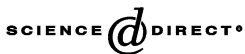


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Some further development on the eigensystem approach for graph isomorphism detection

P.R. He^a, W.J. Zhang^{a,*}, Q. Li^b

^a*Department of Mechanical Engineering, University of Saskatchewan, Saskatoon, Canada, SK S7N 5A9*

^b*Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

Abstract

Many science and engineering problems can be represented by a network, a generalization of which is a graph. Examples of the problems that can be represented by a graph include: cyclic sequential circuit, organic molecule structures, mechanical structures, etc. The most fundamental issue with these problems (e.g., designing a molecule structure) is the identification of structure, which further reduces to be the identification of graph. The problem of the identification of graph is called graph isomorphism. The graph isomorphism problem is an NP problem according to the computational complexity theory. Numerous methods and algorithms have been proposed to solve this problem. Elsewhere we presented an approach called the eigensystem approach. This approach is based on a combination of eigenvalue and eigenvector which are further associated with the adjacency matrix. The eigensystem approach has been shown to be very effective but requires that a graph must contain at least one distinct eigenvalue. The adjacency matrix is not shown sufficiently to meet this requirement. In this paper, we propose a new matrix called adjusted adjacency matrix that meets this requirement. We show that the eigensystem approach based on the adjusted adjacency matrix is not only effective but also more efficient than that based on the adjacency matrix.

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Keywords: Graph theory; Matrix decomposition; Eigenvalues; Eigenvectors; Graph isomorphism; Kinematic chains

*Corresponding author. Tel.: +1 306 966 5478; fax: +1 306 966 5427.

E-mail addresses: peh985@mail.usask.ca (P.R. He), wjz485@enr.usask.ca (W.J. Zhang), mqli@ntu.edu.sg (Q. Li).

1. Introduction

Many science and engineering problems can be represented by a network, a generalization of which is a graph. Examples of the problems that can be represented by a graph include: cyclic sequential circuit, organic molecule structures [1,2], mechanical structures (especially kinematic chains) [3–9], etc. Specifically, in the recent years, graph theory has been successfully applied in the area called bioinformatics and computational biology [10,11]. The most fundamental issue with these problems (e.g., designing a molecule structure) is the identification of structure, which further reduces to be the identification of graph. The problem of the identification of graph is called graph isomorphism (GI). The GI problem is an NP problem according to the computational complexity theory.

The identification of GI is notably an NP (nondeterministic polynomial time) problem in the complexity class. Mathematicians and computer scientists have been working on finding efficient algorithms for GI [12,13]. So far, no known polynomial-time algorithm for GI has been found for general graphs. Excellent progresses have been made towards polynomial-time algorithms for special graphs, such as trees, interval graphs, planar graphs, and permutation graphs [14,15]. In this paper, concern is with general graphs.

The studies regarding the use of the characteristic polynomial of the adjacency matrix (AM) to characterize a graph in terms of isomorphism have a long history in graph theory [16,17]. The applications of the characteristic polynomial to detect isomorphism in kinematic chains have been discussed in [7–9]. The chief merit of this method is its computational simplicity and efficiency. However, this method only provides a necessary condition for GI.

Another stream of studies on GI is to develop a canonical code (if any) for a graph directly based on AM. Since the AM of a graph is always symmetric and has zero diagonal elements, its upper right triangular part is sufficient to describe the graph. Each row in the upper right triangular matrix can be regarded as a binary code, and these binary codes can be combined into an integer number called optimal code. This integer number uniquely corresponds to the graph and the labeling of the vertices of the graph. There exists a unique maximum number defined as max code of the graph [18], and there also exists a unique minimum code defined as min code of the graph [19]. Therefore, one can identify GI by comparing these unique or canonical codes of two graphs. However, the method based on such codes requires an exhaustive search in many worst cases. As a modification of the max code, Tang et al. [20] introduced a degree code, suggesting: first re-label the AM such that the degrees of the vertices of a graph are in a descending order, and then search for the max code based on the re-labeled AM. Note that the degree of a vertex of a graph is defined as the number of edges incident to the vertex. This method can thus reduce the search space for a canonical code. Luo et al. [21] developed an incident degree code approach. The incident degree code of a vertex of a graph is a number combined by the weights of the edges incident to that vertex and the degree codes of the vertices adjacent to that vertex. Suppose vertex i in a graph has a degree m and is connected to its adjacent m vertices with weights $w_{i1}, w_{i2}, \dots, w_{im}$. Each adjacent vertex has its own degree

