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Spectral Technique using Normalized Adjacency Matrices for Graph Matching

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Abstract

Graph matching problem has found many applications in areas as diverse as chemical structure analysis, pattern recognition and bio-informatics. Many works have been reported for matching of graphs with special properties. Also some heuristic approaches exist for generalized graph matching. A new spectral technique based on eigenvalues and eigenvectors of the normalized adjacency matrices of the graphs is proposed in this paper. The methodology is applicable to graphs not having isolated vertices. The methodology has been tested on variety of graphs and has given accurate results.

Keywords: Graph matching, Isomorphism, Spectral technique, Normalized Adjacency Matrix, Eigenvalue, Eigenvector.

IMS Classification No: 05C50

Introduction

Graph matching involves finding out whether two graphs are same/ similar. Two graphs are said to match each other if they are isomorphic. Two graphs are isomorphic if there is a correspondence between their vertex sets that also preserves adjacency.

Thus $G_1 = (V,E)$ is isomorphic to $G_2 = (V',E')$ if there is a bijection $\varphi: v \rightarrow v'$ such that $\langle x,y \rangle \in E$ if and only if $\langle \varphi(x), \varphi(y) \rangle \in E'$. Clearly, isomorphic graphs have same number of vertices and edges.

Graph isomorphism problem could be restated as: Two graphs G_1 and G_2

represented by adjacency matrices A and B are isomorphic if and only if there exist a permutation matrix P such that

$A=PBP^{-1}$ or $A=PBP^{T}$.

Graph matching is a fundamental task in a variety of application domains including shape matching, handwritten character recognition, natural language understanding etc .The work reported in [1] demonstrates the power of combining eigenspace graph decomposition models with clustering techniques. A method for graph matching based on constructing an auxiliary graph by co-joining the two graphs by a layer of indicator vertices and performing continuous time walks on the graphs is proposed in [2].

The problem of determining whether a pair of graphs is isomorphic has been extensively studied in literature. Polynomial time algorithms for graphs with a number of special properties are found in literature. Theoretical results, demonstrating that for all chemical molecules, the problem of isomorphism, automorphism, partitioning, and canonical labeling are polynomial time problems are presented in [3]. The paper also provides polynomial algorithms for planar molecular graphs.

A new approach to the solution of graph isomorphism in [4] suggests a method based on the spectral decomposition of the adjacency matrix. A new metric and weighted spectral distribution methodology, that improves on the raw spectrum by discounting those eigenvalues believed to be unimportant and emphasizing the contribution of those believed to be important for comparing graphs based on the distribution of their internal structure is proposed in [5]. An inexact spectral matching algorithm that embeds the large graphs on a low-dimensional isometric space spanned by a set of eigenvectors of the graph Laplacian is described in [6].

A novel graph matching algorithm, which uses random walks to compute topological features for each node, in order to identify candidate pairs of corresponding nodes in the two graphs is discussed in [7]. A method based on matching of spanning trees is proposed in [8]. The lazy random walks on the graph, which are determined by the heat-kernel of the graph and characterized by the commute times between nodes are used to compute spanning trees which are further matched by tree matching algorithms [8].

A survey of results in spectral graph theory and the inverse eigenvalue problem of a graph are presented in (9), it further examines the connection between these problems and presents some new results on construction of a matrix of minimum rank for a given graph having a special form such as 0-1 matrix or a generalized Laplacian.

The graph matching/ isomorphism problem is still an open problem though some of the algorithms are polynomial time efficient algorithms for special graphs. A new and promising methodology for testing whether two graphs are isomorphic is presented in this paper. The proposed methodology is applicable to graphs without isolated vertices and finds graph isomorphism using eigenvalues of a normalized adjacency matrix. Firstly, the adjacency matrices of graph G_1 and G_2 are found. Next, the square roots of degree of each vertex are taken and they are represented as diagonal matrix. The inverses of these diagonal matrices are obtained.

These inverse diagonal matrices are employed to find normalized adjacency matrix from the adjacency matrix of the graph. If the eigenvalues of the normalized adjacency matrices of the two graphs are the same then the two are isomorphic. Further the eigenvectors corresponding to minimum eigenvalues of the two normalized adjacency matrices are employed for finding the mapping between the vertices of the two graphs. The conceptual technique developed has been implemented using MATLAB. The technique has been used to test more than 100 pairs of graphs having different number of vertices and edges and the proposed methodology correctly predicts the graph isomorphism

The next part of the paper is divided into three sections. Section 2 describes the spectral representation and graph matching methodology. Section 3 presents the experimentation conducted and the results obtained. Section 4 brings up the conclusion and future works.

