions (1a) and (1c). Now using a similar argument for the second row onwards of the $(n-2)(n-1)$-th block, we can fill in the remaining entries.

Hence we see that the number of independent variables, including those in diagonal blocks, is no more than $(n-1)^2+((n-1)(n-2)-1)(2+\cdots+(n-2))+(n-1)(n-2)/2 = n!/(2(n-4)!) +(n-1)^2+1$. From [24] we know that the dimension of the $\mathscr{B}^{[2]}$ polytope is $\frac{n!}{2(n-4)!}+(n-1)^2+1$. This along with the result of the previous paragraph leads to the conclusion that equations (1a)-(1d) define the affine plane spanned by the $P_\sigma^{[2]}$s. $\square$

Corollary 2 $\mathscr{B}^{[2]}$ *is full dimensional in P.*

The following observations are in order.

Observation 2 $Y_{ij,kl} = 0$ *for* $\{i,k\} \in E(G_1), \{j,l\} \notin E(G_2)$ *or* $\{i,k\} \notin E(G_1), \{j,l\} \in E(G_2)$.

Proof Consider (1f) with $l = j$ and $A_{ik} = 0$. The left hand side of the equation reduces to 0 since $Y_{ij,pj} = 0$ for all $p \neq i$. That leads to $\sum_p Y_{ij,kp}\cdot B_{pj} = 0$. This combined with (2b) results in $Y_{ij,kp} = 0$ for any k such that $A_{ik} = 0$ and for all p such that $B_{jp} = 1$.

Next consider a value of l such that $B_{jl} = 0$. Also let $k = i$. So the right hand side of (1f) reduces to zero. That gives $\sum_p A_{ip}\cdot Y_{ij,pl} = 0$ which implies from (2b) that $Y_{ij,pl} = 0$ for all p such that $A_{ip} = 1$ and any l such that $B_{jl} = 0$. $\square$

Observation 3 *$\mathscr{P}_{G_1G_2} \cap \mathscr{B}^{[2]} = \mathscr{B}^{[2]}_{G_1G_2}$ is the convex hull of $P^{[2]}_\sigma$s where σ are the isomorphisms between G_1 and G_2.*

Proof From Corollary 1, we know that $P^{[2]}_\sigma$s are the only $0/1$ points in $\mathscr{P}_{G_1G_2}$ where σ are the isomorphisms between G_1 and G_2. Clearly, $\mathscr{B}^{[2]}_{G_1G_2} \subseteq \mathscr{P}_{G_1G_2} \cap \mathscr{B}^{[2]}$. Let $Y \in (\mathscr{P}_{G_1G_2} \cap \mathscr{B}^{[2]}) \setminus \mathscr{B}^{[2]}_{G_1G_2}$. Since $Y \in \mathscr{B}^{[2]}$ but $Y \notin \mathscr{B}^{[2]}_{G_1G_2}$, we can express Y as a convex combination of $P^{[2]}_\sigma$s such that at least one of these does not correspond to an isomorphism between G_1, G_2. Let such a $P^{[2]}_\sigma$ correspond to some permutation σ_1. So we have $Y_{ij,kl} = 0$ for some ij, kl such that $\sigma_1(i) = j$ and $\sigma_1(k) = l$ i.e., $P^{[2]}_{\sigma_1}(ij,kl) = 1$. This is impossible. Hence $(\mathscr{P}_{G_1G_2} \cap \mathscr{B}^{[2]}) \setminus \mathscr{B}^{[2]}_{G_1G_2} = \emptyset$. □

Consider the feasible region $\mathscr{P}_{G_1G_2}$ after a sequence of $0/1$ assignments to some of the free variables. We have the following corollary to the above observation.

Corollary 3 *Let $x_i = \alpha_i$ for $i = 1, \ldots, k$ be a sequence of k $0/1$ assignments to the free variables x_i (each x_i corresponds to some $Y_{ij,kl}$ in LP-GI). Then $(\mathscr{P}_{G_1G_2}|_{x_1=\alpha_1,\ldots,x_k=\alpha_k})$ $\cap \mathscr{B}^{[2]} = conv(\mathscr{P}^{[2]}_\sigma |$ σ is an isomorphism between G_1, G_2 that respects $x_i = \alpha_i$ for all $i \in \{1, \ldots, k\})$.*

Proof Similar to that of Observation 3. Note that $\sum_i \beta_i y_i = \gamma$ for $\gamma \in \{0,1\}$, $\sum_i \beta_i = 1$, $\beta \geq 0$ implies that $y_i = \gamma$ for all i such that $\beta_i > 0$. □

Observation 4 *Graphs G_1, G_2 are isomorphic if and only if the feasible region of LP-GI shares at least one point with $\mathscr{B}^{[2]}$.*

Proof Let Y be a point in the feasible region of LP-GI such that $Y \in \mathscr{B}^{[2]}$. From Observation 3 Y can be expressed as $\sum_\sigma \alpha_\sigma P^{[2]}_\sigma$ where the sum is over the isomorphisms between G_1 and G_2. Since Y is non-empty, $\alpha_{\sigma'} > 0$ for some isomorphism σ'. Also, since Y respects the constraints given in Observation 2, $P^{[2]}_{\sigma'}$ must also respect these constraints. Hence, $P^{[2]}_{\sigma'}$ belongs to the feasible region of LP-GI and σ' gives an isomorphism between G_1, G_2.

For the other direction, let σ'' be an isomorphism between G_1, G_2. So $P^{[2]}_{\sigma''}$ must respect the constraints implied by Observation 2. All the other constraints of LP-GI are satisfied by every $P^{[2]}_\sigma$. Hence $P^{[2]}_{\sigma''}$ belongs to the feasible region of LP-GI. Also, $P^{[2]}_{\sigma''}$ is a vertex of $\mathscr{B}^{[2]}$. □

Observation 5 *Vertices of $\mathscr{B}^{[2]}$ (i.e., $P^{[2]}_\sigma$) are a subset of the vertices of $\mathscr{P}$.*

Proof Since $\mathscr{P}$ is contained in the unit cube in $\mathbb{R}^{n^2 \times n^2}$, any vertices of the unit cube in $\mathbb{R}^{n^2 \times n^2}$ that are contained in $\mathscr{P}$ must form the vertices of $\mathscr{P}$. Clearly, $P^{[2]}_\sigma$ are such vertices. Hence, $\mathscr{B}^{[2]} \subseteq \mathscr{P}$. □

Observation 6 *The complete set of facet planes of $\mathscr{P}$ is $Y_{ij,kl} = 0 \forall i \neq k, \forall j \neq l$.*

Proof Observe that $Y_{ij,kl} = 0 \forall i \neq k, \forall j \neq l$ are the only bounding planes of polytope $\mathscr{P}$. Hence, these are the only planes that can form the facets of polytope $\mathscr{P}$. However, there is no way to differentiate any one of these from the other. So, if one of these defines a facet, then so must the other. Hence, $Y_{ij,kl} = 0 \forall i \neq k, \forall j \neq l$ is a complete set of facet planes of $\mathscr{P}$. □

From Observations 2,6 we can conclude that the feasible region of LP-GI, if non-empty, is contained inside a face of the polytope $\mathscr{P}$.

4 Facial Structure of $\mathscr{B}^{[2]}$

Volker Kaibel studied the polyhedral combinatorics of the QAP-polytope in his PhD thesis in 1997. Several facets of this polytope were identified in the thesis and finding the remaining facets was left as an open problem. In this paper we identify new families of facets but also prove that the extended list of known facets is still incomplete. For this we give a general inequality such that all the known facets (including the ones that we describe in this paper) are special instances of this inequality. We observe that each of the new facets identified in this paper (Theorems 8 and 9) as well as the facets given in Theorem 7, has a special property: that the complementary set of vertices (QAP-polytope vertices not contained in the facet) are co-planar. Moreover, this plane is parallel to the facet plane.

Among various definitions of the Quadratic Assignment problem (QAP), see [24], one is $min\{\sum_{ij,kl}(A_{ik}B_{jl} + D_{ij,kl})Y_{ij,kl} | Y \in \mathscr{B}^{[2]}\}$ [37] where A, B, D are input matrices. Thus QAP is an optimization problem over $\mathscr{B}^{[2]}$.

4.1 Some Facets of $\mathscr{B}^{[2]}$

In this section we will identify exponentially many new facets of $\mathscr{B}^{[2]}$, in addition to exponentially many already known facets given in [23,24]. 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. If P is the affine span of $\mathscr{B}^{[2]}$ (see Lemma 2), then observe that the facet plane is given by the intersection of P with the plane given by $f(x) = 0$.

All the known facets of $\mathscr{B}^{[2]}$, including the ones that we are going to present in this paper, are special instances of the following general inequality.

$$\sum_{ijkl} n_{ij} n_{kl} Y_{ij,kl} + (\beta - 1/2)^2 \geq (2\beta - 1) \sum_{ij} n_{ij} Y_{ij,ij} + 1/4 \tag{3}$$

where $\beta \in \mathbb{Z}$ and $n_{ij} \in \mathbb{Z}$ for all (ij).

Lemma 3 $\mathscr{B}^{[2]}$ *respects the inequality (3).*

Proof We will show that $P_\sigma^{[2]}$ for every $\sigma \in S_n$ satisfies (3). The same must then hold for their convex combination since (3) defines a half-space, which is convex.

Inequality (3) reduces to $(\sum_i n_{i\sigma(i)} - (\beta - 1/2))^2 \geq 1/4$ for $Y = P_\sigma^{[2]}$. Since $n_{ij}, \beta \in \mathbb{Z}$, the left hand side expression is the square of a positive number whose fractional part is $1/2$. Clearly, this square is at least $1/4$. □

Lemma 3 only proves that the entire $\mathscr{B}^{[2]}$ polytope belongs to the half space described by (3) for any choice of n_{ij} and β. In the following part of this section we will show that for certain choices of these parameters this inequality defines facets of $\mathscr{B}^{[2]}$.

The first set of facets are the instances of (3) where $n_{i_0 j_0} = n_{k_0 l_0} = 1$ for some $(i_0 j_0) \neq (k_0 l_0)$, all other $n_{ij} = 0$, and $\beta = 1$. With these parameters the inequality reduces to $Y_{i_0 j_0, k_0 l_0} \geq 0$.

Theorem 7 *$Y_{i_0 j_0, k_0 l_0} \geq 0$ defines a facet of $\mathscr{B}^{[2]}$ for every i_0, j_0, k_0, l_0 such that $i_0 \neq k_0$ and $j_0 \neq l_0$.*

The above theorem is proved in [24]. We give an alternative proof in section A.2.

The next set of facets are due to $\beta = n_{p_1 q_1} = n_{p_2 q_2} = n_{p_1 q_2} = 1$, $n_{kl} = -1$, and the rest of the n_{ij} are zero. Here p_1, p_2, k are any distinct indices. Similarly q_1, q_2, l are also any distinct indices. There are $n^2(n-1)^2(n-2)^2$ such facets.

Theorem 8 *Inequality $Y_{p_1 q_1, kl} + Y_{p_2 q_2, kl} + Y_{p_1 q_2, kl} \leq Y_{kl,kl} + Y_{p_1 q_1, p_2 q_2}$ defines a facet of $\mathscr{B}^{[2]}$, where p_1, p_2, k are distinct and q_1, q_2, l are also distinct and $n \geq 6$.*

The third set of facets is due to $\beta = n_{i_1 j_1} = \cdots = n_{i_m j_m} = 1$, $n_{kl} = -1$ and the remaining $n_{ij} = 0$. The size of this family is $\sum_{m=3}^{n-3} \frac{n^2(n-1)^2 \ldots (n-m)^2}{m!}$.

Theorem 9 *Inequality $Y_{i_1 j_1, kl} + Y_{i_2 j_2, kl} + \ldots + Y_{i_m j_m, kl} \leq Y_{kl,kl} + \sum_{r<s} Y_{i_r j_r, i_s j_s}$, defines a facet of $\mathscr{B}^{[2]}$, where $i_1, \ldots, i_m, k$ are all distinct and $j_1, \ldots, j_m, l$ are also distinct. In addition, $n \geq 6, m \geq 3$.*

Proofs of theorems 8, 9 appear in sections A.4, A.5, respectively.

The next two sets of facets are established in [24]. Let P_1 and P_2 be disjoint subsets of $[n]$. Similarly let Q_1 and Q_2 also be disjoint subsets of $[n]$. In these facets $n_{ij} = 1$ if $(ij) \in (P_1 \times Q_2) \cup (P_2 \times Q_1)$ and $n_{ij} = -1$ if $(ij) \in (P_1 \times Q_1) \cup (P_2 \times Q_2)$. All other n_{ij} are zero. In the following case $P_2 = Q_1 = \emptyset$.

Theorem 10 *[24, Definition 8.5] Following inequality defines a facet of $\mathscr{B}^{[2]}$*
$(\beta - 1) \sum_{(ij) \in P_1 \times Q_2} Y_{ij,ij} \leq \sum_{(ij),(kl) \in P_1 \times Q_2, i<k} Y_{ij,kl} + (1/2)(\beta^2 - \beta)$
when (i) $\beta + 1 \leq |P_1|, |Q_2| \leq n-3$, (ii) $|P_1| + |Q_2| \leq n - 3 + \beta$, (iii) $\beta \geq 2$.