1 denoted by $d_{i1}, d_{i2}, \dots, d_{im}$. The incident degree code is defined as
 2 $d_{i1}, d_{i2}, \dots, d_{im}, w_{i1}, w_{i2}, \dots, w_{im}$ by following the arrangement $d_{i1} > d_{i2} > \dots > d_{im}$.
 3 If some adjacent vertices have the same degree, the weights of the corresponding
 4 edges should be in a descending order. It is obvious that the method of incident
 5 degree code uses more features of the vertices of a graph than the method of degree
 6 code, and thus the incident degree code method is generally more efficient than the
 7 degree code method. Based on the observation of a generic feature with these code-
 8 based methods, i.e., imposing the constraints on vertices based on the topological
 9 feature of a graph prior to any permutation, Zhang and Li [22] proposed a method
 10 called vertex feature degree (VFD). The VFD method extends the method of incident
 11 degree by adding the body type of vertices into the incident degree code. In general,
 12 therefore, this method can further reduce the searching space for the identification of
 13 graphs. It is noted, however, that all these modified code methods can present the
 14 same defect as the methods of optimal code when the graphs to be detected are
 15 relatively regular or uniform.

16 Partitioning of a graph is another method used for GI. McKay [23] proposed a
 17 canonical labeling algorithm for the GI problem. Suppose that V denotes the vertex
 18 set $\{1, 2, \dots, n\}$ of a graph. A partition π of the set V is a set of disjoint non-empty
 19 subsets of $V: V_1, V_2, \dots, V_m$. An ordered partition of V is a sequence
 20 (V_1, V_2, \dots, V_r) such that $\{V_1, V_2, \dots, V_r\}$ is a partition of V . Each element (called
 21 cell) of a partition of V will be further split until a leaf partition which is a partition
 22 with only singleton sets. There is an automorphism if two distinct leaf partitions
 23 result in the same AMs after re-labeling vertices. If we construct a label for a graph
 24 by concatenating the rows of the AM to form an $n \times n$ binary number, we can then
 25 compute a canonical label for the graph by looking at the label of every
 26 automorphism of the graph, and returning the smallest one. This algorithm is
 27 basically a depth first search of the space of partitions, with the added optimization
 28 to refine each partition before expanding its children. Kim and Kwak [24] proposed
 29 an algorithm of topological ordering of vertices for generating a unique edge list of a
 30 given graph, and used it for the isomorphism test. A specific starting vertex, which
 31 has the highest degree, is used as the root of topological ordering in this algorithm.
 32 According to the distances from a starting vertex, the vertices can be partitioned into
 33 a level structure. Some rules are used to determine the order of vertices in each level.
 34 Renumbering the vertices for the level structure results in a new edge list after the
 35 level structure is ordered completely. This new edge list (or a representative of new
 36 edge lists) is unique for a given graph, and can be used as identifier of isomorphism
 37 problem. However, the challenge also exists with the partition method when graphs
 38 are relatively regular and uniform. This is because the partition method also uses the
 39 degree as the ordering condition.

40 Elsewhere, we proposed a method which is based on a combination of eigenvalue
 41 and eigenvector, as opposed to relevant methods in the literature which only make
 42 use of the eigenvalue. This method is called the eigensystem approach. The
 43 eigensystem approach has been shown to be very effective but requires that a graph
 44 must contain at least one distinct eigenvalue. The AM is not shown sufficiently to
 45 meet this requirement. In this paper, we propose a new matrix called adjusted

adjacency matrix (AAM) that meets this requirement. We show that the eigensystem approach based on the adjusted adjacency matrix is not only effective but also more efficient than that based on the AM.

We arrange the remainder of this paper as follows. Section 2 gives an introduction of the eigensystem method, in which the condition for the eigensystem method to work is discussed. The AAM is proposed in Section 3 to meet this condition. A comparison of the AM-based and the AAM-based eigensystem methods is given in Section 4. The computational complexity of the proposed method is analyzed in Section 5. A conclusion is given in Section 6.

2. The eigensystem approach

We proposed in [25] a new approach based on quadratic forms for GI of the graphs that are simple, connected, undirected, and labeled graphs. The basic idea of this approach is to represent two graphs using two quadratic forms in which the matrices of the two quadratic forms are exactly the AMs of two graphs, and then compare their quadratic surfaces to determine if these two graphs are isomorphic. As it is known, the principal axes of the quadratic surface form a mutually orthogonal set. Assume that there is an orthogonal matrix Ψ . The principal axes of the quadratic surface are chosen as a new co-ordinate system x'_1, x'_2, \dots, x'_n by the transformation

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \Psi \begin{bmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{bmatrix}. \quad (1)$$

