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Research article

Graph isomorphism—*Characterization and efficient algorithms*

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ABSTRACT

The Graph isomorphism problem involves determining whether two graphs are isomorphic and the computational complexity required for this determination. In general, the problem is not known to be solvable in polynomial time, nor to be NP-complete. In this paper, by analyzing the algebraic properties of the adjacency matrices of the undirected graph, we first established the connection between graph isomorphism and matrix row and column interchanging operations. Then, we prove that for undirected graphs, the complexity in determining whether two graphs are isomorphic is at most $\mathcal{O}(n^3)$.

1. Introduction

Graphs are data structures used to represent objects and their relationships [1]. The objects are also sometimes referred to as nodes or vertices, while the relationships are known as edges. Essentially, graphs provide descriptions of items that are interconnected by relations.

Graphs are widely used in machine learning as a tool to predict links and classify nodes [2]. By loading the data into the graph database, the data science library can be used to train a machine learning model and make predictions.

Deciding whether two graphs are isomorphic is a classical algorithmic problem that has been researched since the early days of computing. Graph isomorphism involves determining when two graphs possess the same data structures and data connections [3]. It is widely used in various areas such as social networks, computer information system, image processing, protein structure, chemical bond structure, etc.

Unfortunately, the general graph isomorphism problem is not known to be solvable in polynomial time nor to be NP-complete, and therefore may be in the computational complexity class NP-intermediate [3–5]. An excellent literature review in this area can be found in [3] and also in [4]. In fact, this problem was even viewed as an open problem [6,7].

In this paper, we investigate the graph isomorphism of undirected graphs using the eigenvalues and eigenvectors of the adjacency matrices of the graphs. Eigenvalues and eigenvectors of square matrices have been widely used in many areas.

Eigenvalues are used in computer graphics to perform transformations on objects, such as rotating or scaling. For example, when an image is resized, the eigenvalues of its covariance matrix can be used to preserve its principal components and avoid distortion, because the eigenvectors of the covariance matrix are actually the directions of the axes of the principals components, while eigenvalues are simply the coefficients attached to eigenvectors, which given the amount of variance carried in each principal component [8]. Eigenvalues have also been widely used in signal processing to extract meaningful features from large datasets. For example, in image processing, the eigenvalues of a matrix of pixel intensities can be used to identify the most significant patterns and structures in the image [9]. Google's extraordinary success as a search engine was due to their clever use of eigenvalues and eigenvectors [10]. Claude Shannon utilized eigenvalues to calculate the theoretical limit of channel capacity. The eigenvalues are then essentially the gains of the channel's fundamental modes, which are recorded by the eigenvectors. Eigenvalues have also been employed to analyze the stability of structures and machines, such as determining the natural frequency of a bridge and assessing the likelihood of bridge oscillations or even collapse under specific conditions.

The rest of this paper is organized as follows: In Section 2, the preliminary is provided. Our main results are presented in Section 3. We conclude in Section 4.

2. Preliminary

2.1. Undirected graph and adjacency matrix

An undirected graph is generally represented as a pair $G = (V, E)$, where V is the set of vertices, and $E \subset V \times V$ is the set of

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edges satisfying $(u, v) \in E$ if and only if $(v, u) \in E$. The neighbors of a vertex v is $N(v) = \{w : (v, w) \in E\}$.

In graph theory, we say that $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there exists a bijection between the vertex sets of V_1 and V_2

$$f : V_1 \to V_2$$

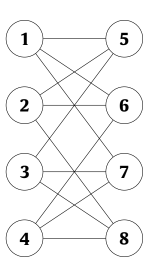
such that any two vertices u and v of G_1 are connected in G_1 if and only if $f(u)$ and $f(v)$ are connected in G_2, i.e., $(u, v) \in E_1$ if and only if $(f(u), f(v)) \in E_2$. If an isomorphism exists between two graphs, then the graphs are called isomorphic and denoted as $G_1 \simeq G_2$, and f is call an *isomorphic function* between G_1 and G_2.

In graph theory, the degree of a vertex v is the number of edges connecting it and denoted as $\deg(v)$. It is obvious that $\deg(v) = |N(v)|$. From the definition of isomorphism, we must have $\deg(v) = \deg(f(v))$, which implies that if $\deg(v) \neq \deg(f(v))$, then we cannot match up the two vertices.

In many applications, each edge E of a graph is associated with a numerical value called a weight, denoted as $w(E)$, which might represent for example costs, lengths or capacities, depending on the problem at hand. In this paper, we consider the weight of all edges to be 1.

