

THE COMPUTATIONAL COMPLEXITY COLUMN

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Perhaps the oldest algorithmic technique used for the Graph Isomorphism problem is the Weisfeiler-Lehman procedure. Invented in the late 1960's, it has attracted research in several directions over the last five decades, and continues to be an actively researched topic. Algorithmists invariably use this procedure in combination with other tools for Graph Isomorphism. Logicians interested in descriptive complexity have found logical characterizations for it. There is a linear programming connection to the Weisfeiler-Lehman procedure, and the Sherali-Adams hierarchy for the natural LP relaxation of a 0-1 integer linear program for Graph Isomorphism turns out to be intimately connected to "higher dimensional" versions of the procedure.

This brief essay, meant as an invitation to the topic, will touch upon these aspects of the Weisfeiler-Lehman procedure. However, it is by no means a complete survey.

THE WEISFEILER-LEHMAN PROCEDURE

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1 Introduction

Two simple, undirected n -vertex graphs $X = (V, E)$ and $X' = (V', E')$ are *isomorphic* if there is a bijection $\pi : V \rightarrow V'$ that maps edges to edges and non-edges to non-edges. I.e.

$$\{u^\pi, v^\pi\} \in E' \leftrightarrow \{u, v\} \in E.$$

The Graph Isomorphism problem is to test if a given pair of graphs X, X' are isomorphic. A generic procedure for the Graph Isomorphism problem builds on a simple *color refinement* procedure. It is an iterative procedure for coloring the vertices of a graph X :

- To begin with, all vertices have the same color.
- In each color refinement step, if two vertices u and v have the same color but their neighborhoods are differently colored (counting color multiplicity), then u and v get fresh different colors.

This iterative procedure stops when the coloring does not refine any further, i.e. it becomes a *stable coloring*.

Color refinement yields a simple isomorphism test when applied to the disjoint union $X \sqcup X'$ of X and X' . In the stable coloring for $X \sqcup X'$, if the number of vertices colored c , for some color c is different in X and X' then they are clearly not isomorphic. But the converse is not always true. For example, if X and X' are two regular nonisomorphic graphs then the stable coloring is just the initial coloring which does not distinguish between any two vertices. Nevertheless, this simple method is a basic tool in many of the current algorithms for Graph Isomorphism. Even practical Graph Isomorphism testing tools like NAUTY [18] are based on color refinement.

The color refinement method dates back to a 1968 paper by Weisfeiler and Lehman [23], where they actually proposed a stronger method of coloring

pairs of vertices. This was subsequently generalized to the k -dimensional Weisfeiler-Lehman method (k -WL for short) for a graph $X = (V, E)$. The k -WL procedure colors k -tuples of vertices of X . Two k -tuple (u_1, \dots, u_k) and (v_1, \dots, v_k) are i -adjacent if $u_j = v_j$ for all $j \neq i$.

- Initially all k -tuples of vertices (u_1, u_2, \dots, u_k) are colored by the isomorphism type of the induced ordered subgraphs. I.e. (u_1, \dots, u_k) and (v_1, \dots, v_k) are colored the same if and only if the map $u_i \mapsto v_i$ is an isomorphism between the respective induced k -vertex subgraphs.
- In a general refinement step, the k -tuples (u_1, \dots, u_k) and (v_1, \dots, v_k) are colored different if for some index i , there are a different number of k -tuples colored c that are i -adjacent to (u_1, \dots, u_k) and (v_1, \dots, v_k) .

The above procedure stops when a stable coloring is reached, which will clearly be in at most $|V|^k$ refinement steps. It turns out that 2-WL coincides with the color refinement procedure.

A graph X is said to be *identified* by color refinement if for any non-isomorphic graph X' , the above procedure distinguishes them. For instance, trees (and forests) are identified by color refinement. Furthermore, Babai, Erdős and Selkow [4] have shown that a random graph is identified by color refinement with high probability; in fact, the stable coloring gives distinct colors to all vertices in a mere two rounds. For larger k , the k -WL method is known to be more powerful. For instance, it follows from [16] that 3-WL succeeds with high probability on random regular graphs. There is a fixed k such that k -WL succeeds on all planar graphs [11]. Furthermore, Grohe has extended this result to all graph classes characterized by excluded minors [12].