The next set of facets, with $Q_1 = \emptyset$, is given by the following theorem.

Theorem 11 *[24, Definition 8.6] Following inequality defines a facet of $\mathscr{B}^{[2]}$*
$-(\beta - 1) \sum_{(ij) \in P_1 \times Q_2} Y_{ij,ij} + \beta \sum_{(ij) \in P_2 \times Q_2} Y_{ij,ij} + \sum_{(ij),(kl) \in P_1 \times Q_2, i<k} Y_{ij,kl} + \sum_{(ij),(kl) \in P_2 \times Q_2, i<k} Y_{ij,kl} - \sum_{(ij) \in P_1 \times Q_2, (kl) \in P_2 \times Q_2} Y_{ij,kl} + (1/2)(\beta^2 - \beta) \geq 0$
where the conditions on the parameters are as given in [24, Definition 8.6].

4.2 Insufficiency of inequality (3)

All the known facets of the polytope $\mathscr{B}^{[2]}$ can be obtained by assigning certain values to the coefficients in (3). It is possible that some hitherto unknown facets of $\mathscr{B}^{[2]}$ could also be obtained by assigning certain other values to these coefficients. A natural question to ask, then, would be "can all the facets of $\mathscr{B}^{[2]}$ be obtained from (3) by setting the coefficients appropriately?". In this section we show that this is not true. There must exist facets that are not instances of (3).

Let R denote that part of the polytope $\mathscr{P}$ which satisfies (3) for all integral values of n_{ab} and β. Clearly $\mathscr{B}^{[2]} \subseteq R$. However, $R \subseteq \mathscr{B}^{[2]}$ would imply that $R = \mathscr{B}^{[2]}$ which will hold if and only if every facet of $\mathscr{B}^{[2]}$ is an instance of (3). The following lemma gives an alternative characterization.

Lemma 4 *We define the row-major vectorization of a $m \times m$ matrix M as a m^2-dimensional vector V with the entry $M(i,j)$ located at $V(m*(i-1)+j)$. Now, let P_σ denote the row-major vectorization of the corresponding permutation matrix. Following statements are equivalent.*

1. Region of $\mathscr{P}$, 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 $\mathscr{B}^{[2]}$.

2. Given any set of permutations I such that $\{P_\sigma^{[2]} | \sigma \in I\}$ is linearly independent, 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 Assume (2).

Let $Y \in P$. There exists a set I of permutations σ such that $P_\sigma^{[2]}$ for $\sigma \in I$ form a linearly independent set and $Y = \sum_{\sigma\in I} \alpha_\sigma P_\sigma^{[2]}$ and $\sum_{\sigma\in I} \alpha_\sigma = 1$. Then $Y \in \mathscr{B}^{[2]}$ if and only if $\alpha_\sigma \geq 0 \forall\ \sigma \in I$ if and only if $\sum_{\sigma\in I} \alpha_\sigma((P_\sigma^T \cdot x)^2 - (2z-1)(P_\sigma^T \cdot x)) + z^2 - z \geq 0$ for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$ if and only if $\sum_{\sigma\in I} \alpha_\sigma(\sum_{ijkl} P_\sigma^{[2]}(ij,kl)x_{ij}x_{kl} - (2z-1)\sum_{ij} P_\sigma^{[2]}(ij,ij)x_{ij} + z^2 - z \geq 0$ for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$ if and only if $\sum_{ijkl} Y_{ij,kl}x_{ij}x_{kl} - (2z-1)\sum_{ij} Y_{ij,ij}x_{ij} + z^2 - z \geq 0$ for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$.

Assume (1).

$\alpha_\sigma \geq 0$ for all $\sigma \in I$ and $\sum_{\sigma\in I} \alpha_\sigma = 1$ if and only if $Y = \sum_{\sigma\in I} \alpha_\sigma P_\sigma^{[2]}, \in \mathscr{B}^{[2]}$ if and only if $\sum_{ijkl} x_{ij}x_{kl}\, Y_{ij,kl} - (2z-1)\sum_{ij} x_{ij}Y_{ij,ij} + z^2 - z \geq 0$ for all $x_{ij}, z \in \mathbb{Z}$ if and only if $\sum_{\sigma\in I} \alpha_\sigma((P_\sigma^T \cdot x)^2 - (2z-1)(P_\sigma^T \cdot x)) + z^2 - z \geq 0$ for all $x \in \mathbb{Z}^{n^2}, z \in \mathbb{Z}$. □

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

Lemma 5 $\sum_\sigma \alpha_\sigma(y_\sigma^2 - y_\sigma) = 0$ *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 $z \in \mathbb{Z}$. Select arbitrary $a \in \mathbb{Z}^{n^2}$, $b \in \mathbb{Z}$ and indices 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 $(S(a'',b)-S(a',b))/4=\sum_{\sigma:\sigma(i)=j}\alpha_\sigma y_\sigma(a,b)$. 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,b,i,j 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 $T(x,z)=\sum_\sigma \alpha_\sigma\ (y_\sigma^2-y_\sigma)$. □

Let $\tilde{P}_\sigma$ be the (n^2+1)-dimensional vector in which the vectorized P_σ constitutes the first n^2 entries and the last entry is 1. Define the rank-1 matrix $\tilde{P}_\sigma^{[2]}$ as the outer product of $\tilde{P}_\sigma$ with its transpose.

Lemma 6 $\{P_\sigma^{[2]}|\sigma\in I\}$ *is linearly independent if and only if* $\{\tilde{P}_\sigma^{[2]}|\sigma\in I\}$ *is linearly independent.*

Proof (If) Suppose $\{P_\sigma^{[2]}|\sigma\in I\}$ is linearly dependent. So there exist coefficients $\alpha_\sigma\in\mathbb{R}$, not all zero, such that $\sum_{\sigma\in I}\alpha_\sigma P_\sigma^{[2]}(ij,kl)=0$ for all i,j,k,l. Since $\tilde{P}_\sigma^{[2]}(ij,n^2+1)=\tilde{P}_\sigma^{[2]}(n^2+1,ij)=P_\sigma^{[2]}(ij,ij)$, we have from the above equation $\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}(ij,n^2+1)=\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}(n^2+1,ij)=0$ for all i,j. Finally, $\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}(n^2+1,n^2+1)=\sum_{\sigma\in I}\alpha_\sigma(1)=\sum_{\sigma\in I}\alpha_\sigma(\sum_j P_\sigma^{[2]}(ij,ij))=0$ where i in the last expression is arbitrary.

(Only if) Follows trivially from the fact that the $n^2\times n^2$ matrix $P_\sigma^{[2]}$ is a submatrix of $\tilde{P}_\sigma^{[2]}$. □

Lemma 7 $\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}=0$ *if and only if* $\sum_{\sigma\in I}\alpha_\sigma q^T\tilde{P}_\sigma^{[2]}q=0\ \forall\ q\in\mathbb{Q}^{n^2+1}$.

Proof (If) Let $f(q)=\sum_{\sigma\in I}\alpha_\sigma q^T\tilde{P}_\sigma^{[2]}q$. So we are given that $f(q)=0\ \forall\ q\in\mathbb{Q}^{n^2+1}$. We can rewrite $f(q)$ as $f(q)=\sum_{\sigma\in I}\alpha_\sigma(vec(\tilde{P}_\sigma^{[2]})^T vec(qq^T))$ which is same as $f(q)=\sum_{\sigma\in I}\alpha_\sigma(\sum_{\sigma(i)=j,\sigma(k)=l}q_{ij}q_{kl}+q_{n^2+1}^2)$. Consider a vector q' with $q'_{n^2+1}=1$ and remaining entries zero. Since $f(q')=0$, we have $\sum_{\sigma\in I}\alpha_\sigma=0$. Next consider a vector q'' with $q''_{ij}=1/q''_{kl}$ for some i,j,k,l such that $\sigma(i)=j$ and $\sigma(k)=l$ for $\sigma\in I$. The remaining entries of q'' are all zero. So $f(q'')=0$ leads to $\sum_{\sigma\in I,\sigma(i)=j,\sigma(k)=l}\alpha_\sigma=0$. The above argument can be repeated for all i,j,k,l such that $\sigma(i)=j$ and $\sigma(k)=l$ for $\sigma\in I$. Thus, $\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}=0$.

(Only if) Consider an arbitrary vector $q\in\mathbb{Q}^{n^2+1}$. We have $f(q)=\sum_{\sigma\in I}\alpha_\sigma($ $\sum_{\sigma(i)=j,\sigma(k)=l}q_{ij}q_{kl}+q_{n^2+1}^2)$ which reduces to $f(q)=\sum_{\sigma\in I}\alpha_\sigma(\sum_{\sigma(i)=j,\sigma(k)=l}q_{ij}q_{kl})$ since we are given that $\sum_{\sigma\in I}\alpha_\sigma=0$. The reduced expression can be rewritten as $f(q)=\sum_{i,j,k,l}\sum_{\sigma\in I,\sigma(i)=j,\sigma(k)=l}\alpha_\sigma q_{ij}q_{kl}$, which is same as $f(q)=\sum_{i,j,k,l}q_{ij}q_{kl}\sum_{\sigma\in I,\sigma(i)=j,\sigma(k)=l}\alpha_\sigma$. But from $\sum_{\sigma\in I}\alpha_\sigma\tilde{P}_\sigma^{[2]}=0$ we know that $\sum_{\sigma\in I,\sigma(i)=j,\sigma(k)=l}\alpha_\sigma=0$ for all i,j,k,l. Hence $f(q)=0$. □

Lemma 8 $\{\tilde{P}_\sigma^{[2]}|\sigma\in I\}$ *is linearly independent if and only if* $\{y_\sigma^2-y_\sigma|\sigma\in I\}$ *is linearly independent.*

Proof Consider $f(q)$ where the first n^2 components of q are $-x$ each and the last component is z. It can be rewritten as $\sum_{\sigma\in I}\alpha_\sigma(z-P_\sigma^T\cdot x)^2=0\ \forall x\in\mathbb{Q}^{n^2},\forall z\in\mathbb{Q}$. 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 5, this is equivalent to $\sum_{\sigma\in I}\alpha_\sigma(y_\sigma^2-y_\sigma)=0\ \forall x\in\mathbb{Q}^{n^2},\forall z\in\mathbb{Q}$. □

Corollary 4 $\{P_\sigma^{[2]}|\sigma \in I\}$ *is linearly independent if and only if* $\{y_\sigma^2 - y_\sigma|\sigma \in I\}$ *is linearly independent.*

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

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 linearly dependent, 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 linearly independent. But α_{σ_2} is negative. Hence we have established that the second statement of Lemma 4 does not hold.

Theorem 12 *Region of* $\mathscr{P}$ *satisfying conditions (3), properly contains* $\mathscr{B}^{[2]}$. *Hence, there exists at least one facet of* $\mathscr{B}^{[2]}$ *which is not an instance of (3).*

5 Partial Ordering on Facet Defining Inequalities

In Section 4 we described several families of facet defining inequalities. In this section we revisit the three exponential sized families and relax some of the conditions so that each family now also includes inequalities that define some of the lower dimensional faces of $\mathscr{B}^{[2]}$. We then define a partial ordering on each family of supporting planes (or inequalities). Note that each facet (or face) defining inequality is also a supporting plane when viewed as an equality. Let X be a supporting plane belonging to one of these three families such that the corresponding inequality is violated by some point p in the feasible region. Also, let the point p does not violate any inequality that lies at a level lower than that of X in the respective ordering. Then we call X a *minimal violated inequality* for point p. We show that given a point in the feasible region that violates an inequality from one of these three families, there always exists a minimal violated inequality for that point. In the next section we give an algorithm for the GI problem that runs in polynomial time if there exists a common minimal violated inequality for all points in the feasible region of LP-GI, that lie outside the polytope $\mathscr{B}^{[2]}$. Recall that if the feasible region is totally confined inside $\mathscr{B}^{[2]}$ then our LP can be made to return a corner point that is a $P_\sigma^{[2]}$ and we can conclude immediately that the given pair is isomorphic.

The first family of inequalities, described in Theorem 9, is given below. Let $i_1, \dots, i_m, k$ be $m+1$ distinct indices. Similarly let $j_1, \dots, j_m, l$ be distinct indices. Let $A = \{(i_1, j_1), \dots, (i_m, j_m)\}$. Then the inequality $Q_1(k,l,A)$ is given by

$$\sum_{(i,j)\in A} Y_{ij,kl} \le Y_{kl,kl} + \sum_{(i,j)\neq(i',j')\in A} Y_{ij,i'j'}. \quad (4)$$

Let $A' \subseteq A$. Then we define $Q_1(k,l,A') \prec Q_1(k,l,A)$. Note that the inequalities in this family corresponding to $|A| = 1$, i.e., $Y_{ij,kl} \le Y_{kl,kl}$ for all $i, j \in [n]$, cannot be violated by any point in $\mathscr{P}$. The same is true for inequalities corresponding to $A = \emptyset$ i.e., $0 \le Y_{kl,kl}$. An inequality corresponding to $m \ge 2$ can however by violated by a point in $\mathscr{P} \setminus \mathscr{B}^{[2]}$. Therefore if an inequality of this class is violated, then there will be a minimal inequality which will be violated and all the lower inequalities will be satisfied. Note that the facets in Theorem 9 require $m \ge 3$. Here we have relaxed that condition to also include the inequalities corresponding to the case of $m = 2$, which define lower dimensional faces of $\mathscr{B}^{[2]}$.

