Revisiting the Graph Isomorphism Problem with Semidefinite Programming

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Abstract

It is well-known that the graph isomorphism problem can be posed as an equivalent problem of determining whether an auxiliary graph structure contains a clique of specific order. However, the algorithms that have been developed so far for this problem are either not efficient or not exact. In this paper, we present a new algorithm which solves this equivalent formulation via semidefinite programming. Specifically, we show that the problem of determining whether the auxiliary graph contains a clique of specific order can be formulated as a semidefinite programming problem, and can thus be (almost exactly) solved in polynomial time. Furthermore, we show that we can determine if the graph contains such a clique by rounding the optimal solution to the nearest integer. Our algorithm provides a significant complexity result in graph isomorphism testing, and also represents the first use of semidefinite programming for solving this problem.

1 Introduction

Graph isomorphism is one of those few fundamental problems in NP whose computational status still remains unknown [1]. Roughly speaking, the graph isomorphism problem asks whether two graphs are structurally identical or not. The problem is clearly in NP. However, it has been neither proven NP-complete nor found to be solved by a polynomial time algorithm. In fact, there is strong evidence that graph isomorphism is not NP-complete since it has been shown that the problem is located in the low hierarchy of NP [2]. This implies that if the problem was NP-complete, then the polynomial time hierarchy would collapse to its second level.

Over the years, algorithms of different nature have been developed to attack the problem. Traditionally, those that draw ideas from group theory turn out to be the most promising. One of these group-theoretic algorithms was proposed by Babai and Luks in 1983 [3]. The algorithm combines a preprocessing procedure proposed by Zemlyachenko et al. [4] with an efficient algorithm for solving graph isomorphism on graphs of bounded degree [5]. Its computational complexity is \(2^{\Omega(\sqrt{n\log n})}\) where \(n\) denotes the number of vertices. Despite decades of active research, no progress had been achieved, and this was the best known algorithm until recently when Babai presented an algorithm that solves the graph isomorphism problem in

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quasi-polynomial time [6]. It should be mentioned that while the complexity status of the graph isomorphism for general graphs remains a mystery, for many restricted graph classes, polynomial time algorithms are known. This is, for example, the case for planar graphs [7], graphs of bounded degree [5], or graphs with bounded eigenvalue multiplicity [8]. It should also be noted that there exist several algorithms which have proven very efficient for graphs of practical interest [9, 10, 11]. Interestingly, these algorithms are very different from the ones that offer the lowest worst case complexities. This indicates that there is a wide gap between theory and practice.

Besides the above algorithms, there are also several scalable heuristics for graph isomorphism which are based on continuous optimization. In these heuristics, the discrete search problem in the space of permutation matrices is replaced by an optimization problem with continuous variables, enabling the use of efficient continuous optimization algorithms. Formally, for any two graphs on \( n \) vertices with respective \( n \times n \) adjacency matrices \( A_1 \) and \( A_2 \), the optimization problem consists in minimizing the function \( \| A_1 - P A_2 P^T \|_F \) over all \( P \in \Pi \), where \( \Pi \) denotes the set of \( n \times n \) permutation matrices, and \( \| \cdot \|_F \) is the Frobenius matrix norm [12]. Therefore, the problem of graph isomorphism can be reformulated as the problem of minimizing the above function over the set of permutation matrices. The two graphs are isomorphic to each other if there exists a permutation matrix \( P \) for which the above function is equal to 0. Note also that other objectives have also been proposed in the literature, this being perhaps the most common. This problem has a combinatorial nature and there is no known polynomial algorithm to solve it. Numerous approximate methods have been developed. Most of these methods replace the space of permutations by the space of doubly-stochastic matrices. Let \( D \) denote the set of \( n \times n \) doubly stochastic matrices, i.e., nonnegative matrices with row and column sums each equal to 1. The convex relaxed problem minimizes the function \( \| A - D A D^\top \|_F^2 \) over all \( D \in D \). There is a polynomial-time algorithm for exactly solving the convex relaxed graph matching problem [13]. However, due to relaxation, even if there exists a doubly stochastic matrix \( D \) for which the objective function is equal to 0, there is no guarantee that the two graphs are isomorphic to each other.

