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ABSTRACT

In this research paper, 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 provides one possible solution to such a problem.

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. Specifically Babai showed that graph isomorphism problem can be solved in ($\exp((\log n)^{O(1)})$ time [2]. For the problem, the previous known best bound was $\exp\left(o(square\ root\ of\ (n \log n\ ))\right)$, where $'n'$ is the number of vertices (Luks, 1982, [8]).There are other research efforts which provide approximate solutions to the problem (i.e. approximate algorithms were designed) [3], [4], [5],[6],[8]. Also, the problem of solving Graph Isomorphism has been attempted using the quadratic non-negative matrix factorization problem[14].

3. POLYNOMIAL TIME ALGORITHMS FOR GRAPH ISOMORPHISM PROBLEM (UNDER SOME CONDITIONS) :

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) [11,12,13] Thus, it is clear that the eigenvectors ofadjacency 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 [7] (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 [10]. 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 Certain 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 [9].

We now formulate the problem of determining the isomorphism of graphs in three equivalent ways. Let the symmetric matrices A and B be the adjacency matrices of two graphs.

- **Quadratic Non-Negative Matrix Factorization**: The problem of determining isomorphism of two graphs boils to determining if a Permutation matrix P exists such that

$$B = P\,A\,P^T \ldots .(1)$$

Such a problem is already being attempted using the approach based on Quadratic Non-Negative Matrix Factorization [14]. The results proposed for such a problem readily apply for determining isomorphism of two graphs.

- **Structured Quadratic Programming Problems**: There is another interesting way of looking at the equation (1). Let the unknown matrix P be given by (in terms of columns)

$$P = [\,P_1\ P_2\ \ldots P_N\,].$$

Since A, B are { 0, 1 } matrices, we have homogeneous, second degree equations (quadratic forms) in the elements of unknown matrix P with coefficients being { 0, 1 } and the bi-variate homogeneous polynomials being equated with values { 0, 1}. Further the variables (i.e. elements of P) are constrained to be { 0, 1 }. Hence, we have structured set of simultaneous quadratic programming problems. The problem boils down to testing if the { 0, 1 } solutions (if they exist) lead to a permutation matrix, P.

- **Algebraic Riccati Equation: Symmetric Permutation Matrix P**
The quadratic matrix equation (non-linear) has resemblance to the Symmetric Algebraic Riccati Equation of the following form

$$X\,C\,X - A\,X - X\,A^T + B = 0$$

(with compatible matrices X, C, A, B), where *the matrice B and C are symmetric and X is the unknown matrix*. As can be readily seen the matrix equation (1) is a *structured symmetric Algebraic Riccati equation* with *P being a symmetric unknown matrix* and $A \equiv 0$.

$The\ known\ algorithms\ for\ solving\ such\ a\ Riccati\ equation\ may\ readily\ apply\ for\ testing\ isomorphism\ of\ two\ graphs\ for\ which\ P\ is\ a\ symmetric\ permutation\ matrix.$ Specifically, there are efforts to determine the non-negative matrix solutions of Riccati equation [15], [16]. It should be kept in mind that the solution of algebraic Riccati equation that is of interest to us is a structured { 0, 1 } matrix.

- **Explicit Solution when the Adjacency Matrices of the graphs are non-singular and are related through "Symmetric" Permutation Matrix:**

- **Algorithm : (If graphs are isomorphic, the algorithm declares them correctly).**

Lemma 2: Under the above assumptions, two graphs with adjacency matrices { B, C } (whose eigenvalues need NOT be distinct) are isomorphic if

$$X = [\,Matrix\ Square\ Root\ (\,B\ C\,)\,]\ C^{-1}$$

is a Permutation matrix.

Proof: We are interested in the solution of following MATRIX EQUATION:

$$X\ C\ X = B,\ where\ \{\,C, B\,\}\ are\ adjacency\ matrices\ of\ graphs\ .$$

$$Multiplying\ on\ both\ sides\ of\ the\ equation\ by\ C,\qquad we\ have\ that$$

$$(X\ C)(\,X\ C\,) =\ B\ C\ .\ Hence,\qquad it\ readily\ folllows\ that$$

$$X\ C = Matrix\ Square\ Root\ (\,B\ C\,).$$

$$Now,\qquad if\ C\ is\ non-singular, X\ can\ readily\ be\ computed\ as$$

$$X = [\,Matrix\ Square\ Root\ (\,B\ C\,)\,]\ C^{-1}$$

The matrix square root is unique only when BC is a positive definite matrix. In the case where the two graphs are isomorphic (with a symmetric permutation matrix P i.e. $P = P^T\ and\ B = P\ C\ P$), *it readily follows that* $B\,C$ *is a positive definite matrix (with B and C being non-singular matrices with the same set of eigenvalues*). It is possible that, the graphs are not isomorphic, but BC is a positive definite matrix. Q.E.D.

Note: In the case of matrix equation, $X\ C\ X = B$, if $B\ C$ is a positive definite matrix, unique solution can be determined using approach similar to Lemma 5.

Remark 2: In view of the above three equivalent problems, the results available for solution of one problem can be utilized in the solution of other problems. For instance, when eigenvalues of A, B are equal and distinct, the algorithm discussed for graph isomorphism can be utilized in other problems.

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 1 of Lemma 3 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 3: 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 1: 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.

Corollary 2: From the above proof, it is clear that if two graphs (with associated adjacency matrices A, B) are isomorphic, the associated quadratic form being same is a necessary condition. The author reasons that it is also a sufficient condition. Thus, an algorithm can easily be designed to check if the associated quadratic forms are same.

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. Efficient algorithms for testing if two graphs are isomorphic are discussed.

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