When precisely are two graphs X and X' *indistinguishable* by color refinement? I.e. for which pair of graphs X and X' does it hold that when we run color refinement on their disjoint union $X \sqcup X'$ and obtain the stable coloring, for any color c the number of vertices colored c is the same in X and X' ? It turns out that there are two nice characterizations of this property. One is logical and descriptive complexity-theoretic. The other is a geometric characterization, based on linear programming. We first explain the linear programming based characterization.

1.1 A linear programming characterization

There is a natural integer programming formulation of the Graph Isomorphism problem.

Let X and X' be two undirected simple graphs on vertex set $[n]$, with adjacency matrices A and B respectively. Suppose the graphs X and X' are isomorphic witness by permutation $\pi : [n] \rightarrow [n]$ that maps X to X' . Let P be the permutation matrix corresponding to π :

$$P_{ij} = 1 \leftrightarrow \pi(i) = j.$$

Then $AP = PB$. Conversely, if $AP = PB$ for a permutation matrix P , then the permutation π corresponding to P is an isomorphism from X to X' . We can express this as a 0-1 integer linear program given in the statement below.

Fact 1. *Let X and X' be two n -vertex graphs with adjacency matrices A and B respectively. An $n \times n$ permutation matrix P encodes an isomorphism π from X to X' if and only if P is a solution to the following 0-1 integer linear program:*

$$\begin{aligned} AP &= PB, \\ \sum_{i=1}^n P_{ij} &= 1, 1 \leq j \leq n, \\ \sum_{j=1}^n P_{ij} &= 1, 1 \leq i \leq n, \\ P_{ij} &\in \{0, 1\}, 1 \leq i, j \leq n. \end{aligned}$$

The above Integer Linear Program (ILP) is feasible if and only if the graphs corresponding to A and B are isomorphic. Notice that the row and column sum being 1, and the P_{ij} taking 0-1 values forces P to be a permutation matrix. A natural LP relaxation of the above ILP is

$$\begin{aligned} AP &= PB, \\ \sum_{i=1}^n P_{ij} &= 1, 1 \leq j \leq n, \\ \sum_{j=1}^n P_{ij} &= 1, 1 \leq i \leq n, \\ P_{ij} &\geq 0, 1 \leq i, j \leq n, \end{aligned}$$

and the solutions to this LP are called *fractional isomorphisms*. Clearly, the fractional isomorphisms P are all doubly stochastic matrices. If we drop the equality constraints given by $AP = PB$, the resulting system of linear

inequalities defines the polytope of all doubly stochastic matrices which, by Birkhoff's theorem, has as its extreme points all the $n!$ many permutation matrices.

We say that the graphs X and X' are fractionally isomorphic if the above LP relaxation has a fractional solution, where A and B are the adjacency matrices of X and X' . The following theorem by Ramana, Schneierman, and Ullman [19] shows a remarkable connection between fractional isomorphisms and the color refinement procedure.

Theorem 2. [19] *The graphs X and X' are fractionally isomorphic if and only if they are indistinguishable by color refinement.*

The proof relies on the Perron-Frobenius theorem and the notion of *equitable partitions* of a graph $X = (V, E)$. It is a partition of the vertex set

$$V = C_1 \sqcup C_2 \sqcup \cdots \sqcup C_r$$

such that the subgraph $X[C_i]$ induced by C_i is regular and the bipartite graph $X[C_i, C_j]$ is semi-regular for all $i \neq j$. For instance the *discrete partition* in which each C_i is a singleton is equitable. As it turns out, at the other extreme we have the equitable partition given by the stable coloring computed by color refinement, which is actually the *coarsest equitable partition*: any other equitable partition is a refinement of the stable coloring.

Let A be the adjacency matrix of graph X . A doubly stochastic matrix P is a *fractional automorphism* of X if $AP = PA$. We can interpret the matrix P as the adjacency matrix of a directed graph G_P with nonnegative weights. An important observation of [19] is that the strongly connected components of the directed graph G_P must form an equitable partition of X . As a consequence, it follows that any fractional automorphism P has to be block diagonal, where the blocks correspond to the stable coloring partition of V .