For a graph with vertex set $V = \{v_1, \ldots, v_n\}$, the adjacency matrix, sometimes also called the connection matrix, is a square $n \times n$ (0, 1)-matrix A such that its element $A_{ij} = A_{ji} = 1$ if there is an edge from vertex v_i to vertex v_j, and 0 if there is no edge, and also $A_{ii} = 1$ for all i, that is 1's on its diagonal elements [11]. The elements of the matrix indicate whether pairs of vertices are adjacent or connected in the graph. If the graph is undirected (i.e., all of its edges are bidirectional), the adjacency matrix is symmetric, that is $A_{ij} = A_{ji}$.

Example 1. For the graph given below, the corresponding adjacency matrix is shown to the right.



$$\Longrightarrow \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Definition 1. Let A be an adjacency matrix of a graph G. We represent the matrix obtained by interchanging the ith and the jth rows and the ith and the jth columns of matrix A as $A[i \leftrightarrow j]$. We will refer to this operation as the (i, j) interchanging for simplicity.

The $A[i \leftrightarrow j]$ operation defined in Definition 1 can be represented in matrix multiplication form as follows:

$$A[i \leftrightarrow j] = E_{ij} A E_{ij}^T$$

where E_{ij} is the matrix derived by interchanging the ith and jth rows of the identity matrix I_n, that is

$$E_{ij} = \begin{array}{c} \begin{matrix} 1 & & i & & j & & n \end{matrix} \\ \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 0 & \cdots & 1 & & \\ & & \vdots & \ddots & \vdots & & \\ & & 1 & \cdots & 0 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix} \begin{matrix} 1 \\ \\ i \\ \\ j \\ \\ n \end{matrix} \end{array}$$

The number of 1's in a row or column of matrix A is referred as the *weight* of that row or column.

2.2. Eigenvalues and eigenvectors

For a square matrix A, a scale λ is called an *eigenvalue* [12] if there exists a vector $\boldsymbol{u}$ such that

$$A\boldsymbol{u} = \lambda \boldsymbol{u} \tag{1}$$

In this case, $\boldsymbol{u}$ is called an *eigenvector* of matrix A associated with eigenvalue λ.

Let A be an $n \times n$ matrix, then the expression

$$\det(xI - A) \tag{2}$$

is a polynomial, called the *characteristic polynomial* of matrix A, and

$$\det(xI - A) = 0 \tag{3}$$

is called the *characteristic equation*. The eigenvalues λ's of A defined in Eq. (1) are solutions of the characteristic equation (3).

It follows from Eq. (3) that if λ is an eigenvalue of A, then there exists a nonzero eigenvector $\boldsymbol{u}$ such that $A\boldsymbol{u} = \lambda\boldsymbol{u}$.

For an $n \times n$ matrix A with characteristic polynomial given by Eq. (2), the *multiplicity* of an eigenvalue λ of A is the number of times λ occurs as a root of that characteristic polynomial.

If A be a real symmetric matrix, then the eigenvalues of A are real numbers and eigenvectors corresponding to distinct eigenvalues are orthogonal.

If A is a real $n \times n$ symmetric matrix, then there exists an orthonormal (orthogonal and unit vector) set of eigenvectors that forms the basis of the n dimensional vector space.

3. Our main results

In this section, we provide theoretical proofs of our main results. Theorem 1 states that the adjacency matrices have the same column and row weights. Based on Theorem 1, we prove in Theorem 2 that two graphs are isomorphic if and only if their corresponding adjacency matrices can be transformed from one to the other through a sequence of column and row interchanging operations. Theorem 3 shows that two graphs are isomorphic if and only if their corresponding adjacency matrices have the same set of eigenvalues.

Theorem 1. *The interchange operations on adjacency matrices will not alter the weight of the columns or rows of the matrix.*

Proof. Let A be an $n \times n$ adjacency matrix of a graph and $1 \leq i, j \leq n$ are two integers, $i \neq j$. The matrix $A[i \leftrightarrow j]$ is derived from matrix A by interchanging the ith and jth rows and columns of A, resulting in the interchanging A_{ii} with A_{jj}, and A_{ij} with A_{ji}.

Since A is a symmetric matrix with diagonal elements equal to 1, these four elements in A remain unchanged. Therefore, the weight of the ith row or column is simply exchanged with the jth row or column. Therefore, the overall weight of the matrix A remains unchanged.

Note that this theorem holds due to the special structure of the adjacency matrix, and it does not hold true in general even for symmetric matrices.