The main contribution of this work is a novel algorithm which attacks efficiently the problem of graph isomorphism. The main tools employed are a compatibility graph, i.e., an auxiliary graph structure that is useful for solving general graph and subgraph isomorphism problems, and a semidefinite programming formulation. Given two graphs of order \( n \), we build their compatibility graph of order \( n^2 \). We show that testing the two graphs for isomorphism is equivalent to determining whether the compatibility graph contains a clique of order \( n \). We show that this problem can be formulated as a semidefinite programming optimization problem, and can thus be (almost exactly) solved in polynomial time with readily available solvers. We show that the two graphs are isomorphic to each other if the optimal value of the semidefinite program is arbitrarily close to \( n(n-1) \). Our algorithm demonstrates the usefulness of semidefinite programming in combinatorial optimization, and provides a significant complexity result in graph isomorphism testing. It should be mentioned that our work is not the first to apply continuous optimization approaches to the problem of determining whether the compatibility graph contains a clique of order \( n \). In a previous study, Pelillo developed a heuristic for computing the clique number of the compatibility graph [14]. However, in contrast to the proposed algorithm, this method provides no guarantees, and may get stuck on some local optimum of the objective function.
2 Preliminaries

In this Section, we first define our notation, and we then introduce the concept of a compatibility graph. We show that the graph isomorphism problem is equivalent to finding if the compatibility graph contains a clique of specific size. We also present the basic concepts of semidefinite programming and an algorithm which is based on Lovász $\vartheta$ number and for almost all classes of graphs can decide if two instances are isomorphic to each other.

2.1 Graph Theory Notation and Terminology

Let $G = (V, E)$ be an undirected and unweighted graph consisting of a set $V$ of vertices and a set $E$ of edges between them. We will denote by $n$ the number of vertices. The adjacency matrix of $G$ is a symmetric matrix $A \in \mathbb{R}^{n \times n}$ defined as follows: $A_{ij} = 1$ if $(i, j) \in E$, and 0 otherwise. Note that since the graph is undirected, $(i, j) \in E$ if and only if $(j, i) \in E$, for all $i, j \in V$. Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic (denoted by $G_1 \cong G_2$), if there is a bijective mapping $\phi : V_1 \to V_2$ such that $(v_i, v_j) \in E_1$ if and only if $(\phi(v_i), \phi(v_j)) \in E_2$.

We next present the notion of a compatibility graph, i.e., a structure that is very useful for solving graph/subgraph isomorphism and maximum common subgraph problems. These auxiliary graph structures have been proposed independently by several authors [15, 16, 17], while they also lie at the core of several algorithms [14, 18, 19]. Furthermore, different authors have used different names to describe them. For instance, compatibility graphs, association graphs, derived graphs, M-graphs, and product graphs are all names that have been coined to describe these structures. In what follows, we will use the name compatibility graph to refer to them. Formally, given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, their compatibility graph $G_c = (V_c, E_c)$ is a graph with vertex set $V_c = V_1 \times V_2$. An edge is drawn between two vertices $(v_1, u_1), (v_2, u_2) \in V_c$ if and only if $v_1 \neq v_2$, $u_1 \neq u_2$ and either $e_1 = (v_1, v_2) \in E_1$ and $e_2 = (u_1, u_2) \in E_2$ or $e_1 \notin E_1$ and $e_2 \notin E_2$. Clearly, there are two types of edges in a compatibility graph: (1) edges that represent common adjacency, and (2) edges that represent common non-adjacency. An example of the compatibility graph that emerges from two $P_3$ graphs is illustrated in Figure 1.

Levi established a relation between isomorphic subgraphs of two graphs and cliques in their compatibility graph [15]. Specifically, if some vertices $(v_1, u_1), (v_2, u_2), \ldots, (v_k, u_k) \in V_c$ form a clique, and are thus pairwise adjacent, then the subgraph in $G_1$ induced by the vertices $v_1, v_2, \ldots, v_k$ is isomorphic to the subgraph in $G_2$ induced by the vertices $u_1, u_2, \ldots, u_k$. The isomorphism is given by the vertices $(v_1, u_1), (v_2, u_2), \ldots, (v_k, u_k) \in V_c$ of the compatibility graph that form the clique, i.e., $\phi(u_1) = v_1, \phi(u_2) = v_2, \ldots, \phi(u_k) = v_k$.

The next Theorem establishes an equivalence between the graph isomorphism problem and the maximum clique problem on the compatibility graph, and corresponds to a sub-instance of Levi’s result. For completeness, we also provide the proof. Note that if $G_1$ and $G_2$ are two graphs of order $n$, the maximum clique of their compatibility graph will consist of at most $n$ vertices.

**Theorem 1.** Let $G_1$ and $G_2$ be two graphs of order $n$, and let $G_c$ be their compatibility graph. Then, $G_1$ and $G_2$ are isomorphic if and only if $G_c$ contains a clique of order $n$, i.e., $\omega(G_c) = n$.