1.2 The convex set of fractional automorphisms

Let $X = (V, E)$ be an undirected graph with adjacency matrix A . The set of all fractional automorphisms P forms a convex set defined by the LP: $AP = PA$ such that $\sum_i P_{ij} = 1$, $\sum_j P_{ij} = 1$, and $P_{ij} \geq 0$, for $1 \leq i, j \leq n$.

Proposition 3. *The fractional automorphisms of X forms a semigroup $\text{FracA}(X)$ under matrix multiplication.*

Proof. If $P_1, P_2 \in \text{FracA}(X)$ are fractional automorphisms of X then we have $AP_1 = P_1A$ and $AP_2 = P_2A$. It follows that

$$AP_1P_2 = P_1AP_2 = P_1P_2A.$$

The semigroup also has the identity matrix I which is the identity element. \square

Since $\text{FracA}(X)$ is a convex set, it is also closed under convex combinations. I.e. if $P_i \in \text{FracA}(X)$, $1 \leq i \leq t$ and α_i , $1 \leq i \leq t$ are nonnegative such that $\sum_i \alpha_i = 1$ then $\sum_i \alpha_i P_i \in \text{FracA}(X)$.

Let $\text{Aut}(X)$ denote the automorphism group of X (we use the same notation $\text{Aut}(X)$ whether we treat its elements as permutations on the vertices or $|V| \times |V|$ permutation matrices). Clearly, $\text{Aut}(X) \subseteq \text{FracA}(X)$.

Proposition 4. *$\text{Aut}(X)$ coincides with $\text{FracA}(X)$ if and only if the stable coloring of the graph X yields the discrete partition.*

Proof. If the stable coloring yields the discrete partition, then by Theorem 2 stated above it follows that the only fractional automorphism of X is the identity matrix which implies $\text{Aut}(X) = \text{FracA}(X)$.

Conversely, suppose $\text{Aut}(X) = \text{FracA}(X)$. Now, suppose the stable coloring is the equitable partition

$$V = C_1 \sqcup C_2 \sqcup \dots \sqcup C_r,$$

is not discrete. Consider the block diagonal doubly stochastic matrix P , with blocks defined by subsets C_1, C_2, \dots, C_r , such that for all $u, v \in C_k$ we have $P_{uv} = \frac{1}{|C_k|}$. As the stable coloring is an equitable partition, it follows that P is a fractional automorphism. Furthermore, P is not in $\text{Aut}(X)$ which contradicts the assumption. \square

If X is a regular graph with no nontrivial automorphisms then $\text{Aut}(X)$ is a proper subset of $\text{FracA}(X)$, because $\text{Aut}(X) = \{1\}$ and $\text{FracA}(X)$ contains $\frac{1}{d}A$, where d is the degree of each vertex in X .

By Birkhoff's theorem we know that the extreme points of the polytope of doubly stochastic matrices are precisely the $n!$ many permutation matrices. As a consequence, for any graph X , all matrices in $\text{Aut}(X)$ are extreme points of $\text{FracA}(X)$. However, in general, the fractional automorphism polytope $\text{FracA}(X)$ may have non-integral extreme points.

For graphs X and X' , let $\text{FracI}(X, X')$ denote the (possibly empty) convex polytope of all fractional isomorphisms from X to X' given by Equation 1. We note that $\text{FracA}(X)P \subseteq \text{FracI}(X, X')$, where P is some fractional solution to Equation 1. Now, there are graphs X (like forests, for instance) such that $\text{FracI}(X, X') \neq \emptyset$ if and only if there is an integral solution in $\text{FracI}(X, X')$ (i.e., X and X' are isomorphic). This will happen if the set of all extreme points of the convex polytope $\text{FracA}(X)$ is precisely $\text{Aut}(X)$. This property

was noticed by Tinhofer [21, 22], and he called such graphs X *compact*. For example, forests are compact. If X is compact, Tinhofer [21, 22] gives an algorithm to compute an isomorphism from X to another graph X' , if it exists, by computing an extreme point solution for the linear program given by Equation 1 [21, 22].