Theorem 2. *Let A_1 and A_2 be the adjacency matrices of graphs G_1 and G_2, respectively. Then G_1 and G_2 are isomorphic if and only if there exists a sequence of interchange operations (i.e., a permutation matrix) that transforms the adjacency matrix A_1 to A_2.*

Proof. Assuming that graph G_1 is isomorphic to graph G_2. Denote their vertices and adjacency matrices as V_1, A_1 and V_2, A_2, respectively. According to the definition of graphic isomorphism, there is an injection $f : V_1 \to V_2$ such that $f(V_1) = V_2$.

Let the vertices of G_1 be $V_1 = \{1, \ldots, n\}$, then the vertex of G_2 can be expressed as $V_2 = \{f(1), \ldots, f(n)\}$. Define $g(i) = f^t(i)$ where $t = \max\{t \mid f^{t-1}(i) < i\}$. Then we can convert the adjacency matrix A_1 of G_1 to the adjacency matrix A_2 of G_2 through the following sequence of interchanging operations:

$$A_2 \leftarrow A_2[i \leftrightarrow g(i)], g(i) < i, i = 1, \ldots, n$$

On the other hand, assume there is a sequence of interchanging operations $A[j, h(j)] \leftrightarrow j \le n$ that transforms A_1 to A_2.

Define $f : V_1 \to V_2$ as follows:

$$f(i) = h^t(i)$$

where $t = \max\{t \mid h^{t-1}(i) > i\}$. Then f is an isomorphic function between G_1 and G_2.

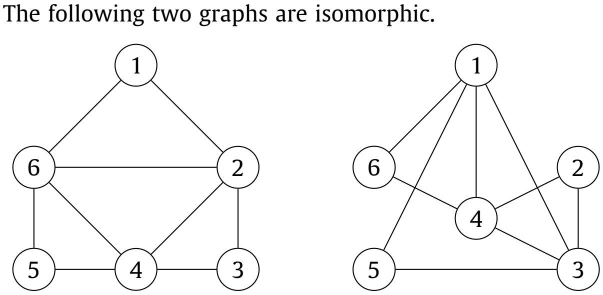
In addition to bridge isomorphism and interchange operations, Theorem 2 also provides an efficient algorithm to transform graph V_1 into its isomorphic counterpart V_2, as presented in Algorithm 1.

Algorithm 1 Transform graph G_1 to its isomorphic counterpart G_2 by transforming adjacency matrices A_1 to A_2

```
Let V_1 = {1, 2, ··· , n}, V_2 = {f(1), f(2), ··· , f(n)}
for i = 1 to n do
    t = f(i)
    for j = 1 to n do
        while t < i do
            t = f(t)
        end while
    end for
    g(i) = t
    A_1 = A_1[i, g(i)]
end for
```

Example 2. In this example, we will demonstrate how to construct a sequence of interchanging operations to convert one graph into another.

The following two graphs are isomorphic.

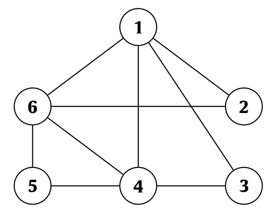


The adjacency matrices of the two graphs A and B are given below:

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

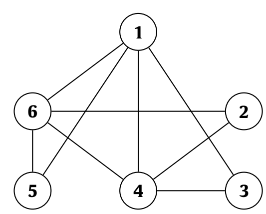
Suppose we want to transfer the vertices of V_1 to $V_2 = \{2, 5, 3, 4, 1, 6\}$. Based on Algorithm 1, we can transform the graph with matrix A to the graph with matrix B through the following sequence of interchanging operations.

(1) $A[1 \leftrightarrow 2]$, which transforms the graph with adjacency matrix A and the following graph and adjacency matrix:



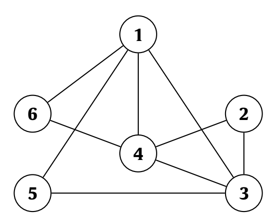
$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

(2) $A[2 \leftrightarrow 5]$, which further transforms the graph with adjacency matrix A and the following graph and adjacency matrix:



$$\begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

(3) $A[3 \leftrightarrow 6]$, which finally transforms the graph and the corresponding adjacency matrix from A to B:



$$\begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

Algorithm 2 Transform graph G_2 back to its isomorphic graph G_1 by transforming adjacency matrices A_2 to A_1

```
Let V_1 = {1, 2, ··· , n}, V_2 = {f(1), f(2), ··· , f(n)}
for i = 1 to n do
    t = f(i)
    for j = 1 to n do
        while t > i do
            t = f(t)
        end while
    end for
    h(i) = t
    A_2 1 = A_2[i, h(i)]
end for
```

Example 3. In this example, we illustrate how to construct the inverse sequence of operations that maps vertices of V_2 in graph G_2 back to the vertices in V_1 of graph G_1.