**Proof.** If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic, then there exists a bijective mapping $\phi : V_1 \to V_2$ such that $(v_i, v_j) \in E_1$ if and only if $(\phi(v_i), \phi(v_j)) \in E_2$. Then, by construction, there are $n$ vertices $(v_1, \phi(v_1)), \ldots, (v_n, \phi(v_n)) \in V_c$ which are connected to each other by an edge, i.e., $(v_1, \phi(v_1)), (v_2, \phi(v_2)), \ldots, (v_{n-1}, \phi(v_{n-1})), (v_n, \phi(v_n)) \in E_c$. These vertices form a clique of order $n$, and therefore, $\omega(G_c) = n$. For the second part, given a compatibility graph $G_c$ that contains a clique of order $n$, let $(v_1, u_1), \ldots, (v_n, u_n) \in V_c$ denote the $n$ vertices that
The set of nodes $V$ compatibility graph $G$ since $|G|_{\text{automorphisms}}$ of $n$ of vertices of the graphs $i$ and $j$ form the clique. By definition, $V_1 = \{v_1, \ldots, v_n\}$ and $V_2 = \{u_1, \ldots, u_n\}$. Then, we can construct a bijective mapping $\phi : V_1 \rightarrow V_2$ as follows: $\phi(v_i) = u_i$. Since $((v_i, \phi(v_i)), (v_j, \phi(v_j))) \in E_c$ for $i \in \{0, \ldots, n\}$, we have that $(v_i, v_j) \in E_1$ if and only if $(\phi(v_i), \phi(v_j)) \in E_2$. Therefore, $G_1$ and $G_2$ are isomorphic to each other.

Note that the number of isomorphisms between two graphs can be exponential to the number of vertices of the graphs $n$. Specifically, if $G_1$ and $G_2$ are isomorphic, then the number of automorphisms of $G_1$ (or of $G_2$) is equal to the number of isomorphisms from $G_1$ to $G_2$. Hence, if, for instance, $G_1$ and $G_2$ are complete graphs on $n$ vertices, i.e., both correspond to the complete graph $K_n$, then the number of isomorphisms between the two graphs is equal to $n!$ since $|\text{Aut}(G_1)| = |\text{Aut}(G_2)| = |\text{Aut}(K_n)| = n!$. Each isomorphism $\phi : V \rightarrow V'$ corresponds to an $n$-clique in the compatibility graph. Therefore, the compatibility graph can contain up to $n!$ cliques. As an example, consider the graphs shown in Figure 1. There are two isomorphisms between $G_1$ and $G_2$. Hence, their compatibility graph contains exactly two cliques of order 3.

We now introduce the following Lemma which we will use in the next Section.

**Lemma 1.** Let $G_1$ and $G_2$ be two graphs of order $n$, and let $G_c$ be their compatibility graph. Then, the vertices of $G_c$ can be grouped into $n$ partitions such that there are no edges between vertices that belong to the same partition.

**Proof.** Let $V_1$ and $V_2$ denote the sets of vertices of $G_1$ and $G_2$, respectively. Then, $V_1 = \{v_1, \ldots, v_n\}$ and $V_2 = \{u_1, \ldots, u_n\}$. Let also $V_c$ and $E_c$ denote the set of vertices and edges of the compatibility graph $G_c$, and $(a, b), (c, d) \in V_c$. Then, by definition, if $a = c$, $((a, b), (c, d)) \notin E_c$. The set of nodes $V_c$ can be decomposed into the following $n$ disjoint sets: $P_1 = \{(v_1, u_1), (v_1, u_2), \ldots, (v_1, u_n)\}$, $P_2 = \{(v_2, u_1), (v_2, u_2), \ldots, (v_2, u_n)\}$, $P_3 = \{(v_3, u_1), (v_3, u_2), \ldots, (v_3, u_n)\}$, $\ldots$, $P_n = \{(v_n, u_1), (v_n, u_2), \ldots, (v_n, u_n)\}$.
Then, $V_c = P_1 \cup P_2 \cup \ldots \cup P_n$. Clearly, there is no edge between each pair of vertices of each partition. This concludes the proof.

2.2 Semidefinite Programming

A semidefinite program (SDP) is the problem of optimizing a linear function over the intersection of the cone of positive semidefinite matrices with an affine space. Semidefinite programming has attracted a lot of attention in recent years since many practical problems in operations research and combinatorial optimization can be modeled or approximated as semidefinite programming problems. For instance, in control theory, SDPs are used in the context of linear matrix inequalities. In graph theory, the problem of computing the Lovász number of a graph can be formulated as a semidefinite program. Given any $\epsilon > 0$, semidefinite programs can be solved within an additive error of $\epsilon$ in polynomial time. There are several different algorithms for solving SDPs. For instance, this can be done through the ellipsoid algorithm [20] or through interior-point methods [21].

