A Geometric Approach to Graph Isomorphism

Pawan Aurora and Shashank K Mehta

Indian Institute of Technology, Kanpur - 208016, India
{paurora,skmehta}@cse.iitk.ac.in

Abstract. We present an integer linear program (IP), for the Graph Isomorphism (GI) problem, which has non-empty feasible solution if and only if the input pair of graphs are isomorphic. We study the polytope of the convex hull of the solution points of IP, denoted by $\mathcal{B}^{[2]}$. Exponentially many facets of this polytope are known. We show that in case of non-isomorphic pairs of graphs if a feasible solution exists for the linear program relaxation (LP) of the IP, then it violates a unique facet of $\mathcal{B}^{[2]}$. We present an algorithm for GI based on the solution of LP and prove that it detects non-isomorphism in polynomial time if the solution of the LP violates any of the known facets.

Keywords: Graph Isomorphism Problem • Linear Programming • Polyhedral Combinatorics

1 Introduction

The graph isomorphism problem (GI) is a well-studied computational problem: Formally, given two graphs G_1 and G_2 on n vertices, decide 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. Without loss of generality, we assume that the vertices in both the graphs are labelled by integers $1, \ldots, n$. Hence $V(G_1) = V(G_2) = [n]$ and each bijection is a permutation of $1, \ldots, n$. It remains one of the few problems that are unlikely to be NP-complete [1] and for which no polynomial time algorithm is known. The fastest known graph isomorphism algorithm for general graphs has running time $2^{O(\sqrt{n \log n})}$ [4].

Several approaches to solve GI have been adopted. Most prominent of these has been the one that finds a canonical labeling of the vertices of the two graphs [3],[5]. For a comprehensive list of all the approaches there are some survey papers on the works published on this problem, such as [6].

Another problem of interest in the present context is Quadratic Assignment Problem (QAP) [8]. The QAP polytope is defined as the convex hull of all the feasible solutions to its linear formulation [9]. The polyhedral combinatorics of this polytope was studied by Volker Kaibel in his PhD thesis [7]. In the thesis he identifies a class of facets of this polytope and the dimension of its affine plane.

In this work we derive an integer linear program for graph isomorphism. Each (integer) solution of this program corresponds to one permutation. The convex hull of these points is denoted by $\mathcal{B}^{[2]}$ when both graphs are $([n], \emptyset)$. The polytope of the corresponding linear program (LP) is denoted by $\mathcal{P}$. We show that each maximally connected region of $\mathcal{P} \setminus \mathcal{B}^{[2]}$ is separated from $\mathcal{B}^{[2]}$ by only one facet. Hence in case of non-isomorphic graph pairs if the linear program is feasible, then the solutions violate exactly one facet of $\mathcal{B}^{[2]}$. Several facets of $\mathcal{B}^{[2]}$ are already known and many new facets are identified in this paper.

We describe an algorithm which is based on the linear program. We show that if the linear program gives a feasible solution for non-isomorphic pair, then the algorithm correctly detects in polynomial time that the pair is non-isomorphic if the solution is separated from $\mathcal{B}^{[2]}$ by any of the described facets. We also show that there must be several additional facets of $\mathcal{B}^{[2]}$ which are yet to be discovered. This is the reason that we cannot yet claim that this algorithm solves the graph isomorphism problem in polynomial time.

2 Integer Linear Program for GI

Define a second-order permutation matrix $P_\sigma^{[2]}$ corresponding to a permutation σ as $(P_\sigma^{[2]})_{ij,kl} = (P_\sigma)_{ij}(P_\sigma)_{kl}$. We call the convex hull of the second-order permutation matrices, the *second-order Birkhoff polytope* $\mathcal{B}^{[2]}$. In [10] a completely positive formulation of *Quadratic Assignment Problem* (QAP) is given. The feasible region of this program is precisely $\mathcal{B}^{[2]}$, see theorem 3 in [10].

Let $\mathcal{B}^{[2]}_{G_1G_2}$ denote the convex hull of the $P_\sigma^{[2]}$ where σ are the isomorphisms between G_1 and G_2. If the graphs are non-isomorphic, then $\mathcal{B}^{[2]}_{G_1G_2} = \emptyset$. Clearly $\mathcal{B}^{[2]} = \mathcal{B}^{[2]}_{G_1G_2}$ when $G_1 = G_2 = ([n], \emptyset)$ or $G_1 = G_2 = K_n$.