Hence, the quadratic form Q with the new variables is

$$\begin{aligned} Q &= [x_1 \ x_2 \ \cdots \ x_n]A \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = [x'_1 \ x'_2 \ \cdots \ x'_n]\Psi^T A \Psi \begin{bmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{bmatrix} \\ &= [x'_1 \ x'_2 \ \cdots \ x'_n]A \begin{bmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{bmatrix} = \lambda_1 x'^2_1 + \lambda_2 x'^2_2 + \cdots + \lambda_n x'^2_n, \end{aligned} \quad (2)$$

where

$$A = \Psi^T A \Psi = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}. \quad (3)$$

In the quadratic form, $1/\sqrt{\lambda_1}, 1/\sqrt{\lambda_2}, \dots, 1/\sqrt{\lambda_n}$ are called the lengths that are commonly referred to as the semiaxes of the quadratic surface. The orthogonal matrix Ψ represents the directions of these semiaxes. As a result, determining whether two graphs are isomorphic or not is equivalent to determining whether or not their quadratic surfaces are isomorphic, i.e., having the same semiaxes of quadratic surfaces and the directions of these semiaxes. Eq. (3) can be written as

$$A = \Psi \Lambda \Psi^T. \quad (4)$$

Eq. (4) indicates that matrix Λ is the eigenvalue matrix of matrix A and matrix Ψ is the normalized eigenvector matrix of matrix A . Detection of isomorphic quadratic surfaces (i.e., isomorphic graphs) can be characterized as the detection of eigenvalues and eigenvectors of graphs. In graph theory, we normally call the eigenvalues of a graph the *spectrum of the graph*, and thus the graphs with the same spectrum are called *cospectral graphs*. It is further noted that in our previous work, we developed the following results based on the AM [25].

Result 1. For two graphs with all distinct eigenvalues, they are isomorphic if and only if they have the same graph spectrum and the equivalent eigenvectors.

Result 2. For two graphs with some coincident eigenvalues, they are isomorphic if they have the same graph spectrum and the equivalent ‘unique’ eigenvectors. This further implies that two graphs are definitely non-isomorphic if their graph spectrums are different or their ‘unique’ eigenvectors are not equivalent. It is noted that a unique eigenvector refers to the eigenvector associated with a distinct eigenvalue.

The above two results imply a very important concept, that is, the equivalent vector or matrix. Suppose the unique eigenvector set X of graph A is $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m]$ and the unique eigenvector set Y of graph B is $Y = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m]$. X and Y are equivalent if there exists a row permutation matrix P such that

$$\mathbf{x}_i = P\mathbf{y}_i \quad \text{for } i = 1, 2, \dots, m. \quad (5)$$

In the following, we describe the procedure to prove whether or not there is a P matrix for a particular problem.

Take a pair of eigenvectors \mathbf{x}_i in X and \mathbf{y}_j in Y . If there is a one-to-one mapping φ_i such that the j th element \mathbf{x}_{ij} in \mathbf{x}_i (which corresponds to the j th vertex of graph A) equals the k th element \mathbf{y}_{jk} in \mathbf{y}_j (which corresponds to the k th vertex of graph B) for all $j = 1, 2, \dots, n$, i.e., $k = \varphi_i(j)$, we can obtain a set of such mappings below

$$\Phi = [\varphi_i(j)] = \begin{bmatrix} \varphi_1(1) & \varphi_1(2) & \cdots & \varphi_1(n) \\ \varphi_2(1) & \varphi_2(2) & \cdots & \varphi_2(n) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_m(1) & \varphi_m(2) & \cdots & \varphi_m(n) \end{bmatrix}, \tag{6}$$

where Φ is an $m \times n$ matrix. If all the rows of Φ in Eq. (6) are the same, there must be a common mapping function among mapping φ_i (for $i = 1, 2, \dots, m$). It is further noted that we can write φ_i into the form of a row permutation matrix, i.e., P in Eq. (5). In this case the P matrix can be obtained. If not all the rows of Φ in Eq. (6) are the same, a common mapping function does not exist. This implies that the P matrix does not exist.