The next are the one-box inequalities, described in Theorem 10. Let P and Q be sets of indices and $\beta \ge 0$ be an integer, then the inequality $Q_2(P,Q,\beta)$ is

$$(\beta-1)\sum_{(ij)\in P\times Q} Y_{ij,ij} \le \sum_{(ij),(kl)\in P\times Q, i<k} Y_{ij,kl} + (\beta^2-\beta)/2. \quad (5)$$

It may be noted that these correspond to facets when $\beta + 1 \le \min\{|P|,|Q|\}, |P| + |Q| \le n-3+\beta, \beta \ge 2$. Here we consider the inequality without these restrictions.

If $P' \subseteq P$ and $Q' \subseteq Q$, then ordering is defined as $Q_2(P',Q',\beta) \prec Q_2(P,Q,\beta)$ and if $0 \le \beta' \le \beta$, then $Q_2(P,Q,\beta') \prec Q_2(P,Q,\beta)$. In this case the lowest level inequalities correspond to $\beta = 0, |P| = |Q| = 2$, i.e., $0 \le \sum_{(ij)\in P\times Q} Y_{ij,ij} + \sum_{(ij),(kl)\in P\times Q, i<k} Y_{ij,kl}$ which cannot be violated.

The last family of inequalities described in Section 4, Theorem 11, is the two-box inequality. Let Q, P_1, and P_2 be index sets such that $P_1 \cap P_2 = \emptyset$ and β be any integer.

Then the inequality $Q_3(P_1,P_2,Q,\beta)$ is

$$\begin{aligned} &-(\beta-1)\sum_{(ij)\in P_1\times Q} Y_{ij,ij} + \beta \sum_{(ij)\in P_2\times Q} Y_{ij,ij} + \sum_{(ij),(kl)\in P_1\times Q, i<k} Y_{ij,kl} \\ &+ \sum_{(ij),(kl)\in P_2\times Q, i<k} Y_{ij,kl} - \sum_{(ij)\in P_1\times Q,(kl)\in P_2\times Q} Y_{ij,kl} + \frac{\beta^2-\beta}{2} \ge 0. \end{aligned} \quad (6)$$

Once again these inequalities define facets of $\mathscr{B}^{[2]}$ when parameters P_1, P_2, Q and β satisfy certain conditions. However, we consider $Q_3(P_1,P_2,Q,\beta)$ without any of these conditions. Note that the inequalities still define planes that support lower dimensional faces of $\mathscr{B}^{[2]}$.

Observe that if $\beta \ge 0$, then $Q_3(P_1,\emptyset,Q,\beta) = Q_2(P_1,Q,\beta)$ and if $\beta < 0$, then $Q_3(\emptyset,P_2,Q,\beta) = Q_2(P_2,Q,-\beta+1)$. Let $i_1 \in P_1$ and $i_2 \in P_2$ be arbitrary indices. Let $P_1' = P_1 \setminus \{i_1\}$ and $P_2' = P_2 \setminus \{i_2\}$. Then we define $Q_3(P_1',P_2',Q,\beta) \prec Q_3(P_1,P_2,Q,\beta)$. The partial ordering will be the transitive closure of this relation. In the case of the 2-box family of inequalities, the inequalities at the lowest level in the partial ordering correspond to one of the following: (a) a 1-box inequality, (b) $Q_3(\emptyset,P_2,Q,\beta)$ where $\beta \ge 0$, or (c) $Q_3(P_1,\emptyset,Q,\beta)$ where $\beta < 0$. The cases (b) and (c) cannot be violated by any point in $\mathscr{P}$. Thus all the inequalities at the lowest level in the partial ordering will be non-violating if all the 1-box inequalities are satisfied by the solution face $\mathscr{P}_{G_1G_2}$.

6 Zero-One Reducibility

Definition 1 Let R be a region in $[0,1]^N$ (unit hypercube in $\mathbb{R}^N$) and let $x_1,\ldots,x_N$ denote the coordinate variables. The region R is said to be zero-one reducible if either $R=\emptyset$ or R is a single point with all $0/1$ coordinates (a corner of the unit hypercube) or there exists some index i and $\alpha\in\{0,1\}$ such that $R|_{x_i=1-\alpha}=\emptyset$ and $R|_{x_i=\alpha}$ is zero-one reducible. See Fig. 3 for an example.

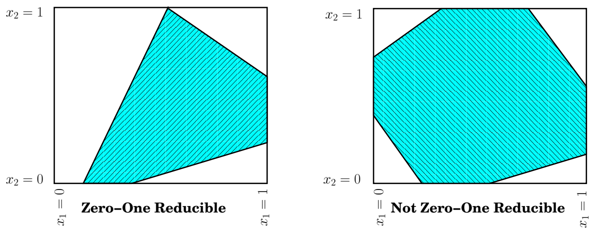

Fig. 3: A 2-dimensional example of zero-one reducibility

Suppose a region $R\subset[0,1]^N$ is zero-one reducible. Then $x_{j_1},x_{j_2},\ldots,x_{j_r}$ is called a reduction sequence if there exist $\alpha_{j_1},\ldots,\alpha_{j_r}\in\{0,1\}$ such that $R|_{x_{j_1}=\alpha_{j_1},\ldots,\,x_{j_{i-1}}=\alpha_{j_{i-1}},\,x_{j_i}=1-\alpha_{j_i}}=\emptyset\;\forall\, i$ and $R|_{x_{j_1}=\alpha_{j_1},\ldots,x_{j_r}=\alpha_{j_r}}=\emptyset$. Suppose $x_{j_1},x_{j_2},\ldots,x_{j_r}$ is a reduction sequence for R. Also suppose that there exists x_j and $\beta_j\in\{0,1\}$ such that $R|_{x_j=1-\beta_j}=\emptyset$. If $x_j\neq x_{j_i}$ for any i, then $x_{j_1},x_{j_2},\ldots,x_{j_r}$ is also a reduction sequence for $R|_{x_j=\beta_j}$. On the other hand, if $j=j_i$, then $x_{j_1},\ldots,x_{j_{i-1}},x_{j_{i+1}},\ldots,x_{j_r}$ is a reduction sequence for $R|_{x_j=\beta_j}$. Hence $R|_{x_j=\beta_j}$ is also zero-one reducible.

From the above observation we can design a polynomial time recursive procedure to detect zero-one reducibility of a given region if we can detect in polynomial time whether the given region is empty or not, which in our case is equivalent to solving LP-GI with additional constraints of the form $x_i=\alpha_i$. The resulting linear program clearly has constraints that are polynomially many in the number of variables, and hence can be solved efficiently using say the ellipsoid method. Given the region R, a sub-routine *SearchVar*() will consider each dimension j and each value $\alpha\in\{0,1\}$ and check if $R|_{x_j=1-\alpha}=\emptyset$. If such j and α are found, then repeat the procedure to detect the zero-one reducibility of $R|_{x_j=\alpha}$.

The idea is to use this procedure to solve the GI problem by reducing the feasible region of LP-GI to empty if the given graphs are non-isomorphic and the region $R=\mathscr{P}_{G_1G_2}$ is zero-one reducible or to the convex hull of $P_\sigma^{[2]}$ for σ corresponding to a subset of G_1,G_2 isomorphisms, if the graphs are isomorphic and the region $R=\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ is zero-one reducible.

6.1 The Search Algorithm

The objective of the algorithm is to check if the feasible region of LP-GI intersects $\mathscr{B}^{[2]}$ or not. We know from Observation 3 that if the feasible region intersects $\mathscr{B}^{[2]}$, then there must be at least one $P_\sigma^{[2]}$ in the region because the entire intersection is the convex hull of $P_\sigma^{[2]}$s that correspond to the isomorphisms between the two graphs. Since $P_\sigma^{[2]}$ are the only $0/1$ points in the feasible region (in the entire $\mathscr{P}$), all we need to detect is whether there is any $0/1$ point in the feasible region $\mathscr{P}_{G_1G_2}$.

Algorithm 1 returns $true$ if the graphs are isomorphic otherwise it returns $false$. It is based on the procedure described above. Parameter Q denotes the equations of the form $x = 0$ and $x = 1$ which are set in the process. $LP(Q)$ represents LP-GI with additional equations Q. The second parameter U denotes the set of variables that are free (not yet set to either zero or one). Initially $Q = Q_0$ is an empty set and $U = U_0$ is the set of all the variables not set in (1b) or implied by Observation 2. The subroutine $SearchVar(Q,U)$ returns a tuple (x,α) when the feasible region of LP-GI with additional conditions Q and $x = 1-\alpha$ is empty. Otherwise it returns either $(null,2)$ (when a $P_\sigma^{[2]}$ is obtained as a corner solution) or $(null,-1)$. A sample run of the procedure is shown in Fig. 4.

```
Function: GISolver(Q,U)
if LP(Q) is infeasible then
|   return false/* Graphs are non-isomorphic */
else
|   if LP(Q) is feasible and U = ∅ then
|   |   return true/* Graphs are isomorphic */
|   else
|   |   (x,α) := SearchVar(Q,U);
|   |   if α = 2 then
|   |   |   return true/* Graphs are isomorphic */
|   |   else
|   |   |   if α = 1 then
|   |   |   |   return GISolver(Q ∪ {x = 1}, U \ {x});
|   |   |   else
|   |   |   |   if α = 0 then
|   |   |   |   |   return GISolver(Q ∪ {x = 0}, U \ {x});
|   |   |   |   else
|   |   |   |   |   Select an arbitrary variable x from U;
|   |   |   |   |   return GISolver(Q ∪ {x = 0}, U \ {x}) ∨ GISolver(Q ∪ {x = 1}, U \ {x});
|   |   |   |   end
|   |   |   end
|   |   end
|   end
end
```

Algorithm 1: Algorithm for searching a $0/1$ solution, one variable at a time

If we view the space searched by GISolver as a tree with (Q_0,U_0) as the root, then those nodes, (Q,U), have two children where $SearchVar(Q,U)$ returns $(null,-1)$. Call them split nodes. All other internal nodes have one child each. Let there be at

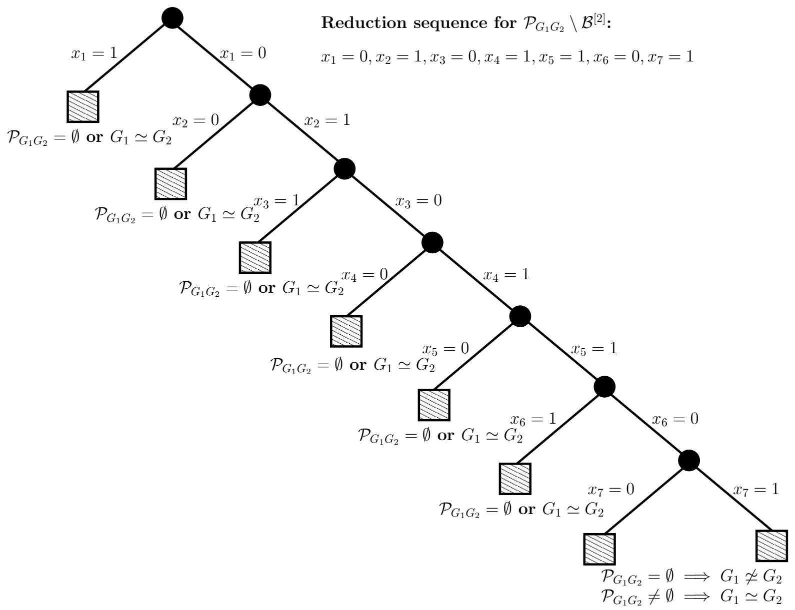

Fig. 4: A sample execution tree of Algorithm 1

most τ split nodes along any path from root to the leaves. Then the time complexity of this algorithm is $O(p(n)2^{\tau})$ where $p(n)$ denotes a polynomial in n. Observe that if the feasible region of $LP(Q_0)$ outside $\mathscr{B}^{[2]}$ is zero-one reducible, then the tree will not have any split nodes and the procedure will require polynomial time.

6.2 $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ is Zero-One Reducible

An important question, which influences the performance of Algorithm 1 is whether a single minimal violated inequality exists for all points in the feasible region of LP-GI that lie outside $\mathscr{B}^{[2]}$. In this section we will assume that such an inequality exists and then we consider three cases where the minimal violated inequality belongs to one of the three families described in Section 5. In each case we show that the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ is zero-one reducible. Subsequently in Section 7 we will drop this assumption and consider the general case.

