Mid-term Exam (Graph Mining – Spring 2024)

Full Name:
Student ID:

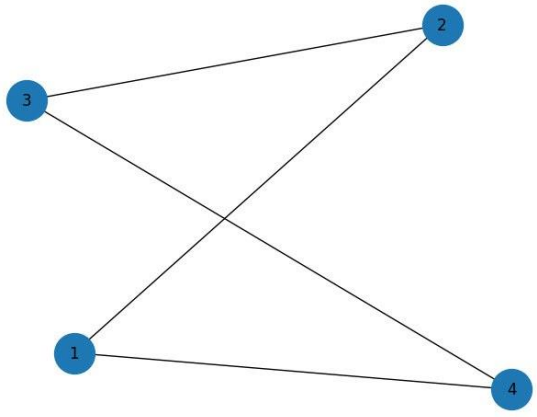
- The formula and solution process should be presented with the answer.
- All the codes must include detail comments in English.

1. Consider an undirected graph G of four nodes given in the following figure, calculate betweenness and closeness centrality of node 1 (5pt)

   Equation betweenness centrality: $B(v_i) = \sum_{s,t \in V} \frac{\sigma(s,t|v_i)}{\sigma(s,t)}$, where $\sigma(s,t)$ is the number of shortest paths from node s to node t, $\sigma(s,t|v_i)$ is the number of shortest paths from node s to node t that passing through node v_i.

   Normalized betweenness centrality: $\bar{B}(v_i) = \frac{B(v_i)}{(n-1)\,(n-2)/2}$ where n is number of nodes.

   Equation closeness centrality: $C(v_i) = \frac{N-1}{\sum_{j=1}^{N-1} d(v_j,v_i)}$, where $d(v_j, v_i)$ is number of nodes in the shortest path between node v_j and node v_i , and N-1 is the number of nodes reachable from v_i.



Ans:

Betweenness centrality of node 1

	$\sigma(s,t)$	$\sigma(s,t\|i)$	$\sigma(s,t\|i)/\sigma(s,t)$
1,2	1	0	0
1,3	2	0	0
1,4	1	0	0
2,3	1	0	0
2,4	2	1	1/2
3,4	1	0	0

$$\bar{B}(v_i) = \frac{B(v_i)}{(n-1)\,(n-2)/2} = \frac{1/2}{(4-1)\,(4-2)/2} = \frac{1/2}{3*2/2} = \frac{1}{6}$$

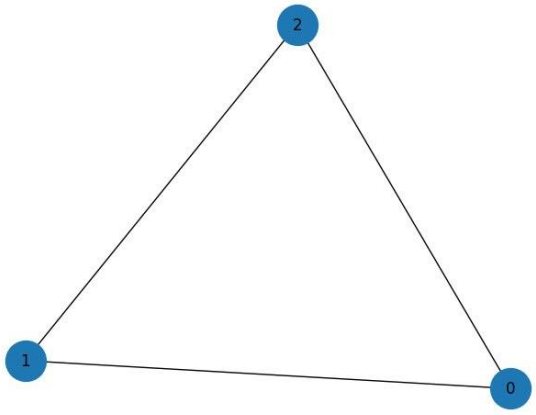
Closeness centrality of node 1

$$C(v_i) = \frac{N-1}{\sum_{j=1}^{N-1} d(v_j v_i,)} = \frac{4-1}{1+2+1} = \frac{3}{4}$$

2. Calculate Eigenvector, Katz and PageRank centrality(10pt)
   a. Consider an undirected graph G of three nodes given in the following figure, calculate Eigenvector, Katz centrality of node 2 with $\alpha = 0.1$, $\beta = 1$, t = 1 (6pt)

   Equation Eigenvector: x_i (t) = $\sum_{v_j \in N(v_i)} A_{ij} x_j(t-1)$, where A is adjacency matrix, t is time, with the centrality at time t = 0 being $x_j(0) = 1\ \forall j$

   Equation Katz: $Katz(G) = \beta(I - \alpha A^T)^{-1}.\mathbf{1}$, where α is damping factor, β is bias constant, I refers to the identity matrix, and **1** is a column vectors of ones. From Katz(G) results, write down the Katz centrality of node 2.



