Graph Isomorphism and Matrix Representations

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Outline
Graph Isomorphism

Definition

Two graphs $G_1$ and $G_2$ are **isomorphic** if there exist one-to-one and onto functions (bijections) $g: V(G_1) \rightarrow V(G_2)$ and $h: E(G_1) \rightarrow E(G_2)$ such that for any $v \in V(G_1)$ and any $e \in E(G_1)$,

$v$ is an endpoint of $e$ if and only if $g(v)$ is an endpoint of $h(e)$.

The pair of functions $g$ and $h$ is called a **graph isomorphism**.

- Roughly speaking, graphs $G_1$ and $G_2$ are isomorphic to each other if they are “essentially” the same.
- More intuitively, if graphs are made of elastic bands (edges) and knots (vertices), then two graphs are isomorphic to each other if and only if one can stretch, shrink and twist one graph so that it can sit right on top of the other graph, vertex to vertex and edge to edge.
- The isomorphism functions $g$ and $h$ will thus provide the one-to-one correspondences for the vertices and the edges respectively.
Example

Show that graphs $G_1$ and $G_2$ below are isomorphic.

Let $g$ and $h$ be given by

$$g(v_1) = w_2, \quad g(v_2) = w_1, \quad g(v_3) = w_4, \quad g(v_4) = w_3,$$

$$h(e_1) = f_2, \quad h(e_2) = f_1, \quad h(e_3) = f_4, \quad h(e_4) = f_3, \quad h(e_5) = f_5$$

which can be alternatively represented in the diagrams below.
Graph Isomorphism Example

\[ V(G_1) \xrightarrow{g} V(G_2) \]

\[ E(G_1) \xrightarrow{h} E(G_2) \]
Graph Isomorphism Example

- We now verify the *preservation of endpoints* under $g$ and $h$

\[
\begin{align*}
e_1 & \triangleq \{v_1, v_2\} \rightarrow f_2 \triangleq \{w_1, w_2\} = \{g(v_1), g(v_2)\} \\
e_2 & \triangleq \{v_2, v_4\} \rightarrow f_1 \triangleq \{w_1, w_3\} = \{g(v_2), g(v_4)\} \\
e_3 & \triangleq \{v_2, v_3\} \rightarrow f_4 \triangleq \{w_1, w_4\} = \{g(v_2), g(v_3)\} \\
e_4 & \triangleq \{v_1, v_4\} \rightarrow f_3 \triangleq \{w_2, w_3\} = \{g(v_1), g(v_4)\} \\
e_5 & \triangleq \{v_3, v_4\} \rightarrow f_5 \triangleq \{w_3, w_4\} = \{g(v_3), g(v_4)\},
\end{align*}
\]

where we used $e \triangleq \{v, w\}$ to indicate that edge $e$ has endpoints $\{v, w\}$.

- Since $g$ and $h$ are obviously one-to-one and onto, the pair $g$ and $h$ thus constitute an isomorphism of graphs $G_1$ and $G_2$, i.e. $G_1$ and $G_2$ are isomorphic, $G_1 \cong G_2$. 

Graph Isomorphism
Example

The vertex bijection is given by $1 \rightarrow 1$, $2 \rightarrow 2$, $3 \rightarrow 4$, $4 \rightarrow 3$
Isomorphic invariant

- Isomorphic graphs are "same" in shapes, so properties on "shapes" will remain invariant for all graphs isomorphic to each other.

- A property $P$ is called an **isomorphic invariant** if and only if, given any graphs isomorphic to each other, all the graphs will have property $P$ whenever any one of the graphs does.

- There are many isomorphic invariants, e.g.

  (a) vertices of a given degree,
  (b) number of edges,
  (c) number of connected components,
  (d) has a circuit of given length,
  (e) number of loops at a vertex,
  (f) number of sets of parallel edges,
  (g) has a Hamiltonian circuit.

- Incidentally, an **isomorphic invariant** is sometimes also referred to as an **isomorphism invariant**.
Isomorphic invariant

Example

Graphs $G_1$ and $G_2$ below are not isomorphic to each other because vertex $v$ of $G_1$ has degree 5 while no vertices of $G_2$ have degree 5.
Isomorphic invariant

Example

Back to example 1. We now explain briefly how we found the isomorphism functions $g$ and $h$ there.

First, since $v_2, v_4$ in $G_1$ and $w_1$ and $w_3$ in $G_2$ are the only vertices of degree 3, $g$ must map $v_2, v_4$ to $w_1, w_3$ or $w_3, w_1$ respectively.

We thus choose $g(v_2) = w_1$ and $g(v_4) = w_3$.

Since $\{v_2, v_4\}$ are the endpoints of $e_2$, we must have $h(e_2) = f_1$ so that the endpoints $\{v_2, v_4\}$ of edge $e_2$ are preserved because $f_1$ has endpoints $\{w_1, w_3\} = \{g(v_2), g(v_4)\}$.