Spectral Properties and Graph Matching Methodology

In literature three different matrix representations are often used for finding the spectral properties of the graphs. The matrix representations of graphs, which are employed for the purpose, are the Adjacency matrices, Laplacian matrices, the signless Laplacian matrices and their normalized forms. In this work the normalized adjacency matrix representation of the graph and its spectral representation is employed for matching of graphs. The eigenvalues and eigenvectors of the two normalized adjacency matrices representing the two graphs are used for correspondence. In the following sub sections the proposed methodology is described in detail.

Normalized Adjacency Matrix

The normalized adjacency matrix of graph is an unique representation that combines the degree information of each vertex and their adjacency information in the graph. The normalized adjacency matrix is obtained from the adjacency matrix of the graph.

Consider an undirected graph G = (V, E) where V is the set of vertices and E is the set of edges. The adjacency matrix of G, A(G), has an entry of one if two vertices u and v, are connected and zero otherwise, this is shown in equation (1).

$$A(G)(u,v) = \begin{cases} 1, \text{if u, v are connected} \\ 0, \text{if u, v are not connected} \end{cases} \quad (1)$$

The diagonal degree matrix, D = diag ($\deg_G 1, \ldots\ldots \deg_G n$), represents the degrees of each vertex of the graph.

The normalized adjacency matrix, L(G) = $\sqrt{D}^{-1} A(G) \sqrt{D}^{-1}$, where $\sqrt{D} = \mathrm{diag}(\sqrt{\deg_G 1}, \ldots\ldots\ldots \sqrt{\deg_G n})$.

The normalized adjacency matrix L associated with graph G is constructed from A by normalizing the entries of A by the vertex degrees of A as described in (2)

$$L(G) = D^{-1/2}AD^{-1/2} \tag{2}$$

L(G) is referred to as normalized adjacency matrix. The normalized adjacency matrix is defined only for graphs without isolated vertices. This is because the degree of the isolated vertex is zero and $D^{-1/2}$ cannot be uniquely determined for such graphs. Hence the proposed methodology is suitable only for graphs without isolated vertices. This normalized adjacency matrix is further processed to extract the spectral properties as described in section 2.2.

Spectral Properties and Graph Matching

The spectral properties of the graph are determined by computing the eigenvalues and eigenvectors. The eigenvalues of the normalized adjacency matrices are known to be invariant under isomorphic transformations. Hence eigenvalues of the normalized adjacency matrices of two isomorphic/ similar graphs are the same. To evaluate graph matching it is proposed to check the equality of eigenvalues of the normalized adjacency matrices of the graphs G_1 and G_2.

Let $L_1=L(G_1)$, be the normalized adjacency matrix of G_1 and $L_2=L(G_2)$, be the normalized adjacency matrix of the graph G_2.The two matrices L_1 and L_2 are equivalent if G_1 and G_2 are isomorphic. When L_1 and L_2 matrices are equivalent they can be shown to be equal matrices by subjecting one of the matrix to elementary matrix transformations. These transformations will also be able to give the mapping between the vertices of the two graphs. This is exemplified by the example in section 3.

The same equality of L_1 and L_2 and mapping between vertices of the two graphs can be obtained by the extracting the spectral properties of the matrices(graphs) The spectral properties of the graphs are found by computing the eigenvalues and eigenvectors of L_1 and L_2.

Let E_1=eigenvalue (L_1) and E_2=eigenvalue (L_2), be the eigenvalues of the normalized adjacency matrices L_1 and L_2. If $E_1=E_2$ then the two graphs G_1 and G_2 are found to be isomorphic and is equivalent to saying L_1 is equivalent to L_2 .

Further let EV_1=eigenvector (L_1) and EV_2=eigenvector (L_2) be the eigenvectors of L_1 and L_2. The correspondence of the vertices is found by matching the values of the eigen vectors corresponding to the minimum eigenvalues of G_1 and G_2.

