

isomorphism  
permutation matrix  
similarity

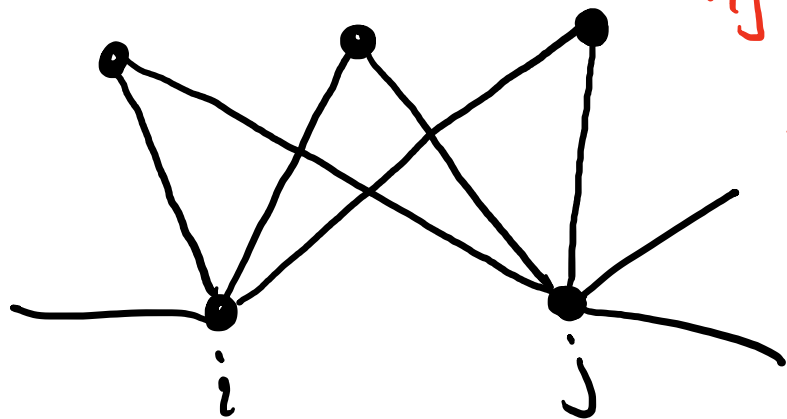
SYSM 6302

CLASS 16

# Similarity

Two nodes can be similar because they

Connect to the same nodes



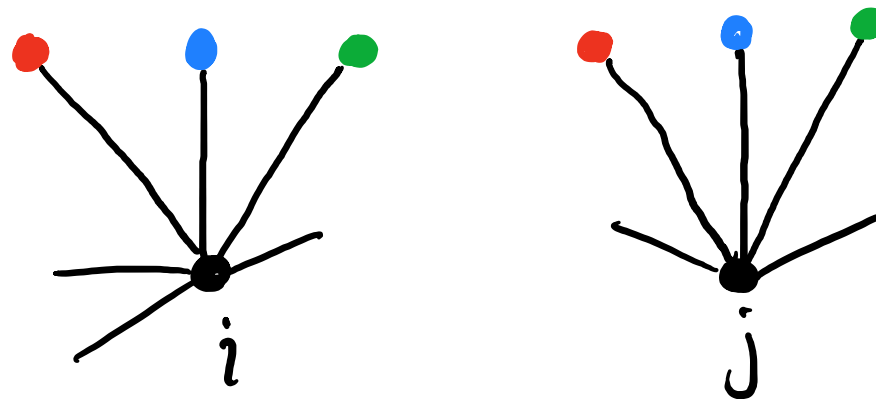
$$\begin{aligned} n_{ij} &= \sum_{k=1}^n A_{ik} A_{jk} \\ &= \sum_{k=1}^n A_{ik} A_{kj} \\ &= [A^2]_{ij} \end{aligned}$$

undirected graph

Structural Equivalence

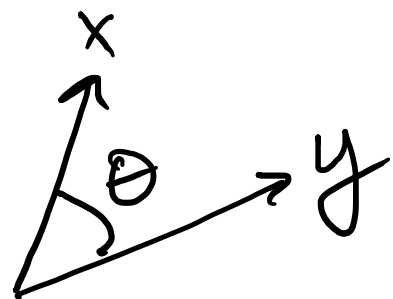
(aka Revenge of Cocitation)

Connect to different nodes, but that are similar



Regular Equivalence

# Cosine Similarity



Similar vectors point in the same direction

$$x \cdot y = |x| |y| \cos \theta$$

$$\cos \theta = \frac{x \cdot y}{|x| |y|}$$

Let  $x = i^{\text{th}}$  row of  $A$   
 $y = j^{\text{th}}$  row of  $A$  ↖  
Connections to node  $i$   
Connections to node  $j$

$$A_{ij} \in \{0, 1\} \Rightarrow A_{ij} = (A_{ij})^2$$

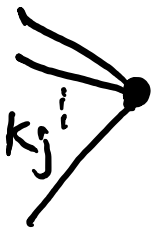
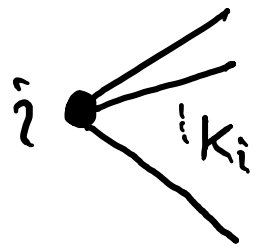
$$0 \leq \sigma_{ij} \leq 1$$

$$\sigma_{ij} = \cos \theta = \frac{x \cdot y}{|x| |y|} = \frac{\sum_{k=1}^n A_{ik} A_{jk}}{\sqrt{\sum_k A_{ik}^2} \sqrt{\sum_k A_{jk}^2}} \stackrel{\downarrow}{=} \frac{n_{ij}}{\sqrt{\sum_k A_{ik}} \sqrt{\sum_k A_{jk}}} = \frac{n_{ij}}{\sqrt{k_i k_j}}$$

# Pearson Correlation Coefficient for Similarity

Compare  $n_{ij}$  to the number of common neighbors expected at random

$$\sigma_{ij} = n_{ij} - \frac{k_i k_j}{n} = \sum_{l=1}^n A_{il} A_{jl} - n \underbrace{\frac{k_i}{n}}_{\langle A_i \rangle} \underbrace{\frac{k_j}{n}}_{\langle A_j \rangle} = \sum_{l=1}^n (A_{il} A_{jl} - \langle A_i \rangle \langle A_j \rangle)$$



