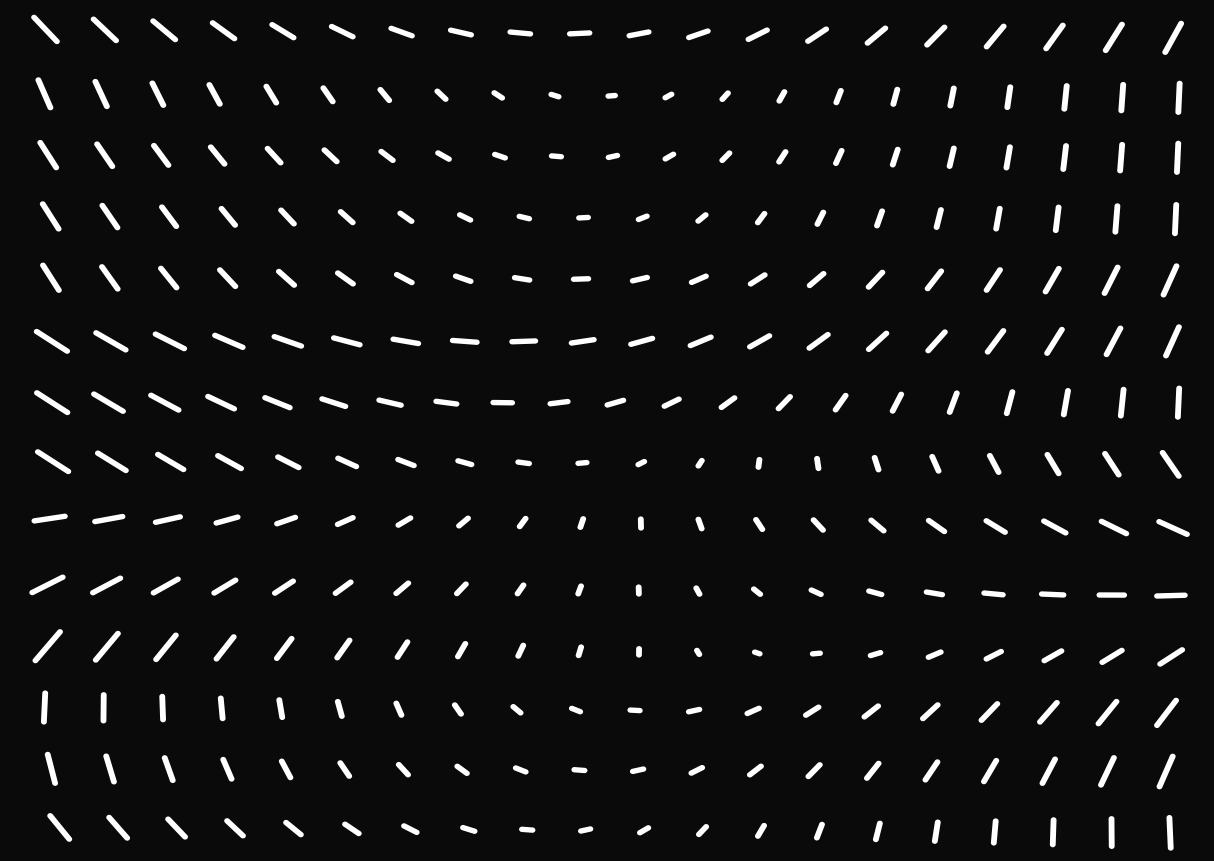
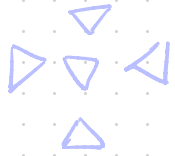
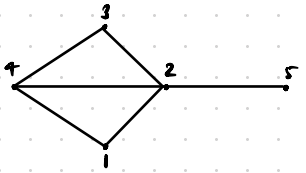


$\frac{6}{6} = 1 \qquad \frac{3}{6} = \frac{1}{2}$





$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$C_{max} = \begin{bmatrix} 1.899 \\ 2.686 \\ 1.899 \\ 2.414 \\ 1 \end{bmatrix} \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix}$

$M^3 = \cdots$

C_{max} (normalized)

(a, c) , (c, a)

(a, a)

a, b

$A = \{a, b, c\}$

$M_{R_1} \hookrightarrow R_1 \quad R$

$$M_{R_1} = \begin{array}{c} \\ a \\ b \\ c \end{array} \begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \end{array}$$

R_1

$R_1 = \{(a, a), (a, c), (b, a), (c, b)\}$

$R \subseteq A \times B$

$R_2 = \{(a, a), (a, c), (b, b), (b, c)\}$

$R_1 \cup R_2 = \{(a, a), (a, c), (c, a), \ldots\}$

$R_1 \odot R_2 = \{(a,b)\}$ $R = \{\}$ $R^n = \{(a,b)\}$

$R_1 = \{(a,c)\}$ $R_1 \odot R_2$ (a,b) b,c $(a, a_1, a_2, \ldots a_{n-2}, b)$

$R_2 = (c,b) = a,b$ a,c $,b$

(a,a) a

$M_R = \{a, a$ b,a

$R = \{(a,a), (a,c)$

$(b,b), (b,a)$

$R^2 = R \odot R S = \{(a,b) \ldots\}$

A^3 $S \otimes R$ (a,a)

a,b b,c

(a,c)

