On the graph isomorphism problem

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Abstract

We relate the graph isomorphism problem to the solvability of certain systems of linear equations and linear inequalities. The number of these equations and inequalities is related to the complexity of the graphs isomorphism and subgraph isomorphim problems.

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1 Introduction

Let $G_1 = (V, E_1), G_2 = (V, E_2)$ be two simple undirected graphs, where V is the set of vertices of cardinality n and $E_1, E_2 \subset V \times V$ the set of edges. G_1 and G_2 are called *isomorphic* if there exists a bijection $\sigma : V \to V$ which induces the corresponding bijection $\tilde{\sigma} : E_1 \to E_2$. The graph isomorphism problem, abbreviated here as *GIP*, is the problem of determination if G_1 and G_2 are isomorphic. Clearly the *GIP* in the class *NP*. It is one of a very small number of problems whose complexity is unknown [4, 6]. For certain graphs it is known that the complexity of *GIP* is polynomial [1, 2, 3, 5, 9, 10].

Let $G_3 = (W, E_3)$, where $\#W = m \le n$. G_3 is called isomorphic to a subgraph of G_2 if there exits an injection $\tau : V_3 \to V_2$ which induces an injection $\tilde{\tau} : E_3 \to E_2$. The subgraph isomorphism, abbreviated here as *SGIP*, is the problem of determination if G_3 is isomorphic to a subgraph of G_2. It is well known that SGIP is *NP-Complete* [4].

In the previous versions of this paper we related the graph isomorphism problem to the solvability of certain systems of linear equations and linear inequalities. It was pointed out to me by N. Alon and L. Babai, that my approach relates in a similar way the SGIP to the solvability of certain systems of linear equations and linear inequalities. Hence $f(n)$, the number of these linear equalities and inequalities for $V = n$, is probably exponential in n. Thus, the suggested approach in this paper does not seem to be the right approach to determine the complexity of the

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GIP. Nevertheless, in this paper we summarize the main ideas and results of this approach. It seems that our approach is related to the ideas and results discussed in [11].

Let $\Omega_n \subset \mathbb{R}_+^{n\times n}$ be the convex set of $n \times n$ doubly stochastic matrices. In this paper we relate the complexity of the *GIP* to the minimal number of supporting hyperplanes determining a certain convex polytope $\Psi_{n,n} \subset \Omega_{n^2}$. More precisely, two graph are isomorphic if certain system of n^2 hyperplanes intersect $\Psi_{n,n}$. More general, if the corresponding system n^2 half spaces intersect $\Psi_{n,n}$ then G_3 is isomorphic to a subgraph of G_2. Hence the minimal number of supporting hyperplanes defining $\Psi_{n,n}$, denoted by $f(n)$, is closely related to the complexity of *SGIP*. We give a larger polytope $\Phi_{n,n}$, characterized by $(4n-1)n^2$ linear equations in n^4 nonnegative variables satisfying

$$\Psi_{n,n} \subset \Phi_{n,n} \subset \Omega_{n^2}. \tag{1.1}$$

In the first version of this paper we erroneously claimed that $\Phi_{n,n} = \Psi_{n,n}$. The error in my proof was pointed out to me by Babai, Melkebeek, Rosenberg and Vavasis. The inequality $\Psi_{n,n} \subsetneqq \Phi_{n,n}$ for $n \geq 4$ is implied by the example of J. Rosenberg.

Thus if two graphs are isomorphic then certain system of n^2 hyperplanes intersect $\Phi_{n,n}$. This of course yields a necessary conditions for GIP and SGIP.

We now outline the main ideas of the paper. Let A, B be $n \times n$ adjacency matrices of G_1, G_2. So A, B are $0-1$ symmetric matrices with zero diagonal. It is enough to consider the case where A and B have the same number of 1's. Let $\mathcal{P}_n$ be the set of $n \times n$ permutation matrices. Then G_1 and G_2 are isomorphic if and only if $PAP^\top = B$ for some $P \in \mathcal{P}_n$. It is easy to see that this condition is equivalent

$$P(A + 2I_n)Q^\top = B + 2I_n \text{ for some } P, Q \in \mathcal{P}_n, \tag{1.2}$$

where I_n is the $n \times n$ identity matrix.

For $C, D \in \mathbb{R}^{n\times n}$ denote by $C \otimes D \in \mathbb{R}^{n^2\times n^2}$ the Kronecker product, see §2. Let $\mathcal{P}_n \otimes \mathcal{P}_n := \{P \otimes Q,\ P, Q \in \mathcal{P}_n\}$. Denote by $\Psi_{n,n} \subset \mathbb{R}_+^{n^2\times n^2}$ the convex set spanned by $\mathcal{P}_n \otimes \mathcal{P}_n$. $\Psi_{n,n}$ is a subset of $n^2 \times n^2$ doubly stochastic matrices. Then the condition (1.2) implies the solvability of the system of n^2 equations of the form $Z(\widehat{A + 2I_n}) = \widehat{B + 2I_n}$ for some $Z \in \Psi_{n,n}$. Here $\widehat{B + 2I_n} \in \mathbb{R}^{n^2}$ is a column vector composed of the columns of $B + 2I_n$. Vice versa, the solvability of $Z(\widehat{A + 2I_n}) = \widehat{B + 2I_n}$ for some $Z \in \Psi_{n,n}$ implies (1.2). The ellipsoid algorithm in linear programming [8, 7] yields that the existence a solution to this system of equations is determined in polynomial time in $\max(f(n), n)$. Similarly, for the SGIP one needs to consider the the solvability of $Z(\widehat{C + 2^{n^2}I_n}) \leq \widehat{B + 2^{n^2}I_n}$ for some $Z \in \Psi_{n,n}$, where C is the adjacency matrix of the graph $\tilde{G}_3 = (V, E_3)$ obtained from G_3 by appending $n - m$ isolated vertices.