If the matching results in less than n/2 matches (empirical value) one of the eigenvector is negated and further matching is obtained and this gives the correspondence between the vertices of the graphs. This aspect of matching is clearly brought out in the example detailed in the subsequent section.

Experimentation

The proposed methodology for the graph matching is implemented using MATLAB. More than hundred graph pairs have been tested and 100% accurate results have been achieved. Among this hundred graphs sixty graph pairs were isomorphic and the remaining graph pairs were non isomorphic. Graphs of different number of vertices have been used for testing. The results are brought out in the bar graphs of figure 1.

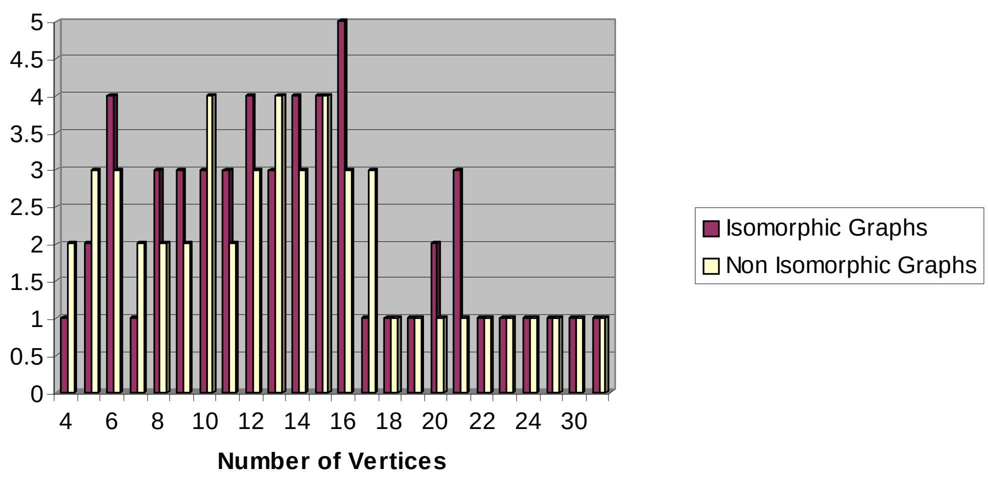

Figure 1: Bar Graph Showing Isomorphic/ Non Isomorphic Graphs Tested.

The mapping of vertices of the isomorphic graphs is obtained by the correspondence of values between the eigenvectors related to the minimum eigenvalues of the normalized adjacency matrices of the two graphs. This is indicated by the example shown below. The two six vertex graphs A and B are shown in Figure 2 below.

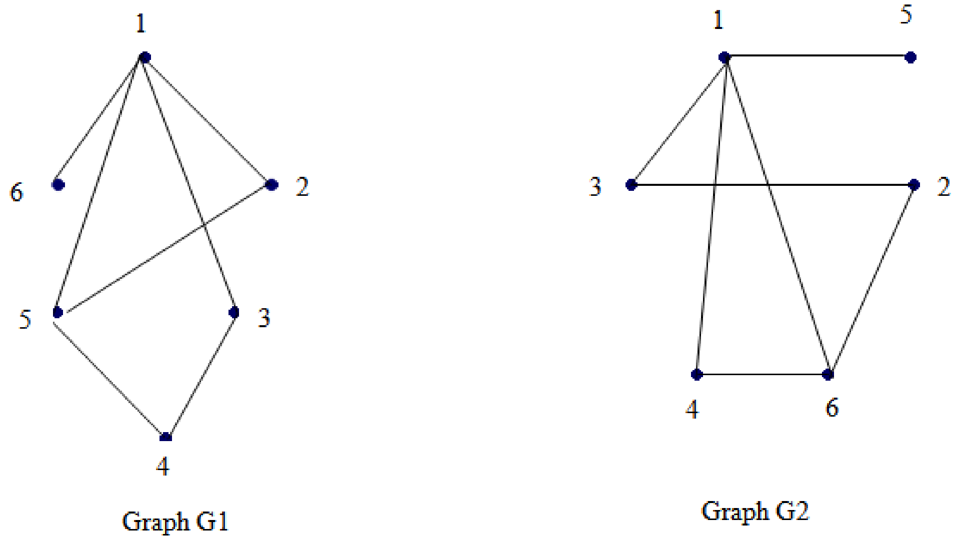

Figure 2: Graphs G_1 and G_2.

