Efficient Algorithm for Graph Isomorphism Problem

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ABSTRACT

In this research paper, two polynomial time algorithms for graph isomorphism problem (i.e. effectively deciding whether two graphs are isomorphic) are discussed under some conditions. The algorithms are essentially based on linear algebraic concepts related to graphs. Also, some new results in spectral graph theory are discussed.

1. INTRODUCTION:

Directed/undirected, weighted/unweighted graphs naturally arise in various applications. Such graphs are associated with matrices such as weight matrix, incidence matrix, adjacency matrix, Laplacian etc. Such matrices implicitly specify the number of vertices/ edges, adjacency information of vertices (with edge connectivity) and other related information (such as edge weights). In recent years, there is explosive interest in capturing networks arising in applications such as social networks, transportation networks, bio-informatics related networks (e.g. gene regulatory networks) using suitable graphs. Thus, NETWORK SCIENCE led to important problems such as community extraction, frequent sub-graph mining etc. In many applications the problem of deciding whether two given graphs are isomorphic (i.e. the two graphs are essentially same upto relabeling the vertices) naturally arises.

This research paper is organized in the following manner. In section 2, relevant research literature is briefly reviewed. In section 3, two polynomial time algorithms, to test if two graphs are isomorphic are discussed. In section 4, interesting results related to spectral graph theory are discussed. The research paper concludes in section 5.

2. REVIEW OF RESEARCH LITERATURE:

L. Babai recently claimed quasi-polynomial time algorithm for determining if two graphs are isomorphic [1] . This is the most recent contribution to the graph isomorphism problem. There are other research efforts which provide approximate solutions to the problem (i.e. approximate algorithms were designed).

3. POLYNOMIAL TIME ALGORITHMS FOR GRAPH ISOMORPHISM PROBLEM:

We now briefly review relevant results from spectral graph theory.

3.1 **Spectral Graph Theory**: Spectral graph theory deals with the study of properties of a graph in relationship to the characteristic polynomial, eigenvalues and eigenvectors of matrices associated with the graph, such as its adjacency matrix or Laplacian matrix.

- An undirected graph has a symmetric adjacency matrix A and hence all its eigenvalues are real. Furthermore, the eigenvectors are orthonormal.

We have the following definition

Definition: An undirected graph's SPECTRUM is the multiset of real eigenvalues of its adjacency matrix, A. Graphs whose spectrum is same are called co-spectral.

Remark 1. It is well known that isomorphic graphs are co-spectral. But co-spectral graphs need not be isomorphic. Thus spectrum being same is only a necessary condition for graphs to be isomorphic (but not sufficient). Thus, it is clear that the eigenvectors of adjacency matrices of isomorphic graphs must be constrained in a suitable manner (orthonormal basis vectors of the symmetric adjacency matrices are some how related for isomorphic graphs).

3.2. Polynomial Time Algorithm to determine cospectral Graphs:

Lemma 1: The problem of determining if two graphs are Co-Spectral is in P (i.e. a polynomial time algorithm exists)

Proof: Since the elements of adjacency matrix are '0's and '1's, the characteristic polynomial of it is a polynomial with integer coefficients. Thus, there exists a polynomial time algorithm [2] (LLL algorithm) to compute the zeroes of such polynomial i.e. spectrum of associated graph. Thus the problem of determining if two graphs are cospectral is in P (class of polynomial time algorithms)………………………………………………………..Q.E.D.

Note: By Perron-Frobenius theorem, the spectral radius of an irreducible adjacency matrix (non-negative matrix) is real, positive and simple. Thus, to check for the necessary condition on isomorphic graphs, a first step is to determine if the spectral radius of two gaphs are exactly same.

Definition: Two graphs are isomorphic, if the vertices of one graph are obtained by relabeling the vertices of another graph.

3.3. Necessary and Sufficient Conditions: Isomorphism of Graphs:

3.3.1 Necessary Conditions: Isomorphism of Graphs.

• The following necessary conditions for isomorphism of graphs with adjacency matrices A, B can be checked before applying the following algorithm

• Check if Trace(A) = Trace(B) and if Determinant(A) = Determinant(B)

• Check if Spectral radius of A, B are same. This can be done using the Jacob's algorithm for computing the largest zero of a polynomial. Since the coefficients of characteristic polynomial are integers, we expect the computational complexity of this task to be smaller. If this step fails, all other zeroes need not be computed.

