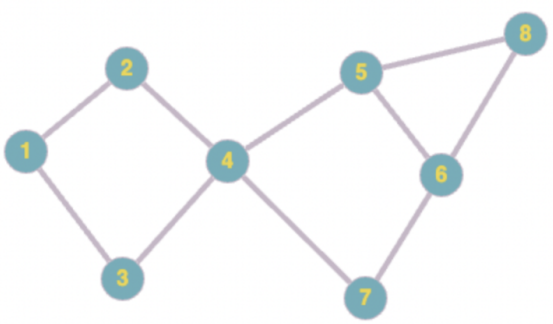
Homework 1

Graph Neural Networks Course

Task 1: Graph Analysis (4 points)

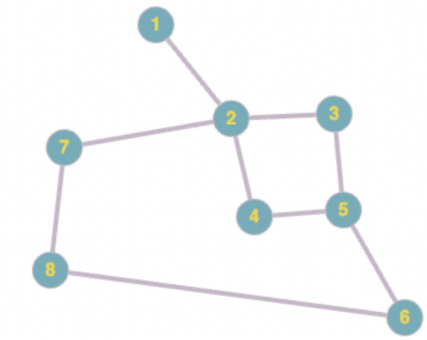
Given a graph:

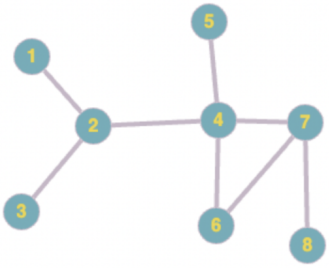


1. Write out the adjacency matrix.
2. Compute the degree for all vertices.
3. Calculate centrality measures:
   - Eigenvector centrality
   - Closeness centrality
   - Neighborhood-based centrality
4. Compute the clustering coefficient for vertices **1, 4, 8**.
5. For vertex pairs **13, 45, 48**, calculate local overlap statistics:
   - Common neighbors
   - Jaccard coefficient
   - Adamic-Adar index
6. Compute Graphlet Degree Vector (GDV) of size 3 for vertices **4, 5, 8**.

Task 2: Kernel Computation (3 points)

Given two graphs:





1. Compute the **Graphlet Kernel** of size 3 (max graphlet size = 3).
2. Compute the **Weisfeiler-Lehman (WL) kernel** with 3 iterations.

You must implement these computations yourself. Using pre-built kernel computation libraries is not allowed. Provide your code and the resulting vectors for each graph.

Task 3: Kernel Validity Proof (3 points)

Prove that the **Graphlet Kernel** is indeed a valid kernel function.

Bonus Task: Katz Index (5 points)

The Katz index for global overlap statistics is defined as:

$$S_{Katz}[u, v] = \sum_{i=1}^{\infty} \beta^i A^i[u, v]$$

Computing an infinite sum directly is problematic. Find an analytical form for the full Katz matrix.

Hint: Use the following theorem:

Theorem: Let X be a square matrix in $\mathbb{R}$. Let λ_1 be the largest eigenvalue of X. Then:

$$(I - X)^{-1} = \sum_{i=1}^{\infty} X^i$$

if and only if $\lambda_1 \leq 1$ and $(I - X)$ is non-singular.