6.3 A Minimal Violated Inequality of Type (4)

Lemma 9 *If all points in the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ violate $Q_1(k,l,A)$ but satisfy $Q_1(k,l,A')$ where $A' = A \setminus \{(i,j)\}$ for each $(i,j) \in A$, then Algorithm 1 terminates in polynomial time.*

Proof Suppose all points in the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ violate an inequality defined by $\sum_{r\in[m]} Y_{i_rj_r,kl} \leq Y_{kl,kl} + \sum_{r<s\in[m]} Y_{i_rj_r,i_s,j_s}$. Consequently, each point in $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ will satisfy $\sum_{r=1}^{m} Y_{i_rj_r,kl} > Y_{kl,kl} + \sum_{r<s} Y_{i_rj_r,i_s,j_s}$. Let a be an arbitrary element of $[m]$ and define $S = [m] \setminus \{a\}$. Then we have the inequality $\sum_{r\in S} Y_{i_rj_r,kl} \leq Y_{kl,kl}$ $+\sum_{r<s\in S} Y_{i_rj_r,i_s,j_s}$ which must be satisfied by every point in the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$. Subtracting the second from the first we have $Y_{i_aj_a,kl} > \sum_{r\in S} Y_{i_rj_r,i_aj_a} \geq 0$. The last inequality is due to the non-negativity condition in the linear program. This implies that during a call of *SearchVar*() when $Y_{i_aj_a,kl}$ will be set to zero in the algorithm, the linear program will either declare it infeasible or return a $P_\sigma^{[2]}$. In the former case, $Y_{i_aj_a,kl}$ will be set to 1. Since a is any arbitrary index, eventually $Y_{i_aj_a,kl}$ will be set to 1 for each $a \in [m]$ in the worst case when we do not encounter any $P_\sigma^{[2]}$. These will force $Y_{kl,kl}$ and $Y_{i_rj_r,i_sj_s} \forall\ r,s \in [m]$ to 1. Then the first inequality will be violated since the left hand side will be m but the right hand side will be $1 + \binom{m}{2}$ where $m \geq 2$. So either we encounter a $P_\sigma^{[2]}$, in which case we conclude that the given graphs are isomorphic, or we deduce that the feasible region does not contain any integer solution, in which case we conclude that the given graphs are non-isomorphic. □

6.4 A Minimal Violated inequality of Type (5)

6.4.1 Restriction to Facets

Similar to a minimal violated inequality we define the notion of a minimal violated *facet* inequality. Here only the facet defining inequalities are considered in the partial ordering. We consider two separate cases. In the first case the minimal violated facet inequality has $max\{|P|,|Q|\} > \beta + 1$, whereas in the second case the minimal violated facet inequality has $|P| = |Q| = \beta + 1$ and $\beta > 2$. The minimal inequalities in the partial ordering correspond to the case when $\beta = 2$ and $|P| = |Q| = 3$. Since we want them to be satisfied by every point in the feasible region, we add all these inequalities to the linear program. Note that the number of these inequalities is polynomial in the size of the graphs, hence adding them to LP-GI will not affect its poly-time solvability.

Lemma 10 *If all points in the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ violate $Q_2(P,Q,\beta)$ but satisfy $Q_2(P',Q',\beta')$ such that either (i) $|P| > \beta + 1$ and $P' = P \setminus \{i\}$ for arbitrary $i \in P$, $Q' = Q, \beta' = \beta$, or (ii) $|Q| > \beta + 1$ and $Q' = Q \setminus \{j\}$ for arbitrary $j \in Q$, $P' = P, \beta' = \beta$, then Algorithm 1 terminates in polynomial time.*

Proof Suppose the inequality $(\beta-1)\sum_{(ij)\in P\times Q} Y_{ij,ij} \leq \sum_{(ij),(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)$ $(\beta^2-\beta)$ is violated. Note that the roles of P and Q can be interchanged without affecting the inequality. Hence it is sufficient to consider only one case, namely, $|P| > \beta + 1$.

$$(\beta-1) \sum_{(ij)\in P\times Q} Y_{ij,ij} > \sum_{(ij),(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2-\beta) \tag{7}$$

Let $i_0 \in P$ and $j_0 \notin Q$. Define $P' = P \setminus \{i_0\}$. Suppose during a call of *SearchVar*() the algorithm forces $Y_{i_0 j_0, i_0 j_0}$ to 1. Since P' and Q both have at least $\beta+1$ elements, every point in the region $\mathscr{P}_{G_1 G_2} \setminus \mathscr{B}^{[2]}$ must satisfy the following inequality

$$(\beta-1) \sum_{(ij)\in P'\times Q} Y_{ij,ij} \leq \sum_{(ij),(kl)\in P'\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2-\beta). \tag{8}$$

(7) minus (8) gives $(\beta-1)\sum_{j\in Q} Y_{i_0 j, i_0 j} > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl}$.

Since $Y_{i_0 j_0, i_0 j_0} = 1$ where $j_0 \notin Q$, $\sum_{j\in Q} Y_{i_0 j, i_0 j} = 0$. The non-negativity condition implies that the right-hand-side is non-negative so we conclude that $0 > 0$. As $Y_{i_0 j_0, i_0 j_0} = 1$ renders the region $\mathscr{P}_{G_1 G_2} \setminus \mathscr{B}^{[2]}$ empty, the algorithm will either encounter a $P^{[2]}_\sigma$ or set $Y_{i_0 j, i_0 j} = 0$ for all $j \notin Q$. As i_0 was an arbitrary element of P, eventually the algorithm will set $Y_{ij,ij} = 0$ for all $i \in P$ and all $j \notin Q$, unless it has encountered a $P^{[2]}_\sigma$, in which case it has already concluded that the given graphs are isomorphic.

Next consider an arbitrary $(i_0 j_0) \in P \times Q$. Suppose algorithm sets $Y_{i_0 j_0, i_0 j_0} = 1$. Let $P' = P \setminus \{i_0\}$. Then the violated inequality (7) reduces to $(\beta-1)(1+\sum_{(ij)\in P'\times Q} Y_{ij,ij}) > \sum_{(ij),(kl)\in P'\times Q, i<k} Y_{ij,kl} + \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl} + \frac{\beta^2-\beta}{2}$.

Subtracting (8) from the above inequality gives $(\beta-1) > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl}$. Since $Y_{i_0 j,kl} = 0$ for all $j \neq j_0$, $\sum_{j\notin Q}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl} = 0$. Adding this term to the right hand side of the inequality we get $(\beta-1) > \sum_{j\in[n]}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl} = \sum_{(kl)\in P'\times Q} Y_{kl,kl}$. From the first part of the proof, $Y_{kl,kl} = 0$ for any $k \in P$ and $l \notin Q$. So we have $\sum_{(kl)\in P'\times Q} Y_{kl,kl} = \sum_{(kl)\in P'\times[n]} Y_{kl,kl} = |P'| > \beta+1-1 = \beta$. It reduces to infeasible $\beta - 1 > \beta$, which leads the algorithm to set $Y_{i_0 j_0, i_0 j_0} = 0$ or conclude that the given pair of graphs are isomorphic. Hence eventually $Y_{ij,ij}$ is set to zero for all $(ij) \in P \times Q$ (assuming that the favorable event of finding a $P^{[2]}_\sigma$ did not occur). Combining with the fact that $Y_{ij,ij} = 0$ for all $i \in P, j \notin Q$, we have $1 = \sum_{j\in[n]} Y_{ij,ij} = 0$ for any $i \in P$. Hence the algorithm will report an empty feasible region and conclude that the graphs are non-isomorphic. At no stage is the algorithm required to invoke two calls, one with $x = 0$ and the other with $x = 1$ for any variable x. So we see that the feasible region is zero-one reducible and the algorithm requires polynomial time. □

Lemma 11 *If all points in the region $\mathscr{P}_{G_1 G_2} \setminus \mathscr{B}^{[2]}$ violate $Q_2(P,Q,\beta)$ where $|P| = |Q| = \beta+1, \beta > 2$ but satisfy $Q_2(P',Q',\beta')$ such that either (i) $P' = P \setminus \{i\}$ for arbitrary $i \in P$, $Q' = Q, \beta' = \beta - 1$, or (ii) $Q' = Q \setminus \{j\}$ for arbitrary $j \in Q$, $P' = P, \beta' = \beta - 1$, then Algorithm 1 terminates in polynomial time.*

Proof The violation of $(\beta-1)\sum_{(ij)\in P\times Q} Y_{ij,ij} \leq \sum_{(ij),(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2 - \beta)$ gives inequality (7), given in the last proof.

Let $i_0 \in P$ and $P' = P \setminus \{i_0\}$. Then every point in the region $\mathscr{P}_{G_1 G_2} \setminus \mathscr{B}^{[2]}$ must satisfy the inequality with parameters $P', Q, \beta - 1$. So we have

$$(\beta-2) \sum_{(ij)\in P'\times Q} Y_{ij,ij} \leq \sum_{(ij),(kl)\in P'\times Q, i<k} Y_{ij,kl} + (1/2)((\beta-1)^2 - (\beta-1)) \tag{9}$$

(7) minus (9) gives

$$\sum_{(ij)\in P'\times Q} Y_{ij,ij} + (\beta-1)\sum_{j\in Q} Y_{i_0 j, i_0 j} > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0 j,kl} + (\beta-1). \tag{10}$$

Since $(\beta-1)\sum_{j\in Q} Y_{i_0j,i_0j} = (\beta-1)-(\beta-1)\sum_{j\notin Q} Y_{i_0j,i_0j}$, the inequality transforms to $\sum_{(ij)\in P'\times Q} Y_{ij,ij} > (\beta-1)\sum_{j\notin Q} Y_{i_0j,i_0j} + \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl} = (|P'|-1)\sum_{j\notin Q} Y_{i_0j,i_0j} + \sum_{j\in Q}\sum_{k\in P'}\sum_{l\in Q} Y_{i_0j,kl}$, because $\beta+1 = |P| = |P'|+1$. For Y is a solution of the LP, $Y_{i_0j,i_0j} = \sum_{l\in[n]} Y_{i_0j,kl}$ for any k. So $|P'|\sum_{j\notin Q} Y_{i_0j,i_0j} = \sum_{k\in P'}\sum_{j\notin Q}\sum_{l\in[n]} Y_{i_0j,kl}$. Plugging this equation in the previous inequality we get $\sum_{(ij)\in P'\times Q} Y_{ij,ij} > -\sum_{j\notin Q} Y_{i_0j,i_0j} + \sum_{k\in P'}\sum_{l\in[n]}\sum_{j\notin Q} Y_{i_0j,kl} + \sum_{k\in P'}\sum_{l\in Q}\sum_{j\in Q} Y_{i_0j,kl}$. Combining the last two terms, ignoring $l\notin Q$ terms due to non-negativity, we get $\sum_{(ij)\in P'\times Q} Y_{ij,ij} > -\sum_{j\notin Q} Y_{i_0j,i_0j} + \sum_{(kl)\in P'\times Q}\sum_{j\in[n]} Y_{i_0j,kl} = -\sum_{j\notin Q} Y_{i_0j,i_0j} + \sum_{k\in P'}\sum_{l\in Q} Y_{kl,kl}$. It simplifies to $\sum_{j\notin Q} Y_{i_0j,i_0j} > 0$.

If the algorithm sets $Y_{i_0j,i_0j} = 1$ for some $j\in Q$, then the above inequality will reduce to $0>0$ making it infeasible. So eventually algorithm will set $Y_{ij,ij} = 0$ for all $(ij)\in P\times Q$, assuming that no $P_\sigma^{[2]}$ is encountered. This will make (7) infeasible. Again we find that the feasible region of LP-GI outside $\mathscr{B}^{[2]}$ is zero-one reducible.

□

Lemmas 10 and 11 lead to the following corollary.

Corollary 5 *If all points in the region $\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ violate $Q_2(P,Q,\beta)$ but satisfy $Q_2(P',Q',\beta')$ such that $Q_2(P',Q',\beta')\prec Q_2(P,Q,\beta)$ and each $Q_2(P,Q,\beta)$ defines a facet of $\mathscr{B}^{[2]}$, then Algorithm 1 terminates in polynomial time.*

6.4.2 General 1*-box Inequality*

Now we withdraw the restriction of (5) to only the facets of $\mathscr{B}^{[2]}$ and consider all the 1-box inequalities given by (5), even those that represent some of the lower dimensional faces of $\mathscr{B}^{[2]}$. These 1-box inequalities have a partial ordering as defined in Section 5.

Lemma 12 *If all points in the region $\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ violate $Q_2(P,Q,\beta)$ but satisfy $Q_2(P',Q',\beta')$ for all $Q_2(P',Q',\beta')\prec Q_2(P,Q,\beta)$, then Algorithm 1 terminates in polynomial time.*

The proof of this lemma is same as that of Lemma 10 while ignoring the restriction $min\{|P|,|Q|\}\geq\beta+1$.

6.5 A Minimal Violated Inequality of Type (6)

In this case we directly consider the unrestricted inequality because the base case of restricted inequality (associated with facets) may not always hold true for all points in $\mathscr{P}$ and their number is not polynomial so that we cannot incorporate them into LP-GI, forcing them to hold true. In the case of unrestricted inequality Q_3 the base cases always hold true provided the feasible region satisfies all the 1-box inequalities. If it fails 1-box inequality, then the minimal violated inequality will be a Q_2 and we can use the previous section's argument to prove polynomiality of the algorithm.