$a,d,$ d,c

(a,c)

$(I - \beta A)^{-1} - I$

common neighbour:

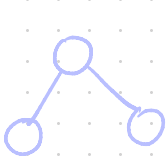
$$N(A) \cap N(B)$$

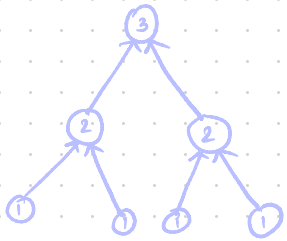
Jaccard coefficient:

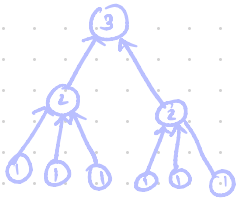
$$\frac{N(A) \cap N(B)}{N(A) \cup N(B)}$$

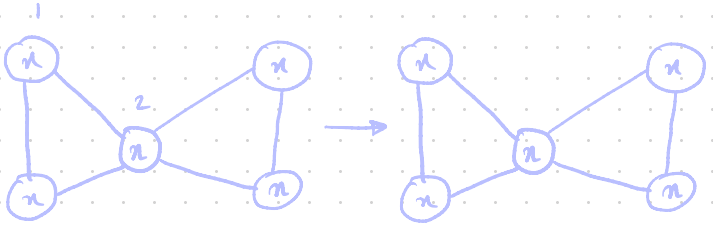
Adamic-Adar:

$$\sum_{c \in N(A) \cap N(B)} \frac{1}{\log(K_c)}$$

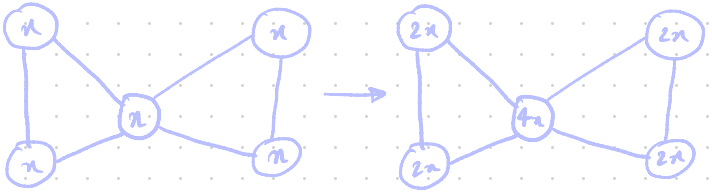


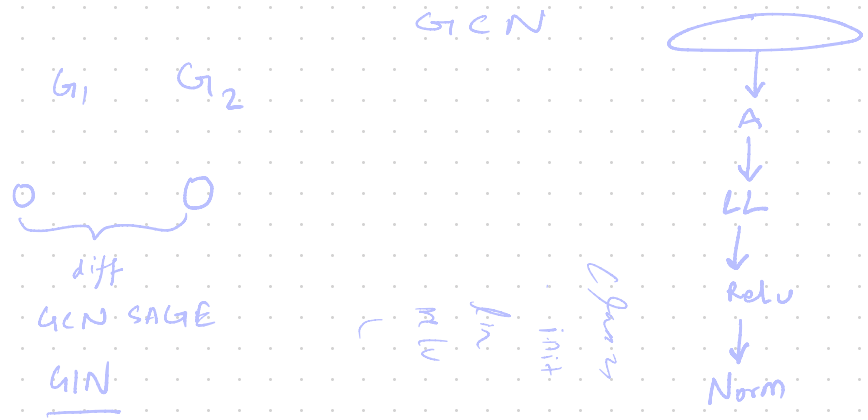






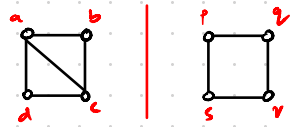
fails for mean/max since
1, 2 are different even though
they have the same embedding




GCN
A
LL
Relu
Norm
Conv
init
forward
self.lin(x)
MLP
lin
G1
G2
diff
GCN SAGE
GIN

Q.3. a)

1.



Mean : a, b, c, d = 1, 1, 1, 1
p, q, r, s = 1, 1, 1, 1

Max : a, b, c, d = 1, 1, 1, 1
p, q, r, s = 1, 1, 1, 1

Sum : a, b, c, d = 3, 2, 3, 2

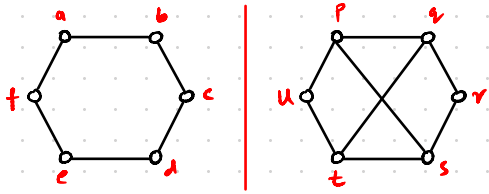
p, q, r, s = 2, 2, 2, 2

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	111
b	111	q	111
c	1111	r	111
d	111	s	111

∴ The Graphs are non-isomorphic

2.



Mean : a, b, c, d, e, f = 1, 1, 1, 1, 1, 1

p, q, r, s, t, u = 1, 1, 1, 1, 1, 1

Max : a, b, c, d, e, f = 1, 1, 1, 1, 1, 1

p, q, r, s, t, u = 1, 1, 1, 1, 1, 1

Sum : a, b, c, d, e, f = 2, 2, 2, 2, 2, 2

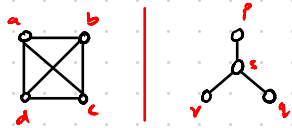
p, q, r, s, t, u = 3, 3, 2, 3, 3, 2

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	111	p	1111
b	111	q	1111
c	11	r	111
d	111	s	1111
e	111	t	1111
f	111	u	111

∴ The Graphs are non-isomorphic.