To provide the necessary and sufficient conditions for graph isomorphism, we need the following well know Lemma from Linear Algebra.

Lemma 2: Every symmetric matrix has UNIQUE spectral representation

Proof: Refer Linear Algebra book [Str] Q.E.D.

Let the adjacency matrices of two given co-spectral graphs be A, B. Suppose the graphs are isomorphic i.e. there exists a permutation matrix P such that

$$B = P\ A\ P^T \text{......................}(1)$$

But, since A is a symmetric matrix, we have that

$$A = F\ D\ F^T$$

where D is the Diagonal matrix of eigenvalues of A and F is an UNIQUE *orthogonal matrix* (i.e. $F^T = F^{-1}$) $whose$ columns are right eigenvectors of A. Also, we have that

$$B = \ G\ D\ G^T \text{.................}(2)$$

Thus, we must have that

$$G = P\ F \quad or \ \ G\ F^T = P.$$

But, we know that a Permutation matrix, P must be DOUBLY STOCHASTIC and *there is precisely one* $p_{ij} = 1$ *in each row and each column.*
Thus, the orthogonal matrices G, F must be related by the above equation i.e. we need to check if P is doubly stochastic and if precisely *one* $p_{ij} = 1$ in each row and each column.
Therefore, the above condition is necessary and sufficient.
Hence, we have proved the following Lemma.

Lemma 3: Given the above Spectral Representations of adjacency matrices A, B (with unique G, F) of two graphs, they are isomorphic if and only if $G\ F^T = P,$ where P is a Permutation matrix.

The computational complexity of checking the above condition leads to a polynomial time algorithm under some conditions. Based on the above results, we summarize the following steps in the algorithm to determine if two graphs are isomorphic.

3.3.2 Polynomial Time Algorithm under some conditions: Algorithmic Steps: Proof of Correctness of the Algorithm: Computational Complexity:

(1) Compute the zeroes of characteristic polynomial of adjacency matrix A as well as B. For matrix A, Determinant(λ I − A) is a polynomial with integer coefficients. A polynomial time algorithm (LLL Algorithm) [2] exists for this problem. If the eigenvalues of A, B are not same, then they are not even cospectral and the algorithm stops. If they are cospectral, proceed to the following step to determine if they are isomorphic graphs.

(2) Compute Spectral representation of adjacency matrices A, B of two given graphs:

$$A = F\ D\ F^T \ \ and \ \ B = \ G\ D\ G^T$$

where D is the common set of eigenvalues and F, G are the unique orthogonal matrices. Efficient polynomial time algorithms exist for this problem when the eigenvalues are rational numbers. Effectively, eigenvectors of A, B are computed in polynomial time. Gaussian Elimination to compute every eigenvector requires $O(N^3)$ Computations (additions, multiplications). Thus, in the worst case, this step requires $O(N^4)$ computations (additions, multiplications) for computing all the eigenvectors.

Note: Research effort motivated by Strassen's algorithm currently requires $O(N^{2.4})$ Computations. Thus the Step (2) requires smaller number of computations.

(3) Determine if $G\ F^T = P$, where P is a Permutation matrix i.e. if P is doubly stochastic and there is precisely *one* $p_{ij} = 1$ *in each row and each column*
Efficient polynomial time algorithms are well known for this problem. This step requires $O(N^2)$ comparisions.

Note: If the eigenvalues of A, B are rational numbers, polynomial time algorithm definitely exists. Even if the eigenvalues are irrational numbers, it is possible that a polynomial time algorithm can be found.

Note: For step 2, Prof. Lovasz informed the author that if we assume that exact real arithmetic can be carried out, polynomial time algorithm exists. He also informed that if we can model the problem in an approximate computing model, polynomial time algorithm exists [3].

Note: Interesting discussion on how non-isomorphic two graphs are is included in [4].
We now utilize Laplacian matrices of graphs to determine if they are isomorphic. This approach leads to **another algorithm for the problem which is more efficient**.