Based on Algorithm 2, we can transform matrix B to matrix A, which transform the vertices $V_2 = \{1, 2, 3, 4, 5, 6\}$ to $V_1 = \{5, 1, 6, 4, 2, 3\}$, through the following interchanging operations:

(1) $B[2 \leftrightarrow 1]$, which transforms B to

$$B_1 = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}$$

(2) $B[5 \leftrightarrow 1]$, which transforms B_1 to

$$B_2 = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}$$

(3) $B[6 \leftrightarrow 3]$, which transforms B_2 to A.

Since the interchange operation is an elementary matrix operation, it does not alter the eigenvalues of the adjacency matrix. Therefore, we have the following corollaries.

Corollary 1. *Let A_1 and A_2 be the adjacency matrices of graphs G_1 and G_2, respectively. If G_1 and G_2 are isomorphic, then their eigenvalues are the same.*

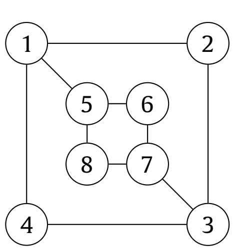
Corollary 2. *Let A_1 and A_2 be the adjacency matrices of graphs G_1 and G_2, respectively. If the eigenvalues of A_1 and A_2 are different, then they are not isomorphic.*

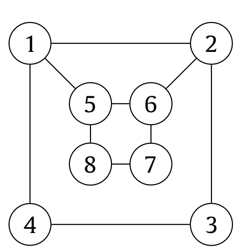
Corollary 3. *Let A and B be $n \times n$ adjacency matrices of two graphs. If the two graphs are isomorphic, then the total number of 1's (corresponding to the edges in the graphs) in the two matrices should be the same.*

From Corollary 3, we can conclude that if the number of 1's of two matrices are different, then the two graphs are not isomorphic.

However, the inverse of Corollary 3 is not true. In other words, even if two matrices have the same number of 1's, they may not be isomorphic, as shown in the following example.

Example 4. For the following two graphs,





their adjacency matrices are

$$G = \begin{bmatrix} 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

$$H = \begin{bmatrix} 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

Matrices G and H contain the same number of 1's. However, due to 0 being an eigenvalue of G but not of H, the two graphs are not isomorphic.

Next, suppose two graphs are isomorphic, based on the definition of graph isomorphism, the corresponding vertices should have the same degree. Moreover, the subsequent vertex should also have the same degree and structure. The vertex and the associated structure are refereed to as the *vertex tree*. Therefore, the corresponding vertices should have the same vertex trees.

Based on this discovery, we can derive Algorithm 3.

Algorithm 3 Derive an isomorphic function to transform graph G_1 to graph G_2

Let G_1 and G_2 be two graphs and their vertex sets are $V_1 = \{v_1, \cdots, v_n\}$ and $V_2 = \{\bar{v}_1, \cdots, \bar{v}_n\}$, respectively.
Derive the degree tree of all the vertex of both graph G_1 and graph G_2.
repeat
  Select a vertex $v \in V_1$.
  if no vertex in V_2 has the same vertex tree as v **then**
    $G_1 \ncong G_2$ and **stop**
  else
    Select a vertex $\bar{v} \in V_2$, that has the same vertex tree as v and map $f : v \to \bar{v}$.
    $V_1 \leftarrow V_1 \backslash \{v\}$ and $V_2 \leftarrow V_2 \backslash \{\bar{v}\}$.
  end if
until $V_1 = \emptyset$, or no $\bar{v} \in V_2$ for the selected v.

This following example shows how Algorithm 3 can be used to define an isomorphic mapping between two graphs.

Example 5. For the two graphs given in Example 2, the degrees for the 6 vertices of graphs A and B are given below:

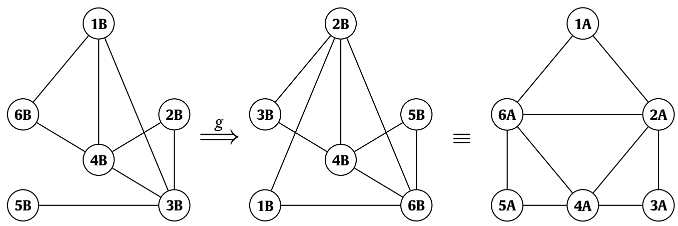
$A : \{2, 4, 2, 4, 2, 4\}$, $B : \{4, 2, 4, 4, 2, 2\}$.