3.



Mean : a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

Max : a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

WL-Test

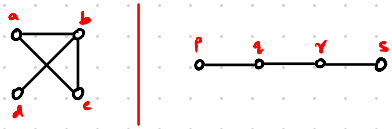
Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	11
b	1111	q	11
c	1111	r	11
d	1111	s	1111

∴ The Graphs are non-isomorphic

Sum: a, b, c, d = 3, 3, 3, 3

p, q, r, s = 1, 1, 1, 3

4.



Mean: a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

Max: a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

Sum: a, b, c, d = 2, 3, 2, 1

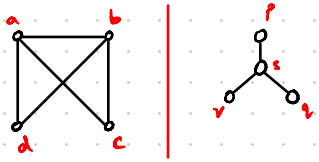
p, q, r, s = 1, 2, 2, 1

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	111	p	11
b	1111	q	111
c	111	r	111
d	11	s	11

∴ The Graphs are non-isomorphic

5.



Mean: a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

Max: a, b, c, d = 1, 1, 1, 1

p, q, r, s = 1, 1, 1, 1

Sum: a, b, c, d = 3, 3, 2, 2

p, q, r, s = 1, 1, 1, 3

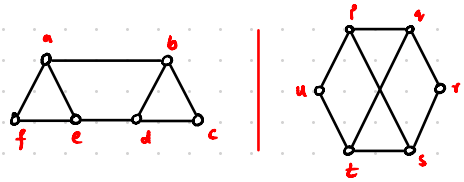
WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	11
b	1111	q	11
c	111	r	11
d	111	s	1111

∴ The Graphs are non-isomorphic

b) GIN fails to differentiate

1)



sum: a, b, c, d, e, f = 3, 3, 2, 3, 3, 2

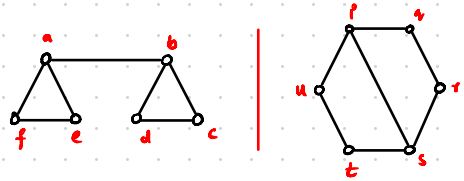
p, q, r, s, t, u = 3, 3, 2, 3, 3, 2

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	1111
b	1111	q	1111
c	111	r	111
d	1111	s	1111
e	1111	t	1111
f	111	u	111

∴ WL-Test fails

2)



Sum: a, b, c, d, e, f = 3, 3, 2, 2, 2, 2

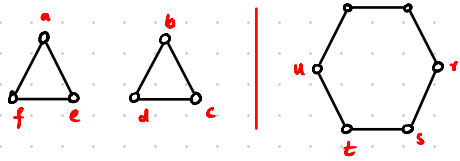
p, q, r, s, t, u = 3, 2, 2, 3, 2, 2

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	1111
b	1111	q	111
c	111	r	111
d	111	s	1111
e	111	t	111
f	111	u	111

∴ WL-Test fails

3)



Sum: a, b, c, d, e, f = 2, 2, 2, 2, 2, 2

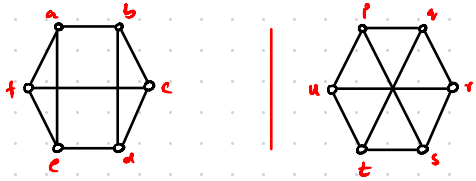
p, q, r, s, t, u = 2, 2, 2, 2, 2, 2

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	111	p	111
b	111	q	111
c	111	r	111
d	111	s	111
e	111	t	111
f	111	u	111

∴ WL-Test fails

4)



sum: a, b, c, d, e, f = 3, 3, 3, 3, 3, 3

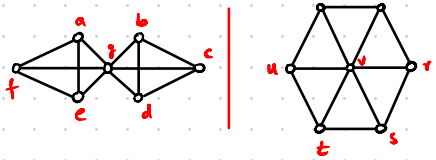
p, q, r, s, t, u = 3, 3, 3, 3, 3, 3

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	1111	p	1111
b	1111	q	1111
c	1111	r	1111
d	1111	s	1111
e	1111	t	1111
f	1111	u	1111

∴ WL-Test fails

5)



Sum: a, b, c, d, e, f, g = 3, 3, 3, 3, 3, 3, 6

p, q, r, s, t, u, v = 3, 3, 3, 3, 3, 3, 6

WL-Test

Graph 1		Graph 2	
Node	Embedding	Node	Embedding
a	11111	p	111111
b	111111	q	111111
c	111111	r	111111
d	111111	s	111111
e	111111	t	111111
f	111111	u	111111
g	111111	v	111111

∴ WL-Test fails

Task → Node clustering

Approach 1:

Create r-ego networks of nodes, augment them, perform graph contrastive learning for clustering

Approach 2:

Create a similarity graph (different from assembly graphs), use this in conjunction with assembly graphs that are already given