Observation 1 *Given a pair of graphs, there exists a linear program (probably with exponentially many conditions) such that the feasible region of the program ($\mathcal{B}^{[2]}_{G_1G_2}$) is non-empty if and only if the graphs are isomorphic.*

Next we will develop an integer linear program such that the convex hull of its feasible points is $\mathcal{B}^{[2]}_{G_1G_2}$. It is easy to verify that for every permutation σ, $Y = P_\sigma^{[2]}$ satisfies equations 1a-1d.

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

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

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

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

Lemma 1. *The solution plane, P, of equations 1a-1d is the affine plane spanned by $P_\sigma^{[2]}$'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 $n!/(2(n-4)!) + (n-1)^2 + 1$.

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

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

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

In [7] it is shown that the dimension of $\mathcal{B}^{[2]}$ polytope is $\frac{n!}{2(n-4)!} + (n-1)^2 + 1$. This claim along with the result of the previous paragraph leads to the conclusion that equations 1a-1d define the affine plane spanned by the $P_\sigma^{[2]}$s. □

Corollary 1. *$\mathcal{B}^{[2]}$ is a full dimensional polytope in P.*

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

Proof. Let Y be a $0/1$ solution of the above system of linear equations. 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 $Y_{ij,ij} = (P_\sigma)_{ij}$.

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

Equations 1a and 1b describe the remaining entries. □

Let $G_1 = ([n], E_1)$ and $G_2 = ([n], E_2)$ be simple graphs on n vertices each. Define a graph $G = (V, E)$, where $V = [n] \times [n]$ and $\{ij, kl\} \in E$ if either $\{i, k\} \in E_1$ and $\{j, l\} \in E_2$ or $\{i, k\} \notin E_1$ and $\{j, l\} \notin E_2$.

Corollary 2. *The only 0/1 solutions of equations 1a-1d and $Y_{ij,kl} = 0$ $\{ij, kl\} \notin E$, are the $P_\sigma^{[2]}$ where σ are the isomorphisms between G_1 and G_2.*

Corollary 2 gives the following integer program for GI.

$$\begin{aligned}
\text{IP-GI:} \quad & \text{Find a point} \quad Y && \\
& \text{subject to} \quad 1a\text{-}1d && \text{(2a)}\\
& Y_{ij,kl} = 0 \quad , \{ij, kl\} \notin E && \text{(2b)}\\
& Y_{ij,kl} \in \{0,1\} \ , \forall\, i,j,k,l &&
\end{aligned}$$

Note This is a feasibility formulation of GI. To formulate an optimization program for GI, replace the conditions 1d by $\sum_i Y_{ij,ij} \leq 1$ and $\sum_j Y_{ij,ij} \leq 1$, and set the objective function to be $\sum_{i,j} Y_{ij,ij}$. The solutions of IP-GI coincide with those solutions of the optimization version where the objective function evaluates to n.

The LP relaxation, LP-GI, is IP-GI with relaxed conditions on the variables. Here we only require that $Y_{ij,kl} \geq 0$ for all i,j,k,l. The condition $Y_{ij,kl} \leq 1$ is implicit for all i,j,k,l. Let $\mathcal{P}_{G_1G_2}$ denote the feasible region of LP-GI. So $\mathcal{B}^{[2]}_{G_1G_2} \subseteq \mathcal{P}_{G_1G_2}$. Define $\mathcal{P} = \mathcal{P}_{G_1G_2}$ where $G_1 = G_2 = ([n], \emptyset)$ or $G_1 = G_2 = K_n$. $\mathcal{P}$ is contained in the unit-cube $\{0,1\}^{n^2 \times n^2}$, so it is a polytope. It is also contained in the plane P, hence it too is a full-dimensional polytope in that plane.

The following observations are in order.

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

Observation 3 *The complete set of facets of $\mathcal{P}$ is $Y_{ij,kl} = 0\, \forall i \neq k\, \forall j \neq l$.*

Observation 4 *Vertices of $\mathcal{B}^{[2]}$ (i.e., $P^{[2]}_\sigma$) are a subset of the vertices of $\mathcal{P}$.*

3 Facial Structure of $\mathcal{B}^{[2]}$

The feasible region of LP-GI for an isomorphic graph pair, G_1, G_2, will always contain at least one point from $\mathcal{B}^{[2]}_{G_1G_2}$. In case of non-isomorphic pair, either the feasible region will be empty or it will be confined to $\mathcal{P} \backslash \mathcal{B}^{[2]}$. While such solutions satisfy the non-negativity conditions, they occur on the wrong side of some of the facets of $\mathcal{B}^{[2]}$. We cannot include the corresponding inequalities into the linear program (even if we know them) and get an exact program for GI because they are exponentially large in number. It is easy to devise an algorithm for GI based on the present LP. Our goal is to identify the facets of $\mathcal{B}^{[2]}$ and using the corresponding inequalities prove that this algorithm will take only polynomial time to detect that the entire LP feasible region is outside $\mathcal{B}^{[2]}$. Hence our first task is to identify all the $\mathcal{B}^{[2]}$ facets. Exponentially many of these facets are already identified in the literature and we will identify exponentially many new facets.