2.3 An Algorithm for Almost all Classes of Graphs

It follows from Lemma 1 that the set of vertices $V_c$ of a compatibility graph can be decomposed into $n$ disjoint sets $P_1, P_2, \ldots, P_n$ such that there is no edge that connects vertices of the same set. Since a compatibility graph can be decomposed into $n$ disjoint sets such that every edge $e \in E_c$ connects a vertex in $P_i$ to one in $P_j$ with $i \neq j$, the minimum number of colors required for a proper coloring of $G_c$ is no more than $n$. Therefore, $\chi(G_c) \leq n$.

For an arbitrary graph $G$, it is well-known that $\omega(G) \leq \chi(G)$. Therefore, a compatibility graph can contain a clique of order $n$ only if $\chi(G_c) = n$. Computing the chromatic number of a graph is in general an NP-complete problem. However, we can compute in polynomial time a real number $\vartheta(G)$ that is “sandwiched” between the clique number and the chromatic number of a graph $G$, that is $\omega(G) \leq \vartheta(G) \leq \chi(G)$ [22]. This number is known as the Lovász number of $G$. Again, a compatibility graph can contain a clique of order $n$ only if $\vartheta(G_c) = \chi(G_c) = n$. However, the fact that $\vartheta(G_c) = \chi(G_c) = n$ does not imply that $\omega(G) = n$. Instead, it may hold that $\omega(G_c) < \vartheta(G_c) = \chi(G_c) = n$. One class of graphs for which the above holds is the family of latin square graphs. Although for the class of compatibility graphs, it may hold that $\omega(G) = n$ whenever $\vartheta(G) = \chi(G) = n$, we do not study this any further, but we leave it as future work.

3 The Main Result

Next, we give a SDP based solution for the graph isomorphism problem. We show that the problem of identifying whether a compatibility graph contains a clique of order $n$ can be expressed as a SDP. For the ease of presentation, we start with a simple formulation where we assume that the rank of the matrix involved in the objective function of the SDP is 1. Unfortunately, this constraint is not convex, and renders the problem NP-hard. We then drop the rank constraint, and show that the emerging SDP can successfully deal with the general case.

3.1 Rank-1 Case

Define a variable $x_i$ for every vertex $i \in V_c$, and let $X = xx^\top$. Let also $m = n^2$. Then, we have that:

$$X = xx^\top \iff X \in S_m, X \succeq 0, \ \text{rank}(X) = 1$$
where $S_m$ is the set of all $m \times m$ real symmetric matrices and $X \succeq 0$ means that the matrix variable $X$ is positive semidefinite. Let also $J$ denote the $m \times m$ matrix of ones. Consider now the following optimization problem:

\[
\begin{align*}
\text{maximize} & \quad \text{trace}(JX) \\
\text{subject to} & \quad \text{trace}(X) = n, \\
& \quad X_{i,j} = 0, \ (i,j) \notin E_c, \\
& \quad X_{i,j} \leq 1, \ (i,j) \in E_c, \\
& \quad X \succeq 0, \\
& \quad \text{rank}(X) = 1.
\end{align*}
\]

We can determine if there is a clique of order $n$ in $G_c$ by solving the above optimization problem. Specifically, if there exists such a clique in $G_c$, the value of the optimal solution to the problem is equal to $n^2$.

**Lemma 2.** The value of problem (1) is no greater than $n^2$.

**Proof.** The value of the objective function of the optimization problem is:

\[
\text{trace}(JX) = \sum_{i=1}^{m} \sum_{j=1}^{m} J_{i,j} X_{i,j} = J_{1,1} X_{1,1} + \ldots + J_{m,m} X_{m,m} = x_1 x_1 + \ldots + x_m x_m
\]

From constraint (1b), it follows that the sum of the diagonal terms of matrix $X$ is equal to $n$, i.e., $x_1 x_1 + x_2 x_2 + \ldots + x_m x_m = n$. We next replace these terms with their sum. Therefore, the objective function of the optimization problem becomes:

\[
\text{trace}(JX) = \sum_{i=1}^{m} \sum_{j=1}^{m} J_{i,j} X_{i,j} = n + x_1 x_2 + \ldots + x_m x_{m-1}
\]

We will next show that in our setting, we can have at most $n$ vertices for which $x_i \neq 0$. It follows from the constraint (1c) that $\forall (i,j) \notin E_c, X_{i,j} = x_i x_j = 0$. Therefore, $\forall (i,j) \notin E_c$, one of the following three conditions holds: (1) $x_i = 0, x_j \neq 0$, (2) $x_i \neq 0, x_j = 0$, (3) $x_i = 0, x_j = 0$. It follows also from Lemma 1 that the vertices of $G_c$ can be grouped into $n$ partitions such that the $n$ vertices that belong to each partition are not connected by an edge. Therefore, there can be at most one vertex $i$ from each partition for which $x_i \neq 0$. It thus turns out that we can have at most $n$ vertices for which $x_i \neq 0$. From these $n$ vertices, we can obtain $n(n-1)$ (ordered) pairs of vertices. For each pair, $X_{i,j} = x_i x_j \leq 1$ holds. Therefore, it follows that:

\[
\text{trace}(JX) = \sum_{i=1}^{m} \sum_{j=1}^{m} J_{i,j} X_{i,j} \leq n + n(n-1) = n^2
\]

This proves the Lemma.