Based on the degree information, we can derive the following mapping g, which transforms graph B to graph A:

(1) Since the degree of node 1_B is 4, it can only be mapped to one of the nodes in $\{2_A, 4_A, 6_A\}$. Let us map node 1_B to node 2_A, i.e., define $g(1_B) = 2_A$.
(2) Node 2_B has degree 2, so it can only be mapped to a node in $\{1_A, 3_A, 5_A\}$. Define $f(2_B) = 5_A$.

(3) Similarly, node 3_B has degree 4, and can only be mapped to the remaining nodes that have degree 2, $\{2_A, 4_A, 6_A\}$. However, since we have mapped node 1_B to 2_A, we can only map node 3_B to 4_A or 6_A. Let us select 6_A, i.e., $g(3_B) = 6_A$.
(4) Finally, we define $g(4_B) = 4_A, g(5_B) = 1_A, g(6_B) = 3_A$.

The above process can be demonstrated through the following figure:

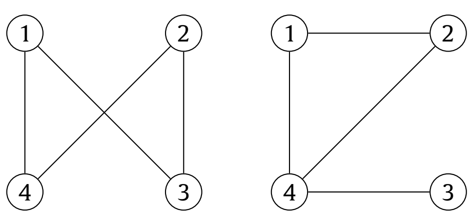


Corollary 4. *The corresponding rows and columns of the adjacency matrices of two isomorphic graphs have the same distribution of 0's and 1's.*

Example 6. Let

$$A = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

The corresponding graphs are



Since the weight sequence of the rows for matrix A is 3, 3, 3, 3, and for matrix B is 3, 3, 2, 4, which are different, therefore, the graphs corresponding to matrices A and B are not isomorphic. In fact, it can also be verified that the characteristic polynomials for matrix A is $x^4 - 4x^3 + 2x^2 + 4x - 3$ and for matrix B is $x^4 - 4x^3 + 2x^2 + 2x$, which is different from that of A. Therefore, the two graphs cannot be isomorphic, and there does not exist an orthogonal matrix P that satisfies the equation $PAP^T = B$ to make matrices A and B equivalent.

The inequivalence of these two graphs can also be confirmed because the weights of the rows and columns in their adjacency matrices are different.

Theorem 3. *Let A and B, the adjacency matrices of graphs G_1 and G_2, respectively, have the same column/row weight. Then G_1 and G_2 are isomorphic if and only if their adjacency matrices have the same characteristic polynomial (the same eigenvalues).*

Sketch of Proof. The necessity of this theorem is straightforward based on Theorem 2. Therefore, we only need to prove the sufficiency part.

We will use the induction method to prove this theorem. For $n = 2$, if A and B have the same characteristic polynomial, then it is apparent that $A = B$; therefore, $P = I$ is sufficient.

Suppose the result holds true for $n - 1$, we need to prove that it is also true for n.

Without loss of generality, we may assume that the first rows/columns of A and B have the same weight since, otherwise, we only need a single interchange operation, denoted as P_1, such that the weight of the first row/column of matrix $P_1AP_1^T$ is the same as that of matrix B.

Let

$$P_1AP_1^T = \begin{bmatrix} 1 & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix}, \quad B = \begin{bmatrix} 1 & B_{12} \\ B_{12}^T & B_{22} \end{bmatrix} \tag{4}$$

Based on our assumption, it can be easily derived from Eq. (4) that A_{12} and B_{12} have the same weight, which implies that A_{22} and B_{22} also have the same row/column weight sequence.

Since both A_{22} and B_{22} are matrices of order $n-1$, there exists a $(n-1) \times (n-1)$ permutation matrix P_2 such that

$$P_2A_{22}P_2^T = B_{22}.$$

Define

$$P = \begin{bmatrix} 1 & 0 \\ 0 & P_2 \end{bmatrix} P_1$$

then we have

$$\begin{aligned} PAP^T &= \begin{bmatrix} 1 & 0 \\ 0 & P_2 \end{bmatrix} P_1AP_1^T \begin{bmatrix} 1 & 0 \\ 0 & P_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & P_2 \end{bmatrix} \begin{bmatrix} 1 & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & P_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & A_{12} \\ P_2A_{12}^T & P_2A_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & P_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & A_{12}P_2^T \\ P_2A_{12}^T & P_2A_{22}P_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & A_{12}P_2^T \\ P_2A_{12}^T & B_{22} \end{bmatrix} \end{aligned}$$

Since the weight sequence of A is the same as the B and B_{22} is the same as that of A_{22}, it implies that $A_{12}P_2^T = B_{12}$. Therefore, we have

$$PAP^T = \begin{bmatrix} 1 & B_{12} \\ B_{12}^T & B_{22} \end{bmatrix} = B \tag{5}$$

and P is a permutation matrix, which concludes the proof of the theorem.