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 that facet. All the known facets of $\mathcal{B}^{[2]}$ are special instances of a 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).

The first set of facets are the instances of this inequality 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 $\beta = 1$.

Theorem 5. *$Y_{i_0 j_0, k_0 l_0} \geq 0$ defines a facet of $\mathcal{B}^{[2]}$ 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 proven in [7].

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 set of indices. Similarly q_1, q_2, l are also any set of distinct indices.

Theorem 6. *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 $\mathcal{B}^{[2]}$, 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 $n_{ij} = 0$.

Theorem 7. *Inequality $Y_{i_1 j_1, kl} + Y_{i_2 j_2, kl} + \ldots + Y_{i_m j_m, kl} \leq Y_{kl,kl} + \sum_{r \neq s} Y_{i_r j_r, i_s j_s}$, defines a facet of $\mathcal{B}^{[2]}$, where $i_1, \ldots, i_m, k$ are all distinct and $j_1, \ldots, j_m, l$ are also distinct. In addition, $n \geq 6, m \geq 3$.*

Theorems 6,7 appear with proof in [2] as Theorems 10,17 respectively.

The next two sets of facets are established in [7]. 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 8. *[7, Definition 8.5] Following inequality defines a facet of $\mathcal{B}^{[2]}$*
$(\beta - 1) \sum_{(ij) \in P_1 \times Q_2} Y_{ij,ij} \leq \sum_{(ij) \neq (kl) \in P_1 \times Q_2, i<k} Y_{ij,kl} + (1/2)(\beta^2 - \beta)$
when $\beta + 1 \leq |P_1|, |Q_2| \leq n - 3$;$|P_1| + |Q_2| \leq n - 3 + \beta$; $\beta \geq 2$.

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

Theorem 9. *[7, Definition 8.6] Following inequality defines a facet of $\mathcal{B}^{[2]}$*
$-(\beta - 1) \sum_{(ij) \in P_1 \times Q_2} Y_{ij,ij} + \beta \sum_{(ij) \in P_2 \times Q_2} Y_{ij,ij} + \sum_{(ij) \neq (kl) \in P_2 \times Q_2, i<k} Y_{ij,kl} + \sum_{(ij) \neq (kl) \in P_1 \times Q_2, i<k} Y_{ij,kl} - \sum_{(ij) \in P_1 \times Q_2, (kl) \in P_2 \times Q_2} Y_{ij,kl} + (1/2)(\beta^2 - \beta) \geq 0$
where the conditions on the parameters are as given in [7, Definition 8.6].

From Observations 3, 4 and Theorem 5 we have the following result.

Theorem 10. *All facet defining planes of $\mathcal{P}$ also define facets of $\mathcal{B}^{[2]}$ and all vertices of $\mathcal{B}^{[2]}$ are also vertices of $\mathcal{P}$. Besides, the dimensions of the two polytopes are same (both are full dimensional polytopes in plane P).*

Let the sets of vertices and the facet planes of $\mathcal{B}^{[2]}$ be denoted by $V(\mathcal{B}^{[2]})$ and $F(\mathcal{B}^{[2]})$ respectively. Similarly denote the respective sets for $\mathcal{P}$.

Since $V(\mathcal{B}^{[2]}) \subset V(\mathcal{P})$, $\mathcal{B}^{[2]}$ is contained in $\mathcal{P}$. $F(\mathcal{P})$ is a subset of $F(\mathcal{B}^{[2]})$ and these facet planes are $Y_{ij,kl} = 0$ planes so we refer to them as *zero-planes* and the corresponding facets as *trivial facets* of $\mathcal{B}^{[2]}$. Each facet $X \in F(\mathcal{B}^{[2]}) \setminus F(\mathcal{P})$ partitions $\mathcal{P}$ into two parts because the two polytopes are of the same dimension. One part contains $\mathcal{B}^{[2]}$. We will refer to the other part of $\mathcal{P}$ by a *pocket*. Note that the points on the facet X do not belong to the pocket. The non-$P_\sigma^{[2]}$ vertices of $\mathcal{P}$ do not belong to X since it is a facet of $\mathcal{B}^{[2]}$ and it is the convex-hull of the $P_\sigma^{[2]}$s belonging to it. Clearly only non-$P_\sigma^{[2]}$ vertices must occur in the pockets. In the following lemma we will show that these pockets do not overlap, hence each vertex of $V(\mathcal{P}) \setminus V(\mathcal{B}^{[2]})$ belongs to a unique pocket.