2 Logical perspective

Immerman and Lander [15] wrote a seminal paper introducing a first-order logic based approach to understanding the color refinement procedure. In order to state their results precisely, we will require some basic definitions from their paper.

The first-order language of graphs is built from variables x_i , the binary edge relation E and equality $=$, along with the usual logical connectives and quantifiers \forall and \exists . The quantifiers range over the vertex set of a given graph. Occasionally, it is useful to consider vertex colored graphs, where the colors are defined by unary predicates.

For any given language \mathcal{L} (either first-order or a suitable extension of it, usually), we say that graphs G and H are \mathcal{L} -equivalent iff for all sentences $\varphi \in \mathcal{L}$ we have

$$G \models \varphi \leftrightarrow H \models \varphi.$$

A k -*valuation* over graph G is an assignment u of vertices to variables x_1, x_2, \dots, x_k . Suppose u and v are k -valuations for graphs G and H respectively. We say that G, u and H, v are \mathcal{L} -equivalent iff for all formulas $\varphi \in \mathcal{L}$ with free variables from x_1, \dots, x_k

$$G, u \models \varphi \leftrightarrow H, v \models \varphi.$$

We say that \mathcal{L} k -characterizes G iff for all graphs H , and all k -valuations u and v over G and H respectively, if G, u and H, v are \mathcal{L} -equivalent then there is an isomorphism extending the correspondence given by (u, v) .

2.1 The first-order language \mathcal{C}_k

The language \mathcal{L}_k is defined to be first-order formulas which use k variables. The language \mathcal{C}_k is defined to be first-order formulas with k variables, where the formulas use *counting quantifiers*: For example, the formula $(\exists^i x)\varphi(x)$ means there are at least i vertices v such that $\varphi(v)$ is true.

It turns out that the language \mathcal{C}_2 precisely corresponds to color refinement.

Theorem 5. [15] *Given a graph $G = (V, E)$, let \bar{f} denote the stable coloring of V produced by color refinement. let v_1 and v_2 be two vertices of G . The following conditions are equivalent:*

- $\bar{f}(v_1) = \bar{f}(v_2)$.
- For each formula $\varphi(x) \in \mathcal{C}_2$

$$G \models \varphi(v_1) \leftrightarrow G \models \varphi(v_2).$$

The proof is by an inductive argument on the number of color refinement rounds which corresponds to the quantifier depth of the formula φ . I.e. v_1 and v_2 are indistinguishable by color refinement in r rounds precisely when \mathcal{C}_2 formulas $\varphi(x)$ of quantifier depth r cannot distinguish between v_1 and v_2 . An important tool in analyzing the power of \mathcal{C}_2 is the following *two-player pebble game*. For a pair of graphs G and H the \mathcal{C}_2 -game on them is defined as follows: there are two pairs of pebbles $(g_1, h_1), (g_2, h_2)$:

1. The first player takes a pebble, say g_i , and chooses a subset A of vertices from one of the graphs. The second player has to choose a subset B of vertices from the other graph such that $|A| = |B|$.
2. The first player places h_i on some vertex in B and the second player has to respond by placing g_i on some vertex in A .

The first player wins iff the subgraph induced by g_1, g_2 is not the same as that induced by h_1, h_2 . Otherwise, the second player wins.

The above theorem actually shows that $\bar{f}(v_1) = \bar{f}(v_2)$ iff the first player has a winning strategy in the above game played on two copies of G with g_1 placed on v_1 in the first copy and h_1 placed on v_2 in the second copy.

The Immerman-Lander theorem combined with Theorem 2 gives a beautiful three-way characterization of graphs G and H that are indistinguishable by color refinement. This can be briefly summarized as below:

Theorem 6. [19, 15] *The following statements are equivalent:*

- *Graphs G and H are indistinguishable by color refinement.*
- *Graphs G and H are indistinguishable by formulas in \mathcal{C}_2 .*
- *Graphs G and H are fractionally isomorphic.*

Immerman and Lander [15] also generalize their result to show that graphs G and H are indistinguishable in \mathcal{C}_k if and only if they are indistinguishable by $(k - 1)$ -WL (the $(k - 1)$ -dimensional Weisfeiler-Lehman procedure).