We now survey briefly the contents of this paper. In §2 we introduce the needed concepts from linear algebra to give the characterization of $\Phi_{n,n}$ in terms of $(4n-2)n^2$ linear equations in n^4 nonnegative variables. This is done for the general set $\Phi_{m,n}$, which contains $\Psi_{m,n}$, the convex hull of $\mathcal{P}_m \otimes \mathcal{P}_n$. §3 discusses the permutational similarity of $A, B \in \mathbb{R}^{n\times n}$ and permutational equivalence of $A, B \in \mathbb{R}^{n\times m}$. We show the second main result that the permutational similarity and equivalence is equivalent to solvability of the corresponding system of equations discussed above. In §4 we deduce the complexity results claimed in this paper.

This paper generated a lot of interest. I would like to thank all the people who sent their comments to me.

2 Tensor products of doubly stochastic matrices

For $m \in \mathbb{N}$ denote $\langle m \rangle := \{1, \ldots, m\}$. For $\mathcal{A} \subset \mathbb{R}$ denote by $\mathcal{A}^{m\times n}$ the set of $m \times n$ matrices $A = [a_{ij}]_{i,j=1}^{m,n}$ such that each $a_{ij} \in \mathcal{A}$. Recall that $A = [a_{ij}] \in \mathbb{R}_+^{m\times m}$ is called doubly stochastic if

$$\sum_{j=1}^{m} a_{ij} = \sum_{j=1}^{m} a_{ji} = 1, \quad i = 1, \ldots, m. \tag{2.1}$$

Since the sum of all rows of A is equal to the sum of all columns of A it follows that at most $2m-1$ of above equations are linearly independent. It is well known that any $2m-1$ of the above equation are linearly independent. Let $\mathbf{1} := (1, \ldots, 1)^\top \in \mathbb{R}_+^m$. Note that $A = [a_{ij}] \in \mathbb{R}^{m\times m}$ satisfies (2.1) if and only if and $A\mathbf{1} = A^\top \mathbf{1} = \mathbf{1}$.

Denote by Ω_m the set of doubly stochastic matrices. Clearly, Ω_m is a convex compact set. Birkhoff theorem claims that the set of the extreme points of Ω_m is the set of permutations matrices $\mathcal{P}_m \subset \{0,1\}^{m\times m}$.

Lemma 2.1 *Denote by $\Lambda_m \subset \mathbb{R}_+^{m\times m}$ the set of nonnegative matrices satisfying the conditions $A\mathbf{1} = A^\top\mathbf{1} = a\mathbf{1}$ for some $a \ge 0$ depending on A. Then Λ_m is a multiplicative cone:*

$$\Lambda_m + \Lambda_m = \Lambda_m, \ a\Lambda_m \subset \Lambda_m \textit{ for all } a \ge 0, \ \Lambda_m \cdot \Lambda_m = \Lambda_m.$$

Furthermore, $A = [a_{ij}] \in \mathbb{R}_+^{m\times m}$ is in Λ_m if and only if the following $2(m-1)$ equalities hold.

$$\sum_{j=1}^{m} a_{ij} = \sum_{j=1}^{m} a_{ji} = \sum_{j=1}^{m} a_{1j} \textit{ for } i = 2, \ldots, m. \tag{2.2}$$

Proof. The fact that Λ_m is a cone is straightforward. Since $I_m \in \Lambda_m$ we deduce the equality $\Lambda_m \cdot \Lambda_m = \Lambda_m$. Observe next that the conditions (2.2) imply that $A\mathbf{1} = a\mathbf{1}$, where a is the sum of the elements in the first row. Also the sum of the elements in each column except the first is equal to a. Since the sum of all elements of A is ma it follows that the sum of the elements in the first column is also a, i.e $A^\top\mathbf{1} = a\mathbf{1}$. □

For $A = [a_{ij}] \in \mathbb{R}^{m\times m}, B = [b_{kl}] \in \mathbb{R}^{n\times n}$ denote by $A \otimes B \in \mathbb{R}^{mn\times mn}$ the tensor product of A and B. The rows and columns of $A \otimes B$ are indexed by double indices (i,k) and (j,l), where $i,j = 1, \ldots m, \ k,l = 1, \ldots, n$. Thus

$$A \otimes B = [c_{(i,k)(j,l)}] \in \mathbb{R}^{mn\times mn}, \tag{2.3}$$

where $c_{(i,k)(j,l)} = a_{ij}b_{kl}$ for $i,j = 1, \ldots, m, \ k,l = 1, \ldots, n$.