Ans:

Eigenvector: x_i (t) = $\sum_{v_j \in N(v_i)} A_{ij} x_j(t-1)$

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

$$x_j(0) = 1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

x_2 (1) = $\sum_{v_j} A_{2j} x_j(0) = (1*1) + (0*1) + (1*1) = 2$

Explanation:

The first element 1*1 represents the presence of a connection from node 2 to node 0

The second element 1*0 represents the presence of a connection from node 2 to node 2

The third element 1*1 represents the presence of a connection from node 2 to node 1

$$Katz(G) = \beta(I - \alpha A^T)^{-1}.\mathbf{1}$$

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

$$A^T = A$$

$$Katz(G) = 1\left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - 0.1\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}\right)^{-1} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & -0.1 & -0.1 \\ -0.1 & 1 & -0.1 \\ -0.1 & -0.1 & 1 \end{bmatrix}^{-1} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{det}\begin{bmatrix} 1 & -0.1 & -0.1 \\ -0.1 & 1 & -0.1 \\ -0.1 & -0.1 & 1 \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

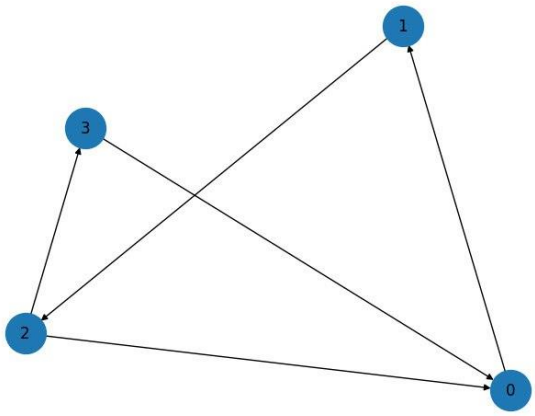
$$= \frac{1}{1 + (-0.1)^3 + (-0.1)^3 - (-0.1)^2 - (-0.1)^2 - (-0.1)^2}\begin{bmatrix} 0.99 & 0.11 & 0.11 \\ 0.11 & 0.99 & 0.11 \\ 0.11 & 0.11 & 0.99 \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \frac{1}{1 - 0.001 - 0.001 - 0.01 - 0.01 - 0.01}\begin{bmatrix} 0.99 & 0.11 & 0.11 \\ 0.11 & 0.99 & 0.11 \\ 0.11 & 0.11 & 0.99 \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \frac{1}{0.968}\begin{bmatrix} 0.99 & 0.11 & 0.11 \\ 0.11 & 0.99 & 0.11 \\ 0.11 & 0.11 & 0.99 \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{0.99}{0.968} & \frac{0.11}{0.968} & \frac{0.11}{0.968} \\ \frac{0.11}{0.968} & \frac{0.99}{0.968} & \frac{0.11}{0.968} \\ \frac{0.11}{0.968} & \frac{0.11}{0.968} & \frac{0.99}{0.968} \end{bmatrix} * \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\text{Katz(node 2)} = \frac{0.11}{0.968} + \frac{0.99}{0.968} + \frac{0.11}{0.968} = \frac{1.21}{0.968} = 1.25$$

b. Consider a directed graph G of four nodes given in the following figure, calculate PageRank centrality of all nodes, with β = 0.85 (4pt)
Equation PageRank centrality of node i: $x_i = \sum_{(j,i)\in E} x_j + \beta$, where x_j is PageRank score of all pages j that point to page i



Ans:

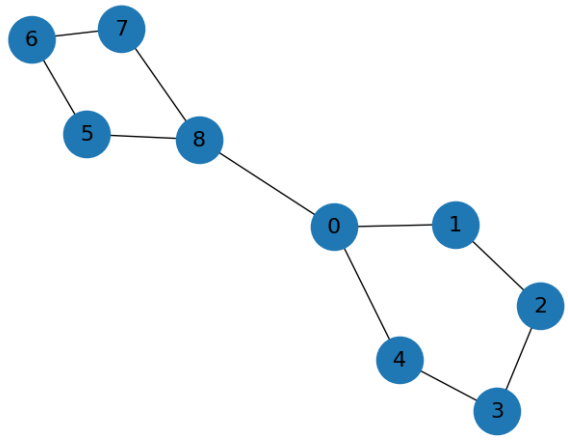
PageRank score equally 4 pages

$$x_0 = \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{pmatrix}$$

$$E = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$x_i = \sum_{(j,i)\in E} x_j + \beta = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{pmatrix} + 0.85 = \begin{pmatrix} 0.5 \\ 0.25 \\ 0.25 \\ 0.25 \end{pmatrix} + 0.85 = \begin{pmatrix} 1.35 \\ 1.1 \\ 1.1 \\ 1.1 \end{pmatrix}$$

3. Consider an undirected graph G of nine nodes given in the following figure. There are two communities in the graph: A = {0, 1, 2, 3, 4} and B = {5, 6, 7, 8}. (10pt)



a. Calculate Min-cut and Normalized cut measurements of A and B.

Ans:

Min_cut (A, B) = 1 N_cut(A, B) = $\frac{1}{1+5} + \frac{1}{1+4} = \frac{11}{30}$

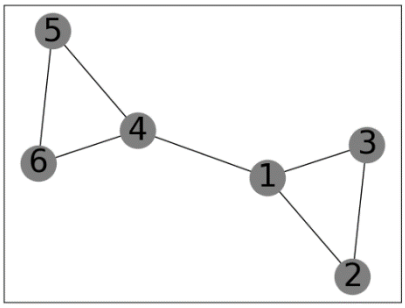
b. Calculate conductance of A and B using the equation (1).

$$conductance(A,B) = \frac{cut(A,B)}{\min\left(assoc(A,V), assoc(B,V)\right)} (1)$$

where $assoc(A,V)$ and $assoc(B,V)$ is the total connection from nodes in A and B to all nodes in the graph, respectively. $cut(A,B)$ is the number of cut between 2 communities A and B.

Ans: Conductance (A, B) = $\frac{1}{\min(6,5)} = \frac{1}{5} = 0.2$

4. Consider an undirected graph G of six nodes given in the following figure. Apply the Equation (1) to calculate the clustering C_i of each node i and Equation (2) to calculate the average clustering in the graph G. (10pt)



Equation (1): $C_i = \frac{2L_i}{d_i(d_i-1)}$ (1)

where d_i is the degree of node i and L_i is number of edges between neighbors of node i.

Equation (2): $\langle C \rangle = \frac{1}{N}\sum_{i=0}^{N} C_i$ (2)

Ans:

Clustering node 1: $C_1 = \frac{2L_1}{d_1(d_1-1)} = \frac{2.1}{3.(3-1)} = 0.333$

Clustering node 2: $C_2 = \frac{2L_2}{d_2(d_2-1)} = \frac{2.1}{2.(2-1)} = 1$

Clustering node 3: $C_3 = \frac{2L_3}{d_3(d_3-1)} = \frac{2.1}{2.(2-1)} = 1$

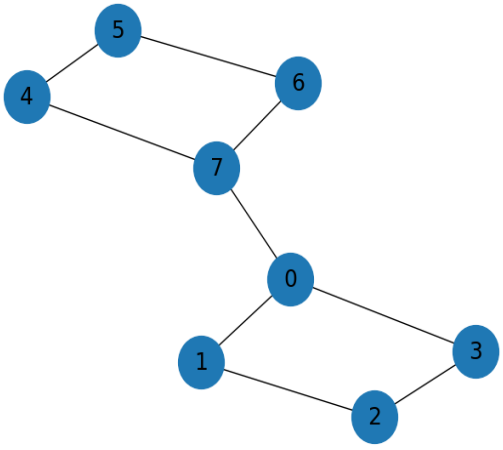
Clustering node 4: $C_4 = \frac{2L_4}{d_4(d_4-1)} = \frac{2.1}{3.(3-1)} = 0.33$

Clustering node 5: $C_5 = \frac{2L_5}{d_5(d_5-1)} = \frac{2.1}{2.(2-1)} = 1$

Clustering node 6: $C_6 = \frac{2L_6}{d_6(d_6-1)} = \frac{2.1}{2.(2-1)} = 1$

Average Clustering $\langle C \rangle = 0.7778$.