2.2 Weisfeiler-Lehman and Graph Isomorphism

Coming back to the color refinement procedure as an algorithm for Graph Isomorphism, it is natural to ask for which graphs does it give the correct answer. We say that color refinement succeeds on a graph G iff for any nonisomorphic graph H , color refinement distinguishes between G and H . Equivalently, G and H are isomorphic iff they are indistinguishable in \mathcal{C}_2 . As already noted, color refinement succeeds on forests, and also on random graphs with high probability. In [2, 20] the class of graphs on which color refinement succeeds is completely characterized. In particular, these graphs can also be efficiently recognized. However, the problem of precisely characterizing the class of graphs on which k -WL succeeds remains open, for $k \geq 3$.

In this connection, it is natural to wonder if k -WL for some k could be powerful enough to solve Graph Isomorphism on all instances. It is easy to see that $k = n$ succeeds. We have already noted that for each n -vertex graph G there is a first-order formula using n variables that is true on G and not on any nonisomorphic graph H . Whether a smaller k succeeds remained open until the seminal paper by Cai, Fürer, and Immerman [7] in which they showed a lower bound of $k = \Omega(n)$. More precisely, they proved the following result.

Theorem 7. [7] *There exists a sequence of nonisomorphic graph pairs $\{G_n, H_n\}_n$ such that G_n and H_n have $\Theta(n)$ vertices, but G_n and H_n are indistinguishable by n -WL.*

It is interesting to note that the graphs G_n and H_n , ingeniously constructed, are actually very simple instances of Graph Isomorphism. That is to say, they are vertex-colored graphs with at most 4 vertices of each color, and the problem is to check if G_n and H_n have a *color-preserving* isomorphism. Such instances of Graph Isomorphism (with bounded size color classes) are easily solved in polynomial time by simple group-theoretic techniques from [10].

Since the k -WL procedure takes essentially n^k time, it is clear from this theorem that the Weisfeiler-Lehman procedure alone is not enough to get an efficient algorithm for Graph Isomorphism.

Nevertheless, it is often a crucial component in many algorithms for Graph Isomorphism. For instance, Lindell's logspace algorithm for Tree Isomorphism (and Canonization) [17] is essentially a clever logspace implementation of color refinement on trees. Another appealing paper in this direction is due to Grohe and Verbitsky [14]. They note that if graphs from a graph class \mathcal{C} can be identified in \mathcal{C}_k for small k using a formula of logarithmic quantifier

depth, then it is possible to find efficient *parallel algorithms* for isomorphism (and even canonization) for such graphs. Using their method they could show that planar graph isomorphism can be solved in the parallel circuit class AC^1 (which is contained in NC^2). Similarly, they show that bounded treewidth graph isomorphism is in the circuit class TC^1 (also contained in NC^2). Recent work with much more complicated algorithms has improved these upper bounds to logarithmic space.

Remark 8. *The Immerman-Lander theorem has also driven a lot of research in the study of new extensions of first-order logic. There is interesting work of Dawar et al [8] using a rank operator based extension of first-order logic.*

Remark 9. *Finally, we briefly mention that the technique of Individualization of vertices combined with Weisfeiler-Lehman is a powerful tool for obtaining efficient isomorphism algorithms. Originally, it was introduced by Zemlyachenko as a “degree reduction trick” yielding the $2^{O(\sqrt{n \ln n})}$ time isomorphism algorithm [5]. It also plays a significant role in Babai’s recent breakthrough algorithm [6].*

3 More linear programming

This section is essentially based on the work of Atserias and Maneva [3] in which they consider the different levels of the Sherali-Adams LP relaxation hierarchy of Equation 1 and shows a close relationship to k -dimensional Weisfeiler-Lehman for $1 \leq k \leq n$. We will state their main result and point to some questions that arise from their work. We begin with defining the Sherali-Adams relaxation.