If we arrange the indices (i,k) in the lexicographic order then $A \otimes B$ has the following block matrix form called the *Kronecker product*

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1m}B \\ a_{21}B & a_{22}B & \dots & a_{2m}B \\ \vdots & \vdots & \dots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mm}B \end{bmatrix}. \tag{2.4}$$

For simplicity of the exposition we will identify $A \otimes B$ with the block matrix (2.4) unless stated otherwise. Note that any other ordering of $\langle m \rangle \times \langle n \rangle$ induces a different representation of $A \otimes B$ as $C \in \mathbb{R}^{mn \times mn}$, where $C = P(A \otimes B)P^\top$ for some permutation matrix $P \in \mathcal{P}_{mn}$.

Recall that $A \otimes B$ is bilinear in A and B. Furthermore

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) \text{ for all } A, C \in \mathbb{R}^{m \times m},\ B, D \in \mathbb{R}^{n \times n}. \tag{2.5}$$

Proposition 2.2 *Let $A \in \Omega_m, B \in \Omega_n$. Then $A \otimes B \in \Omega_{mn}$.*

Proof. Clearly $A \otimes B$ is a nonnegative matrix. Assume the representation (2.3). Then

$$\sum_{j,l=1}^{m,n} c_{(i,k)(j,l)} = \sum_{j,l=1}^{m,n} a_{ij} b_{kl} = (\sum_{j=1}^{m} a_{ij})(\sum_{l=1}^{n} b_{kl}) = 1 \cdot 1 = 1,$$
$$\sum_{j,l=1}^{m,n} c_{(j,l)(i,k)} = \sum_{j,l=1}^{m,n} a_{ji} b_{lk} = (\sum_{j=1}^{m} a_{ji})(\sum_{l=1}^{n} b_{lk}) = 1 \cdot 1 = 1.$$

□

Lemma 2.3 *Denote by $\Psi_{m,n} \subset \Omega_{mn}$ the convex hull spanned by $\Omega_m \otimes \Omega_n$, i.e. all doubly stochastic matrices of the form $A \otimes B$, where $A \in \Omega_m,\ B \in \Omega_n$. Then the extreme points of $\Psi_{m,n}$ is the set $\mathcal{P}_m \otimes \mathcal{P}_n$, i.e. each extreme point is of the form $P \otimes Q$, where $P \in \mathcal{P}_m, Q \in \mathcal{P}_n$.*

Proof. Use Birkhoff's theorem and the bilinearity of $A \otimes B$ to deduce that $\Psi_{m,n}$ is spanned by $\mathcal{P}_m \otimes \mathcal{P}_n$. Clearly $\mathcal{P}_m \otimes \mathcal{P}_n \subset \mathcal{P}_{mn}$. Since Birkhoff's theorem implies that $\mathcal{P}_{mn}$ are extreme points of Ω_{mn} it follows that $\mathcal{P}_m \otimes \mathcal{P}_n \subset \mathcal{P}_{mn}$ are convexly independent. □

Theorem 2.4 *Let $\Phi_{m,n}$ be the convex set of $mn \times mn$ nonnegative matrices characterized by $2mn+(2n-2)m^2+(2m-2)n^2$ linear equations of the following form. View $C \in \mathbb{R}^{mn \times mn}$ as a matrix with entries $c_{(i,k)(j,l)}$ where $i, j = 1, \dots, m,\ k, l = 1, \dots, n$. Then $C \in \mathbb{R}_+^{mn \times mn}$ belongs to $\Phi_{m,n}$ if the following equalities hold.*

$$\sum_{j,l=1}^{m,n} c_{(i,k),(j,l)} = \sum_{j,l=1}^{m,n} c_{(j,l)(i,k)} = 1,\ i = 1,\ldots,m,\ k = 1,\ldots,n, \tag{2.6}$$

$$\sum_{j=1}^{m} c_{(i,k)(j,l)} = \sum_{j=1}^{m} c_{(1,k)(j,l)},\ \sum_{j=1}^{m} c_{(j,k)(i,l)} = \sum_{j=1}^{m} c_{(1,k)(j,l)} \tag{2.7}$$

$$\text{where } i = 2,\ldots,m \text{ and } k,l = 1,\ldots,n,$$

$$\sum_{l=1}^{n} c_{(i,k)(j,l)} = \sum_{l=1}^{n} c_{(i,1)(j,l)},\ \sum_{l=1}^{n} c_{(i,l)(j,k)} = \sum_{l=1}^{n} c_{(i,1)(j,l)} \tag{2.8}$$

$$\text{where } k = 2,\ldots,n \text{ and } i,j = 1,\ldots,m.$$

Furthermore

$$\Psi_{m,n} \subset \Phi_{m,n} \subset \Omega_{mn} \tag{2.9}$$

Proof. The conditions (2.6) state that $C \in \Omega_{mn}$. We now show the conditions $\Psi_{m,n} \subseteq \Phi_{m,n}$. Let $A \in \Omega_m, B \in \Omega_n$ and consider the Kronecker product (2.4). Then for $i,j \in \langle m\rangle$, the (i,j) block of $A \otimes B$ is $a_{ij}B \in \Lambda_n$. Since Λ_n is a cone, it follows that for any $C \in \Psi_{m,n}$, having the block form $C = [C_{ij}],\ C_{ij} \in \mathbb{R}_+^{n\times n},\ i,j \in \langle m\rangle$, each $C_{ij} \in \Lambda_n$. Lemma 2.1 yields the conditions for each $i,j \in \langle m\rangle$. Since $A \otimes B = P(B \otimes A)P^\top$ we also deduce the conditions (2.7) for each $k,l \in \langle n\rangle$. □

Lemma 2.5 $\Psi_{2,2} = \Phi_{2,2}$.