Lemma 13 *If all points in the region* $\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ *violate* $Q_3(P_1,P_2,Q,\beta)$ *but satisfy* $Q_3(P_1',P_2',Q,\beta)$ *where* $P_1'=P_1\setminus\{i\}$ *for arbitrary* $i\in P_1$ *and* $P_2'=P_2\setminus\{j\}$ *for arbitrary* $j\in P_2$ *and also satisfy all* $Q_2(P,Q,\beta)$*, then Algorithm 1 terminates in polynomial time.*

Proof Given that a 2-box inequality (P_1,P_2,Q,β) is violated, every point in $\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ satisfies

$$\begin{aligned}&-(\beta-1)\sum_{(ij)\in P_1\times Q}Y_{ij,ij}+\beta\sum_{(ij)\in P_2\times Q}Y_{ij,ij}+\sum_{(ij),(kl)\in P_1\times Q,i<k}Y_{ij,kl}\\&+\sum_{(ij),(kl)\in P_2\times Q,i<k}Y_{ij,kl}-\sum_{(ij)\in P_1\times Q,(kl)\in P_2\times Q}Y_{ij,kl}+\frac{\beta^2-\beta}{2}<0.\end{aligned}\tag{11}$$

Let $i_0\in P_1$ and $i_0'\in P_2$ be two arbitrary indices. Let $P_1'=P_1\setminus\{i_0\}$ and $P_2'=P_2\setminus\{i_0'\}$. Then every point in $\mathscr{P}_{G_1G_2}\setminus\mathscr{B}^{[2]}$ must also satisfy the inequality corresponding to (P_1',P_2',Q,β). We have

$$\begin{aligned}&-(\beta-1)\sum_{(ij)\in P_1'\times Q}Y_{ij,ij}+\beta\sum_{(ij)\in P_2'\times Q}Y_{ij,ij}+\sum_{(ij),(kl)\in P_1'\times Q,i<k}Y_{ij,kl}\\&+\sum_{(ij),(kl)\in P_2'\times Q,i<k}Y_{ij,kl}-\sum_{(ij)\in P_1'\times Q,(kl)\in P_2'\times Q}Y_{ij,kl}+\frac{\beta^2-\beta}{2}\geq 0.\end{aligned}\tag{12}$$

Case 1: In the algorithm when $Y_{i_0j_0,i_0'j_0'}$ is set to 1, where $j_0,j_0'\in Q, j_0\neq j_0'$, (11) minus (12) gives $0<0$ which is absurd. Hence algorithm will set $Y_{ij,i'j'}=0$ for all $i\in P_1,i'\in P_2,j,j'\in Q$, assuming no $P_\sigma^{[2]}$ is encountered.

Case 2: When *SearchVar*() sets $Y_{i_0j_0,i_0'j_0'}=1$, where $j_0\notin Q,j_0'\in Q$. Then (11) minus (12) gives $\beta+\sum_{(i,j)\in P_2'\times Q}Y_{ij,ij}<0$, where we used the result of the previous case, i.e., $Y_{ij,kl}=0$ for all $ij\in P_1\times Q$ and $kl\in P_2\times Q$. Note that it is impossible if $\beta\geq 0$.

Case 3: When *SearchVar*() sets $Y_{i_0j_0,i_0'j_0'}=1$, where $j_0\in Q,j_0'\notin Q$. Then (11) minus (12) gives $-(\beta-1)+\sum_{(i,j)\in P_1'\times Q}Y_{ij,ij}<0$, which is impossible if $\beta\leq 1$.

If $\beta\geq 0$, then combining the results of cases 1 and 2 we see that the algorithm sets $Y_{ij,kl}=0$ for all $i\in P_1,k\in P_2,j\in[n],l\in Q$ which is same as setting $Y_{ij,ij}=0$ for all $ij\in P_2\times Q$. Similarly we can see that if $\beta<0$, then the algorithm will set $Y_{ij,ij}=0$ for all $(ij)\in P_1\times Q$. Here we assume that no $P_\sigma^{[2]}$ is ever encountered during a call to *SearchVar*().

Plugging these values in inequality (11) we have following simplified cases

$$0\leq\beta\leq 1:\text{Impossible. Recall that }\beta\in\mathbb{Z}.\tag{13}$$

$$\beta\leq -1:\beta\sum_{(ij)\in P_2\times Q}Y_{ij,ij}+\sum_{(ij),(kl)\in P_2\times Q,i<k}Y_{ij,kl}+\frac{\beta^2-\beta}{2}<0.\tag{14}$$

$$\beta\geq 2:-(\beta-1)\sum_{(ij)\in P_1\times Q}Y_{ij,ij}+\sum_{(ij),(kl)\in P_1\times Q,i<k}Y_{ij,kl}+\frac{\beta^2-\beta}{2}<0.\tag{15}$$

The inequality (15) clearly violates $Q_2(P_1,Q,\beta)$ whereas the inequality (14) violates $Q_2(P_2,Q,1-\beta)$. But we have assumed that all the Q_2 inequalities are satisfied by the feasible region. This leads to a contradiction and hence at this stage the algorithm will find no solution outside $\mathscr{B}^{[2]}$ and conclude that the graphs must be non-isomorphic, unless a $P_\sigma^{[2]}$ was encountered during a call to *SearchVar*(), in which case the graphs must be isomorphic.

For the completeness sake we will prove that these inequalities cannot hold true even if we assume that only those Q_2 inequalities that are associated with facets hold true. For this we need the following additional restrictions: (i) $|P_1|,|P_2| \geq 3$, (ii) if $\beta \geq 0$ and $\min\{|Q|,|P_1|\} \geq \beta+1$ then $|Q|+|P_1|+3 \leq n+\beta$, (iii) if $\beta < 0$ and $\min\{|Q|,|P_2|\} \geq 2-\beta$ then $|Q|+|P_2|+3 \leq n+1-\beta$.

We will first consider inequality (15). If $|P_1|,|Q| \geq \beta+1$, then (15) implies that the 1-box inequality corresponding to (P_1,Q,β) is violated. But that is not possible due to the assumption that all Q_2 inequalities associated with facets hold true for the feasible region. So the only case that needs to be considered is $\min\{|P_1|,|Q|\} \leq \beta$.

First assume that $|P_1| \leq |Q|$. Consider the identity $\sum_{(ij),(kl)\in P_1\times Q, i<k} Y_{ij,kl} = |P_1|(|P_1|-1)/2 + \sum_{(ij),(kl)\in P_1\times \overline{Q}, i<k} Y_{ij,kl} - (|P_1|-1)\sum_{(ij)\in P_1\times \overline{Q}} Y_{ij,ij}$. Plugging into the inequality (15) gives $-(\beta-1)\sum_{(ij)\in P_1\times Q} Y_{ij,ij} + |P_1|(|P_1|-1)/2 + \sum_{(ij),(kl)\in P_1\times \overline{Q}, i<k} Y_{ij,kl} - (|P_1|-1)\sum_{(ij)\in P_1\times \overline{Q}} Y_{ij,ij} + \beta(\beta-1)/2 < 0$. But the left hand side of the inequality is greater than or equal to $-(\beta-1)\sum_{i\in P_1, j\in[n]} Y_{ij,ij} + (\beta(\beta-1)+|P_1|(|P_1|-1))/2 = ((\beta-|P_1|)^2-(\beta-|P_1|))/2 \geq 0$ since $\sum_{i\in P_1, j\in[n]} Y_{ij,ij} = |P_1|$ and $\beta, |P_1|$ are both integral. Hence we find that inequality (15) is impossible. The case of $|Q| \leq |P_1|$, is handled similarly since P_1 and Q have similar role. So we conclude that inequality (15) is impossible.

In case of inequality (14) we rewrite it by replacing β by $-(\gamma-1)$. We get $-(\gamma-1)\sum_{(ij)\in P_2\times Q} Y_{ij,ij} + \sum_{(ij),(kl)\in P_2\times Q, i<k} Y_{ij,kl} + (1/2)(\gamma^2-\gamma) < 0$, where $\gamma \geq 2$. We can now use the same argument as above to establish that (14) is also impossible. □

Theorem 13 *Algorithm 1 solves the Graph Isomorphism problem in polynomial time if there exists a common minimal violated inequality of type 4, 5 or 6 for all points in the feasible region of LP-GI outside $\mathscr{B}^{[2]}$, namely $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$.*

7 The General Case

In the general case we consider the situation when more than one non-trivial minimal facets are required to separate $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ from $\mathscr{B}^{[2]}$. The assumption here is that $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ is separable from $\mathscr{B}^{[2]}$ exclusively by the presently known facets (described in Section 4). Let these minimal facets be $F_1,\ldots,F_{k_0}$ and the regions separated by them be $R_1,R_2,\ldots$ respectively. Clearly these regions need not be mutually exclusive and $\cup_i R_i = \mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$.

So we have the region of $\mathscr{P}_{G_1G_2}$ outside $\mathscr{B}^{[2]}$, divided into subregions such that for each subregion there exists a common minimal violated inequality of type 4, 5 or 6. In this section we describe a procedure that solves the Graph Isomorphism problem in $O(k_0(2n)^{k_0})$ time.

From Section 6 we know that each R_i as defined above, is zero-one reducible. Let $x_{i1}, x_{i2}, \ldots$ be a reduction sequence for region R_i, for each i. Let $\alpha_{i1}, \alpha_{i2}, \ldots \in \{0,1\}$ be the respective values. So we have $R_i|_{x_{i1}=\alpha_{i1}, x_{i2}=\alpha_{i2}, \ldots} = \emptyset$. Also, $R_i|_{x_{i1}=\overline{\alpha_{i1}}} = \emptyset$ for all $i \in [k]$. Clearly, $(\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]})|_{x_{11}=\overline{\alpha_{11}}, x_{21}=\overline{\alpha_{21}}, \ldots, x_{k1}=\overline{\alpha_{k1}}} = \emptyset$. Note that for isomorphic graphs, $\mathscr{P}_{G_1G_2}$ reduces to the convex hull of $\mathscr{P}_\sigma^{[2]}$s for those σ that correspond to the isomorphisms between G_1 and G_2 and are consistent with $x_{11} = \overline{\alpha_{11}}, x_{21} = \overline{\alpha_{21}}, \ldots, x_{k1} = \overline{\alpha_{k1}}$. So in this case $\mathscr{P}_{G_1G_2}|_{x_{11}=\overline{\alpha_{11}}, x_{21}=\overline{\alpha_{21}}, \ldots, x_{k1}=\overline{\alpha_{k1}}} \subseteq \mathscr{B}_{G_1G_2}$.

We will now use the above information to devise a procedure for the Graph Isomorphism problem.

7.1 A Generalized Algorithm for GI

In this section we will describe an extended procedure for the general case. This procedure subsumes Algorithm 1.

7.1.1 k-SearchVar()

Recall that the procedure *SearchVar*() in Algorithm 1 returns a variable x and a $0/1$ value α such that $x = 1 - \alpha$ makes the linear program infeasible. We modify this procedure to now consider all subsets of k variables and return a subset $x_1, x_2, \ldots, x_k$ with the respective values $\alpha_1, \alpha_2, \ldots \alpha_k$ such that the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ becomes empty on setting $x_i = 1 - \alpha_i$ for all $i \in [k]$. For non-isomorphic graphs the linear program becomes infeasible when such an assignment is found. However, for isomorphic graphs the feasible region of LP-GI need not become empty even if all the subregions do become empty. The feasible region in this case is reduced to the convex hull of a subset of the isomorphisms between the input pair that survive the assignments to the k variables (Corollary 3). So an optimization step is included that would optimize a random direction over this convex hull, thus detecting one of its corners, which will be a $P_\sigma^{[2]}$ where σ is an isomorphism. The invoking procedure can then declare isomorphism and terminate.

The new procedure must also ensure that the assignments $x_i = 1 - \alpha_i$ are consistent with the conditions (1c)-(1d) for all $i \in [k]$, i.e., the assignment must not lead to a solution outside the plane P. We will refer to this modified procedure as *k-SearchVar*(). Clearly, *SearchVar*() is same as 1-*SearchVar*().

7.1.2 The Procedure

The number k_0 of minimal violating inequalities that separate the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$, is unknown. So we first determine the value of k_0 by invoking *k-SearchVar*() for $k = 1, 2, \ldots, k_0$ until a combination of k_0 variables and respective k_0 values either renders the linear program infeasible or concludes that G_1 and G_2 are isomorphic. Subsequent procedure is given in Algorithm 2.

At each step (one full execution of the *While* loop) we reduce the given problem on N variables with parameter k to N problems with strictly smaller parameter (less

```
Data: Q: set of constraints; U: set of unassigned variables
Result: true if the given pair of graphs are isomorphic; false if the given pair of graphs are
        non-isomorphic
Function: k-GISolver(Q,U)
if LP(Q) is infeasible then
    return false/* Graphs are non-isomorphic */
else
    if LP(Q) is feasible and U = ∅ then
        return true/* Graphs are isomorphic */
    else
        while LP(Q) is feasible do
            (x, α, k) := k-SearchVar(Q,U);
            if k = −1 then
                return true/* Graphs are isomorphic */
            end
            for i := 1 to k do
                val := k-GISolver(Q ∪ {x_i = ᾱ_i}, U \ {x_i});
                if val = true then
                    return true/* Graphs are isomorphic */
                end
                Q := Q ∪ {x_i = α_i};
                U := U \ {x_i};
            end
            if OPT(LP(Q)) = P_σ^[2] then
                return true/* Graphs are isomorphic */
            end
        end
        return false/* Graphs are non-isomorphic */
    end
end
```

Algorithm 2: Algorithm for searching a $0/1$ solution, k variables at a time

than or equal to $k-1$) because each reduced problem has at least one of the regions R_i missing from the feasible region of LP-GI. Each iteration of the *While* loop makes assignments to k variables. Figure 5 shows the result of the complete run of the *While* loop. When the *While* loop terminates, each of the regions R_i would be empty.