Consider any 0-1 integer linear program

$$\begin{aligned} Ax &\geq b, \\ x_i &\in \{0, 1\}, \forall x_i. \end{aligned}$$

Let P_{int} denote the convex polytope which is the convex hull of solutions $x \in \{0, 1\}^n$ of the above integer linear program.

Its LP relaxation, where the integral constraints are replaced by $0 \leq x_i \leq 1$, also defines a convex polytope P . Clearly,

$$P \supseteq P_{int}.$$

In the special case when $P = P_{int}$ we can use linear programming to find integral solutions. Otherwise, one approach to understanding P_{int} is by

defining a sequence of relaxations that “interpolate” P and P_{int} . In particular, the *Sherali-Adams* hierarchy is defined by a sequence of “approximating” polytopes

$$P = P_1 \supseteq P_2 \supseteq \dots \supseteq P_n = P_{int},$$

where the k^{th} polytope in the sequence is obtained as follows from P :

For all subsets $I \in \binom{[n]}{\leq k-1}$, and all partitions $I = I_1 \sqcup I_2$, each inequality $\sum_{j=1}^n A_{ij}x_j \geq 0$ is multiplied by $\prod_{i \in I_1} x_i \prod_{j \in I_2} (1 - x_j)$. Overall, this yields a system of polynomial inequalities, where each polynomial’s degree is at most k in each inequality.

Next, in each polynomial inequality, each monomial is “flattened” into a multilinear monomial by repeatedly replacing x_i^2 with x_i . This yields a system of multilinear polynomial inequalities, where each polynomial has degree at most k . Then, each monomial $\prod_{i \in A} x_i$ is replaced by a new variable y_A , and a fresh constraint $y_\emptyset = 1$ is included. This results in an LP Q_k in variables $y_A, A \in \binom{[n]}{\leq k}$. Finally, the polytope $P_k \subseteq \mathbb{R}^n$ is defined by projecting Q_k to the n variables y_A such that $|A| = 1$. Clearly, the LP defining P_k requires the variables $y_A, A \in \binom{[n]}{\leq k}$ and is of size $n^{O(k)}$.

By examining the integral solutions it is clear that $P_{int} \subseteq P_k$. Since the constraints of P_k are only tighter we have $P_k \subseteq P_1$. Furthermore, it turns out that $P_{int} = P_n$. Thus, the hierarchy is finite. Thus, if $P_k = P_{k+1}$ for some $k < n$, it follows that $P_k = P_{int}$.

Following [3], we consider the Sherali-Adams hierarchy corresponding to the 0-1 integer linear program defined in Fact 1. Let that polytope be denoted by P_{int}^{gi} , and let P^{gi} denote its LP relaxation given in Section 1, which defines fractional isomorphisms. The Sherali-Adams relaxations yields the following sequence of polytopes:

$$P^{gi} = P_1^{gi} \supseteq P_2^{gi} \supseteq \dots \supseteq P_n^{gi} = P_{int}^{gi}.$$

Let X and X' be two n -vertex graphs with adjacency matrices A and B , and consider the above Sherali-Adams relaxation hierarchy. Say that X and X' are *fractionally k -isomorphic* if and only if the polytope P_k^{gi} is nonempty. Thus, X and X' are fractionally n -isomorphic precisely when they are isomorphic. We now state the main result of Atserias and Maneva [3].

Theorem 10. [3] *Let X and X' be two n -vertex graphs with adjacency matrices A and B . For any $k \geq 0$, if X and X' are fractionally $k+1$ -isomorphic then X and X' are indistinguishable by $k+1$ -dimensional Weisfeiler-Lehman. Furthermore, if X and X' are indistinguishable by $k+1$ -dimensional Weisfeiler-Lehman, then X and X' are fractionally k -isomorphic.*

In [13] it is shown that the interleaving of fractional k -isomorphism and k -WL for different k is, in fact, a strict interleaving, except for equality at the first level, given by Theorem 2.

We recall from Section 1 Tinhofer's definition of compact graphs. A graph X is compact iff $P^{gi} = P_{int}^{gi}$.

An intriguing open question is the complexity of recognizing compact graphs. For the general case we have the following simple complexity-theoretic upper bound.