Proof. Let $D = [d_{pq}]_{p,q=1}^4 \in \Phi_{2,2}$. Since

$$F_{11} := \begin{bmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{bmatrix}, F_{12} := \begin{bmatrix} d_{13} & d_{14} \\ d_{23} & d_{24} \end{bmatrix} \in \Lambda_2$$

it follows that

$$d_{11} = d_{22} = a,\ d_{12} = d_{21} = b,\ d_{13} = d_{24} = c,\ d_{14} = d_{23} = d.$$

Since

$$G_{11} := \begin{bmatrix} d_{11} & d_{13} \\ d_{31} & d_{33} \end{bmatrix}, G_{12} := \begin{bmatrix} d_{12} & d_{14} \\ d_{32} & d_{34} \end{bmatrix} \in \Lambda_2$$

it follows that

$$d_{31} = c,\ d_{32} = d,\ d_{33} = a,\ d_{34} = b.$$

Since

$$F_{21} := \begin{bmatrix} d_{31} & d_{32} \\ d_{41} & d_{42} \end{bmatrix}, F_{22} := \begin{bmatrix} d_{33} & d_{34} \\ d_{43} & d_{44} \end{bmatrix} \in \Lambda_2$$

it follows that

$$d_{41} = d,\ d_{42} = c,\ d_{43} = b,\ d_{44} = b.$$

So $a,b,c,d \geq 0$ and $a+b+c+d = 1$. This set has 4 extreme points which form the set $\mathcal{P}_2 \otimes \mathcal{P}_2$. □

The following result was communicated to me by J. Rosenberg. Recall that $P \in \mathcal{P}_n$ is called a *cyclic* permutation if $\sum_{i=1}^n P^i$ is a matrix whose all entries are equal to 1.

Lemma 2.6 *Let $P, Q \in \mathcal{P}_n$ be cyclic permutations. Then the block matrix $D = \frac{1}{n}[P^i Q^j]_{i,j=1}^n$ belongs to $\Phi_{n,n}$. If $P \neq Q^i$ for $i = 1, \ldots, n-1$ then $D \notin \Psi_{n,n}$. In particular $\Psi_{n,n} \subsetneqq \Phi_{n,n}$ for $n \geq 4$. For $n = 3$ each D of the above form is in $\Psi_{3,3}$.*

Proof. Since $P^i, Q^j \in \Omega_n$ it follows that $P^i Q^j \in \Omega_n$ for $i, j = 1, \ldots, n$. Hence the conditions (2.8) and (2.6) are satisfied. It is left to show the conditions (2.7). Denote $A^i = [a_{kp}^{(i)}]_{k,p=1}^n, B^j = [b_{pl}^{(j)}]_{p,l=1}^n \in \Omega_n$. View $D = [c_{(i,k)(j,l)}]$. Then

$$c_{(i,k)(j,l)} = \frac{1}{n} \sum_{p=1}^{n} a_{kp}^{(i)} b_{pl}^{(j)}, \quad i, j, k, l = 1, \ldots, n. \tag{2.10}$$

Since $\sum_{j=1}^n b_{pl}^{(j)} = 1$ for $p, l = 1, \ldots, n$ and $A^i \in \Omega_n$ we obtain $\frac{1}{n}\sum_{j=1} c_{(i,k)(j,l)} = \frac{1}{n}\sum_{p=1}^n a_{kp}^{(i)} = \frac{1}{n}$. In a similar way we deduce that $\sum_{j=1}^n c_{(j,k)(i,l)} = \frac{1}{n}$. So $D \in \Phi_{n,n}$.

Suppose that $D \in \Psi_{n,n}$. Observe that $P^n Q^n = I_n I_n = I_n$. Assume D as a convex combination of some extreme points $U \otimes V \in \mathcal{P}_n \otimes \mathcal{P}_n$ with positive coefficients. Express $U \otimes V$ as a block matrix $[(U \otimes V)_{ij}]_{i,j=1}^n$. Suppose furthermore that $(U \otimes V)_{nn} \neq 0_{n \times n}$. Then $V = I_n$. Hence there exists $j \in \langle n-1 \rangle$ such $PQ^j = I$, i.e $P = Q^{n-j}$. If P is not a power of Q we deduce that $D \notin \Psi_{n,n}$. For $n \geq 4$ it is easy to construct such two permutations. For example, let P and Q are represented by the cycles

$$1 \to 3 \to 2 \to 4 \to \ldots \to n \to 1, \; 1 \to 2 \to 3 \to 4 \to \ldots \to n \to 1.$$

If $n = 3$ then one has only two cycles R and R^2. A straightforward calculation show that if $P, Q \in \{R, R^2\}$ the $D \in \Psi_{3,3}$. □

Note that the system (2.6) has $2mn - 1$ linear independent equations. Since any permutation matrix is an extreme point in Ω_{mn} we deduce.

Corollary 2.7 *The convex set $\Phi_{m,n} \subset \mathbb{R}_+^{mn \times mn}$ is given by at most $2((n-1)m^2 + (m-1)n^2 + mn) - 1$ linear equations. It contains all the extreme points $\mathcal{P}_m \otimes \mathcal{P}_n$ of $\Psi_{m,n}$.*

It is interesting to understand the structure of the set $\Phi_{m,n}$ and to characterize it extreme points. It is easy to characterize the following larger set.

