1 Question 1

Let $G(n,p)$ be the Erdős–Rényi random model. It starts with a fixed number n of vertices and each pair of distinct vertices in the graph is connected by an edge with a probability p, independent of other pairs. This probability is the same for all pairs of vertices. So the distribution of the degree of a node is the binomial distribution $B(n-1,p)$ as a sequence of $n-1$ independent Bernoulli steps (the number of possibilities for the node) of parameter p. Consequently the expected degree of a node is $m=(n-1)p$.

- $n=25, p=0.2 \implies m=4.8$.
- $n=25, p=0.4 \implies m=9.6$.

2 Question 2

We consider G_1, G_2 and G_3 defined in the handout. The respective adjacency matrices are

$$A_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, A_3 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Sum and mean operations are permutation-invariant, meaning they produce the same output regardless of the order of nodes in the input graph. For exemple, in G_1 the center node should be different from the others in term of representation. And using a fully connected layer would lead to a different result depending on the place of this node in the matrix, because it's generally not permutation invariant.

3 Question 3

When using "mean" operator for the readout function, we observe that all the rows of the node representations matrix are equal, whether the operator used for neighborhood aggregation operator. Each graph has the same representation. Otherwise, all the rows are different.
Message passing:
Since all the graphs are cycle graphs, and the feature matrix is uniform (full of ones), $\mathbf{Z}_{\text{sum}}$ gives as output a matrix where all the rows (representing nodes) are equal. All the nodes have the same representation. That's because all the nodes are surrounded by similar neighborhood and have the same feature. All the degrees are equal so $\mathbf{Z}_{\text{mean}}$ gives the same result as $\mathbf{Z}_{\text{sum}}$. So the message passing operator does not affect the structure of the output.
Readout:
The readout gives a representation for each graph. It's logical that "mean" and "sum" behave differently because all the graphs have different number of nodes n. Given the result of the aggregator (message passing) which does not differentiate nodes, the "mean" is going to give equal rows between each graphs because the size n has no effect in the "mean" operator, whereas the "sum" completely depends on the size n.

4 Question 4

We consider two graphs with the same degree sequence but are not isomorphic . They can never be distinguished by the GNN model which only uses "sum" operator.
It is explained by the equality between the number of nodes $n = 8$ and the degree sequences $deg = [3,2,2,2,2,1,1,1]$ of G_1 and G_2. So we almost retrieve the case of the question 3 except n is constant, so the "sum" does not distinguish graphs.

References

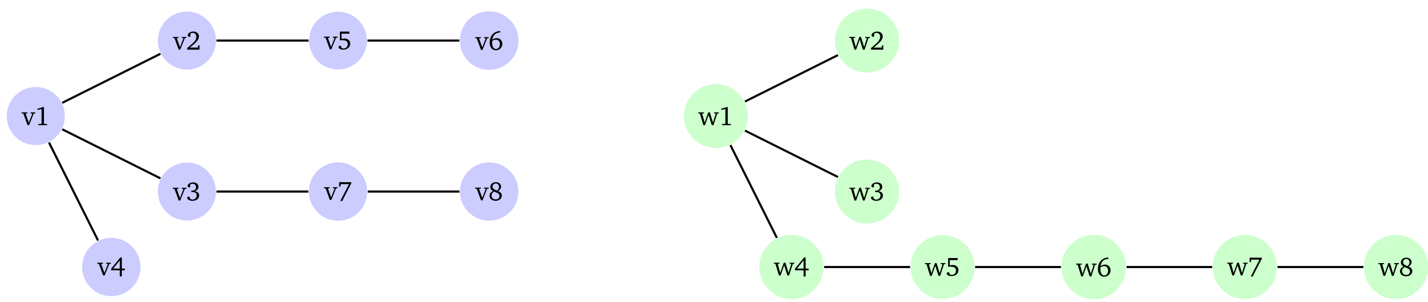

Figure 1: Non-isomorphic graphs with same representation