5. Consider an undirected graph G of eight nodes given in the following figure with two communities: A = {0, 1, 2, 3} and B = {4, 5, 6, 7}. Apply the Equation (1) to calculate the modularity Q of the two communities. (10pt)



$$Q = \frac{1}{2m}\sum_{i,j}\left(A_{ij} - \frac{d_i d_j}{2m}\right)\cdot\delta(v_i, v_j) \quad (1)$$

$$\delta(v_i, v_j) = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are in the same community.} \\ 0 & \text{otherwise.} \end{cases}$$

where m is the number of edges, A is the adjacency matrix of G, d_i is the degree of node v_i

Ans:

$$Q = \frac{1}{2 \times m}\sum_{i,j}\left(A_{ij} - \frac{d_i d_j}{2m}\right) \cdot \delta(v_i, v_j)$$

$$Q = \frac{1}{2 \times 9}\left[\left(1 - \frac{d_0 d_1}{18}\right) + \left(1 - \frac{d_1 d_2}{18}\right) + \left(1 - \frac{d_2 d_3}{18}\right) + \left(1 - \frac{d_3 d_0}{18}\right) + \left(1 - \frac{d_7 d_4}{18}\right) + \left(1 - \frac{d_4 d_5}{18}\right) + \left(1 - \frac{d_5 d_6}{18}\right) + \left(1 - \frac{d_6 d_7}{18}\right)\right]$$

$$Q = \frac{1}{2 \times 9}\left[\left(1 - \frac{3 \times 2}{18}\right) + \left(1 - \frac{2 \times 2}{18}\right) + \left(1 - \frac{2 \times 2}{18}\right) + \left(1 - \frac{2 \times 3}{18}\right) + \left(1 - \frac{3 \times 2}{18}\right) + \left(1 - \frac{2 \times 2}{18}\right) + \left(1 - \frac{2 \times 2}{18}\right) + \left(1 - \frac{2 \times 3}{18}\right)\right]$$

$$Q = \frac{1}{2 \times 9}\left[4\left(1 - \frac{3 \times 2}{18}\right) + 4\left(1 - \frac{2 \times 2}{18}\right)\right] = 0.3209$$

6. Consider an undirected graph G of eight nodes given in the following figure, calculate Jaccard's coefficient (JC), Adamic-Adar (AA) index of node 2 and node 6 (10pt)

   Equation JC: score (x, y) = $\frac{|N(x) \cap N(y)|}{|N(x) \cup N(y)|}$, where N(x), N(y) are neighbor nodes of node x, y respectively

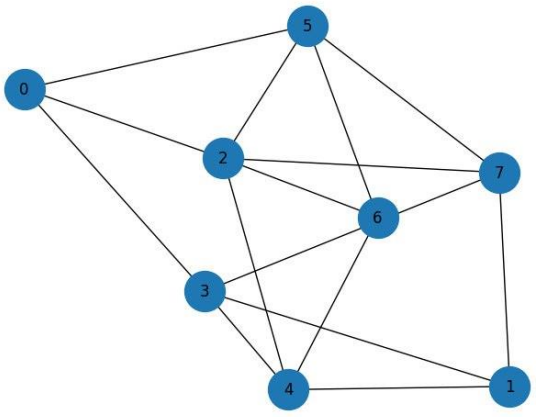
   Ans:

   $$JC(2,6) = \frac{|\{5,7,4\}|}{|\{5,7,4,0,3\}|} = \frac{3}{5+5-3} = \frac{3}{7}$$

   Equation AA: score (x, y) = $\sum_{u \in N(x) \cap N(y)} \frac{1}{\log |N(u)|}$, with log(4) ≈ 0.6

   Ans:

   $$AA(2,6) = = \sum_{u \in N(x) \cap N(y)} \frac{1}{\log |N(u)|} = \frac{1}{\log |N(4)|} + \frac{1}{\log |N(5)|} + \frac{1}{\log |N(7)|} = \frac{3}{\log (4)} = \frac{3}{0.6} = 5$$



7. Consider an undirected graph G of four nodes given in the following figure, calculate Katz Index with L = 2, β = 0.5 (5pt)