Lemma 2.8 *Let $\Theta_{m,n}$ be the convex set of $mn \times mn$ nonnegative matrices characterized by $2mn + (2n-2)m^2$ linear equations of the following form. View $C \in \mathbb{R}^{mn \times mn}$ as a matrix with entries $c_{(i,k)(j,l)}$ where $i, j = 1, \ldots, m, \; k, l = 1, \ldots, n$. Then $C \in \mathbb{R}_+^{mn \times mn}$ belongs to $\Theta_{m,n}$ if the equalities (2.6) and (2.8) hold. Then $\Phi_{m,n} \subset \Theta_{m,n} \subset \Omega_{mn}$. Furthermore, any $C = [C_{ij}]_{i,j=1}^m \in \Theta_{m,n}$ is of the following form*

$$C_{ij} = a_{ij} D_{ij}, \; D_{ij} \in \Omega_n, \; i, j = 1, \ldots, m, \; A = [a_{ij}]_{i,j=1}^m \in \Omega_m. \tag{2.11}$$

In particular, the extreme points of $\Theta_{m,n}$ are of the the above form where $A \in \mathcal{P}_m, D_{ij} \in \mathcal{P}_n$ for $i, j = 1, \ldots, n$.

Proof. Observe first that C in the block from $C = [C_{ij}]$, $C_{ij} \in \mathbb{R}^{n\times n}$ where $C_{ij} \in \mathbb{R}^{n\times n}_+$. Conditions (2.8) equivalent to the assumptions that $C_{ij} \in \Lambda_n$. Hence $C_{ij} = f_{ij}D_{ij}$ for some $D_{ij} \in \Omega_n$ and $f_{ij} \geq 0$. If $f_{ij} = 0$ we can choose any $D_{ij} \in \Omega_n$. If $f_{ij} > 0$ then D_{ij} is a unique doubly stochastic matrix. Let $F = [f_{ij}] \in \mathbb{R}^{m\times m}$. Then the conditions (2.6) are equivalent to the condition that $F \in \Omega_m$. Thus the conditions (2.8) and (2.6) are equivalent to the statement that $C = [f_{ij}D_{ij}]$ where each $D_{ij} \in \Omega_n$ and $F = [f_{ij}] \in \Omega_m$.

Since the extreme points of Ω_n are $\mathcal{P}_n$ we deduce that any extreme point of $\Theta_{m,n}$ is of the block form $C = [f_{ij}P_{ij}]$ where each $P_{ij} \in \mathcal{P}_n$. Since the extreme points of Ω_m are $\mathcal{P}_m$ it follows that the extreme points of $\Theta_{m,n}$ are of the form $E = [E_{ij}]$ satisfying the following conditions. There exists a permutation $\sigma : \langle m\rangle \to \langle m\rangle$ such that $E_{i\sigma(i)} \in \mathcal{P}_n$ for $i = 1, \ldots, m$ and $E_{ij} = 0_{m\times m}$ otherwise. □

3 Permutational similarity and equivalence of matrices

For $A \in \mathbb{R}^{n\times n}$ denote by $\operatorname{tr} A$ the *trace* of A. Recall that $\langle A, B\rangle$, the standard inner product on $\mathbb{R}^{n\times n}$, is given by $\operatorname{tr} AB^\top$.

We say that $A, B \in \mathbb{R}^{n\times n}$ are permutationally similar, and denote it by $A \sim B$ if $B = PAP^\top$. Clearly, if $A \sim B$ then A and B have the same characteristic polynomial, i.e. $\det(xI_n - A) = \det(xI_n - B)$. In what follows we need the following three lemmas. The proof of the first two straightforward and is left to the reader.

Lemma 3.1 *Let $A = [a_{ij}], B = [b_{ij}] \in \mathbb{R}^{n\times n}$. Assume $A \sim B$. Then the following conditions hold.*

$$P(a_{11}, \ldots, a_{nn})^\top = (b_{11}, \ldots, b_{nn})^\top \text{ for some } P \in \mathcal{P}_n, \tag{3.1}$$

$$R(a_{12}, \ldots, a_{1n}, a_{21}, a_{23}, \ldots, a_{2n}, \ldots, a_{n1}, \ldots, a_{n(n-1)})^\top = \tag{3.2}$$

$$(b_{12}, \ldots, b_{1n}, b_{21}, b_{23}, \ldots, b_{2n}, \ldots, b_{n1}, \ldots, b_{n(n-1)})^\top \text{ for some } R \in \mathcal{P}_{n^2-n}.$$

Lemma 3.2 *Assume that $A, B \in \mathbb{R}^{n\times n}$ satisfy the conditions (3.1) and (3.2). Then $\operatorname{tr}(A + tI_n)(A + tI_n)^\top = \operatorname{tr}(B + tI_n)(B + tI_n)^\top$ for each $t \in \mathbb{R}$.*

Lemma 3.3 *Let $A = [a_{ij}], B = [b_{ij}] \in \mathbb{R}^{n\times n}$ satisfy the conditions (3.1) and (3.2). Fix $t \in R$ such that $t \neq a_{ij} - a_{kk}$ for each $i, j, k \in \langle n\rangle$ such that $i \neq j$. Then the following conditions are equivalent.*