The adjacency matrices of G_1 and G_2 are given below.

$$\mathrm{Adj}(G_1)\begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \mathrm{Adj}(G_2)\begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

The normalized adjacency matrices L_1 and L_2 are computed and depicted in the following.

$$L_1=\mathrm{NAM}(G_1)=\begin{bmatrix} 0 & 0.3536 & 0.3536 & 0 & 0.2887 & 0.5000 \\ 0.3536 & 0 & 0 & 0 & 0.4082 & 0 \\ 0.3536 & 0 & 0 & 0.5000 & 0 & 0 \\ 0 & 0 & 0.5000 & 0 & 0.4082 & 0 \\ 0.2887 & 0.4082 & 0 & 0.4082 & 0 & 0 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$L_2=\mathrm{NAM}(G_2)=\begin{bmatrix} 0 & 0 & 0.3536 & 0.3536 & 0.5000 & 0.2887 \\ 0 & 0 & 0.5000 & 0 & 0 & 0.4082 \\ 0.3536 & 0.5000 & 0 & 0 & 0 & 0 \\ 0.3536 & 0 & 0 & 0 & 0 & 0.4082 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 \\ 0.2887 & 0.4082 & 0 & 0.4082 & 0 & 0 \end{bmatrix}$$

If matrix L_2 is subjected to the elementary transformation listed in equation 3 sequentially it results in the matrix L'_2 depicted below. This transformed matrix is the same as L_1. Now if the row/column number of L_1 are mapped and the original (before transformation) row/column number of L'_2 we get the mapping of the vertices of the isomorphic graphs. These results are obtained more succinctly by using spectral characteristic of L_1 and L_2

$$R_2 \leftrightarrow R_4,\ R_5 \leftrightarrow R_6 \text{ and } C_2 \leftrightarrow C_4,\ C_5 \leftrightarrow C_6 \tag{3}$$

$$L'_2=NAM(G2)=\begin{bmatrix} 0 & 0.3536 & 0.3536 & 0 & 0.2887 & 0.5000 \\ 0.3536 & 0 & 0 & 0 & 0.4082 & 0 \\ 0.3536 & 0 & 0 & 0.5000 & 0 & 0 \\ 0 & 0 & 0.5000 & 0 & 0.4082 & 0 \\ 0.2887 & 0.4082 & 0 & 0.4082 & 0 & 0 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The eigenvalues of L_1 and L_2 are [-0.8567,-0.5760,-0.2143,0.2449,0.4021,1.00] and [-0.8567,-0.5760,-0.2143,0.2449,0.4021,1.00].

These eigenvalues are equal, hence G_1 and G_2 are isomorphic. The minimum eigenvectors of L_1 and L_2, namely MinEig1 and Min Eig2 are computed and are enlisted below.

MinEig1= [-0.5300 0.0334 0.4958 -0.4747 0.3889 0.3093]

MinEig2= [-0.5300 -0.4747 0.4958 0.0334 0.3093 0.3889]

Mapping of the vertices are obtained from the above vectors and are enlisted below.

$$\text{Mapping of Vertices}\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 4 & 3 & 2 & 6 & 5 \end{bmatrix}$$

Hence the proposed methodology checks for matching of graphs and further enlists the matching vertices of the two graphs

Conclusion

In the present work a new spectral technique using normalized adjacency matrices for graph matching is presented. The method makes use of eigenvalues of the two normalized adjacency matrices of the graphs. Further if the vertices of the two graphs have the same eigenvalues then the two graphs are declared to be similar/isomorphic. Further the eigenvectors corresponding to minimum eigenvalues are employed for finding the correspondence between the vertices of the graph. A MATLAB program is developed to implement this methodology. The program is tested for more than hundred pairs of graphs for different numbers of vertices and 100% results have been achieved. This methodology has proved to be correct and efficient for a large number of graphs. Further the use of normalized adjacency matrix representation of the graph has proven beneficial as it contains not only the adjacency information but the degree of each vertex stated explicitly. This representation is also simple for computation purpose and holds a lot of promise for other graph theoretic applications.

The graph matching methodology presented here can be employed for various pattern-matching applications in the domains of image processing, chemical structure analysis etc.

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