   Equation: score (x, y) = $\sum_{l=1}^{L} \beta^l |paths_{xy}^{(l)}| = \beta A_{xy} + \beta^2 A_{xy}^2 + \ldots + \beta^L A_{xy}^L$, where $A^2 = A * A$, which A is adjacency matrix

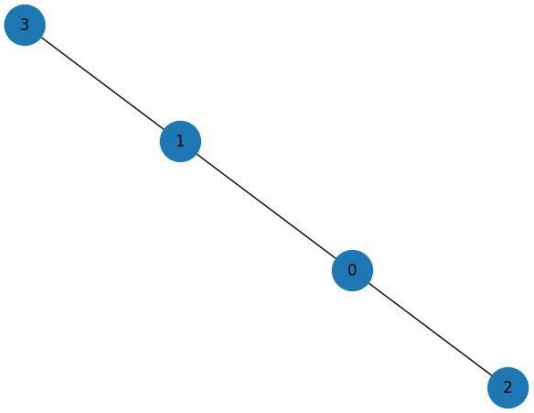
   Ans:

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

$$(\mathrm{x,y}) = \sum_{l=1}^{L} \beta^l \left| paths_{xy}^{(l)} \right| = \beta A_{xy} + \beta^2 A_{xy}^2 = 0.5 \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} +$$

$$0.5^2 \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}^2 = \begin{pmatrix} 0 & 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0 & 0.5 \\ 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \end{pmatrix} + 0.25 \begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} 0 & 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0 & 0.5 \\ 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0.5 & 0 & 0 & 0.25 \\ 0 & 0.5 & 0.25 & 0 \\ 0 & 0.25 & 0.25 & 0 \\ 0.25 & 0 & 0 & 0.25 \end{pmatrix} = \begin{pmatrix} 0.5 & 0.5 & 0.5 & 0.25 \\ 0.5 & 0.5 & 0.25 & 0.5 \\ 0.5 & 0.25 & 0.25 & 0 \\ 0.25 & 0.5 & 0 & 0.25 \end{pmatrix}$$



8. Consider an undirected graph G of three nodes given in the following figure, calculate Hitting time of node 1 and node 2 (5pt).

   Equation Hitting time: score (x , y) = $-\mathrm{H}_{x,y} = -\frac{1}{|N(x)|}\sum_k (1 + \mathrm{H}_{k,y})$,

   where H(k, y) = 1 + $\sum_m \mathrm{p}_{mj} H(m, y)$ when k≠y, otherwise H(k, y) = 0, p_{mj} is the element in the row m-th and column j-th of the matrix, P= AD^{-1},which P is a transition matrix, A is adjacency matrix and D is degree matrix.

   Ans:

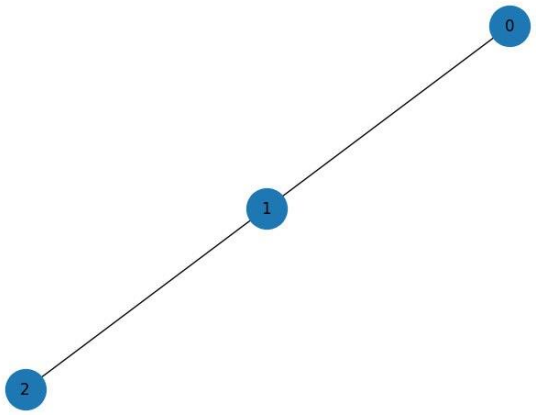
$$A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

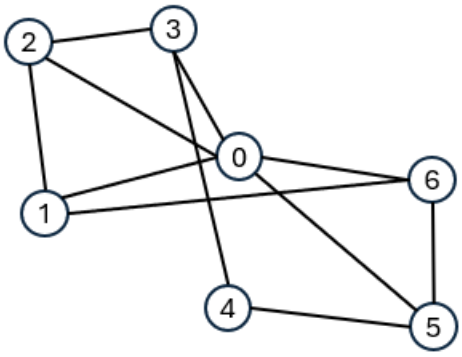
$$P = AD^{-1} = \begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix} * \frac{1}{detD}\begin{bmatrix}1 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 1\end{bmatrix} = \begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix} * \frac{1}{2}\begin{bmatrix}2 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 1\end{bmatrix} = \begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix} * \begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & \frac{1}{2}\end{bmatrix} = \begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0.5\\ 0 & 1 & 0\end{bmatrix}$$