1. *$A \sim B$.*

2. *$B + tI_n = P(A + tI_n)Q^\top$ for some $P, Q \in \mathcal{P}_n$.*

Proof. Suppose that *2* holds. Hence there exists two permutations $\sigma, \eta : \langle n\rangle \to \langle n\rangle$ such that

$$b_{ij} + t\delta_{ij} = a_{\sigma(i)\eta(j)} + t\delta_{\sigma(i)\eta(j)} \quad \text{for all } i, j \in \langle n\rangle.$$

Assume that $\sigma \neq \eta$. Then there exists $i \neq j \in \langle n\rangle$ such that $\sigma(i) = \eta(j) = k$. Hence $b_{ij} = a_{kk} + t$. The condition (3.2) implies that $b_{ij} = a_{i_1j_1}$ for some $i_1 \neq j_1 \in \langle n\rangle$.

So $t = a_{i_1 j_1} - a_{kk}$, which contradicts the assumptions of the lemma. Hence $\sigma = \eta$ which is equivalent to $P = Q$. Thus

$$B + tI_n = P(A + tI_n)P^\top = PAP^\top + tI_n \Rightarrow B = PAP^\top.$$

Reverse the implication in the above statement to deduce *2* from *1*. □

We recall standard facts from linear algebra.

Lemma 3.4 *Let $X = [x_{lj}]_{l,j=1}^{n,m} = [\mathbf{x}_1\ \mathbf{x}_2 \ldots \mathbf{x}_m] \in \mathbb{R}^{n\times m}$, where $\mathbf{x}_1, \ldots, \mathbf{x}_m \in \mathbb{R}^n$ are the m columns of X. Denote by $\hat{X} \in \mathbb{R}^{mn}$ the column vector composed of the columns of X, i.e. $(\hat{X})^\top = (\mathbf{x}_1^\top, \mathbf{x}_2^\top, \ldots, \mathbf{x}_m^\top)$. Let $A = [a_{ij}] \in \mathbb{R}^{m\times m}, B = [b_{kl}] \in \mathbb{R}^{n\times n}$. Consider the linear transformation of $\mathbb{R}^{m\times n}$ to itself given by $X \mapsto BXA^\top = [(BXA^\top)_{ki}]_{k,i=1}^{n,m}$:*

$$(BXA^\top)_{ki} = \sum_{j,l=1}^{m,n} a_{ij} b_{kl} x_{lj}, \quad k = 1, \ldots, n,\ i = 1, \ldots, m. \tag{3.3}$$

Then this linear transformation is represented by the Kronecker product $A \otimes B$. That is,

$$\widehat{BXA^\top} = (A \otimes B)\hat{X} \quad \text{for all } X \in \mathbb{R}^{n\times m}. \tag{3.4}$$

Proof. Observe first that $BX = [B\mathbf{x}_1\ B\mathbf{x}_2 \ldots B\mathbf{x}_m]$. This shows (3.4) in the case $A = I_m$. Consider now the case $B = I_n$. A straightforward calculation shows that $(A \otimes I_n)\hat{X} = \widehat{XA^\top}$. Since $A \otimes B = (A \otimes I_n)(I_m \otimes B)$ we deduce the equality (3.4). □

Theorem 3.5 *Let $A = [a_{ij}], B = [b_{ij}] \in \mathbb{R}^{n\times n}$. The following conditions are equivalent.*

1. *$A \sim B$.*
2. *The following conditions hold.*
   - *(a) The conditions (3.1) and (3.2) hold.*
   - *(b) Fix $t \in R$ such that $t \neq a_{ij} - a_{kk}$ for each $i, j, k \in \langle n\rangle$ such that $i \neq j$. Then there exists $Z \in \Psi_{n,n}$ satisfying $Z(\widehat{A + tI_n}) = \widehat{B + tI_n}$.*

Proof. Assume *1*. So $B + tI_n = P(A + tI_n)P^\top$ for some $P \in \mathcal{P}_n$ and each $t \in \mathbb{R}$. Use Lemma 3.4 to deduce that $(P \otimes P)(\widehat{A + tI_n}) = \widehat{B + tI_n}$. Hence the condition *2b* holds. Lemma 3.1 yields the conditions (3.1) and (3.2).

Assume *2*. Use Lemma 3.2 yields that $\operatorname{tr}(A + tI_n)(A + tI_n)^\top = \operatorname{tr}(B + tI_n)(B + tI_n)^\top$. We claim that

$$\max_{P,Q\in\mathcal{P}_n} \operatorname{tr} P(A + tI_n)Q^\top(B + tI_n)^\top = \max_{Y\in\Psi_{n,n}} (\widehat{B + tI_n})^\top Y(\widehat{A + tI_n}). \tag{3.5}$$

To find the maximum on the right-hand side it is enough to restrict the maximum on the right-hand side to the extreme points of $\Psi_{n,n}$. Lemma 2.3 yields that the extreme points of $\Psi_{n,n}$ are $\mathcal{P}_n \otimes \mathcal{P}_n$. Let $Y = Q \otimes P \in \mathcal{P}_n \otimes \mathcal{P}_n$. (3.4) yields that

$$(\widehat{B + tI_n})^\top Y(\widehat{A + tI_n}) = \operatorname{tr} P(A + tI_n)Q^\top(B + tI_n)^\top.$$

Compare the above expression with the left-hand side of (3.5) to deduce the equality in (3.5).

