Lab session 6: Deep Learning for Graphs

1 Question 1 :

> What accuracy do you expect from such an architecture when the number of columns of Z is chosen to be larger than the number of nodes in the graph? Please explain your answer.

If the number of columns of Z is large, the architecture might face issues finding generally valid rules for assembly of outputs, caused by an overfitting. We can expect an poorer accuracy from such an architecture, in the cases where the number of columns of Z is chosen to be larger than the number of nodes in the graph. The reason we would have overfitting is that, if no regularisation is applied, Z will reconstruct the adjacency matrix quite completely and we will have redundant information.

2 Question 2 :

> Besides randomly sampling node attributes for unattributed graphs, can you think of another possible initialisation of X from which each node can be uniquely identified?

Another possible initialisation of X could be to use a list of direct neighbors associated with a hard limit on the number of features such that a pair of nodes can have the same features only if they are connected with the exact same neighbors.

3 Question 3 :

> What is the expected number of edges in Erdos-Rényi random graphs with $n = 15$ nodes and edge probabilities $p = 0.2$ and $p = 0.4$?
> And what is the variance of the number of edges in these two Erdos-Rényi random graph models?

For a random graph with n vertices and edge probability p, the expected number of edges in Erdos-Rényi random graph models can be written as :

$E[X] = \frac{n(n-1)}{2}p$ We therefore have :

- For p = 0.2 :
  $E[X|p = 0.2] = \frac{201}{2}0.2 = 21$
- For p = 0.4 :
  $E[X|p = 0.4] = \frac{201}{2}0.4 = 42$

The variance of the number of edges in these two Erdos-Rényi random graph mode can be computed as :

$Var[X] = E[X](1 - p) = \frac{n(n-1)}{2}p(1 - p)$
We therefore have :

- For p = 0.2 :
  $Var[X|p = 0.2] = 16.8$
- For p = 0.4 :
  $Var[X|p = 0.4] = 25.2$

4 Question 4 :

Assume that for a set of three graphs we receive the following matrix Z

$$Z = \begin{bmatrix} 0.21 & 0.95 & 0.4 \\ 0.4 & 0.12 & 0.68 \\ 0.89 & 0.34 & 1.31 \\ 0.68 & 0.08 & 0.5 \\ 0.62 & 0.18 & 0.1 \\ 0.89 & 0.34 & 1.31 \\ 0.81 & 0.2 & 1.29 \\ 0.89 & 0.34 & 1.31 \\ 0.61 & 0.14 & 0.31 \end{bmatrix}$$

where rows 1, 2 and 3 correspond to nodes in the first graph G1, rows 4, 5, 6 and 7 correspond to nodes in G2 and the remaining two rows correspond to nodes in G3. Compute the representations of the three graphs (i.e., zG1, zG2 and zG3) for each one of the following three readout functions: (i) sum, (ii) mean, and (iii) max. Which of these functions is able to distinguish these graphs best?

By computing the representations of $zG1$,$zG2$ and $zG3$, we obtain :

i.Sum

$ZG1sum = [0.7, -0.49, 2.39]$
$ZG2sum = [3.0, 0.4, 2.0]$
$ZG3sum = [1.5, 0.2, 1.0]$

ii.Mean

$ZG1mean = [0.23, -0.16, 0.8]$
$ZG2mean = [0.75, 0.1, 0.5]$
$ZG3mean = [0.75, 0.1, 0.5]$

i.Max

$ZG1max = [0.89, 0.34, 1.31]$
$ZG2max = [0.89, 0.34, 1.31]$
$ZG3max = [0.89, 0.34, 1.31]$

We therefore note that the max function don't allow to differentiate any of the 3 graphs. The mean function only differentiate $G1$ from $G2$ and $G3$, but the two latter are not differentiated between each other. We can conclude that the sum function is the one that distinguish these graphs.