It is noted that the mapping function $\varphi_i(j)$ could be a many-to-many relationship (i.e., given j vertex in graph A more than one vertex in graph B corresponds to j ; more than one vertex in graph A may correspond to one vertex in graph B). We call this kind of mapping function $\varphi_i(j)$ the group-to-group mapping function. Table 1 gives an example. Take $\varphi_1(j)$ as an example. We can find that the vertex group (2, 6, 8, 12) in graph A has a many-to-many relationship with the vertex group (2, 6, 8, 10) in graph B . Table 1 also shows that the mapping function φ_i ($i = 1, 2, \dots, m$) may be different with respect to i . The many-to-many mapping implies more options of correspondence between two graphs. In particular, if the size of a many-to-many group is 3 the number of possible mappings will be 6. Let us denote S_i as all mapping options for mapping function i . A common mapping set or function (S_c) is defined by $S_c = S_1 \cap S_2 \cap S_3 \cap \dots \cap S_m$. Table 1 shows an example of common mapping function. We further note that the common mapping function

Table 1
The concept of group-to-group mapping function φ_i and its common mapping

$i = 1$	j	1, 7	2, 6, 8, 12	3, 5, 9, 11	4, 10								
	$\varphi_1(j)$	1, 11	2, 4, 8, 10	3, 5, 7, 9	6, 12								
$i = 2$	j	1, 7	2, 6	8, 12	3, 5, 9, 11	4	10						
	$\varphi_2(j)$	1, 11	8, 10	2, 4	3, 5, 7, 9	12	6						
$i = 3$	j	1	7	2, 6	8	12	3, 9	5, 11	4, 10				
	$\varphi_3(j)$	1	11	8, 10	4	2	3, 9	5, 7	6, 12				
$i = 4$	j	1, 7	2	6	8, 12	3	9	5	11	4, 10			
	$\varphi_4(j)$	1, 11	8	10	2, 4	3	9	7	5	6, 12			
Common mapping	j	1	7	2	6	8	12	3	9	5	11	4	10
	$\varphi(j)$	1	11	8	10	4	2	3	9	7	5	12	6

1 for the example shown in Table 1 contains one vertex only in each subgroup. This
 3 means that the common mapping function contains one option only. In such a case,
 5 we actually have reached a one-to-one correspondence between two graphs; that is to
 7 say two concerned graphs are isomorphic. It is possible that a common mapping
 function has a many-to-many relationship. For example, if we remove mapping φ_2
 (the 2nd row) from Table 1, then the common mapping is not a one-to-one
 relationship (see the last column in Table 1).

9 An algorithm which is able to search all the possibilities of subdivisions in attempt
 to find a one-to-one common mapping for all group-to-group mappings has been
 11 developed in [25]. When the algorithm ends without finding any one-to-one
 mapping, we can conclude that the P matrix does not exist and therefore two
 13 corresponding graphs are not isomorphic.

15 3. Adjusted adjacency matrix of graph

17 The eigensystem approach so far discussed requires that there exists at least one
 distinct eigenvector in the AM of a graph. Nevertheless, this condition is not always
 19 satisfied with AM as representation of a graph. The primary objective of the present
 paper is to provide a solution to this problem. Our general idea is to define a new
 21 matrix to represent a graph. This new matrix must have at least one distinct
 eigenvalue. The new matrix is defined by extending the AM of a graph, and is given
 23 as follows:

$$25 \quad a_{ij} = \begin{cases} \text{same as the adjacency matrix,} & i \neq j, \\ n\text{-degree}(v_i) \neq 0, & i = j. \end{cases}$$

27 We call the new matrix the AAM. The difference between an AM and an AAM is
 29 that all elements on the principal diagonal of the AM are zero but nonzero of the
 AAM. It is easy to see that AAM is unique and sufficient to represent a graph.
 31 Therefore, the isomorphism of two graphs can be studied based on their AAMs. We
 have the following theorem for the AAM.

33 **Theorem.** *The AAM of a connected graph with n vertices will have at least one distinct*
 35 *eigenvalue, i.e., n which is the total number of vertices in this graph.*

37 **Proof.** Consider the matrix

$$39 \quad B = \frac{1}{n} M,$$

41 where M is an AAM of a connected graph. To prove that n is a distinct eigenvalue of
 matrix M , we only need to prove that matrix B has a unique eigenvalue 1. It is easy
 43 to see that matrix B has two properties:

- 45 (1) $b_{ij} \geq 0$;
 (2) $\sum_{i=1}^n b_{ij} = \sum_{j=1}^n b_{ij} = 1$; $i = 1, 2, \dots, n$; $j = 1, 2, \dots, n$.