**Theorem 2.** If $G_c$ contains a clique of order $n$, problem (1) can attain its largest possible value.

**Proof.** Let us assume that $G_c$ contains a clique of order $n$, and let $S$ be the set of vertices that form the $n$-clique. We set $x_i = 1$ for $i \in S$, and $x_j = 0$ for $j \in V_c \setminus S$. Clearly, since $J_{i,j} = 1$ for
each $i, j \in S$, there are $n(n - 1)$ (ordered) pairs of vertices, and for each of those pairs, we have that $x_i x_j = 1$. Therefore, the objective value of problem (1) is equal to:

$$\text{trace}(JX) = n + n(n - 1) = n^2$$

By Lemma 2, the objective value is equal to the largest possible value of problem (1). Furthermore, all the constraints hold. Specifically, $\text{trace}(X) = |S| = n$, and $X_{i,j} \neq 0$ only if $i, j \in S$ (with $i \neq j$). Moreover, since matrix $X$ corresponds to the outer product of a vector and itself, it is symmetric, positive semidefinite and of rank 1.

**Theorem 3.** If $G_c$ contains no clique of order $n$, the optimal solution of problem (1) takes some value no greater than $n + (n - 1)(n - 2)$.

**Proof.** As described above, Lemma 1 implies that we can have at most $n$ vertices for which $x \neq 0$. Furthermore, since $G_c$ does not contain any $n$-clique, for each subset of vertices $S \subset V_c$ with $|S| = n$, there is at least one pair of vertices $i, j$ for which $(i, j) \notin E_c$. Then, to satisfy the condition that $X_{i,j} = 0$ if $(i, j) \notin E_c$, either $x_i = 0$ or $x_j = 0$. Hence, there can be at most $n - 1$ vertices for which $x \neq 0$. Then, the objective value of the problem is equal to:

$$\text{trace}(JX) = x_1 x_1 + \ldots + x_m x_m$$
$$= n + x_1 x_2 + \ldots + x_{m-1} x_m$$
$$\leq n + (n - 1)(n - 2)$$
$$< n^2$$

The first inequality follows from the fact that $x_i x_j \leq 1$ for any $i, j$ with $i \neq j$ (from constraint (1d)), and as mentioned above there are at most $n - 1$ vertices for which $x \neq 0$. □

### 3.2 General Case

Rank constraints in semidefinite programs are usually hard. Specifically, it turns out that problem (1) is a nonconvex problem in $X \in S_m$. If we simply drop the rank constraint, we obtain the following relaxation:

\[
\begin{align*}
\text{maximize} \quad & \text{trace}(JX) \\
\text{subject to} \quad & \text{trace}(X) = n, \quad \text{(2a)} \\
& X_{i,j} = 0, \ (i, j) \notin E_c, \quad \text{(2b)} \\
& X_{i,j} \leq 1, \ (i, j) \in E_c, \quad \text{(2c)} \\
& X \succeq 0. \quad \text{(2d)} 
\end{align*}
\]

which is a semidefinite program in $X \in S_m$. Clearly, the optimal value of problem (2) is an upper bound of the optimal value of problem (1).

We will next show that in case $G_c$ contains one or more cliques of order $n$, then the optimal value of problem (2) is equal to the optimal value of problem (1) (i.e., equal to $n^2$). Furthermore, we will show that if $G_c$ contains no cliques, then the optimal value of the problem is not greater than $n(n - 1)$.

Let $v_i \in \mathbb{R}^d$ be the vector representation of vertex $i \in V_c$, and $U = [v_1, \ldots, v_m]^\top \in \mathbb{R}^{m \times d}$ a matrix whose $i^{th}$ row contains the vector representation of vertex $i \in V_c$. Then, $X = U U^\top$.