The following recurrence sums up the performance of Algorithm 2. Here $T(1)$ is $O(N)$ since each R_i is zero-one reducible. The value of $T(k)$ gives the number of times LP-GI is solved. So the final time complexity will be $poly(N) \cdot T(k)$.

$$T(k) \leq N \cdot T(k-1) + \binom{N}{k} 2^k + \binom{N-k}{k} 2^k + \ldots + \binom{k}{k} 2^k \tag{16}$$

On solving the above recurrence, we get $T(k) = O(k \cdot (2N)^k)$. Note that the cost of finding the value of k can be absorbed in this. So $T(k)$ gives the total cost of the procedure.

The following lemma justifies that Algorithm 2 solves the GI problem in $O(k \cdot (2N)^k)$ steps.

Lemma 14 *Algorithm 2 decides in $O(k \cdot (2N)^k)$ steps if the input pair of graphs is isomorphic or not, where k is the number of subregions into which $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ is*

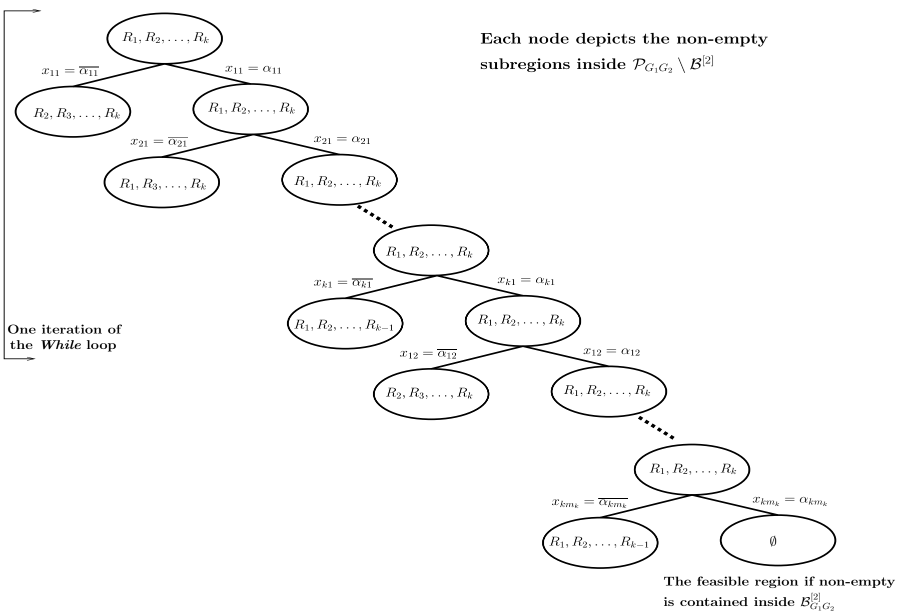

Fig. 5: Execution of Algorithm 2

divided such that each subregion has a common minimal violated inequality of type 4, 5 or 6.

Proof First we will show that the algorithm does not wrongly declare isomorphic graphs as non-isomorphic. Let $\mathscr{P}_{\sigma}^{[2]}$ be a point in the feasible region for a given pair of isomorphic graphs. Note that the algorithm only assigns values to those variables that appear in the reduction sequences of the subregions of $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$. Let $\gamma_{ij} \in \{0,1\}$ be the values that these variables take in $\mathscr{P}_{\sigma}^{[2]}$. Since the algorithm pursues both the paths corresponding to $x_{ij} = \alpha_{ij}$ and $x_{ij} = \overline{\alpha_{ij}}$ for every x_{ij}, there must exist an assignment that corresponds to γ_{ij}, and for this assignment the linear program returns a non-empty feasible solution. Hence in this case the algorithm cannot output *non-isomorphic*.

What remains to be shown now is that the algorithm outputs *non-isomorphic* when the graphs are not isomorphic. In this case $\mathscr{P}_{G_1G_2} = \cup_i R_i$. Since the algorithm assigns the variables in the zero-one reduction sequences of each of these regions, at the end all the final restricted regions (due to various variable assignments) will be empty. Hence the algorithm will correctly characterize this case as non-isomorphic.

The recurrence relation (16) now gives the worst case number of assignments as $O(k \cdot (2n)^k)$. □

Theorem 14 *Algorithm 2 solves the graph isomorphism problem in $O(k \cdot 2^k \cdot N^{k+c})$ time where $N = O(n^4)$ is the number of variables in LP-GI and k is the number of subregions into which $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ is divided such that each subregion has a* *common minimal violated inequality of type 4, 5 or 6. Here $O(N^c)$ denotes the cost of running the LP solver.*

Remark: There is a situation that appears to lead to a conflict in building a k-dimensional zero-one reduction sequence for a general case. In case x_{11} and x_{21} are same but $\alpha_{11} = \overline{\alpha_{21}}$, then $\mathscr{P}_{G_1G_2}|_{x_{11}=\overline{\alpha_{11}},x_{21}=\overline{\alpha_{21}},\dots,x_{k1}=\overline{\alpha_{k1}}}$ is not well defined. However this does not cause any difficulty. To understand consider the $k = 2$ case. Suppose the respective sequences are $x = \alpha, y = \beta, \dots$ and $x = \overline{\alpha}, z = \gamma, \dots$. Then $\mathscr{P}_{G_1G_2}|_{x=\alpha,y=\overline{\beta}} = \emptyset$ and $\mathscr{P}_{G_1G_2}|_{x=\overline{\alpha},z=\overline{\gamma}} = \emptyset$. So we will have two $k = 1$ order problems namely $\mathscr{P}_{G_1G_2}|_{x=\overline{\alpha}}$ and $\mathscr{P}_{G_1G_2}|_{x=\alpha}$. Therefore there is no conflict.

Finally we present a bound for k for some special cases.

7.1.3 A Bound for k

Suppose the region $\mathscr{P}_{G_1G_2} \setminus \mathscr{B}^{[2]}$ violates an inequality of type 4. Note that when the left hand side of this inequality takes its maximum value of m, the right hand side has a value of $\binom{m}{2} + 1$. Clearly, less than $\sqrt{m}$ variables $Y_{ij,kl}$ can be assigned a value of 1 before the violated inequality becomes infeasible. So *k-SearchVar*() cannot return a value of k larger than $\sqrt{m}$. Next consider the case when the portion of the feasible region outside $\mathscr{B}^{[2]}$ violates an inequality of type 5. Using a similar argument we get a bound of $\sqrt{m\beta}$ on the value of k. Here $m = min\{|P|, |Q|\}$. Finally, for a violated inequality of type 6, we have $k = O(\sqrt{|Q||\beta|})$ where $|\beta|$ is the absolute value of β.

8 Experiments

We present the results of the experiments conducted to determine the value of k for non-isomorphic pairs of graphs chosen from two families that are believed to be hard for GI. The two graph families are (i) strongly regular graphs and (ii) CFI-graphs. A d-regular n vertex graph is said to be (n, d, λ, μ)-strongly regular if all adjacent pairs of vertices have λ common neighbors and all non-adjecent pairs of vertices have μ common neighbors. CFI is short for Cai-Fürer-Immerman and these graphs are named so since they use a construction given by Cai, Fürer and Immerman in [13].

The purpose of these experiments is to show the polynomiality of our algorithm on instances taken from the above mentioned classes of graphs, rather than compare its running time with softwares like *nauty*. As it stands, our running time is prohibitive and is not comparable to any practical software.

8.1 Strongly Regular Graphs

The following quote from [6], sums up the relevance of strongly regular graphs to the graph isomorphism problem.

> ”Strongly regular graphs, while not believed to be Graph Isomorphism (GI) complete, have long been recognized as hard cases for GI, and, in this author’s view, present some of the core difficulties of the general GI problem.”

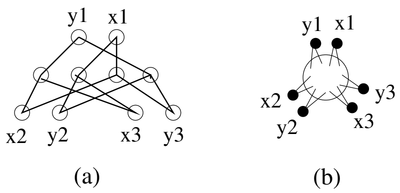

Fig. 6: (a) CFI Gadget F_3, (b) Symbolic F_3

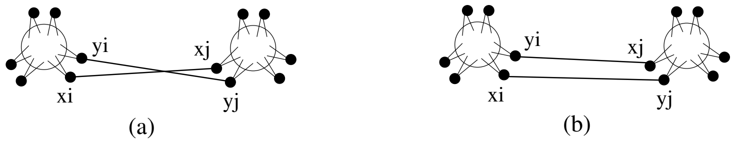

Fig. 7: (a) A Regular Bond, (b) A Twisted Bond

The best known graph isomorphism algorithm for strongly regular graphs runs in time that is slightly better than that for general graphs. In [42], Spielman had given an algorithm with time exponential in $\tilde{O}(n^{1/3})$. This was recently improved by Babai et. al. to $exp(\tilde{O}(n^{1/5}))$ [8]. Recall that the best algorithm for general graphs runs in $exp(\tilde{O}(n^{1/2}))$ time.

8.2 The Cai-Fürer-Immerman construction

CFI graphs are formed by replacing each vertex of degree k in some base graph with the CFI gadget F_k. We will refer to the instance of F_k used for a vertex u by u-gadget. We experiment with CFI graphs having 3-regular graphs as base graphs. Figure 6(a) shows the gadget F_3 where $x_1, y_1, x_2, y_2, x_3, y_3$ are the interface vertices and the remaining vertices are internal vertices. Figure 6(b) shows the same gadget by suppressing the internal vertices. An edge, $\{u, v\}$ in the base graph is replaced by a bond. Figure 7(a) shows a regular-bond between the u-gadget and the v-gadget as a pair of edges $\{x'_i, x''_j\}$ and $\{y'_i, y''_j\}$ for some i, j. Here x'_i, y'_i are i-th interface vertices of the u-gadget and x''_j, y''_j are j-th interface vertices of the v-gadget. Figure 7(b) shows a twisted bond. Here the edges are $\{x'_i, y''_j\}$ and $\{x''_j, y'_i\}$.

Figure 8(a) shows the CFI graph with K_4 as base graph. Figure 8(b) shows the same graph with one of the bonds replaced by a twisted bond. Such pairs are non-isomorphic. We use such pairs for experiments.

The linear program LP-GI has $\Theta(n^4)$ variables. Hence we are required to keep n low in our experiments. We consider two variants of CFI graphs having fewer vertices than the standard construction but with the inherent difficulty preserved. Whenever the standard CFI graph turns out to be too large for our experiments, we use these variants. These variants are formed by contracting edges in the bonds as shown in figures 9(b) and 9(c). Observe that a p-vertex 3-regular base graph results in a $10 \times p$-

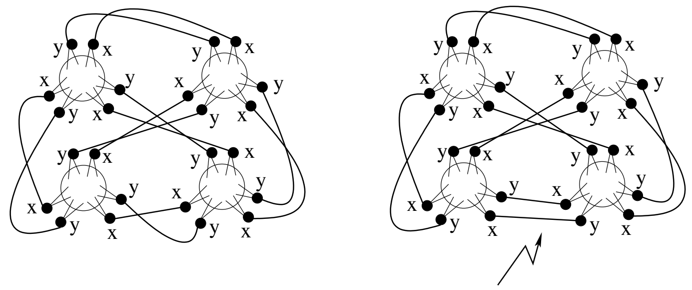

Fig. 8: (a) CFI Graph based on K_4, (b) Same graph but with one Twisted Bond

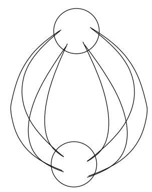

Fig. 9: Bonds: (a) Standard, (b) After one level of contraction, (c) After two levels of contractions

vertex standard CFI graph whereas these variants give $7 \times p$ and $4 \times p$ vertex graphs respectively.

8.3 Experimental setup

We use the GNU Linear Programming Kit (GLPK) version 4.52 to solve LP-GI in our algorithm on graphs taken from the two families described above. The linear program is specified using the GNU MathProg Modeling Language (GMPL). The model file takes its data from a separate file. So for every pair of non-isomorphic graphs we have a separate data file whereas the model file is common. The algorithm is implemented in C language making use of the appropriate GLPK APIs. The experiments are run on a desktop computer running ubuntu 14.04 and having 16 GiB RAM with Intel® Core^{TM} i7-4770 CPU @ $3.40GHz \times 8$ processors. However, no parallelization is done. For the linear program, the default primal simplex algorithm is used and maximum 100000 iterations are allowed. If a program fails to converge in these many iterations, then it is taken to have a feasible solution.

The strongly regular graphs are taken from the collection available at [41]. We take 10 distinct pairs of non-isomorphic graphs for each (n,d,λ,μ). Wherever that many are not available, all possible distinct pairs are taken. The largest graph used has 50 vertices.