3.4 **Cholesky Decomposition: Another Algorithm for Graph Isomorphism**:

Let { G1,G2 } be diagonal matrices with vertex degrees of the two graphs. Also, let {A1,A2} be the adjacency matrices of those graphs. Hence, by definition, the Laplacian matrices of the graphs { L1,L2 } are given by

$$L_1 = \ G_1 - A_1 \ \ and \ \ L_2 = G_2 - A_2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

It is well known that the Laplacian matrix of a graph is positive semi-definite. Thus, Cholesky Decomposition of Laplacian matrix exists (which is not necessarily unique). Such a decomposition can be computed efficiently. Thus, we have that

$$L_1 = N_1 N_1^T \ \ and\ L_2 = N_2 N_2^T, \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (4)$$

where N_1 and N_2 are lower triangular matrices.
If the graphs are isomorphic, we readily have that

$$L_2 = PLP^T = P\ N_1 N_1^T\ P^T = N_2 N_2^T \ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ldots. (5)$$

Hence, it follows that

$$N_2 = PN_1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Thus, a necessary and sufficient condition for the graphs to be isomorphic is that

$$N_2 N_1^{-1} = P \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. (7)$$

where P must be a Permutation matrix which is doubly stochastic and there is precisely *one* $p_{ij} = 1$ *in each row and each column.*

Hence, we have proved the following Lemma.

Lemma 4: Given the Cholesky Decomposition of Laplacian matrices of two graphs, they are isomorphic if and only if $N_2 N_1^{-1} = P$, where P is a Permutation matrix.

As in the case of algorithm in 3.3.2, the above test for graph isomorphism leads to another algorithm for graph isomorphism. This algorithm is known to be more efficient.
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4. Spectral Graph Theory: Interesting Proof of a Known Result:

Fact: While the adjacency matrix depends on the vertex labeling, its spectrum is a graph invariant.

We now provide an interesting proof of the above fact. In fact, the corollary of Lemma 5 is a much stronger result. We need the following well known theorem.

• **Rayleigh's Theorem**: The local optima of the quadratic form associated with a symmetric matrix A on the unit Euclidean hypersphere (i.e.$\{ X : X^T X = 1 \}$) occur at the eigenvectors with the corresponding value of the quadratic form being the eigenvalue.

Lemma 5. Eigenvalues of the adjacency matrix of an undirected graph, A are invariant under relabeling of the vertices.

Proof: By Rayleigh's theorm, eigenvalues of A are the local optimum of the associated quadratic form evaluated on the unit hypersphere. Thus, we need to reason that the quadratic form remains invariant under relabeling of the vertices. We have that

$$X^T A\, X = \sum_{i=1}^{N}\sum_{j=1}^{N} a_{ij} x_i x_j = x_1 \left(x_{i_1} + x_{i_2} + \cdots x_{i_k}\right) + x_2\left(x_{j_1} + x_{j_2} + \cdots x_{j_l}\right)$$
$$+ \cdots + x_N\left(x_{N_1} + x_{N_2} + \cdots + x_{N_m}\right)$$

where, for instance, $\{ i_1, i_2, \ldots . i_k\}$ are the vertices connected to the vertex 1 (one) (and similarly other vertices).

Now, from the above expression, it is clear that the quadratic form remains invariant under relabeling of the vertices. Specifically, relabeling just reorders the expressions.Thus, the eigenvalues of A remain invariant under relabeling of vertices **Q. E..D**

Corollary: Since the quadratic form remains invariant under relabeling of the vertices, the local optima of the quadratic form over various constraint sets remain invariant. For instance, the stable values (i.e. local optima of quadratic form associated with a symmetric matrix over the unit hypercube) remain same under relabeling of the vertices of graph.

Note: Consider a Homogeneous multi-variate polynomial associated with, say, a FULLY SYMMETRIC TENSOR. The local optima of such a homogenous form over various constraint sets such as Euclidean Unit Hypersphere, multi-dimensional hypercube remain invariant under relabeling of nodes of a non-planar graph. Effectively relabeling of vertices, reorders the monomials (terms in multivariate polynomial).

4.CONCLUSION:

In this research paper, results in spectral graph theory of structured graphs are discussed. An efficient algorithm for testing if two graphs are isomorphic is discussed.

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