Therefore, matrix B is a doubly stochastic matrix, and it has a largest eigenvalue 1 and an eigenvector $[1 \ 1 \ \dots \ 1]^T$ corresponding to the largest eigenvalue [26]. Since the associated graph of matrix M (also matrix B) is strongly connected (for each entry (i, j) in matrix M there exists an integer k), matrix B is an irreducible matrix. More exactly, matrix B is an irreducible nonnegative matrix according to property (1) of the matrix. It is known that an irreducible nonnegative matrix with a nonzero principal diagonal is primitive [27], and an $n \times n$ nonnegative primitive matrix has a unique eigenvalue, 1, which is the largest among all its eigenvalues [28]. According to the definition of matrix B , we can conclude that matrix M has a distinct eigenvalue n (which is the largest), and the eigenvector associated with that eigenvalue is $[1 \ 1 \ \dots \ 1]^T$. \square

An example shown in Fig. 1 may help to explain this theorem further. Fig. 1 shows a five-vertex graph and its AAM. The AAM of the graph has the graph spectrum $\Lambda = \text{diag}(5.0000, 3.6180, 3.6180, 1.3820, 1.3820)$ in which 5.0000 is the only distinct eigenvalue and its associated eigenvector has the same element 1 (or 0.4472 as a normalized value).

The advantage of the AAM of a graph is also that the GI detection based on AAM is more efficient than that based on AM in the sense that two nonisomorphic cospectral graphs based on AM may not be the cospectral graph based on AAM and the converse is not true. This is, however, just a conjecture. More work needs to be done to prove this conjecture. Examples supporting the conjecture will be discussed in the next section.

4. Comparison of AAM- and AM-based methods

4.1. Graphs not cospectral on AM and AAM

Fig. 2 includes two graphs, and their spectrums based on AM are

$$A_a = \text{diag}(3, 2, 1.4142, 1.4142, 1, 0, 0, -1, -1.4142, -1.4142, -2, -3),$$

$$A_b = \text{diag}(3, 2, 2, 1, 0, 0, 0, 0, -1, -2, -2, -3).$$

Since the spectrums between the two graphs are different these two graphs are not cospectral. Therefore, these two graphs are not isomorphic. The spectrums of the

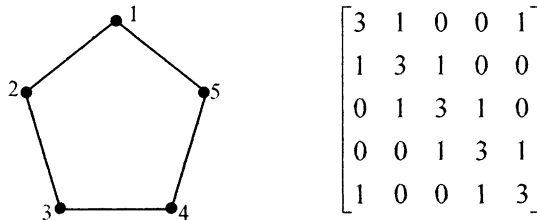


Fig. 1. A five-vertex graph and its AAM.

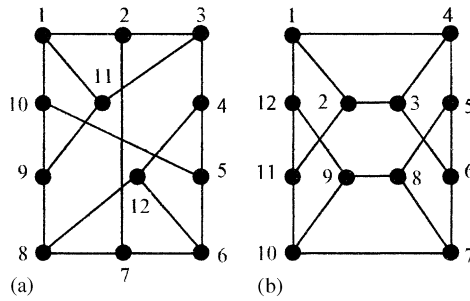


Fig. 2. Two non-isomorphic graphs.

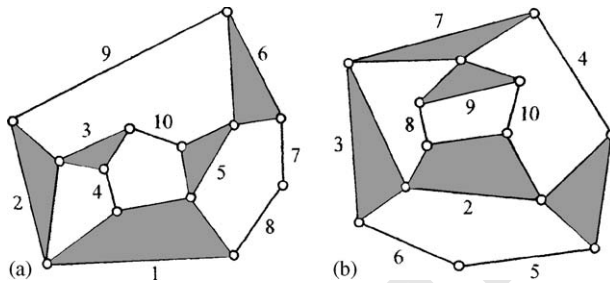


Fig. 3. Two cospectral kinematic chains based on AM.

two graphs based on AAM are shown below:

$$A'_a = \text{diag}(12, 11, 10.4142, 10.4142, 10, 9, 9, 8, 7.5858, 7.5858, 7, 6),$$

$$A'_b = \text{diag}(12, 11, 11, 10, 9, 9, 9, 9, 8, 7, 7, 6).$$

It is clear that these two graphs are not cospectral based on AAM also.

4.2. Graphs cospectral on AM but not on AAM

There are two cospectral kinematic chains on AM shown in Fig. 3, and their spectrums based on AM are as follows:

$$A_a = A_b = \text{diag}(2.7523, 1.6037, 1.1354, 1.0000, 0.4528, 0.0000, \\ -0.9182, -1.5279, -2.0693, -2.4289).$$

However, their graph spectrums based on AAM are

$$A'_a = \text{diag}(10.0000, 9.2295, 8.7930, 8.5509, 7.6967, 7.5416, 6.7547, 5.9379, 5.1341, 4.3617)$$

$$A'_b = \text{diag}(10.0000, 9.3134, 8.7685, 8.2729, 8.0000, 7.4351, 6.8406, 5.8922, 5.0782, 4.3990),$$

respectively, and they are clearly not cospectral.