Corollary 5. *Let A and B be $n \times n$ adjacency matrices of two graphs that have the same set of eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, all with single multiplicity. Let u_i and v_i be the normalized (length equal to 1) eigenvector corresponding to eigenvalue λ_i with respect to matrix A and B, respectively. Let $U = [u_1 \cdots u_n]$, $V = [v_1 \cdots v_n]$, $i = 1, \ldots, n$, and $P = V^TU$, then P is a permutation matrix such that*

$$PAP^T = B \tag{6}$$

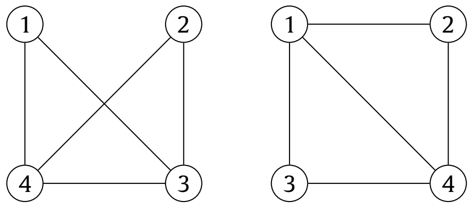
Proof. Without loss of generality, we may assume $\lambda_1 > \lambda_2 > \cdots > \lambda_n$. It is well-known that the normalized eigenvectors u_i and v_i are both bases of their corresponding 1-dimensional subgroups. Therefore, both U and V are unique. Therefore, $P = V^TU$ is also unique. Based on Theorem 3, we have

$$PAP^T = B$$

It follows from Theorem 2 that P is a permutation matrix. □

The following two examples demonstrate how to derive a permutation matrix P for matrices A and B that satisfies Eq. (6) using Corollary 5.

Example 7. For the following two graphs:



their corresponding adjacency matrices are

$$A = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$$

The eigenvalues for the two matrices are 0, 1, $\frac{3-\sqrt{17}}{2}$, $\frac{3+\sqrt{17}}{2}$. Based on Corollary 5, there exists a permutation matrix P such that $PAP^T = B$.

To derive such a permutation matrix P, we first construct the orthonormal matrices from eigenvectors corresponding to the eivenvalues sequence listed above for matrices A and B as follows:

$$U = \begin{bmatrix} \frac{\sqrt{17+\sqrt{17}}(\sqrt{17}-1)}{8\sqrt{17}} & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{17-\sqrt{17}}(\sqrt{17}+1)}{8\sqrt{17}} \\ \frac{\sqrt{17+\sqrt{17}}(\sqrt{17}-1)}{8\sqrt{17}} & \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{17-\sqrt{17}}(\sqrt{17}+1)}{8\sqrt{17}} \\ \frac{\sqrt{17+\sqrt{17}}}{2\sqrt{17}} & 0 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{17-\sqrt{17}}}{2\sqrt{17}} \\ \frac{\sqrt{17+\sqrt{17}}}{2\sqrt{17}} & 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{17+\sqrt{17}}}{2\sqrt{17}} \end{bmatrix}$$

$$V = \begin{bmatrix} -\frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{17-\sqrt{17}}}{2\sqrt{17}} & \frac{\sqrt{17+\sqrt{17}}}{2\sqrt{17}} \\ 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{17-\sqrt{17}}(\sqrt{17}+1)}{8\sqrt{17}} & \frac{\sqrt{17+\sqrt{17}}(\sqrt{17}-1)}{8\sqrt{17}} \\ 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{17-\sqrt{17}}(\sqrt{17}+1)}{8\sqrt{17}} & \frac{\sqrt{17+\sqrt{17}}(\sqrt{17}-1)}{8\sqrt{17}} \\ \frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{17-\sqrt{17}}}{2\sqrt{17}} & \frac{\sqrt{17+\sqrt{17}}}{2\sqrt{17}} \end{bmatrix}$$

While neither of these two matrices is close to a permutation matrix, we have

$$P = VU^T = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

which is the permutation matrix such that

$$PAP^T = B$$

Similar to the previous example, in the next example, we can easily derive a permutation matrix for matrices A and B that satisfies Eq. (6).

