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Lab session # 5
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## Question 1

Generalisation of DeepWalk:

- For a directed graph, we can generate the path following the direction of edge. More concretely, for a given node, select among its out edges .
- For a weighted graph, one natural idea is to select one edge with a probability proportional to its weight.

## Question 2

If we apply this architecture to a graph containing only nodes and no edges, it becomes a vanilla fully connected network. In this case, $\hat{A} = I$ and $Z^0 = f(X\ W^0), Z^1 = f(Z^0\ W^1)$. It is a standard form of fully-connected network.

## Question 3

The receptive field is $2$. Passing a message passing layer means that the node receives the information from its neighbors. Therefore, in a GCN architecture with k message passing layers, the receptive field is $k$.

## Task 12

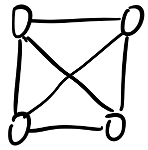
If we initialize all features to the same value, most of features are not helpful. It acts as if there is only one feature. That's why the training and test accuracy degrades, compared to the random initialisation.

## Question 4

The node representation in $Z^1$ is the same for nodes with the same structure in graph. Therefore, we notice that the features of 4 nodes in $K_4$ are the same and the three nodes in $S_4$ of degree 1 also have same features.

If we randomly sample the node features $X$, the node representation would be all different, even for nodes with same structure in graph.

You can find the calculation details in the next two pages.

$K_4$: 

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

$$\tilde{D} = \mathrm{diag}(4, 4, 4, 4)$$

$$\tilde{D}^{-\frac{1}{2}} = \mathrm{diag}\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)$$

$$\hat{A} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \quad Z^0 = f(\hat{A} X W^0) \quad X = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad W^0 = \begin{bmatrix} -0.8 & 0.5 \end{bmatrix}$$

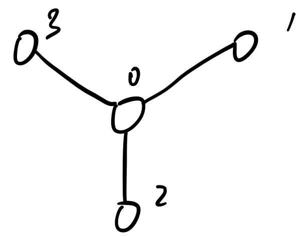
$$XW^0 = \begin{bmatrix} -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \end{bmatrix} \quad \hat{A}XW^0 = \begin{bmatrix} -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \end{bmatrix} \quad Z^0 = f(\hat{A}XW^0) = \begin{bmatrix} 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \end{bmatrix}$$

$$Z^1 = f(\hat{A} Z^0 W^1) \qquad W^1 = \begin{bmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{bmatrix}$$

$$Z^0 W^1 = \begin{bmatrix} -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \end{bmatrix} \qquad \hat{A} Z^0 W^1 = \begin{bmatrix} -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \end{bmatrix}$$

$$\boxed{Z^1 = \begin{bmatrix} 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \end{bmatrix}}$$

$S_4$:




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

$$\tilde{D} = \mathrm{diag}(4, 2, 2, 2)$$

$$\tilde{D}^{-\frac{1}{2}} = \mathrm{diag}\left(\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$$

$$\hat{A} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} \quad Z^0 = f(\hat{A} X W^0) \quad X = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad W^0 = \begin{bmatrix} -0.8 & 0.5 \end{bmatrix}$$

$$\hat{A} = \begin{bmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2} \end{bmatrix} \quad XW^0 = \begin{bmatrix} -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \end{bmatrix} \quad \hat{A}XW^0 = \begin{bmatrix} -0.2(1+3\sqrt{2}) & \frac{1}{8}(1+3\sqrt{2}) \\ -0.2(2+\sqrt{2}) & \frac{1}{8}(2+\sqrt{2}) \\ -0.2(2+\sqrt{2}) & \frac{1}{8}(2+\sqrt{2}) \\ -0.2(2+\sqrt{2}) & \frac{1}{8}(2+\sqrt{2}) \end{bmatrix}$$

$$Z^0 = f(\hat{A}XW^0) = \begin{bmatrix} 0 & \frac{1}{8}(1+3\sqrt{2}) \\ 0 & \frac{1}{8}(2+\sqrt{2}) \\ 0 & \frac{1}{8}(2+\sqrt{2}) \\ 0 & \frac{1}{8}(2+\sqrt{2}) \end{bmatrix} \quad W^1 = \begin{bmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{bmatrix}$$

$$Z^0 W^1 = \begin{bmatrix} -\frac{1}{20}(1+3\sqrt{2}) & \frac{3}{40}(1+3\sqrt{2}) & \frac{1}{16}(1+3\sqrt{2}) \\ -\frac{1}{20}(2+\sqrt{2}) & \frac{3}{40}(2+\sqrt{2}) & \frac{1}{16}(2+\sqrt{2}) \\ -\frac{1}{20}(2+\sqrt{2}) & \frac{3}{40}(2+\sqrt{2}) & \frac{1}{16}(2+\sqrt{2}) \\ -\frac{1}{20}(2+\sqrt{2}) & \frac{3}{40}(2+\sqrt{2}) & \frac{1}{16}(2+\sqrt{2}) \end{bmatrix}$$

$$\hat{A}Z^0W^1 = \begin{bmatrix} -\frac{1}{80}(7+9\sqrt{2}) & \frac{3}{160}(7+9\sqrt{2}) & \frac{1}{64}(7+9\sqrt{2}) \\ -\frac{1}{80}(10+3\sqrt{2}) & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \\ -\frac{1}{80}(10+3\sqrt{2}) & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \\ -\frac{1}{80}(10+3\sqrt{2}) & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \end{bmatrix}$$

$$\boxed{Z^1 = f(\hat{A}Z^0W^1) = \begin{bmatrix} 0 & \frac{3}{160}(7+9\sqrt{2}) & \frac{1}{64}(7+9\sqrt{2}) \\ 0 & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \\ 0 & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \\ 0 & \frac{3}{160}(10+3\sqrt{2}) & \frac{1}{64}(10+3\sqrt{2}) \end{bmatrix}}$$