$$H(1,2) = 1 + \sum_{m} \mathrm{p}_{mj} H(m,y) = 1 + 0 = 1\ (m = y)$$

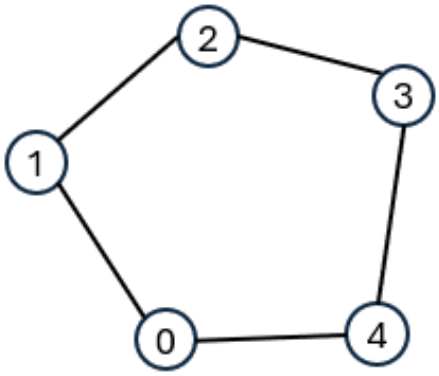
score (1 , 2) = $-\mathrm{H}_{x,y} = -\frac{1}{|N(x)|}\sum_k \left(1 + \mathrm{H}_{k,y}\right) = -\frac{1}{2}(1+1) = -1$



9. Consider two undirected graphs G_1 and G_2 below, calculate the graph edit distances from G_1 to G_2. The set of elementary operations: vertex insertion, vertex deletion, edge insertion, and edge deletion. In addition, the cost of insertion and deletion is 2 and 1, respectively. (5pt)



G_1



G_2

Ans:

Remove node 5 and 6: cost 2.

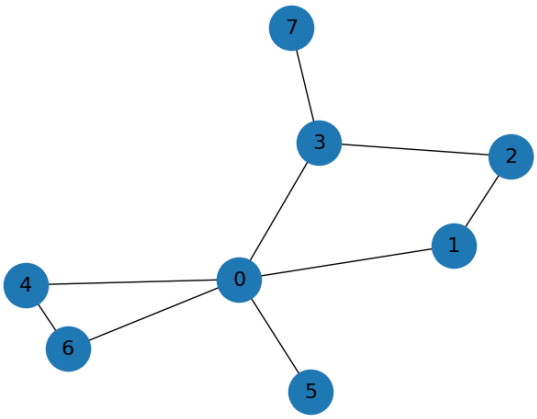
Delete Edges (0,5), (0,6), (1,6), (4,5), and (5,6): cost 5.

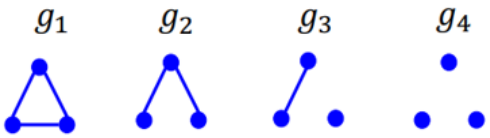
Add edge (0,4): cost 2.

Hence, the cost distance = 2+5+2 = 9.

10. Consider an undirected graph G of eight nodes in the left side and four graphlets kernel g_1, g_2, g_3, g_4 in the right side of following figure. Answer two question below: (10pt)
    a. Count the number of the kernel sub-graphs of limited size 3.

b. Make a feature vector for graph G based on these graphlets kernel.





Ans:

a. Count subgraph:

$N(g_1)$=1:
(0, 4, 6)

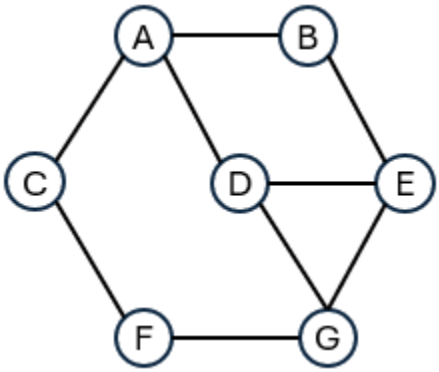
$N(g_2)$=14:
(0, 1, 2), (0, 1, 3), (0, 1 ,4), (0, 1, 6),
(0, 3, 2), (0, 3, 4), (0, 3, 5), (0, 3, 7),
(0, 4, 5), (0, 5, 1), (0, 5, 6), (0, 6, 3),
(2, 1, 3),
(3, 2, 7)