Fig. 4 shows other two pairs of kinematic chains with 10 bars that are not isomorphic. Each pair of the kinematic chains is cospectral based on AM but is not cospectral based on AAM. Fig. 5 shows that two graphs are two cospectral trees with eight vertices. They are absolutely nonisomorphic trees but have the same graph spectrum based on AM:

$$A_a = A_b = \text{diag}(2.3028, 1.3028, 0.0000, 0.0000, 0.0000, 0.0000, -1.3028, -2.3028).$$

However, they have different spectrums based on AAM, i.e.,

$$A'_a = \text{diag}(8.0000, 7.7226, 7.0000, 7.0000, 7.0000, 6.4932, 4.8390, 1.9452),$$

$$A'_b = \text{diag}(8.0000, 7.6458, 7.0000, 7.0000, 7.0000, 7.0000, 4.0000, 2.3542).$$

Two tree graphs are thus not isomorphic. Fig. 6 shows another two examples

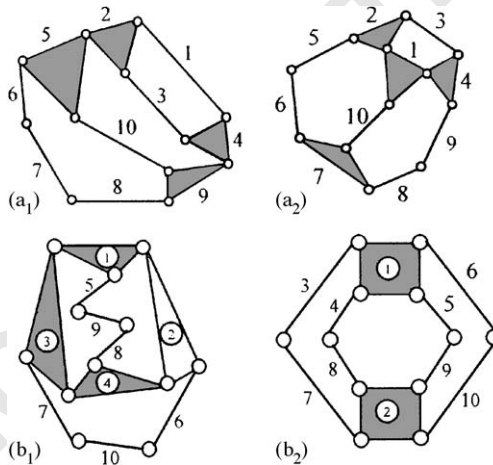


Fig. 4. Two pairs of cospectral kinematic chains based on AM.

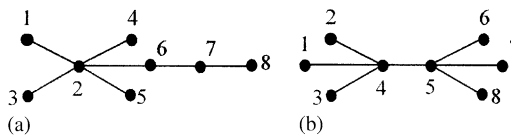


Fig. 5. Two cospectral trees with eight vertices based on AM.

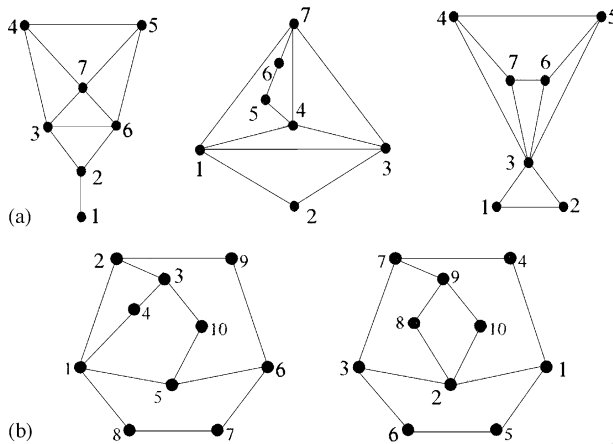


Fig. 6. Two groups of cospectral graphs based on AM.

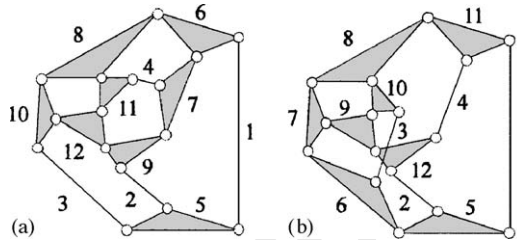


Fig. 7. Two cospectral non-isomorphic kinematic chains both with 12 bars.

where the graphs, respectively, in Fig. 6(a) and (b) are cospectral based on AM but not cospectral based on AAM and therefore they are not isomorphic. It is worth to mention that for all the graphs listed in [16,17], we have checked that they are not cospectral based on AAM. Intuitively, therefore, using AAM seems more efficient than using AM for detection of GI.