For CFI graphs used in the experiments, the base graph is always a three regular graph. Apart from one graph, which is the 3-dimensional cube, all other base graphs are $2k$-cycles with chords. The vertices are labeled from $1 \dots 2k$ and an edge is present between two vertices having labels u, v iff $u - v \equiv \pm 1 \pmod{2k}$ or $u - v \equiv k \pmod{2k}$. We select those values of k for which the number of vertices in at least one of the three variants stays within 56.

8.4 Results

Results of experiments with non-isomorphic pairs of strongly regular graphs appear in Table 1 whereas the results of experiments with non-isomorphic pairs of CFI graphs are presented in Table 2. In all the cases of both the graph families we observe that the feasible region is always zero-one reducible (i.e., $k = 1$). However, due to the large size of the linear program, we could only experiment with graphs of modest sizes. The results are encouraging if not conclusive.

Table 1

Class	Pair	No. of iterations of LP-GI	Class	Pair	No. of iterations of LP-GI	Class	Pair	No. of iterations of LP-GI
(16,6,2,2)	1-2	96	(29,14,6,7)	2-5	406	(37,18,8,9)	4-5	666
(25,12,5,6)	1-2	300	(29,14,6,7)	3-4	406	(40,12,2,4)	1-2	480
(25,12,5,6)	1-3	300	(29,14,6,7)	3-5	406	(40,12,2,4)	1-3	480
(25,12,5,6)	1-4	300	(29,14,6,7)	4-5	406	(40,12,2,4)	1-4	480
(25,12,5,6)	1-5	300	(35,18,9,9)	1-2	630	(40,12,2,4)	1-5	480
(25,12,5,6)	2-3	300	(35,18,9,9)	1-3	630	(40,12,2,4)	2-3	480
(25,12,5,6)	2-4	300	(35,18,9,9)	1-4	630	(40,12,2,4)	2-4	480
(25,12,5,6)	2-5	300	(35,18,9,9)	1-5	630	(40,12,2,4)	2-5	480
(25,12,5,6)	3-4	300	(35,18,9,9)	2-3	630	(40,12,2,4)	3-4	480
(25,12,5,6)	3-5	300	(35,18,9,9)	2-4	630	(40,12,2,4)	3-5	480
(25,12,5,6)	4-5	300	(35,18,9,9)	2-5	630	(40,12,2,4)	4-5	480
(26,10,3,4)	1-2	260	(35,18,9,9)	3-4	630	(45,12,3,3)	1-2	540
(26,10,3,4)	1-3	260	(35,18,9,9)	3-5	630	(45,12,3,3)	1-3	540
(26,10,3,4)	1-4	260	(35,18,9,9)	4-5	630	(45,12,3,3)	1-4	540
(26,10,3,4)	1-5	260	(36,14,4,6)	1-2	504	(45,12,3,3)	1-5	540
(26,10,3,4)	2-3	260	(36,14,4,6)	1-3	504	(45,12,3,3)	2-3	540
(26,10,3,4)	2-4	260	(36,14,4,6)	1-4	504	(45,12,3,3)	2-4	540
(26,10,3,4)	2-5	260	(36,14,4,6)	1-5	504	(45,12,3,3)	2-5	540
(26,10,3,4)	3-4	260	(36,14,4,6)	2-3	504	(45,12,3,3)	3-4	540
(26,10,3,4)	3-5	260	(36,14,4,6)	2-4	504	(45,12,3,3)	3-5	540
(26,10,3,4)	4-5	260	(36,14,4,6)	2-5	504	(45,12,3,3)	4-5	540
(28,12,6,4)	1-2	336	(36,14,4,6)	3-4	504	(50,21,8,9)	1-2	1050
(28,12,6,4)	1-3	336	(36,14,4,6)	3-5	504	(50,21,8,9)	1-3	1050
(28,12,6,4)	1-4	336	(36,14,4,6)	4-5	504	(50,21,8,9)	1-4	1050
(28,12,6,4)	2-3	336	(37,18,8,9)	1-2	666	(50,21,8,9)	1-5	1050
(28,12,6,4)	2-4	336	(37,18,8,9)	1-3	666	(50,21,8,9)	2-3	1050
(28,12,6,4)	3-4	336	(37,18,8,9)	1-4	666	(50,21,8,9)	2-4	1050
(29,14,6,7)	1-2	406	(37,18,8,9)	1-5	666	(50,21,8,9)	2-5	1050
(29,14,6,7)	1-3	406	(37,18,8,9)	2-3	666	(50,21,8,9)	3-4	1050
(29,14,6,7)	1-4	406	(37,18,8,9)	2-4	666	(50,21,8,9)	3-5	1050
(29,14,6,7)	1-5	406	(37,18,8,9)	2-5	666	(50,21,8,9)	4-5	1050
(29,14,6,7)	2-3	406	(37,18,8,9)	3-4	666			
(29,14,6,7)	2-4	406	(37,18,8,9)	3-5	666			

Table 1: Results of experiments with non-isomorphic strongly regular graphs from [41]. In all cases we observe that the feasible region is zero-one reducible.

Base Graph	CFI Construction	n	No. of iterations of LP-GI
2×2 cycle	factor-4	16	144
2×3 cycle	factor-4	24	408
2×4 cycle	factor-4	32	2592
3-dim cube	factor-4	32	2592
2×5 cycle	factor-4	40	8400
2×2 cycle	factor-10	40	1440
2×3 cycle	factor-7	42	1650
2×6 cycle	factor-4	48	20256
2×4 cycle	factor-7	56	13752
3-dim cube	factor-7	56	19184

Table 2: Results of experiments with non-isomorphic graph pairs that use the CFI construction. In all cases we observe that the feasible region is zero-one reducible.

9 Conclusions

In this paper we presented our attempt at tackling the Graph Isomorphism problem. In the process of finding a polynomial time solution to this problem we discovered the role of the Quadratic Assignment Problem (QAP)-polytope. We were successful in showing that a polynomial time solution exists under certain geometric constraints.

We conclude by describing a couple of open problems where we believe that the approach described in this paper can be useful.

9.1 Open Problems

9.1.1 GI belongs to co-NP?

It is easy to see that GI belongs to the class NP. To verify that two graphs are isomorphic, all we need is a permutation σ and verification takes $O(n^2)$ time. However, does a certificate exist that can be used to verify *quickly* (i.e., in poly-time) that the given graphs are non-isomorphic, remains an open problem.

In this paper we have seen that the feasible region of LP-GI, $\mathscr{P}_{G_1G_2}$, is sandwiched between the polytopes $\mathscr{P}$ and $\mathscr{B}^{[2]}$, for non-isomorphic graphs. So there exists a minimal set of facet defining inequalities of $\mathscr{B}^{[2]}$ that separates $\mathscr{P}_{G_1G_2}$ from $\mathscr{B}^{[2]}$. Adding these to LP-GI would make it infeasible. So our certificate for a given pair of non-isomorphic graphs G_1, G_2, is a description of these inequalities. Clearly, if we can show that the resulting linear program can be solved in polynomial time by the ellipsoid method, then we can establish that GI also belongs to the class co-NP.

Alternatively, we could use the fact that for non-isomorphic graphs $\mathscr{P}_{G_1G_2} \cap \mathscr{B}^{[2]} = \phi$. Since both $\mathscr{P}_{G_1G_2}$ and $\mathscr{B}^{[2]}$ are bounded convex regions in $\mathbb{R}^{n^2\times n^2}$, we have from the *Hyperplane Separation Theorem* a non-zero vector $a \in \mathbb{R}^{n^2\times n^2}$, a constant $b \in \mathbb{R}$ such that $a^T x > b, \forall x \in \mathscr{B}^{[2]}$ and $a^T x < b, \forall x \in \mathscr{P}_{G_1G_2}$. Given the values of a, b, we can use LP-GI to verify that $\mathscr{P}_{G_1G_2}$ lies on one side of the hyperplane $a^T x = b$. This step would take polynomial time as long as the values of a, b are not too large. However, we also need to verify that $\mathscr{B}^{[2]}$ lies on the other side of this hyperplane to be totally convinced that the given graphs are non-isomorphic. At this point it is not clear if this step could also be done in polynomial time.

9.1.2 The Graph Automorphism Problem

The graph automorphism problem is the problem of determining if a graph G has a non-trivial automorphism i.e., an isomorphism from the graph to itself other than the one given by the identity permutation. This problem is clearly in the complexity class NP. However, it is not known if the complementary problem is also in NP. In this case we need a certificate using which we can in poly-time say that the graph has only the trivial automorphism (or the graph is rigid). Observe that in the case of rigid graphs, the feasible region of LP-GI (with $G_1 = G_2 = G$), $\mathscr{P}_{GG}$, intersects $\mathscr{B}^{[2]}$ at only one point and that is the $P_\sigma^{[2]}$ corresponding to the identity permutation σ_I. Also, observe that by adding any one of the constraints $Y_{ii,jj} \leq 1-\varepsilon$ for $i < j$ and some $\varepsilon > 0$, to LP-GI, the feasible region totally disconnects from $\mathscr{B}^{[2]}$. So, again from the Hyperplane Separation Theorem, we have for every $i < j$, a non-zero vector $a_{ij} \in \mathbb{R}^{n^2 \times n^2}$, a constant $b_{ij} \in \mathbb{R}$ such that $a_{ij}^T x > b_{ij}, \forall\, x \in \mathscr{B}^{[2]}$ and $a_{ij}^T x < b_{ij}, \forall\, x \in \{\mathscr{P}_{GG} \cap (Y_{ii,jj} \leq 1-\varepsilon)\}$. So our problem reduces to that of verifying in polynomial time if in all the cases $i < j$, the feasible region $\mathscr{P}_{GG} \cap (Y_{ii,jj} \leq 1-\varepsilon)$ lies on the non-$\mathscr{B}^{[2]}$ side of the corresponding hyperplane.

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A Proofs of Theorems 7, 8 and 9

A.1 A Criterion for Facets

The following lemma gives a method to establish a facet.

Let X be a set of vectors in $\mathbb{R}^N$. Then $LS(X)$ denotes the subspace of $\mathbb{R}^N$ spanned by the vectors in X. Also, $ES(X)$ denotes the affine span of X, i.e., $\{\sum_{x\in X} a_x \cdot x | a_x \in \mathbb{R}, \sum_{x\in X} a_x = 1\}$.

Lemma 15 *Let V be the set of vertices of a polytope such that the affine span 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 $V \setminus S \neq \emptyset$. Also, let a vertex $v_0 \in V \setminus S$ be such that $V \subset LS(\{v_0\} \cup S)$. Then the affine plane of S defines a facet, i.e., $f(x) \geq 0$ defines a facet (intersection of $f(x) = 0$ plane with the affine plane of V is the facet plane).*

Proof Let $d = Dim(LS(V))$. Since the origin does not belong to $ES(V)$, $Dim(ES(V)) = d-1$. We are given that $V \subset LS(\{v_0\} \cup S)$. Hence $Dim(LS(S)) \geq d-1$. Again, origin does not belong to $ES(S)$, implying $Dim(ES(S)) \geq d-2$. Note that V is not contained in $ES(S)$ because $f(x) \neq 0\ \forall x \in V \setminus S$. So $Dim(ES(S)) < Dim(ES(V)) = d-1$. So we conclude that $Dim(ES(S)) = d-2$. Hence $ES(S)$ is a hyper-plane in the space defined by $ES(V)$. □

Corollary 6 *Let V and S are as defined in Lemma 15. Further, the origin does not belong to $ES(V)$. Let $G = (V \setminus S, E)$ be a graph with the property that $\{u, v\} \in E$ iff $u - v \in LS(S)$. If G is connected, then (i) S is a facet, (ii) points in $V \setminus S$ are co-planar. In particular, the plane is $f(x) = const$.*

Proof (i) Since G is connected, there exists a simple path in G between every pair of vertices. Let us fix an arbitrary vertex as v_0. Now consider any vertex u in $V(G) \setminus \{v_0\}$. There must exist a simple path between u and v_0 via some vertices $u_1, u_2, \ldots, u_k$. Since $\{u, u_1\}, \{u_1, u_2\}, \ldots, \{u_k, v_0\}$ are edges on this path and $u - v \in LS(S)$ for $\{u, v\} \in E$, we have $u - u_1, u_1 - u_2, \ldots, u_k - v_0 \in LS(S)$. So $u - v_0 \in LS(S)$ or $u \in LS(S \cup \{v_0\})$. Thus $V \subset LS(S \cup \{v_0\})$. The claim now follows from Lemma 15.

(ii) Let $u, v \in V \setminus S$. Since G is connected, there is a path $u_1, \ldots, u_k$ in G where $u = u_1$ and $v = u_k$. So we have $u - v \in LS(S)$ or $u - v = \sum_{v_j \in S} \alpha_j v_j$. So $f(u) - f(v) = f(u - v) = \sum_{v_j \in S} \alpha_j f(v_j) = 0$. □

We say that a permutation σ' is a transposition of another permutation σ (or that σ and σ' are transpositions of each other) if the images of the two permutations differ at two indices, i.e., if there are two distinct indices x, y such that $\sigma(x) = \sigma'(y), \sigma(y) = \sigma'(x)$ and $\sigma(z) = \sigma'(z)$ for all $z \in [n] \setminus \{x, y\}$.