$N(g_3)$=23:
(0, 1, 7),
(0, 4, 2), (0, 4, 7),
(0, 5, 2), (0, 5, 7),
(0, 6, 2), (0, 6 ,7),
(1, 2, 4), (1, 2, 5), (1, 2, 6), (1, 2, 7),
(2, 3, 5), (2, 3, 4), (2, 3, 6),
(3, 7, 1), (3, 7, 4), (3, 7, 5), (3, 7, 6),
(4, 6, 5), (4, 6, 1), (4, 6, 2), (4, 6, 3), (4, 6, 7)

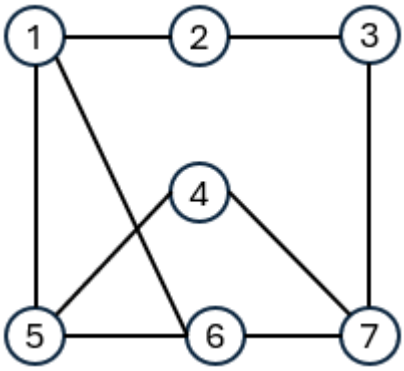
$N(g_4)$=17
(0, 2, 7),
(1, 3, 4), (1, 3, 5), (1, 3, 6),
(1, 5, 6), (1, 5, 7), (1, 6, 7),
(2, 4, 7), (2, 5, 7), (2, 5, 6), (2, 6, 7),
(3, 4, 5), (3, 5, 6),
(4, 1, 5), (4, 2, 5), (4, 5, 7)
(5, 6, 7)

b. $f_G = (1, 14, 23, 17)$

11. Consider two undirected graphs in the following figure: G_1 on the left and G_2 on the right. (10pt)
    a. Conduct Weisfeiler-Lehman (WL) relabeling process with the maximum degree 3.
    b. Make feature vectors for the graphs based on frequency of the WL subgraphs in question a. Then calculate the similarity of graph G_1 and G_2 using equation (1).



G_1



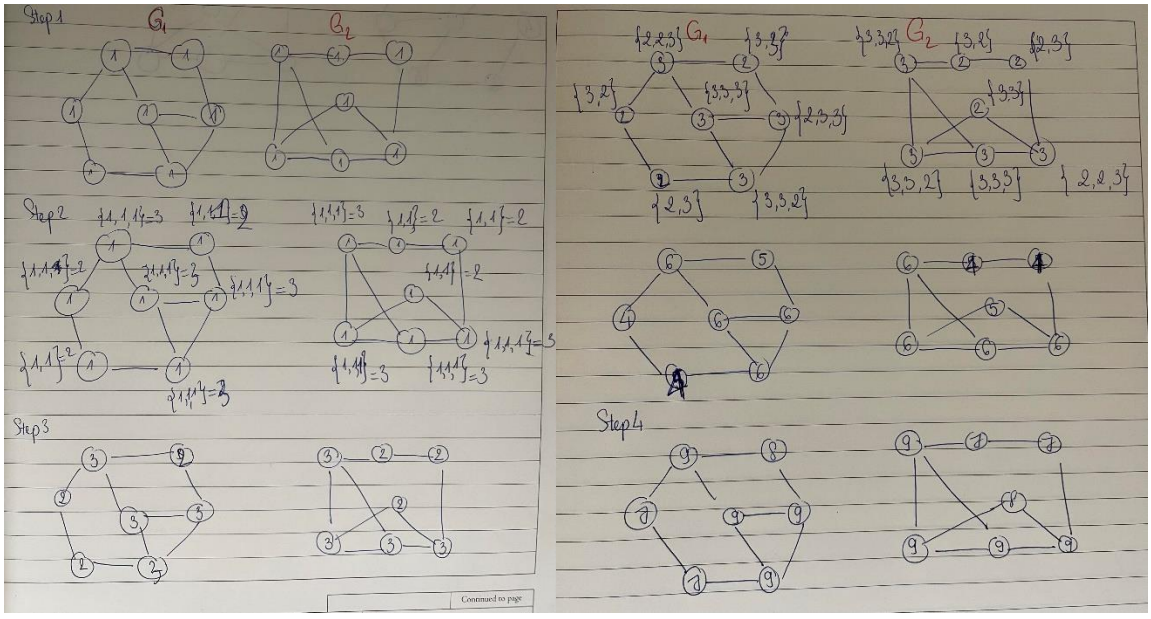
G_2

Cosine Similarity equation 1: $cosine(WL_{G_1}, WL_{G_2}) = \frac{WL_{G_1}.WL_{G_2}}{\|WL_{G_1}\|\|WL_{G_2}\|}$.

where WL_{G_1} and WL_{G_2} is feature vectors of WL subgraph G_1 and G_2. "." denotes the dot product and "|| ||" denotes the Euclidean norm.