4.3. Graphs cospectral on both AM and AAM

We have observed that not all nonisomorphic graphs (which are cospectral based on AM) are not cospectral based on AAM. Fig. 7 shows two non-isomorphic kinematic chains with 12 bars. The spectrums of the two graphs based on AM are

$$A_a = A_b = \text{diag}(2.7580, 1.7668, 1.5713, 1.4142, 0.6350, 0.4150, 0, -0.9815, -1.4142, -1.5382, -2, -2.6264)$$

and the spectrums based on AAM are

$$A'_a = A'_b = \text{diag}(12, 11.2652, 10.8953, 10.8019, 10.1955, 9.7365, 9.4450, 8.4181, 7.7701, 7.7530, 7.2414, 6.4779).$$

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Further examination of these two graphs shows their ψ matrices below, respectively,

$$\psi'_a = \begin{bmatrix} 0.2887 & -0.3236 & -0.3028 & -0.5211 & 0.0967 & 0.2312 & 0.4179 & -0.1984 & -0.2544 & -0.2319 & -0.1831 & 0.1408 \\ 0.2887 & -0.3236 & -0.3028 & 0.5211 & 0.0967 & 0.2312 & -0.4179 & -0.1984 & -0.2544 & 0.2319 & -0.1831 & 0.1408 \\ 0.2887 & -0.3623 & 0.4756 & 0.0000 & -0.4582 & -0.3010 & -0.0000 & 0.3017 & -0.3751 & -0.0000 & 0.0071 & 0.1639 \\ 0.2887 & 0.4688 & -0.1858 & -0.0000 & -0.6210 & 0.1652 & 0.0000 & -0.3446 & -0.0975 & 0.0000 & 0.3467 & 0.0302 \\ 0.2887 & -0.4457 & -0.0685 & 0.0000 & -0.2216 & 0.2193 & -0.0000 & 0.1636 & 0.7187 & 0.0000 & 0.2042 & -0.1766 \\ 0.2887 & 0.0362 & -0.2025 & -0.4179 & 0.2405 & -0.2802 & -0.2319 & 0.1504 & -0.1514 & 0.5211 & 0.3010 & -0.3192 \\ 0.2887 & 0.2390 & -0.3118 & -0.0000 & -0.1172 & -0.5365 & -0.0000 & 0.0753 & 0.3254 & 0.0000 & -0.5395 & 0.2412 \\ 0.2887 & 0.1667 & 0.2307 & -0.2319 & 0.3080 & 0.0990 & -0.5211 & 0.0356 & 0.1152 & -0.4179 & 0.1933 & 0.4232 \\ 0.2887 & 0.0362 & -0.2025 & 0.4179 & 0.2405 & -0.2802 & 0.2319 & 0.1504 & -0.1514 & -0.5211 & 0.3010 & -0.3192 \\ 0.2887 & -0.0127 & 0.4944 & 0.0000 & 0.1320 & -0.1399 & 0.0000 & -0.6408 & 0.1177 & 0.0000 & -0.2239 & -0.4006 \\ 0.2887 & 0.3542 & 0.1454 & 0.0000 & -0.0042 & 0.4930 & 0.0000 & 0.4697 & -0.1080 & -0.0000 & -0.4170 & -0.3476 \\ 0.2887 & 0.1667 & 0.2307 & 0.2319 & 0.3080 & 0.0990 & 0.5211 & 0.0356 & 0.1152 & 0.4179 & 0.1933 & 0.4232 \end{bmatrix}$$

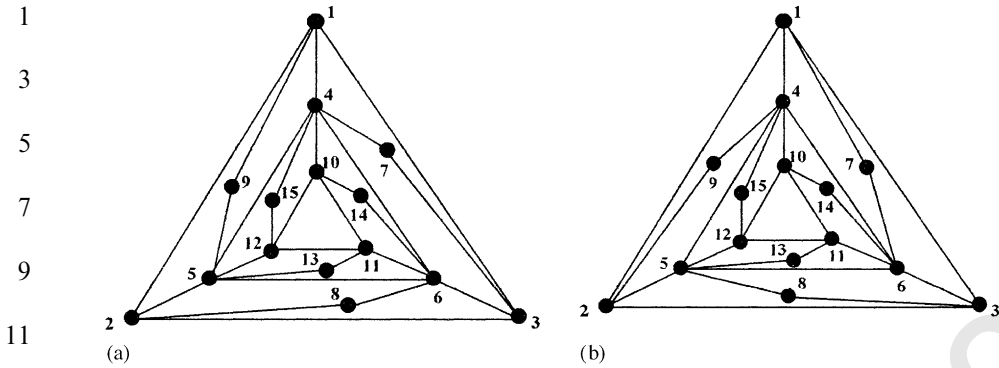


Fig. 8. Two cospectral nonisomorphic graphs with 15 vertices.