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 $i = 1, \ldots, 6$. Following is a useful identity.

Lemma 16 *Let $\Sigma = \{\sigma_1, \ldots, \sigma_6, \sigma_1', \ldots, \sigma_6'\}$ be a set of permutations as defined above. Then $\forall\ i, j, k, l \in [n]$, $\sum_{\sigma \in \Sigma} sign(\sigma) P_\sigma^{[2]}(ij, kl) = 0$.*

Proof All we need to show is that $\forall\, i,j,k,l\ \sum_{\sigma\in\Sigma,\sigma(i)=j,\sigma(k)=l} sign(\sigma)=0$. So from the definition of σ_is we have $sign(\sigma_1)=sign(\sigma_4)=sign(\sigma_5)=-sign(\sigma_2)=-sign(\sigma_3)=-sign(\sigma_6)$. Also, $\forall i\ sign(\sigma_i)=-sign(\sigma_i')$ leading to $\sum_{\sigma\in\{\sigma_1,\ldots,\sigma_6\}} sign(\sigma)=0$ as well as $\sum_{\sigma\in\{\sigma_1',\ldots,\sigma_6'\}} sign(\sigma)=0$. Let us assume that $\sigma_i(x)=d$ and $\sigma_i(y)=e$. So, $\sigma_i'(x)=e$ and $\sigma_i'(y)=d$, for all $i\in\{1,\ldots,6\}$. We consider the following six cases.
Case (i). $i\in\{k_1,k_2,k_3\}$, $k\in\{x,y\}$: here the only interesting scenario is when $j\in\{a,b,c\}$ and $l\in\{d,e\}$ since otherwise none of the permutations in Σ would contribute anything to the sum. Now, depending on l we either get contributions from two permutations in $\{\sigma_1,\ldots,\sigma_6\}$ or we get contributions from two permutations in $\{\sigma_1',\ldots,\sigma_6'\}$. Moreover, these permutations must be transpositions of each other. W.l.o.g. let $i=k_1, j=a, k=x, l=d$. So the contributing permutations are σ_1,σ_2. Note that these are transpositions of each other.
Case (ii). $\{i,k\}\subset\{k_1,k_2,k_3\}$: here we get contributions from two permutations, one from σ_i, say σ_1 w.l.o.g. and the other σ_1'. Clearly these are transpositions of each other.
Case (iii). $\{i,k\}=\{x,y\}$: depending on j,l we have either contributions from $\{\sigma_1,\ldots,\sigma_6\}$ or contributions from $\{\sigma_1',\ldots,\sigma_6'\}$.
Case (iv). $i\in\{k_1,k_2,k_3\}$, $k\in[n]\setminus\{k_1,k_2,k_3,x,y\}$: we get contributions from two permutations from σ_i and the corresponding two permutations from σ_i'. Clearly their signs cancel each other.
Case (v). $i\in\{x,y\}$, $k\in[n]\setminus\{k_1,k_2,k_3,x,y\}$: depending on j we have either $\{\sigma_1,\ldots,\sigma_6\}$ contributing to the sum or $\{\sigma_1',\ldots,\sigma_6'\}$ contributing to the sum.
Case (vi). $\{i,k\}\cap\{k_1,k_2,k_3,x,y\}=\emptyset$: here we have all the twelve permutations contributing to the sum and hence their signs add up to zero. □

A.2 Facets Due to the Non-negativity Constraint

In this section V will denote the set of the vertices of $\mathscr{B}^{[2]}$, i.e., $\{P_\sigma^{[2]}|\sigma\in S_n\}$ and S will denote $\{P_\sigma^{[2]}|\ f(P_\sigma^{[2]})=0\}$.

Theorem 15 *The non-negativity constraint $Y_{ij,kl}\geq 0$, defines a facet of $\mathscr{B}^{[2]}$ 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 $P_\sigma^{[2]}$. 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 $E=\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}$ such that σ, σ' are transpositions of each other. 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 $P_{\sigma_1}^{[2]}$ and $P_{\sigma_1'}^{[2]}$ be a pair of matrices in $V\setminus S$ where σ and σ' are transpositions of each other. 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 16. Observe that all the $P_\sigma^{[2]}$s corresponding to these ten permutations belong to S. Hence we can express $P_{\sigma_1}^{[2]}-P_{\sigma_1'}^{[2]}$ in terms of vertices in S using the identity in Lemma 16. From Corollary 6 the inequality defines a facet. □

From Observations 6, 5 and Theorem 15 we have the following result.

Theorem 16 *All facet defining planes of $\mathscr{P}$ also define facets of $\mathscr{B}^{[2]}$ and all vertices of $\mathscr{B}^{[2]}$ are also vertices of $\mathscr{P}$. Besides, the dimensions of the two polytopes are the same (both are full dimensional polytopes in plane P).*

We will use the following lemma to show that the graph under consideration is connected, hence the name. This is required to prove that certain inequality defines a facet of $\mathscr{B}^{[2]}$, as shown in Corollary 6.

A.3 The Connection Lemma

Lemma 17 *(1) Let X be a set of vertices $P_\sigma^{[2]}$ 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 $[n]\setminus\{1,2,\ldots,a\}$ such that $|\cup_i I_i|\leq n-a-b$. Let $G=(X,E)$ be a graph in which $\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}\in E$ iff σ and σ' are transpositions of each other. Then G is connected.*

(2) Let X be a set of vertices $P_\sigma^{[2]}$ 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 $\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}\in E$ iff 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 $I\subseteq\{a+b+1,a+b+2,\ldots,n\}$. Hence the $P_\sigma^{[2]}$ corresponding to the identity permutation belongs to X.

Given any vertex $P_{\sigma_0}^{[2]}\in X$, we will show that there is a path from $P_{\sigma_0}^{[2]}$ to $P_{\sigma:\sigma(i)=i}^{[2]}$ in G. Starting from $P_{\sigma_0}^{[2]}$, suppose the path has been built up to $P_\sigma^{[2]}$ for some σ 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 $\sigma(j)\in\{a+1,\ldots,a+b\}$. Consider the permutation σ' which is the transposition of σ with respect to the indices i,j. $P_{\sigma'}^{[2]}$ is also in X and $\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}$ is an edge. Extend the path to $P_{\sigma'}^{[2]}$. 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 the indices in $a+b+1,\ldots,n$ 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 the vertices corresponding to the permutations generated in the process, all 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 $1\le i\le b$. So without loss of generality we can assume that $P_{\sigma:\sigma(i)=i}^{[2]}$ belongs to X. To prove the claim we will show that starting from any arbitrary vertex $P_{\sigma_0}^{[2]}\in X$ there is a path from $P_{\sigma_0}^{[2]}$ to $P_{\sigma:\sigma(i)=i}^{[2]}$. While tracing this path, the current permutation σ 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 either $a+k>a+b$ or $a+k\le a+b$ and $\sigma(a+i)\neq x_k$, then perform transposition on indices $a+i$ and $a+k$ resulting into the new permutation σ' that is "closer" to the identity and $P_{\sigma'}^{[2]}\in X$.

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, $P_{\sigma'}^{[2]}$ and $P_{\sigma''}^{[2]}$, belong to X. So the path extends by edges $\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}$ and $\{P_{\sigma'}^{[2]},P_{\sigma''}^{[2]}\}$. Further, σ'' is closer to the identity.

Thus the path eventually reaches the identity. □

A.4 A Polynomial Sized Family of Facets

Theorem 17 *Inequality $Y_{p_1q_1,kl}+Y_{p_2q_2,kl}+Y_{p_1q_2,kl}\le Y_{kl,kl}+Y_{p_1q_1,p_2q_2}$, defines a facet of $\mathscr{B}^{[2]}$, where p_1,p_2,k are distinct and q_1,q_2,l are also distinct and $n\ge 6$.*

Proof The set of vertices which satisfy the inequality strictly is the union of $X_1=\{P_\sigma^{[2]}|\sigma(p_1)=q_1,\sigma(p_2)=q_2,\sigma(k)\neq l\}$ and $X_2=\{P_\sigma^{[2]}|\sigma(p_1)\neq q_1,\ \sigma(p_1)\neq q_2,\ \sigma(p_2)\neq q_2,\ \sigma(k)=l\}$. 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 $\{P_\sigma^{[2]},P_{\sigma'}^{[2]}\}$ where σ is a transposition of σ'. From Lemma 17 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 $\{P_{\alpha_1}^{[2]},P_{\alpha_2}^{[2]}\}$ to G making the graph connected, where $P_{\alpha_1}^{[2]}$ is an arbitrary member of X_1 and α_2 is defined below. 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 $p_1\to a,p_2\to q_1,k\to l,i_2\to b,r\to q_2$. At all other indices the images of α_1 and α_2 coincide. Observe that $P_{\alpha_2}^{[2]}\in X_2$.

Now we will show that for each edge $\{P_{x'}^{[2]},P_{y'}^{[2]}\}$ of the graph, $P_{x'}^{[2]}-P_{y'}^{[2]}$ belongs to $LS(S)$. We begin with the edge $\{P_{\alpha_1}^{[2]},P_{\alpha_2}^{[2]}\}$. 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 16. 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 16 $P_{\alpha_1}^{[2]}-P_{\alpha_2}^{[2]}$ 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 $\{P_{\sigma_1}^{[2]},P_{\sigma'_1}^{[2]}\}$ 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

$k_2 = p_2$. Also, define k_3 as the index different from p_1, p_2, k, such that $\sigma_1(k_3) = \sigma_1'(k_3)$. Note that such an index must exist since $n \geq 6$. 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 16, $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma_1'} \in LS(S)$.

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 16 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: $x = p_2, y = r$; $x = \sigma_1^{-1}(q_1), y = \sigma_1^{-1}(q_2)$; 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 16. The remaining two cases are proved 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 since $n \geq 6$, the pair u, v always exists. Rest of the indices have the same images in the two permutations. To show that after dropping the edges 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 an edge of the third type. 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 graph after deleting both types of edges, 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. Note that $\{P^{[2]}_{\sigma}, P^{[2]}_{\alpha_1}\}$ is an edge of the first type. The remaining edges $\{P^{[2]}_{\alpha_1}, P^{[2]}_{\alpha_2}\}$ and $\{P^{[2]}_{\alpha_2}, P^{[2]}_{\sigma'}\}$ are covered in Case (2).

Case (2) Subcase $\{p_1, p_2, r = \sigma^{-1}(q_2)\} \cap \{x, y\} = \emptyset$: In this case define $k_1 = p_1, k_2 = p_2, k_3 = r$. See that $\sigma_2, \ldots, \sigma_6$ and $\sigma_2', \ldots, \sigma_6'$ belong to S.

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 16 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. □

A.5 An Exponential Sized Family of Facets

Consider the following inequality

$$Y_{i_1 j_1, kl} + Y_{i_2 j_2, kl} + \ldots + Y_{i_m j_m, kl} \leq Y_{kl, kl} + \sum_{r<s} Y_{i_r j_r, i_s j_s} \tag{17}$$

where $n \geq 6, 3 \leq m \leq n-3$, indices $i_1, \ldots, i_m, k$ are distinct and $j_1, \ldots, j_m, l$ are also distinct. In the rest of this section we will show that inequality (17) also defines a facet of $\mathscr{B}^{[2]}$.

We will continue to use S to denote the set of vertices of $\mathscr{B}^{[2]}$ for which the given inequality is tight. Let T denote the set of remaining vertices. 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 18 *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 established from Lemma 17(2).

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 16. Vertices corresponding to each of these permutations belong to S. Hence from Lemma 16, $P^{[2]}_{\sigma_1} - P^{[2]}_{\sigma'_1} \in LS(S)$. □

Corollary 7 *Given any $P^{[2]}_{\sigma*}$ in T_1, each $P^{[2]}_{\sigma}$ in T_1 belongs to $LS(\{P^{[2]}_{\sigma*}\} \cup S)$.*

Lemma 19 *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. 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 16 $P^{[2]}_{\sigma_1} \in LS(T_1 \cup S)$.

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 $LS(T_1 \cup S)$. □

Lemma 20 *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 19.

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 19, $P^{[2]}_{\sigma} \in LS(S \cup T_1)$. □

Lemma 21 *Let $n \geq 6$. Given any $P^{[2]}_{\sigma}$ in $T_{3,r}$ with $r > 2$, it can be expressed as a linear combination of elements in $T_1 \cup S$.*

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 19 as the base case, Lemma 16 gives that $P^{[2]}_{\sigma_1} \in LS(T_1 \cup S)$. □

Similarly the following lemma can also be proved.

Lemma 22 *Let $n \geq 6$. Given any $P^{[2]}_{\sigma}$ in $T_{2,r}$ with $r > 3$, it can be expressed as a linear combination of elements in $T_1 \cup S$.*

Lemmas 19-22 lead to the following corollary.

Corollary 8 *If $n \geq 6$, then $T_2 \cup T_3 \subset LS(T_1 \cup S)$.*

Theorem 18 *If $n \geq 6$, then inequality (17) defines a facet of $\mathscr{B}^{[2]}$.*

Proof From corollaries 7 and 8 every vertex in T can be expressed as a linear combination of a fixed vertex in T and the vertices in S. Now the result follows from Lemma 15. □