Fact 11. *Given an n -vertex graph X as input, we can decide if X is compact in coNP.*

Proof. This follows because testing integrality of every vertex of the polytope P^{gi} for X is in coNP. We use the fact that, as the polytope P^{gi} is itself defined by a small LP, testing if a point is a vertex can be done in polynomial time. \square

It is shown in [1] that the problem of checking if X is compact is P -hard under logspace reductions. Apart from this we do not have any complexity lower bound for the problem. It is open whether the problem is coNP-hard.

Similar to compactness, we can define a notion of k -compactness w.r.t. the k -level of the Sherali-Adams relaxation.

Definition 12. *A graph X is k -compact if $P_k^{gi} = P_{int}^{gi}$.*

Analogous to Tinhofer's observation [21, 22] we note the following.

Theorem 13. *If X is an n -vertex graph that is k -compact then given any other n -vertex graph X' there is an $n^{O(k)}$ time algorithm to check if X and X' are isomorphic.*

Proof. Let A and B be the adjacency matrices of X and X' respectively. Let $P_k^{gi}(A)$ and $P_k^{gi}(B)$ denote the polytopes given by the k^{th} level of the Sherali-Adams hierarchy for X and X' . As per definition $P_k^{gi}(A)$ is the projection of another polytope $\hat{P}_k^{gi}(A)$, where $\hat{P}_k^{gi}(A)$ is defined by an LP of size $n^{O(k)}$ on the variables y_S , for every subset $S \subseteq [n]$ of size at most $k - 1$. The variables $y_{\{i\}}$ equal x_i , $1 \leq i \leq n$ and $P_k^{gi}(A)$ is defined by projection to these n variables. Suppose X and X' are isomorphic and π is an isomorphism. Let Q be the corresponding permutation matrix. Then we have

$$Q^T A Q = B.$$

I.e. $AQ = QB$. The permutation π extends to all subsets of $[n]$ naturally, where $\pi(S) = \{\pi(i) \mid i \in S\}$. It is easy to see that an $\binom{[n]}{\leq k}$ -vector v (of values

to $y_S, |S| \leq k - 1$) is in $\hat{P}_k^{gi}(A)$ iff the vector $u = \pi(v)$ is in $\hat{P}_k^{gi}(B)$, where $u_S = v_{\pi(S)}$ for all $S : |S| \leq k - 1$. As $P_k^{gi}(A)$ and $P_k^{gi}(B)$ are obtained by projecting to the n variables $y_{\{i\}}$, it follows that

$$\pi(P_k^{gi}(A)) = P_k^{gi}(B).$$

Hence, if X is k -compact and X' is isomorphic to X , then X' is also k -compact.

Now, consider the polytope $S_k(X, X')$ obtained as the k^{th} level of the Sherali-Adams relaxation of the integer linear program in Fact 1. Assuming X is k -compact, we show that if $S_k(X, X')$ is nonempty that all its vertices are integral. That would immediately yield an $n^{O(k)}$ time isomorphism test because the size of the LP is $n^{O(k)}$. Let P be an extreme point of $S_k(X, X')$. Suppose P is not integral. We know that $AP = PB$ and P is doubly stochastic. Since $Q^T A Q = B$, it follows that $APQ^T = PQ^T A$. Hence, PQ^T is a fractional automorphism of A (which is not integral because Q is a permutation matrix and P is not integral). Since X is compact, we can write PQ^T as a convex combination of integral automorphisms of X . I.e.

$$PQ^T = \sum_{i=1}^N \lambda_i P_i,$$

where $\sum_i \lambda_i = 1$ and $0 \leq \lambda_i < 1$ for all i , P_i are permutation matrices and $AP_i = P_i A$ for all i . The nonzero λ_i are strictly less than 1 because we have assumed PQ^T is fractional.

Hence,

$$P = \sum_{i=1}^N \lambda_i P_i Q.$$

Now, $AP_i Q = P_i A Q = P_i Q B$ for all i . Hence, $P_i Q$ are all integral isomorphisms from X to X' . This contradicts the extremality of P for the polytope $S_k(X, X')$. \square

Characterizing k -compact graphs is an interesting open problem.

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