Assume that the maximum in the left-hand side of (3.5) is achieved for $P_*, Q_* \in \mathcal{P}_n$. Use Cauchy-Schwarz inequality to deduce that

$$\operatorname{tr} P_*(A+tI_n)Q_*^\top(B+tI_n)^\top \leq$$
$$((\operatorname{tr} P_*(A+tI_n)(A+tI_n)^\top P_*^\top)\operatorname{tr}(B+tI_n)(B+tI_n)^\top)^{\frac{1}{2}} = \operatorname{tr}(B+tI_n)(B+tI_n)^\top.$$

Equality holds if and only if $B+tI_n = P_*(A+tI_n)Q_*^\top$. The assumption *2b* yields the opposite inequality

$$\operatorname{tr}(B+tI_n)(B+tI_n)^\top = (\widehat{B+tI_n})^\top Z(\widehat{A+tI_n}) \leq$$
$$\max_{Y\in\Psi_{n,n}} (\widehat{B+tI_n})^\top Y(\widehat{A+tI_n}) = \operatorname{tr} P_*(A+tI_n)Q_*^\top(B+tI_n)^\top.$$

Hence $B+tI_n = P_*(A+tI_n)Q_*^\top$. Lemma 3.3 implies that $A \sim B$. □

The proof of the above theorem yields.

Corollary 3.6 *Assume that the conditions* 2 *of Theorem 3.5 holds. Let* $\Psi_{n,n}(A,B)$ *be the set of all* $Z \in \Psi_{n,n}$ *satisfying the condition* $Z(\widehat{A+tI_n}) = \widehat{B+tI_n}$. *Then all the extreme points of this compact convex set are of the form* $P \otimes P \in \mathcal{P}_n \otimes \mathcal{P}_n$ *where* $PAP^\top = B$.

$A, B \in \mathbb{R}^{n\times n}$ are called *permutationally equivalent*, denoted as $A \approx B$, if $B = PAQ^\top$ for some $P \in \mathcal{P}_n, Q \in \mathcal{P}_m$. The arguments of the proof of Theorem 3.5 yield.

Theorem 3.7 *Let* $A, B \in \mathbb{R}^{n\times m}$. *The following conditions are equivalent.*

1. $A \approx B$.
2. $\operatorname{tr} AA^\top = \operatorname{tr} BB^\top$ *and there exists* $Z \in \Psi_{m,n}$ *satisfying* $Z\widehat{A} = \widehat{B}$. *That is, view the entries of* Z *as* $z_{(i,k),(j,l)}$ *where* $i, j \in \langle m\rangle, k, l \in \langle n\rangle$. *Then these* m^2n^2 *nonnegative variables satisfy* $2((n-1)m^2 + (m-1)n^2 + mn)$ *conditions (2.6-2.8) and the* mn *conditions:*

$$\sum_{j,l=1}^{m,n} z_{(i,k)(j,l)}a_{lj} = b_{ki} \text{ for } k = 1,\ldots,n,\ i = 1,\ldots,m. \tag{3.6}$$

Corollary 3.8 *Assume that the conditions* 2 *of Theorem 3.7 holds. Let* $\Psi_{m,n}(A,B)$ *be the set of all* $Z \in \Psi_{m,n}$ *satisfying the condition* $Z\widehat{A} = \widehat{B}$. *Then all the extreme points of this compact convex set are of the form* $Q\otimes P \in \mathcal{P}_m \otimes \mathcal{P}_n$ *where* $PAQ^\top = B$.

4 GIP and SGIP

4.1 Graph isomorphisms

Theorem 4.1 *Assume that* $\Psi_{n,n}$ *is characterized by* $f(n)$ *number of linear equalities and inequalities. Then isomorphism of two simple undirected graphs* $G_1 = (V, E_1)$, $G_2 = (V, E_2)$ *where* $\#V = n$ *is decidable in polynomial time in* $\max(f(n), n)$.

Proof. Let $A, B \in \{0,1\}^{n\times n}$ be the adjacency matrices of G_1, G_2 respectively. Recall that A, B are symmetric and have zero diagonal. G_1 and G_2 are isomorphic if and only if $A \sim B$. It is left to show that the conditions *2* of Theorem 3.5 can be verified in polynomial time in $\max(f(n), n)$. *2a* means that G_1 and G_2 have the same degree sequence. This requires at most $4n^2$ computations. Assume that *2a* holds. Note that $t = 2$ satisfies the first part of the condition *2b*. The existence of $Z \in \Psi_{n,n}$ satisfying $Z(\widehat{A + 2I_n}) = \widehat{B + 2I_n}$ is equivalent to the solvability of $f(n) + n^2$ linear equations and inequalities in n^4 nonnegative variables. The ellipsoid method [8, 7] yields that the existence or nonexistence of such $X \in \Psi_{n,n}$ is decidable in polynomial time in $\max(f(n), n)$. □

Theorem 4.2 *Assume that $\Psi_{n,n}$ is characterized by $f(n)$ number of linear equalities and inequalities. Then the isomorphism of two simple directed graphs $G_1 = (V, E_1)$, $G_2 = (V, E_2)$, (self-loops allowed), where $\#V = n$ is decidable in polynomial time in* $\max(f(n), n)$.