Next we need to map $v_1, v_3$ to $w_2, w_4$ or $w_4, w_2$ respectively.

If we choose $w_2 = g(v_1)$ we must have $w_4 = g(v_3)$.

Thus the edge $e_1$ joining $v_1$ and $v_2$ should be mapped to the edge $f_2$ joining $g(v_1) = w_2$ and $g(v_2) = w_1$, i.e. $f_2 = h(e_1)$, etc.
Matrices

- A **matrix** is a rectangular array of numbers (sometimes symbols or expressions) placed at the intersections of rows with columns.
- These numbers are called the *elements* of the matrix.
- A **m-by-n** matrix has $m$ rows and $n$ columns and $m \times n$ is called the *size* of the matrix.
- A squared matrix has the number of rows equal to the number of columns, for instance $n \times n$.
- Usually, the elements of a matrix are denoted by a variable with two subscripts, one for its row and one for its column, e.g.,
  - To represent the element at the third row and fifth column of a matrix $A = (a_{ij})_{m \times n}$, we use
    - $a(3, 5)$ or, equivalently,
    - $a_{35}$
Matrix Operations

- Matrices of the same size can be **added** \((A + B)\) or **subtracted** \((A - B)\) element by element.
- The **scalar multiplication** \(kA\) of a matrix \(A\) and a number \(k\) is given by multiplying every element of \(A\) by \(k\).
- **Multiplication** of two matrices is defined only if the number of columns of the left matrix is the same as the number of rows of the right matrix, that is, given \(A_{m\times n}\) and \(B_{n\times p}\), then \(A_{m\times n} \times B_{n\times p} = C_{m\times p}\).
Matrix Operations

- The elements of $C = (c_{ij})$ are given by dot product (sum of element by element products) of the corresponding row ($i$th) of $A$ and the corresponding column ($j$th) of $B$, that is if

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i1} & a_{i2} & \cdots & a_{in} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$ and $B = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1j} & \cdots & b_{1p} \\ b_{21} & b_{22} & \cdots & b_{2j} & \cdots & b_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nj} & \cdots & b_{np} \end{bmatrix}$

then matrix $C = A \times B$ has $m$ rows and $p$ columns

$$C = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1j} & \cdots & c_{1p} \\ c_{21} & c_{22} & \cdots & c_{2j} & \cdots & c_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ c_{i1} & c_{i2} & \cdots & c_{ij} & \cdots & c_{ip} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mj} & \cdots & c_{mp} \end{bmatrix}$$
Matrix Operations

where

\[ c_{ij} = (a_{i1}, a_{i2}, \cdots, a_{in}) \cdot (b_{1j}, b_{2j}, \cdots, b_{nj}) = a_{i1}b_{1j} + a_{i2}b_{2j} + \cdots + a_{in}b_{nj} \]

or, using summation notation, this can be written much more concisely as

\[ c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj} \]

If \( A = (a_{ij}) \) and \( B = (b_{ij}) \) are two \( n \times n \) matrices, the product of \( A \) and \( B \), i.e. \( AB \), is always possible and it is another \( n \times n \) squared matrix

\[ C = (c_{ij}) \] in which \( c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj} \).
Matrix Operations

Example

Let 2 × 2 (i.e. 2 by 2) matrices $A$ and $B$ be given respectively by

$$A = \begin{bmatrix} 2 & -1 \\ 5 & 3 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 7 & 4 \\ 1 & -2 \end{bmatrix}.$$

Find $A + B$, $AB$ and $A^2$.

Solution.

$$A + B = \begin{bmatrix} 2 + 7 & -1 + 4 \\ 5 + 1 & 3 - 2 \end{bmatrix} = \begin{bmatrix} 9 & 3 \\ 6 & 1 \end{bmatrix}$$

$$AB = \begin{bmatrix} 2 & -1 \\ 5 & 3 \end{bmatrix} \times \begin{bmatrix} 7 & 4 \\ 1 & -2 \end{bmatrix} = \begin{bmatrix} 2 \times 7 + (-1) \times 1 & 2 \times 4 + (-1) \times (-2) \\ 5 \times 7 + 3 \times 1 & 5 \times 4 + 3 \times (-2) \end{bmatrix}$$

$$= \begin{bmatrix} 13 & 10 \\ 38 & 14 \end{bmatrix}$$

$$A^2 = \begin{bmatrix} 2 & -1 \\ 5 & 3 \end{bmatrix} \times \begin{bmatrix} 2 & -1 \\ 5 & 3 \end{bmatrix} = \begin{bmatrix} 2 \times 2 + (-1) \times 5 & 2 \times (-1) + (-1) \times 3 \\ 5 \times 2 + 3 \times 5 & 5 \times (-1) + 3 \times 3 \end{bmatrix}$$

$$= \begin{bmatrix} -1 & -5 \\ 25 & 4 \end{bmatrix}$$
Matrix Operations

Example

Let $3 \times 3$ matrices $A$ and $B$ be given by

$$A = \begin{bmatrix} 2 & -1 & 13 \\ 5 & 3 & -6 \\ 11 & 0 & 10 \end{bmatrix} \quad B = \begin{bmatrix} 7 & 4 & -8 \\ 1 & -2 & 0 \\ 9 & -4 & -3 \end{bmatrix}$$