Lemma 3. *All pockets are disjoint.*

Proof. Polytope $\mathcal{P}$ is the intersection of half spaces $(Y_{ij,kl} \geq 0) \cap P$ in the underlying space P. Let I be the index set such that P is contained in the plane $Y_{pq,rs} = 0$ for all $(pq, rs) \in I$. Hence a point $Z \in P$ belongs to the interior of $\mathcal{P}$ if and only if $Z_{ij,kl} > 0$ for all $(ij, kl) \notin I$. Each pocket K is bounded by some zero planes, $(Y_{ij,kl} = 0) \cap P$, and one facet plane $X \in F(\mathcal{B}^{[2]}) \setminus F(\mathcal{P})$. So all pockets are full dimensional in P. By definition the points of X do not belong to K. Let $\tilde{K}$ denote the interior of pocket K, which is a subset of the interior of $\mathcal{P}$.

Let K_1 and K_2 be two distinct pockets which are separated from $\mathcal{B}^{[2]}$ by facet planes X_1 and X_2 respectively.

Let $Z \in K_1 \cap K_2$. Assume that $Z \notin \tilde{K_2}$ but belongs to $\tilde{K_1}$. Then Z is a point on a face of K_2 which is in the intersection of some zero planes. Let $B(Z, \epsilon)$ be an infinitesimally small ball in P centered at Z with radius ϵ. For small enough radius $B(Z, \epsilon) \subset \tilde{K_1}$. This is absurd because Z being on the intersection of some zero planes, there is a point in the ball which has at least one coordinate negative, which is not possible in the interior of K_1. Hence any zero plane bounding one pocket does not intersect the interior of the other pocket. We also know that $X_1 \cap K_2 = X_2 \cap K_1 = \emptyset$. Hence the interior of either pocket contains no bounding point of the other pocket.

Above argument shows that either $\tilde{K_1} = \tilde{K_2}$ or $\tilde{K_1} \cap \tilde{K_2} = \emptyset$. The former implies $K_1 = K_2$, which is not true. We deduce that the interiors of the pockets are disjoint.

Then the point Z must belong to a face in each pocket. These faces must be due to the intersection of some of the zero planes in P. Once again consider a ball $B(Z, \epsilon)$ in P. Let $B'(Z, \epsilon)$ denote the subset of the ball where all the non-I coordinates are positive. Then for a small enough ϵ, $B'(Z, \epsilon)$ must belong to the interior of $\tilde{K_1}$ as well as of $\tilde{K_2}$. This implies that $\tilde{K_1} \cap \tilde{K_2} \neq \emptyset$. But that is not true as shown in the previous paragraph. So we conclude that $K_1 \cap K_2$ must be empty. □

Corollary 3. *Each pocket is a maximal connected region of $\mathcal{P} \setminus \mathcal{B}^{[2]}$. And there is a one to one correspondence between facets of $F(\mathcal{B}^{[2]}) \setminus F(\mathcal{P})$ and the pockets.*

Each vertex of $V(\mathcal{P}) \setminus V(\mathcal{B}^{[2]})$ belongs to a unique pocket. So we have the following combinatorial result.

Corollary 4. $|F(\mathcal{B}^{[2]}) \setminus F(\mathcal{P})| \leq |V(\mathcal{P}) \setminus V(\mathcal{B}^{[2]})|$.

Lemma 4. *The feasible region of LP-GI for non-isomorphic graphs, if non-empty, lies entirely in a unique pocket.*

Proof. Let the feasible region span multiple pockets. Let these include the pocket of the non-trivial facet X_1. By the definition of the feasible region, it cannot cross the boundary of $\mathcal{P}$ hence it must cross X_1 to enter another pocket. But X_1 is a part of $\mathcal{B}^{[2]}$ so the feasible region contains at least one point of $\mathcal{B}^{[2]}$. This implies that the graphs are isomorphic, falsifying the assumption. □

Corollary 5. *Every point in the feasible region of LP-GI for non-isomorphic graphs violates only one of the non-trivial facets of* $\mathcal{B}^{[2]}$.