Ans:

a.



b. Based on the WL relabeling process in (a), the number of WL subgraphs in G_1 is as follows:

The number of label "1": 7

The number of label “2”: 3

The number of label “3”: 4

The number of label “4”: 2

The number of label “5”: 1

The number of label “6”: 4

The number of label “7”: 2

The number of label “8”: 1

The number of label “9”: 4

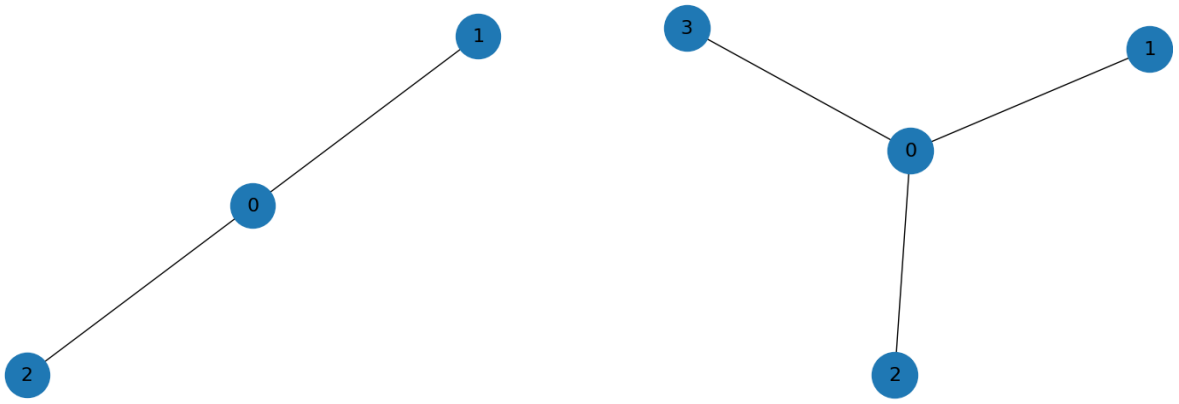
Therefore, the feature vector for G_1 is: (7,3,4,2,1,4,2,1,4)

Similarly, the feature vector for G_2 is: (7,3,4,2,1,4,2,1,4)

The similarity of G_1 and G_2 is

$$\frac{7*7+3*3+4*4+2*2+1*1+4*4+2*2+1*1+4*4}{\sqrt{7^2+3^2+4^2+2^2+1^1+4^2+2^2+1^2+4^2}.\sqrt{7^2+3^2+4^2+2^2+1^1+4^2+2^2+1^2+4^2}}=1$$

12. Consider an undirected graph G_1 and G_2 in the following figure. Make feature vectors of graphs G_1 and G_2 using the shortest path kernel and calculate similarity of graphs using the cosine similarity. (10pt)



G_1 G_2

Ans:

All shortest path Floyd-transformed S_1 of G_1:

+ 0 – 1: 1.

+ 0 – 2: 1

+ 1 – 2: 2

⇨ Frequencies of length 1: 2
Frequencies of length 2: 1

All shortest path Floyd-transformed S_2 of G_2:

+ 0 – 1: 1.

+ 0 – 2: 1

+ 0 – 3: 1

+ 1 – 2: 2

+ 1 – 3: 2

+ 2 – 3: 2

⇨ Frequencies of length 1: 3
Frequencies of length 2: 3

The feature vector of S_1 = (2, 1)

The feature vector of S_2 = (3, 3)

The similarity = $\frac{2*3+1*3}{\sqrt{4+1}.\sqrt{9+9}} = \frac{9}{\sqrt{5}\sqrt{18}} \approx 0.9847$