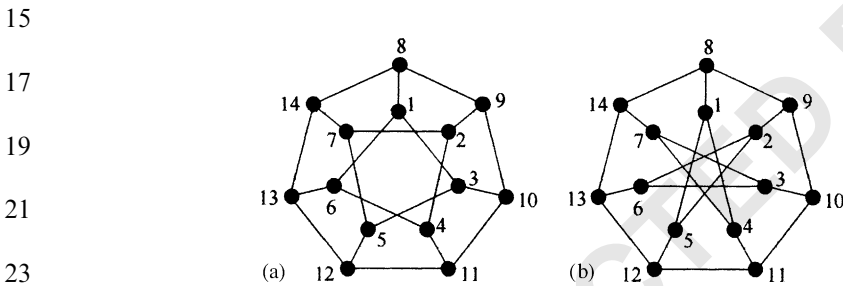


Fig. 9. Two cospectral isomorphic graphs with 14 vertices.

We can apply our proposed method outlined in Section 2 to this problem, and can conclude that there is no common mapping between two eigenvector sets. Thus, there is no permutation matrix P ; in other words, the AAMs of two graphs are not equivalent. Therefore, these two kinematic chains are not isomorphic.

Fig. 8 shows two graphs with fifteen vertices. They are cospectral both based on AM and AAM. Applying the procedure described in Section 2, we can show that there is no matrix P either based on AM or on AAM. Therefore, we can conclude that the two graphs are not isomorphic.

Fig. 9 shows two graphs that are cospectral based on AM and are isomorphic. We can apply our proposed procedure to this problem and can conclude that they are isomorphic based on AAM also.

5. Computational complexity of the approach

We now analyze the computational complexity of the eigensystem approach for GI. The time complexity for a single detecting loop with the proposed algorithm is dominated by eigendecomposition of AAMs, comparisons of eigenvalues and the eigenvectors corresponding to the distinct eigenvalues between graphs. The time cost

1 for the comparisons of eigenvalues–eigenvectors of two graphs is mainly for sorting
 3 eigenvalues and sorting each eigenvector corresponding to a distinct eigenvalue.
 5 Once the common mapping has a many-to-many relationship (i.e., a group-to-group
 7 mapping), a recursive procedure of the eigensystem approach has to be performed,
 9 which consists of several similar detecting loops.

As it is known, in general, the computational complexity of eigendecomposition
 7 with a $N \times N$ matrix is $O(N^3)$, while the computational complexity of sorting
 9 problem for N elements is $O(N \log N)$. The time complexity of comparisons of
 11 eigenvalues–eigenvectors is thus

$$T = \text{sorting eigenvalues} + \text{number of eigenvectors compared} \\ * \text{sorting an eigenvector}, \quad (7)$$

13 where the number of eigenvectors compared is N for N vertex graph in the worst
 15 case. The computational complexity of comparisons of eigenvalues–eigenvectors,
 17 therefore, is bounded by $O(N^2 \log N)$. Finally, the computational complexity of a
 19 single detecting loop by the eigensystem approach can be bounded by $O(N^3)$.
 21 Suppose that a determination of whether two graphs are isomorphic or not could be
 23 made after M detecting loops, then the complexity of the eigensystem approach for
 25 GI is $O(MN^3)$.

23 6. Conclusion

25 GI is a common problem in many science and engineering applications. The study
 27 on efficient algorithms for GI has a long history, and many methods have been
 29 proposed in the literature. In [25], we proposed a new method for GI. This new
 31 method is based on a combination of eigenvalues and eigenvectors which are further
 33 associated with the adjacency matrix (AM) of a graph. The new method is called the
 35 eigensystem approach. In [29] we further improved this method yet left only one
 37 requirement on this method; that is, the AM of a graph must contain at least one
 39 distinct eigenvalue.

33 We observed that the AM cannot ensure this requirement and therefore we define
 35 a new matrix representation for a graph, which may be closely related to the AM but
 37 meets that requirement. This paper presented such a matrix called adjusted
 39 adjacency matrix (AAM). We proved that the AAM can meet that requirement
 41 and showed that the eigensystem approach based on the AM [25,29] can be readily
 43 migrated to the one based on the AAM. We conducted the computational
 45 complexity for the eigensystem approach based on the AAM. There are the
 following conclusions that can be derived from the paper:

- 41 (1) The AAM of a graph contains at least one distinct eigenvalue.
- 43 (2) The algorithm based on the AAM is more efficient than that based on the AM
 because of a proposed conjecture.
- 45 (3) We have so far not found any counterexample for the eigensystem approach

1 based on the AAM.

3 (4) The computational complexity of the eigensystem approach based on the AAM
 5 is bounded by $O(MN^3)$, where N is the number of vertices in a graph, and M is
 7 the level of a recursive algorithm in the method can go in searching a common
 9 mapping function.

11 We further suggest a conjecture based on our experience in many case studies: two
 13 cospectral graphs based on the AM may not be cospectral based on the AAM;
 15 whereas the converse is not true.

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