3.1 There are more Facets

All the known facets of $\mathcal{B}^{[2]}$ are instances of a general inequality $\sum_{i,j,k,l} n_{ij}n_{kl}$ $Y_{ij,kl} + (\beta - 1/2)^2 \geq (2\beta - 1)\sum_{ij} n_{ij}Y_{ij,ij} + 1/4$. It is possible that there are more instances of this inequality which are also facets. Could there be facets of this polytope which are not the instances of this inequality. The answer to this question is in the affirmative. In [2, Section 5] we prove this claim.

In the following section we will show that a simple algorithm can be devised using LP-GI which can detect non-isomorphism in polynomial time, whenever the solution of a non-isomorphic pair belongs to a pocket corresponding to one of the facets described in this section. Hence it is essential to identify the remaining facets to determine how effective this algorithm is.

4 The Algorithm

We have seen that the feasible region of the linear program LP-GI strictly contains $\mathcal{B}^{[2]}_{G_1G_2}$. Therefore if the feasible region of LP-GI is empty, then we can conclude that the graphs are non-isomorphic. But no conclusion can be derived in case LP-GI has a solution. In this section we propose an exact algorithm for graph isomorphism and show that if the solution is confined to any pocket which corresponds to any known facet (discussed in the previous section), then the time complexity of the algorithm is polynomial.

Let E denote the set of equations (2a-2b) and some additional equations of the form $Y_{ij,kl} = 0$ or $Y_{ij,kl} = 1$. Let U denote the set of *live* variables which are not yet set to a fixed value (0 or 1) in E. Let $LP(E,U)$ denote the linear program involving the equations E and inequalities $Y_{ij,kl} \geq 0$ for each $Y_{ijkl} \in U$. Let $SearchVar(E,U)$ be a subroutine which takes one variable Y_{ijkl} from U at a time and finds if the linear program is infeasible on setting this variable to 0 (then returns $(Y_{ij,kl}, 0)$) or on setting it to 1 (then returns $(Y_{ij,kl}, 1)$). If the program is feasible for each assignment of each variable, then it returns $(null, -1)$.

Initially E_0 denotes the system of equations (2a-2b) and U_0 is the set of variables which are live with respect to equations (2a-2b). The main algorithm $GISolver$ given in Algorithm 1 is called with parameters E_0 and U_0.

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

Algorithm 1: Algorithm for GI

If we view the space searched by GISolver as a tree with (E_0, U_0) as the root, then those nodes, (E, U), have two children where $SearchVar(E, U)$ returns $(null, -1)$. Call them split nodes. All other internal nodes have one child. Let there be at 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.

4.1 Algorithm 1 is polynomial time for Pockets of the known facets

In this subsection we will show that if the feasible region of the linear program for a non-isomorphic pair is confined to a pocket corresponding to any of the known facets, then the algorithm will detect it in polynomial time. We will show that in these cases no split nodes will occur in the search-tree generated by the algorithm and hence τ will be zero.

Lemma 5. *$\tau = 0$ when the feasible region lies in a pocket defined by any facet in Theorem 7 with $m > 3$.*

Proof. Suppose the solution of a non-isomorphic pair is contained in the pocket of $\sum_{r\in[m]} Y_{i_rj_r,kl} \leq Y_{kl,kl} + \sum_{r<s\in[m]} Y_{i_rj_r,i_s,j_s}$, then the solutions will satisfy $\sum_{r=1}^{m} Y_{i_rj_r,kl} > Y_{kl,kl} + \sum_{r<s} Y_{i_rj_r,i_s,j_s}$. From Corollary 5, the solutions cannot violate any other facet. Let a be an arbitrary element of $[m]$ and define $S = [m]\setminus\{a\}$. Then we have a facet due to $\sum_{r\in S} Y_{i_rj_r,kl} \leq Y_{kl,kl} + \sum_{r<s\in S} Y_{i_rj_r,i_s,j_s}$ which must be satisfied by the solutions. 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 when $Y_{i_aj_a,kl}$ will be set to zero in the algorithm, the linear program will declare it infeasible. Hence $Y_{i_aj_a,kl}$ will be set to 1. Since a is any arbitrary index, eventually $Y_{i_aj_a,kl}$ will be set to 1 for each $a \in [m]$. 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 $m \geq 4$. □