Proof. Let $A, B \in \{0,1\}^{n\times n}$ be the adjacency matrices of G_1, G_2 respectively. Apply part *2* of Theorem 3.5 with $t = 2$ to deduce the theorem. □

The application of part *2* of Theorem 3.5 yields.

Theorem 4.3 *Assume that $\Psi_{n,n}$ is characterized by $f(n)$ number of linear equalities and inequalities. Let $A, B \in \mathbb{R}^{n\times n}$. Then permutational similarity of A and B is decidable in polynomial time in* $\max(f(n), n)$ *and the entries of A and B.*

Let $G = (V_1 \cup V_2, E)$ be an undirected simple bipartite graph with the set of vertices divided to two classes V_1, V_2 such that $E \subset V_1 \times V_2$. Assume that $\#V_1 = n, \#V_2 = m$ and identify V_1, V_2 with $\langle n\rangle, \langle m\rangle$ respectively. Then G is represented by the incidence matrix $A = [a_{ij}] \in \{0,1\}^{n\times m}$ where $a_{ij} = 1$ if and only if the vertices $i \in \langle n\rangle, j \in \langle m\rangle$ are connected by an edge in E. Let $H = (V_1 \cup V_2, F)$ be another bipartite graph with the incidence matrix $B \in \{0,1\}^{n\times m}$. If $m \neq n$ then G and H are isomorphic if and only if $A \approx B$. If $m = n$ G and H are isomorphic if and only if either $A \approx B$ or $A \approx B^\top$. Theorem 3.7 yields.

Theorem 4.4 *Assume that $\Psi_{m,n}$ is characterized by a $g(m, n)$ number of linear equalities and inequalities. The isomorphism of two simple undirected bipartite graphs $G_1 = (V_1 \cup V_2, E_1)$, $G_2 = (V_1 \cup V_2, E_2)$ where $\#V_1 = n, V_2 = m$ is decidable in polynomial time in* $\max(g(m, n), n + m)$.

Theorem 4.5 *Assume that $\Psi_{m,n}$ is characterized by $g(m, n)$ number of linear equalities and inequalities. Let $A, B \in \mathbb{R}^{n\times m}$. Then permutational equivalence of A and B is decidable in polynomial time in* $\max(g(m, n), n + m)$ *and the entries of A and B.*

We now remark that if we replace in Theorem 3.5 and Theorem 3.7 the sets $\Psi_{n,n}$ and $\Psi_{m,n}$ by the sets $\Phi_{n,n}$ and $\Phi_{m,n}$ respectively, we will obtain necessary conditions for permutational similarity and equivalence, which can be verified in polynomial time.

4.2 Subgraph isomorphism

Theorem 4.6 *Assume that $\Psi_{n,n}$ is characterized by $f(n)$ number of linear equalities and inequalities. Let $G_3 = (W, E_3), G_2 = (V, E_2)$ be two simple undirected graphs, where $\#W = m \le \#V = n$. Then the problem of determining if G_3 is isomorphic to a subgraph of G_2 is decidable in polynomial time in* $\max(f(n), n)$.

Proof. Add $n - m$ isolated vertices to G_3 to obtain the graph $\tilde{G}_3$ on n vertices. Let $C, B \in \{0,1\}^{n\times n}$ be the adjacency matrices of $\hat{G}_3, G_2$ respectively. We claim that G_3 is isomorphic to a subgraph of G_2 if and only if

$$Z(\widehat{C + 2^{n^2} I_n}) \le \widehat{B + 2^{n^2} I_n} \text{ for some } Z \in \Psi_{n,n}. \tag{4.1}$$

Assume first that G_3 is isomorphic to a subgraph of G_2. This is equivalent to the statement that $PCP^\top \le B$ for some $P \in \mathcal{P}_n$. (That is in each place where $PCP^\top$ has entry 1, then B has entry 1 at the same place.) As $PP^\top = I$ we deduce that (4.1) holds for $Z = P \otimes P$.

Assume that (4.1) is satisfied. Let

$$Z = \sum_{P,Q\in\mathcal{P}_n} w(P,Q) P\otimes Q,\ w(P,Q) \ge 0 \text{ for each } P, Q \in \mathcal{P}_n \text{ and } \sum_{P,Q\in\mathcal{P}_n} w(P,Q) = 1.$$

Hence there exists $P_*, Q_* \in \mathcal{P}_n$ such that $w(P_*, Q_*) \ge \frac{1}{(n!)^2}$. (4.1) yields that

$$\frac{1}{(n!)^2} Q_*(C + 2^{n^2} I_n) P_*^\top \le B + 2^{n^2} I_n.$$

Since $n = 2^{n-1}$ for $n = 1, 2$ and $n < 2^{n-1}$ for $2 < n$ it follows that $n! < 2^{\frac{n(n-1)}{2}}$ for $n > 2$. Hence $(n!)^2 < 2^{n^2}$ for $n \ge 1$. Since all offdiagonal elements of B are at most 1 it follows that $P_* = Q_*$. Hence $P_* C P_*^\top \le (n!)^2 B$. Thus if $P_* C P_*^\top$ has 1 in the place (i, j) then B can not have zero in the place (i, j). That is B has 1 in the place (i, j). Therefore G_3 is isomorphic to a subgraph of G_2. □

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