**Lemma 3.** The value of problem (2) is no greater than $n^2$. 7
Proof. The objective value of problem (2) is equal to:

\[
\text{trace}(JX) = \sum_{i=1}^{m} \sum_{j=1}^{m} J_{i,j} X_{i,j} = J_{1,1} X_{1,1} + \ldots + J_{m,m} X_{m,m} = \langle v_1, v_1 \rangle + \ldots + \langle v_m, v_m \rangle
\]

From constraint (2b), it follows that the sum of the diagonal terms of matrix \(X\) is equal to \(n\), i.e., \(\langle v_1, v_1 \rangle + \langle v_2, v_2 \rangle + \ldots + \langle v_m, v_m \rangle = n\). We next replace these terms with their sum. Therefore, the objective function of the optimization problem becomes:

\[
\text{trace}(JX) = \sum_{i=1}^{m} \sum_{j=1}^{m} J_{i,j} X_{i,j} = n + \langle v_1, v_2 \rangle + \ldots + \langle v_m, v_{m-1} \rangle
\]  

(3)

From Lemma 1, it follows that the set of vertices \(V_c\) can be decomposed into \(n\) disjoint sets \(P_1, P_2, \ldots, P_n\) such that there is no edge that connects vertices of the same set. Then, from constraint (2c), it follows that the vector representations of vertices that belong to the same partition are pairwise orthogonal. Let \(v_1, v_2, \ldots, v_n\) denote the vector representations of the vertices that belong to partition \(P_1\), \(v_{n+1}, v_{n+2}, \ldots, v_{2n}\) denote the representations of the vertices that belong to partition \(P_2\), and so on.

Let \(w_1, w_2, \ldots, w_n\) be the sum of the representations of the vertices that belong to partitions \(P_1, P_2, \ldots, P_n\), respectively. Then, \(w_1 = v_1 + v_2 + \ldots + v_n\), \(w_2 = v_{n+1} + v_{n+2} + \ldots + v_{2n}\), and so on. Given two partitions (e.g., partitions \(P_1\) and \(P_2\)), the sum of the inner products of all pairs of vectors is equal to:

\[
\langle w_1, w_2 \rangle = \langle v_1 + v_2 + \ldots + v_n, v_{n+1} + v_{n+2} + \ldots + v_{2n} \rangle = \langle v_1, v_{n+1} \rangle + \langle v_1, v_{n+2} \rangle + \ldots + \langle v_n, v_{2n} \rangle
\]  

(4)

From the Cauchy-Schwarz inequality, it is known that \(\langle v, u \rangle \leq \sqrt{\langle v, v \rangle \langle u, u \rangle}\). Hence, for two partitions (e.g., partitions \(P_1\) and \(P_2\)), we have that:

\[
\langle w_1, w_2 \rangle \leq \sqrt{\langle w_1, w_1 \rangle \langle w_2, w_2 \rangle} = \sqrt{||w_1||^2 ||w_2||^2}
\]  

(5)

Now, since the inner product of each pair of vectors of a partition is equal to 0, for each partition (e.g., partition \(P_1\)), we have that:

\[
||w_1||^2 = \langle w_1, w_1 \rangle = \langle v_1 + \ldots + v_n, v_1 + \ldots + v_n \rangle = \langle v_1, v_1 \rangle + \ldots + \langle v_n, v_n \rangle
\]

Therefore, from constraint (2b), it follows that:

\[
||w_1||^2 + \ldots + ||w_n||^2 = n
\]  

(6)
Now, from Equation (3), we have:

\[
\text{trace}(JX) = n + \langle v_1, v_2 \rangle + \ldots + \langle v_n, v_{n-1} \rangle \\
= n + \langle w_1, w_2 \rangle + \ldots + \langle w_n, w_{n-1} \rangle \\
\leq n + \sqrt{\|w_1\|^2 \|w_2\|^2 + \ldots + \|w_n\|^2 \|w_{n-1}\|^2} \\
\leq n + \frac{\|w_1\|^2 + \|w_2\|^2 + \ldots + \|w_n\|^2 \|w_{n-1}\|^2}{2} \\
= n + \frac{(n-1)\|w_1\|^2 + (n-\|w_1\|^2) + \ldots + (n-1)\|w_n\|^2 + (n-\|w_n\|^2)}{2} \\
= n + \frac{(n-2)\|w_1\|^2 + n + \ldots + (n-2)\|w_n\|^2 + n}{2} \\
= n + \frac{(n-2)n + n^2}{2} \\
= n + \frac{2n^2 - 2n}{2} \\
= n^2
\]

The second equality follows from Equation (4), and the first inequality from Equation (5). The last inequality follows from the well-known inequality of arithmetic and geometric means, while the fourth equality follows from Equation (6). \(\square\)

Clearly, a solution to problem (1) is also a solution to problem (2). Hence, if the compatibility graph \(G_c\) contains a clique of order \(n\), the rank-1 solution that was presented above is also an optimal solution in this case. However, if \(G_c\) contains multiple cliques of order \(n\), there is an optimal solution of higher rank as shown below.

**Theorem 4.** If \(G_c\) contains \(d\) cliques of order \(n\), we can construct an optimal solution to problem (2) as follows: We assign a vector \(v_i \in \mathbb{R}^d\) to each vertex \(i \in V_c\). We consider a feature space with a feature corresponding to each one of the \(d\) cliques. If vertex \(i\) participates in the \(j^{th}\) clique, then the \(j^{th}\) component of \(v_i\) is set equal to \(\frac{1}{\sqrt{d}}\).