Lemma 6. *$\tau = 0$ when the feasible region lies in a pocket defined by any facet in Theorem 8 with $|P| > \beta + 1$ or $|Q| > \beta + 1$.*

Proof. Assume that the inequality $(\beta-1)\sum_{(ij)\in P\times Q} Y_{ij,ij} \leq \sum_{(ij)\neq(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2-\beta)$ is violated and $|P| > \beta + 1$. We have

$$(\beta-1)\sum_{(ij)\in P\times Q} Y_{ij,ij} > \sum_{(ij)\neq(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2-\beta) \qquad (4)$$

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 $Y_{i_0j_0,i_0j_0}$ to 1. Since P' and Q both have at least $\beta + 1$ elements, the solution must satisfy the inequality

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

(4) minus (5) gives $(\beta-1)\sum_{j\in Q} Y_{i_0j,i_0j} > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl}$.

Since $Y_{i_0j_0,i_0j_0} = 1$ where $j_0 \notin Q$, $\sum_{j\in Q} Y_{i_0j,i_0j} = 0$. The non-negativity condition implies that the right-hand-side is non-negative so we conclude that $0 > 0$. As $Y_{i_0j_0,i_0j_0} = 1$ renders the problem infeasible, the algorithm will set $Y_{i_0j,i_0j} = 0$ 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 $j \notin Q$.

Next consider an arbitrary $(i_0j_0) \in P\times Q$. Suppose algorithm sets $Y_{i_0j_0,i_0j_0} = 1$. Let $P' = P \setminus \{i_0\}$. Then the violated inequality (4) reduces to $(\beta-1)(1 + \sum_{(ij)\in P'\times Q} Y_{ij,ij}) > \sum_{(ij)\neq(kl)\in P'\times Q, i<k} Y_{ij,kl} + \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl} + \frac{\beta^2-\beta}{2}$.

Subtracting (5) from the above inequality gives $(\beta-1) > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl}$. Since $Y_{i_0j,kl} = 0$ for all $j \neq j_0$, $\sum_{j\notin Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl} = 0$. Adding this term to the right hand side of the inequality we get $(\beta-1) > \sum_{j\in[n]}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl} = \sum_{(kl)\in P'\times Q} Y_{kl,kl}$. From the first part of the proof, $Y_{kl,kl} = 0$ for any $k \in P$ and $l \notin Q$. So we have $\sum_{(kl)\in P'\times Q} Y_{kl,kl} = |P'| > \beta+1-1 = \beta$. It reduces to infeasible $\beta - 1 > \beta$, which leads the algorithm to set $Y_{i_0j_0,i_0j_0} = 0$. Hence eventually $Y_{ij,ij}$ is set to zero for all $(ij) \in P \times Q$. 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 algorithm will report non-isomorphic pair. □

Lemma 7. $\tau = 0$ *when the feasible region lies in a pocket defined by any facet in Theorem 8 with* $|P| = |Q| = \beta + 1$ *and* $\beta > 2$.

Proof. The violation of $(\beta - 1)\sum_{(ij)\in P\times Q} Y_{ij,ij} \le \sum_{(ij)\neq(kl)\in P\times Q, i<k} Y_{ij,kl} + (1/2)(\beta^2 - \beta)$ gives inequality (4), given in the last proof.

Let $i_0 \in P$ and $P' = P \setminus \{i_0\}$. Then the solution must satisfy the facet with parameters $P', Q, \beta - 1$. So we have

$$(\beta-2)\sum_{(ij)\in P'\times Q} Y_{ij,ij} \le \sum_{(ij)\neq(kl)\in P'\times Q, i<k} Y_{ij,kl} + (1/2)((\beta-1)^2 - (\beta-1)) \quad (6)$$

(4) minus (6) gives

$$\sum_{(ij)\in P'\times Q} Y_{ij,ij} + (\beta-1)\sum_{j\in Q} Y_{i_0j,i_0j} > \sum_{j\in Q}\sum_{(kl)\in P'\times Q} Y_{i_0j,kl} + (\beta-1). \quad (7)$$

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 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 $(ij) \in P \times Q$. This will make (4) infeasible and the algorithm will report that the graphs are non-isomorphic. □

Lemmas 6 and 7 lead to the following corollary.

Corollary 6. $\tau = 0$ *if the solution for a non-isomorphic pair is confined to a pocket defined by one of the facets given in Theorem 8 except when* $\beta = 2$ *and* $|P| = |Q| = 3$.