Find the product matrix $AB$.

$$AB = \begin{bmatrix} 2 & -1 & 13 \\ 5 & 3 & -6 \\ 11 & 0 & 10 \end{bmatrix} \times \begin{bmatrix} 7 & 4 & -8 \\ 1 & -2 & 0 \\ 9 & -4 & -3 \end{bmatrix}$$
The Adjacency Matrix

- Given a directed (undirected) graph $G$ of $n$ vertices $v_1, \cdots, v_n$, we can represent the graph by an $n \times n$ matrix $A$ over $\mathbb{N}$, i.e.

\[
A = \begin{bmatrix}
  a_{11} & \cdots & a_{1n} \\
  \vdots & \ddots & \vdots \\
  a_{n1} & \cdots & a_{nn}
\end{bmatrix}, \quad a_{ij} \in \mathbb{N}
\]

in which the element $a_{ij}$

- is the number of arrows from $v_i$ to $v_j$ if $G$ is a directed graph, or
- $a_{ij}$ is the number of edges connecting $v_i$ to $v_j$ if $G$ is an undirected graph.

- This matrix $A$ is then said to be the adjacency matrix of the graph $G$.

- We note that a matrix is essentially just a table, and an adjacency matrix basically represents a table of nonnegative integers which correspond to the number of edges between different pair of vertices.
The adjacency matrix of digraph on the right is

\[
A = \begin{bmatrix}
1 & 0 & 0 \\
1 & 1 & 2 \\
1 & 0 & 0
\end{bmatrix}
\]
The Adjacency Matrix

Example

The adjacency matrix of graph on the right is

\[
A = \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 2 \\
1 & 2 & 0
\end{bmatrix}
\]
Theorem

Let $G$ be a directed or undirected graph of $n$ vertices $v_1, v_2, \ldots, v_n$, and $A$ be the adjacency matrix of $G$. Then for any positive integer $m$, the $(i, j)$-th entry of $A^m$ is equal to the number of walks of length $m$ from $v_i$ to $v_j$, where $i, j = 1, 2, \ldots n$.

Proof.

- Let $S_m$ denote the statement that $(i, j)^{th}$ entry of $A^m$ is equal to the number of walks of length $m$ from $v_i$ to $v_j$.
- Then for $m = 1$, $S_1$ is true because the adjacency matrix $A$ is defined that way.
- For the induction purpose we now assume $S_k$ is true with $k \geq 1$.
- Let $B = (b_{ij}) \overset{\text{def}}{=} A^k$, then $b_{sj} = \text{the number of walks of length } k \text{ from } v_s \text{ to } v_j$ due to the induction assumption. Hence
Number of Walks

Proof.

\[(i, j)\text{-th element of } A^{k+1} = (i, j)\text{-th element of } AB \]
\[= a_{i1}b_{1j} + a_{i2}b_{2j} + \ldots + a_{is}b_{sj} + \ldots + a_{in}b_{nj} \]

the number of walks of length \(k + 1\) from \(v_i\) to \(v_j\)
that have \(v_s\) as their 2nd vertex

\[= \text{the number of walks of length } k + 1 \text{ from } v_i \text{ to } v_j \]
(taking any vertex as the 2nd vertex)

i.e. \(S_{k+1}\) is true.

Hence \(S_m\) is true for all \(m \geq 1\), and the proof of the theorem is thus completed. \(\square\)
Number of Walks

Example

Consider the digraph on the right, which has the adjacency matrix $A$ below

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

Since

$$A^2 = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 2 & 1 & 0 \end{bmatrix}$$

we see there are exactly 2 walks of length 2 that start at $v_3$ and end at $v_1$. 
Number of Walks

Since

\[
A + A^2 + A^3 = \begin{bmatrix}
1 & 1 & 0 \\
1 & 0 & 0 \\
1 & 1 & 0
\end{bmatrix} + \begin{bmatrix}
2 & 1 & 0 \\
1 & 1 & 0 \\
2 & 1 & 0
\end{bmatrix} + \begin{bmatrix}
3 & 2 & 0 \\
2 & 1 & 0 \\
3 & 2 & 0
\end{bmatrix} = \begin{bmatrix}
6 & 4 & 0 \\
4 & 2 & 0 \\
6 & 4 & 0
\end{bmatrix}
\]

has only 0’s in the third column, we conclude that no vertex can reach \(v_3\) via a walk of nonzero length.