**Proof.** If vertices \(i, j \in V_c\) participate in all \(d\) cliques of \(G_c\), then \(\langle v_i, v_j \rangle = 1\). Otherwise, \(\langle v_i, v_j \rangle < 1\). From the above, it is clear that \(X_{i,j} \leq 1\), \(\forall (i,j) \in E_c\). If a vertex \(i\) participates in no clique, then \(v_i\) is a zero vector, and \(\langle v_i, v_j \rangle = 0\), \(\forall j \in V_c\). Furthermore, if two vertices \(i\) and \(j\) participate in one or more cliques, but \((i, j) \notin E_c\), then the two vertices participate in different cliques and they have no common components taking nonzero values, and thus \(\langle v_i, v_j \rangle = 0\). Therefore, \(X_{i,j} = 0\), \(\forall (i,j) \notin E_c\). Furthermore, we have that:

\[
\text{trace}(X) = \langle v_1, v_1 \rangle + \ldots + \langle v_m, v_m \rangle = \sum_{i=1}^{d} (v_i^1 v_1^1 + \ldots + v_i^m v_m^1)
\]

where \(v^i\) denotes the \(i^{th}\) component of vector \(v\). Since each clique contains \(n\) vertices, there are \(n\) vectors whose \(i^{th}\) component is nonzero and equal to \(\frac{1}{\sqrt{d}}\). Hence, it follows that:

\[
\text{trace}(X) = \sum_{i=1}^{d} n \frac{1}{\sqrt{d}} = n
\]
Since each clique contains $n$ vertices, there are $n(n-1)$ pairs of vertices $i,j \in V_c$ such that $(i,j) \in E_c$. Furthermore, since these vertices participate in a clique, their component that corresponds to that clique is equal to $\frac{1}{\sqrt{d}}$, and therefore, the product of these components is equal to $\frac{1}{d}$. Since there are $n(n-1)$ such pairs for each clique, it follows that:

$$\text{trace}(JX) = n + \sum_{i=1}^{d} n(n-1) \frac{1}{d} = n + n(n-1) = n^2$$

This concludes the proof.

Figure 2 illustrates how an optimal solution is constructed for the compatibility graph of Figure 1. There are two cliques of order 3 in this graph. Therefore, we assign a 2-dimensional vector to each of its vertices.
Theorem 5. If $G_c$ contains no clique of order $n$, the optimal solution of problem (2) takes some value no greater than $n(n - 1)$.

Proof. From the Cauchy-Schwarz inequality, it is known that $\langle v, u \rangle \leq \sqrt{\langle v, v \rangle \langle u, u \rangle}$. Furthermore, for nonzero vectors, equality holds if and only if $v$ and $u$ are linearly dependent (i.e., either $v$ is a multiple of $u$ or the opposite). As shown above, by applying the Cauchy-Schwarz inequality, we obtain:

$$\text{trace}(JX) = n + \langle v_1, v_2 \rangle + \ldots + \langle v_m, v_{m-1} \rangle$$
$$= n + \langle w_1, w_2 \rangle + \ldots + \langle w_n, w_{n-1} \rangle$$
$$\leq n + \sqrt{||w_1||^2||w_2||^2 + \ldots + ||w_n||^2||w_{n-1}||^2}$$

Equality (between the last two quantities) holds if and only if the $n$ vectors $w_1, w_2, \ldots, w_n$ are pairwise linearly dependent. Let us assume that these vectors are pairwise linearly dependent. Then, without loss of generality, let us also assume that the $i^{th}$ component of the first vector $w_1$ is nonzero. Since the vectors are linearly dependent, then the $i^{th}$ component of all the other vectors $w_2, \ldots, w_n$ is also nonzero. Since each vector is equal to the sum of orthogonal vectors (sum of representations of vertices of each partition), for all $n$ partitions there exists some vector (corresponding to some vertex of that partition) whose $i^{th}$ component is nonzero. Then, there exist $n$ vectors whose $i^{th}$ component is nonzero, and hence the inner product of every pair of these vectors is nonzero. That means that every pair of these vertices is connected by an edge (from constraints (2c) and (2d)). Hence, these vertices form a clique of order $n$. We have reached a contradiction since $G_c$ does not contain a clique of order $n$. Therefore, the objective function is:

$$\text{trace}(JX) = n + \langle v_1, v_2 \rangle + \ldots + \langle v_m, v_{m-1} \rangle$$
$$= n + \langle w_1, w_2 \rangle + \ldots + \langle w_n, w_{n-1} \rangle$$
$$< n + \sqrt{||w_1||^2||w_2||^2 + \ldots + ||w_n||^2||w_{n-1}||^2}$$
$$\leq n + \frac{||w_1||^2 + ||w_2||^2 + \ldots + ||w_n||^2||w_{n-1}||^2}{2}$$
$$= n^2$$