Lemma 5 and Corollary 6 imply that by adding additional inequalities corresponding to the base cases of facets in Theorems 7 and 8 to the constraints of LP-GI we can detect non-isomorphic graph pairs if their solution falls in any pocket defined by the facets given in Theorems 7 and 8. Moreover the facets in Theorem 6 can all be added to LP-GI. The additional inequalities will be polynomial in number ($O(n^8)$), hence the modified LP-GI can be solved in polynomial time. Note that the facets given in Theorem 5 are already part of LP-GI.

Lemma 8. $\tau = 0$ *when the feasible region lies in a pocket defined by any facet in Theorem 9 subject to restrictions: (i)* $|P_1|, |P_2| \ge 3$*, (ii) if* $\beta \ge 0$ *and* $\min\{|Q|, |P_1|\} \ge \beta + 1$ *then* $|Q| + |P_1| + 3 \le n + \beta$*, (iii) if* $\beta < 0$ *and* $\min\{|Q|, |P_2|\} \ge 2 - \beta$ *then* $|Q| + |P_2| + 3 \le n + 1 - \beta$.

Proof. Given that a 2-box facet (P_1, P_2, Q, β) is violated by the solution face, every solution point satisfies

$$\begin{aligned} &-(\beta-1)\sum_{(ij)\in P_1\times Q} Y_{ij,ij} + \beta \sum_{(ij)\in P_2\times Q} Y_{ij,ij} + \sum_{(ij)\neq(kl)\in P_1\times Q, i<k} Y_{ij,kl} \\ &+ \sum_{(ij)\neq(kl)\in P_2\times Q, i<k} Y_{ij,kl} - \sum_{(ij)\in P_1\times Q, (kl)\in P_2\times Q} Y_{ij,kl} + \frac{\beta^2-\beta}{2} < 0. \end{aligned} \tag{8}$$

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 all the solutions must satisfy the inequality corresponding to the 2-box facet of (P'_1, P'_2, Q, β). We have

$$\begin{aligned} &-(\beta-1)\sum_{(ij)\in P'_1\times Q} Y_{ij,ij} + \beta \sum_{(ij)\in P'_2\times Q} Y_{ij,ij} + \sum_{(ij)\neq(kl)\in P'_1\times Q, i<k} Y_{ij,kl} \\ &+ \sum_{(ij)\neq(kl)\in P'_2\times Q, i<k} Y_{ij,kl} - \sum_{(ij)\in P'_1\times Q, (kl)\in P'_2\times Q} Y_{ij,kl} + \frac{\beta^2-\beta}{2} \geq 0. \end{aligned} \tag{9}$$

Case 1: In the algorithm when $Y_{i_0 j_0, i'_0 j'_0}$ is set to 1, where $j_0, j'_0 \in Q, j_0 \neq j'_0$, (8) minus (9) gives $0 < 0$ which is absurd. Hence algorithm will set $Y_{ij,i'j'} = 0$ for all $i \in P_1, i' \in P_2, j, j' \in Q$.

Case 2: When the algorithm sets $Y_{i_0 j_0, i'_0 j'_0} = 1$, where $j_0 \notin Q, j'_0 \in Q$. Then (8) minus (9) gives $\beta + \sum_{(i,j)\in P'_2\times Q} Y_{ij,ij} < 0$, where we used the result of the previous case. Note that it is impossible if $\beta \geq 0$.

Case 3: When the algorithm sets $Y_{i_0 l_0, i'_0 l'_0} = 1$, where $l_0 \in Q, l'_0 \notin Q$. Then (8) minus (9) gives $-(\beta-1) + \sum_{(i,j)\in P'_1\times Q} Y_{ij,ij} < 0$, which is impossible if $\beta < 0$.

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 $ij \in P_1 \times Q$.

Plugging these values in inequality (8) we have following simplified cases

$$\beta < 0 : \beta \sum_{(ij)\in P_2\times Q} Y_{ij,ij} + \sum_{(ij)\neq(kl)\in P_2\times Q, i<k} Y_{ij,kl} + \frac{\beta^2-\beta}{2} < 0. \tag{10}$$

$$\beta \geq 0 : -(\beta-1) \sum_{(ij)\in P_1\times Q} Y_{ij,ij} + \sum_{(ij)\neq(kl)\in P_1\times Q, i<k} Y_{ij,kl} + \frac{\beta^2-\beta}{2} < 0. \tag{11}$$

In the remainder we will prove that neither of these inequalities can be satisfied by the solution of the linear program in the subsequent phase of the algorithm. Hence, at this stage, the algorithm will find no solution and conclude that the graphs are non-isomorphic.