Example 8. Let

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

The eigenvalues for A and B are $1, 1-\sqrt{2}, 1+\sqrt{2}$. The corresponding orthonormal matrices generated from the eigenvectors of matrices A and B are:

$$U = \begin{bmatrix} -\frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad V = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{\sqrt{2}}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

While neither of these two matrices is a permutation matrix, we can derive a permutation matrix

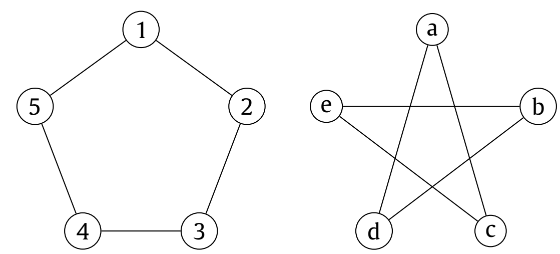
$$P = VU^T = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

such that

$$PAP^T = B$$

Corollary 5 provides an efficient algorithm to derive a permutation matrix P for matrices A and B such that $PAP^T = B$, where A and B have the same set of eigenvalues with single multiplicity. In case that the multiplicity of some eigenvalues is not single, even though the existence of such a permutation is known, the matrix derived this way may or may not be a permutation matrix anymore. Example 9 below shows that matrix derived this way is a permutation matrix that satisfies Eq. (6), while the matrix derived in Example 10 is not even a permutation matrix.

Example 9. Consider the following two graphs:



There corresponding adjacency matrices are:

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix}$$

The two adjacency matrices have the same set of eigenvalues: 3, $\frac{1+\sqrt{5}}{2}$, $\frac{1+\sqrt{5}}{2}$, $\frac{1-\sqrt{5}}{2}$, $\frac{1-\sqrt{5}}{2}$, where both $\frac{1+\sqrt{5}}{2}$ and $\frac{1-\sqrt{5}}{2}$ are duplicate eigenvalues. The corresponding orthonormal matrices derived from the eigenvectors for matrices A and B are

$$U = \begin{bmatrix} \frac{\sqrt{5}}{5} & \frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & \frac{\sqrt{5-\sqrt{5}}}{2\sqrt{5}} & -\frac{5\sqrt{2}+\sqrt{10}}{20} & -\frac{5\sqrt{2}+\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & \frac{\sqrt{5+\sqrt{5}}}{2\sqrt{5}} & -\frac{\sqrt{5+\sqrt{5}}}{2\sqrt{5}} & -\frac{5\sqrt{2}+\sqrt{10}}{20} & \frac{5\sqrt{2}-\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & -\frac{\sqrt{5+\sqrt{5}}}{2\sqrt{5}} & -\frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & \frac{5\sqrt{2}-\sqrt{10}}{20} & \frac{5\sqrt{2}-\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & \frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & 0 & \frac{\sqrt{10}}{5} & -\frac{5\sqrt{2}+\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & \frac{5\sqrt{2}-\sqrt{10}}{20} & \frac{\sqrt{10}}{5} \end{bmatrix}$$

and

$$V = \begin{bmatrix} \frac{\sqrt{5}}{5} & \frac{\sqrt{5+\sqrt{5}}}{2\sqrt{2}} & -\frac{\sqrt{5-\sqrt{5}}}{2\sqrt{5}} & -\frac{5\sqrt{2}+\sqrt{10}}{20} & \frac{5\sqrt{2}-\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & \frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & 0 & \frac{\sqrt{10}}{5} & -\frac{5\sqrt{2}+\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & -\frac{\sqrt{5-\sqrt{5}}}{\sqrt{20}} & \frac{\sqrt{5-\sqrt{5}}}{2\sqrt{2}} & -\frac{5\sqrt{2}+\sqrt{10}}{20} & -\frac{5\sqrt{2}+\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & -\frac{\sqrt{5+\sqrt{5}}}{2\sqrt{5}} & -\frac{\sqrt{5+\sqrt{5}}}{\sqrt{20}} & \frac{5\sqrt{2}-\sqrt{10}}{20} & \frac{5\sqrt{2}-\sqrt{10}}{20} \\ \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5+\sqrt{5}}}{\sqrt{20}} & \frac{5\sqrt{2}-\sqrt{10}}{20} & \frac{\sqrt{10}}{5} \end{bmatrix}$$

respectively. It can be clearly seen that neither U nor V is even an integer matrix. However, it can be verified that

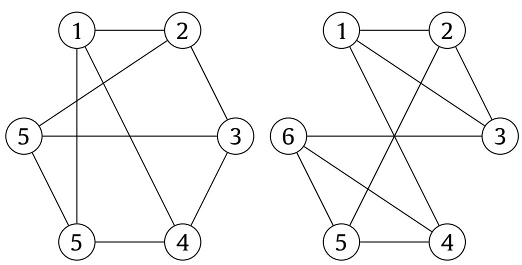
$$P = VU^T = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

is a permutation matrix such that

$$PAP^T = B$$

However, when the multiplicities of some eigenvectors are not single, the result presented in Example 9 may not always be true. In other words, we may not always be able to derive a permutation matrix that transforms matrix A to matrix B, as shown in the following example.