We will now establish an upper bound on the value of the objective function. We have that:

$$\text{trace}(JX) = n + \langle v_1, v_2 \rangle + \ldots + \langle v_m, v_{m-1} \rangle$$
$$= n + \langle w_1, w_2 \rangle + \ldots + \langle w_n, w_{n-1} \rangle$$
$$= n + \sum_{i=1}^{d} (w_1^i w_2^i + \ldots + w_n^i w_{n-1}^i)$$

where $w_i^i$ denotes the $i^{th}$ component of vector $w$. We also have that:

$$\text{trace}(X) = \langle v_1, v_1 \rangle + \langle v_2, v_2 \rangle + \ldots + \langle v_m, v_m \rangle$$
$$= \langle w_1, w_1 \rangle + \langle w_2, w_2 \rangle + \ldots + \langle w_n, w_n \rangle$$
$$= \sum_{i=1}^{d} (w_1^i w_1^i + w_2^i w_2^i + \ldots + w_n^i w_n^i) = n$$

Since $G_c$ contains no cliques of order $n$, for each component $i$ of $w_1, w_2, \ldots, w_n$, at most $n - 1$ out of these $n$ vectors can have a nonzero value. Hence, for each $i \in \{1, 2, \ldots, d\}$, at least one
of the following $n$ components $w_1^i, w_2^i, \ldots, w_n^i$ is equal to zero. Therefore, for each $i$, at most $(n-1)(n-2)$ of the terms of the following summation are nonzero:

$$
\text{trace}(JX) = n + \sum_{i=1}^{d} (w_1^i w_2^i + \ldots + w_n^i w_{n-1}^i)
$$

where $z_i$ denotes the contribution of the $i^{th}$ component to the above summation, i.e., $z_i = w_1^i w_2^i + \ldots + w_n^i w_{n-1}^i$. Let us assume that for a given $i$, $w_j^i$ is equal to zero. Then, we have that:

$$
z_i = w_1^i w_2^i + \ldots + w_d^i w_{d-1}^i + \ldots + w_n^i w_{n-1}^i
$$

where $z_i$ denotes the contribution of the $i^{th}$ component to the above summation, i.e., $z_i = w_1^i w_2^i + \ldots + w_n^i w_{n-1}^i$. Let us assume that for a given $i$, $w_j^i$ is equal to zero. Then, we have that:

$$
z_i = w_1^i w_2^i + \ldots + w_d^i w_{d-1}^i + \ldots + w_n^i w_{n-1}^i
$$

The inequality follows from the fact that for two scalars $a$ and $b$, $\frac{a^2 + b^2}{2} \geq ab$ always holds. Furthermore, the last equality holds since we have assumed that $w_j^i = 0$. From Equation (8), we have:

$$
\text{trace}(JX) = n + \sum_{i=1}^{d} (w_1^i w_2^i + \ldots + w_n^i w_{n-1}^i)
$$

The inequality follows from Equation (9), while the last equality follows from Equation (7). This concludes the proof.

Note that problem (2) has a strictly feasible solution, i.e., a solution that satisfies the positive semidefiniteness requirement strictly. For instance, by setting $X_{i,i} = \frac{1}{n}$ for $i \in 1, \ldots, m$ and $X_{i,j} = 0$ for $i, j \in 1, \ldots, m$ with $i \neq j$, we obtain a positive definite feasible solution, i.e., $X > 0$ and all constraints are satisfied. Therefore, strong duality holds [23]. There is an algorithm that for any $\epsilon > 0$, returns a rational closer than $\epsilon$ to the solution of problem (2) in time bounded by a polynomial in $n$ and $\log(1/\epsilon)$ [21]. We can thus find a number closer than $\frac{1}{2}$ to the optimal value of problem (2) in time polynomial in $n$. By comparing this number with $n^2$, we can answer if the compatibility graph contains a clique of order $n$ or not.
4 Conclusion

In this paper, we have presented an algorithm for the graph isomorphism problem. The algorithm capitalizes on previous results that transform the problem into an equivalent problem of determining whether there exists a clique of specific order in an auxiliary graph structure. We have shown that the answer to the above question can be given by solving a semidefinite program. Given the frequent use of semidefinite programming in the design of algorithms [24, 25, 26], it seemed worthwhile to investigate its effectiveness in addressing the graph isomorphism problem. The results of this paper constitute a first step in this direction. This paper still leaves some open questions. Studying the dual of the proposed semidefinite program is perhaps the most interesting of them.

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References