We will first consider inequality (11). If $\beta \leq 1$ then clearly (11) is violated. So assume that $\beta \geq 2$. Next if $|P_1|, |Q| \geq \beta + 1$, then (11) implies that the 1-box facet corresponding to (P_1, Q, β) is violated. But that is impossible since the solution can violate at most one non-trivial facet. That leaves us the case when $\min\{|P_1|, |Q|\} \leq \beta$.

First assume that $|P_1| \leq |Q|$. Consider the identity $\sum_{ij \neq kl \in P_1 \times Q, i<k} Y_{ij,kl} = |P_1|(|P_1|-1)/2 + \sum_{ij \neq kl \in P \times \overline{Q}, i<k} Y_{ij,kl} - (|P_1|-1)\sum_{ij \in P_1 \times \overline{Q}} Y_{ij,ij}$. Plugging into the inequality (11) gives $-(\beta-1)\sum_{ij \in P_1 \times Q} Y_{ij,ij} + |P_1|(|P_1|-1)/2 + \sum_{ij \neq kl \in P_1 \times \overline{Q}, i<k} Y_{ij,kl} - (|P_1|-1)\sum_{ij \in P_1 \times \overline{Q}} Y_{ij,ij} + \beta(\beta-1)/2 < 0$. But the left hand side of the above inequality is at least $-(\beta-1)\sum_{i \in P_1, j \in [n]} Y_{ij,ij} + \sum_{ij \neq kl \in P_1 \times \overline{Q}, i<k} Y_{ij,kl} + (\beta(\beta-1) + |P_1|(|P_1|-1))/2 \geq ((\beta-|P_1|)^2 - (\beta-|P_1|))/2 \geq 0$ 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 (11) is impossible.

The case of $|Q| \leq |P_1|$, is handled similarly since P_1 and Q have similar role. In case of inequality (10) we rewrite it by replacing β by $-(\gamma-1)$. We get $-(\gamma-1)\sum_{(ij) \in P_2 \times Q} Y_{ij,ij} + \sum_{(ij) \neq (kl) \in P_2 \times Q, i<k} Y_{ij,kl} + (1/2)(\gamma^2 - \gamma) < 0$. We can now use the same argument as above to establish that (10) is also impossible. □

Theorem 11. *Algorithm 1, using modified LP-GI, detects non-isomorphic graph pairs in polynomial time if the solution is confined to a pocket due to any of the facets described in Theorems 7,8 and a subset of facets described in Theorem 9.*

5 Conclusion

We have formulated GI as a geometric problem. The next challenge in establishing that GI is in class P lies in identifying the remaining facets of $\mathcal{B}^{[2]}$ and proving that the corresponding τ is at most $O(\log n)$. This does not contradict the fact that QAP is an NP-hard problem since in the present approach for GI, unlike QAP, the polytope of the linear program is not $\mathcal{B}^{[2]}$.

References

1. Vikraman Arvind and Jacobo Torán. Isomorphism testing: Perspective and open problems. *Bulletin of the EATCS*, 86:66–84, 2005.
2. P. K. Aurora and S. K Mehta. New Facets of the QAP-Polytope. *ArXiv e-prints*, September 2014.
3. László Babai and Ludek Kucera. Canonical labelling of graphs in linear average time. In *FOCS*, pages 39–46, 1979.
4. László Babai and Eugene M. Luks. Canonical labeling of graphs. In *STOC*, pages 171–183, 1983.
5. László Babai, Paul Erdös, and Stanley M. Selkow. Random graph isomorphism. *SIAM J. Comput.*, pages 628–635, 1980.
6. Scott Fortin. The graph isomorphism problem. Technical report, University of Alberta, 1996.
7. V. Kaibel. *Polyhedral Combinatorics of the Quadratic Assignment Problem.* PhD thesis, Faculty of Mathematics and Natural Sciences, University of Cologne, 1997.
8. T.C. Koopmans and M.J. Beckmann. Assignment problems and the location of economic activities. Technical report, Cowles Foundation, Yale University, 1955.
9. Eugene L. Lawler. The quadratic assignment problem. *Management Science*, 9(4):586–599, 1963.
10. Janez Povh and Franz Rendl. Copositive and semidefinite relaxations of the quadratic assignment problem. *Discrete Optimization*, 6(3):231–241, 2009.