$\frac{k_i}{n-1} \approx \frac{k_i}{n}$  : probability of connecting node  $i$  to any other node at random

$k_j$  : number of "tries" to connect  $i$  to  $j$

$\langle A_i \rangle$   $\langle A_j \rangle$   
 ↑  
 average of elements in row  $i$

$$= \sum_{l=1}^n (A_{il} - \langle A_i \rangle)(A_{jl} - \langle A_j \rangle)$$

$$= \text{COV}(A_i, A_j)$$

$$r_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}} \sqrt{\sigma_{jj}}} \quad , \quad -1 \leq r_{ij} \leq 1$$

# Regular Equivalence

$$\sigma_{ij} = \alpha \sum_{k=1}^n A_{ik} \sum_{l=1}^n A_{jl} \sigma_{kl}$$

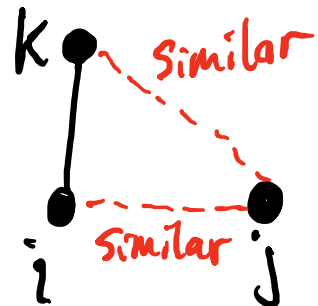
similarity of nbers of i and j  
 sum over nbers of i  
 sum over nbers of j

$$\Rightarrow \sigma = \alpha A \sigma A$$

matrix!

nodes are not similar to themselves!

$$\sigma_{ij} = \alpha \sum_{k=1}^n A_{ik} \sum_{l=1}^n A_{jl} \sigma_{kl} + \delta_{ij} \Rightarrow \sigma = \alpha A \sigma A + I$$




$$\sigma_{ij} = \alpha \sum_{k=1}^n A_{ik} \sigma_{kj} + \delta_{ij} \Rightarrow \sigma = \alpha A \sigma + I$$

Alternate definition

$$\Rightarrow \sigma = (I - \alpha A)^{-1}$$

**Isomorphism** - a one-to-one mapping between graphs.

Graphs  $G_1 \neq G_2$ ,  $\phi: V(G_1) \rightarrow V(G_2)$  is an isomorphism  


if vertices  $u, v \in G_1$  are adjacent  $\Rightarrow \phi(u), \phi(v) \in G_2$  are adjacent

→ Two graphs are isomorphic if an isomorphism exists

→  $\phi^{-1}$  is the inverse isomorphism  $\phi^{-1}: V(G_2) \rightarrow V(G_1)$

→ Necessary conditions: same # nodes, # edges, degree sequence/distribution

→ Isomorphism of  $G$  to itself: automorphism (a strict notion of similarity)

**Permutation Matrix** – square matrix formed by swapping rows of the identity matrix.

Diagram illustrating a permutation mapping  $\pi(1, 2, 3, 4) = (2, 4, 1, 3)$ :

- Element in 1st spot goes to 3rd spot (indicated by a blue arrow from 1 to 3).
- Element in 2nd spot goes to 1st spot (indicated by a blue arrow from 2 to 1).

The corresponding permutation matrix  $P$  is:

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

Labels for the matrix rows and columns:

- Rows: 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup>
- Columns: 1<sup>st</sup> element, 2<sup>nd</sup> element, 3<sup>rd</sup>, 4<sup>th</sup>

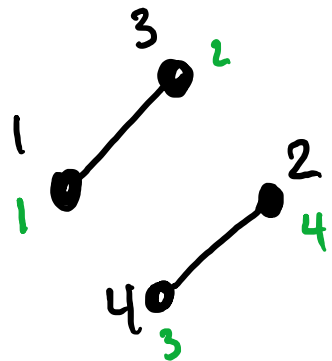
→  $P$  is orthogonal, i.e.,  $P^{-1} = P^T$

→ A permutation matrix defines an isomorphism in matrix form (on the adjacency)

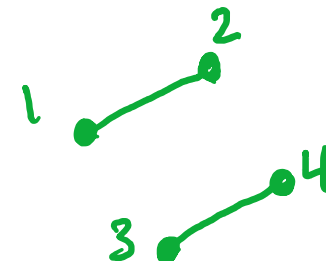
↳  $G_1 \cong G_2$  are isomorphic  $\iff$  there exists a permutation matrix,  $P$ , such that  $PA_1P^T = A_2$

$$\pi(1,2,3,4) = (1,3,4,2)$$

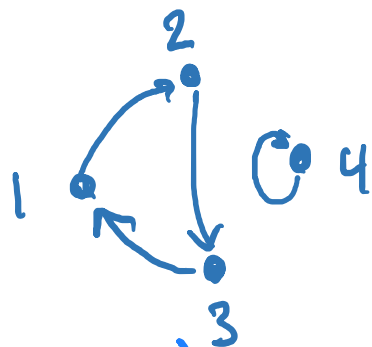
$$P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$



$$A_1 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$



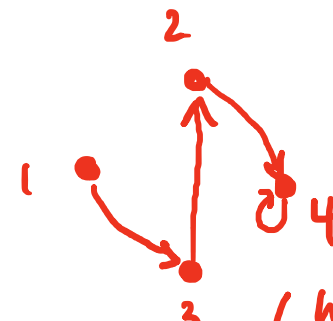
$$A_2 = P A_1 P^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



(has no meaning)

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

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



(has no meaning)