Example 10. For the following two graphs



their corresponding adjacency matrices are given below:

$$A = \begin{bmatrix} 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The eigenvalues of these two matrices are $-1, -1, 1, 1, 4, 2$, where both -1 and 1 are eigenvalues of multiplicity 2. Based on this order, we derive the orthonormal matrices from the eigenvectors of matrices A and B as follows:

$$U = \begin{bmatrix} -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{1}{2} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} \\ -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{1}{2} & \frac{\sqrt{3}}{6} \\ -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{3}}{3} & 0 & -\frac{\sqrt{3}}{3} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{3}}{3} & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$V = \begin{bmatrix} -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{1}{2} & \frac{\sqrt{3}}{6} \\ -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{1}{2} & \frac{\sqrt{3}}{6} \\ -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{3}}{3} & 0 & -\frac{\sqrt{3}}{3} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{1}{2} & -\frac{\sqrt{3}}{6} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{1}{2} & -\frac{\sqrt{3}}{6} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{3}}{3} & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

It can be verified that

$$VU^T = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

is not even an integer matrix, let alone a permutation matrix.

However, it is easy to verify that we can construct a permutation matrix P from the 6×6 identity matrix through 3 consecutive row interchanging operations: $(3, 5), (3, 6), (1, 5)$, that is for

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

we have

$$PAP^T = B$$

Based on Theorem 3, we can derive the following corollary.

Corollary 6. *The complexity in determining whether two undirected graphs are isomorphic is at most $\mathcal{O}(n^3)$.*

Proof. The proof of this corollary follows from the well-known result, which says that the complexity in finding the eigenvalues of each matrix is at most $\mathcal{O}(n^3)$.

4. Conclusion

In this paper, we analyzed the isomorphic problem of undirected graphs and presented two major theorems to characterize it. Specifically, we proved that determining whether two undirected graphs are isomorphic has a complexity of at most $\mathcal{O}(n^3)$. Additionally, we also designed algorithms to convert between isomorphic graphs along with multiple examples.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

[1] Graph (discrete mathematics). [Online]. Available: https://en.wikipedia.org/wiki/Graph_(discrete_mathematics).

[2] Z. Blumenfeld, Graph machine learning: An overview – key concepts for getting started. [Online]. Available: https://towardsdatascience.com/graph-machine-learning-an-overview-c996e53fab90.

[3] M. Grohe, P. Schweitzer, The graph isomorphism problem, Commun. ACM 63 (11) (2020) 128–134, [Online]. Available: http://dx.doi.org/10.1145/3372123.

[4] B.D. McKay, A. Piperno, Practical graph isomorphism, ii, J. Symbolic Comput. (2014) 94–112, [Online]. Available: http://dx.doi.org/10.1016/j.jsc.2013.09.003.
[5] Graph isomorphism problem. [Online]. Available: https://en.wikipedia.org/wiki/Graph_isomorphism_problem.
[6] R. Karp, Reducibilities among combinatorial problems, in: R. Miller, J. Thatcher (Eds.), Complexity of Computer Computations, Plenum Press, New York, 1972, pp. 85–103.
[7] M. Garey, D. Johnson, Computers and Intractability: A Guide To the Theory of NP-Completeness, Freeman, 1979.
[8] Principal component analysis part 1: The different formulations. [Online]. Available: https://towardsdatascience.com/principal-component-analysis-part-1-the-different-formulations-6508f63a5553.
[9] How are eigenvalues used in real life?.
[10] Applications of eigenvalues and eigenvectors. [Online]. Available: https://www.intmath.com/matrices-determinants/8-applications-eigenvalues-eigenvectors.php.
[11] Adjacency matrix. [Online]. Available: https://mathworld.wolfram.com/AdjacencyMatrix.html.
[12] D. Margalit, J. Rabinoff, Interactive linear algebra. [Online]. Available: https://textbooks.math.gatech.edu/ila/ila.pdf.