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Lab session # 5
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1 Question 1

If G consists of M disconnected complete graphs K_2, then we expect the cosine similarities of the embeddings within connected components (i.e., within the K_2 graphs) to be higher than the cosine similarities of embeddings across different connected components.
This is because the *DeepWalk* algorithm performs short random walks on the graph to generate node embeddings. Within a connected component like K_2, the two nodes will frequently co-occur within the same short random walks. This will make their embeddings more similar to each other compared to embeddings of nodes from different connected components that never appear together.

2 Question 2

According to [2], the complexity of the *DeepWalk* algorithm for γ random walks of length t with the window size w and representation size d is :

$$C = \mathcal{O}\big(\gamma|V|tw(d + d\log(|V|)\big)$$

For the spectral clustering, according to [1], the base cost is $\mathcal{O}(|V|^3)$. However we need to have the d embeddings only, hence there are d matrix-vector multiplications. The complexity is then :

$$C = \mathcal{O}\big(|V|^3 + d|V|^2\big)$$

3 Question 3

For this 1-layer GNN, if we consider no self-loops, a vertex with no edge would be completely stuck to evolve. Otherwise, we still aggregate the information of all the neighbours so the difference isn't remarkable here.
However, for the 2-layer GNN, the first layer aggregates information only from these neighbors. Then the second layer aggregates information from the same neighbors again. But these neighbors have no other edges, so their first states contain no new information from further hops. So the node effectively sees the same neighborhood in both layers. The model doesn't propagate information beyond 1 hop.

4 Question 4

4.1 Star graph S_4

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

$$\tilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

Now, let's compute $\tilde{D}^{-\frac{1}{2}} \cdot \tilde{A}$:

$$\tilde{D}^{-\frac{1}{2}} \cdot \tilde{A} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

Hence :

$$\hat{A} = \tilde{D}^{-\frac{1}{2}} \cdot \tilde{A} \cdot \tilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & \frac{1}{2} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{1}{2} & 0 \\ \frac{\sqrt{2}}{4} & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

With X and W^0 :

$$X = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad W^0 = \begin{bmatrix} \frac{1}{2} & -\frac{1}{5} \end{bmatrix}$$

$$X \cdot W^0 = \begin{bmatrix} \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \end{bmatrix}$$

$$\hat{A} \cdot X \cdot W^0 = \begin{bmatrix} \frac{1}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{4} & \frac{1}{2} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{1}{2} & 0 \\ \frac{\sqrt{2}}{4} & 0 & 0 & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \end{bmatrix} = \begin{bmatrix} \frac{1+3\sqrt{2}}{8} & -\frac{1+3\sqrt{2}}{20} \\ \frac{2+\sqrt{2}}{8} & -\frac{2+\sqrt{2}}{20} \\ \frac{2+\sqrt{2}}{8} & -\frac{2+\sqrt{2}}{20} \\ \frac{2+\sqrt{2}}{8} & -\frac{2+\sqrt{2}}{20} \end{bmatrix}$$

Finally,

$$Z^0 = ReLU(\hat{A} \cdot X \cdot W^0) = \begin{bmatrix} \frac{1+3\sqrt{2}}{8} & 0 \\ \frac{2+\sqrt{2}}{8} & 0 \\ \frac{2+\sqrt{2}}{8} & 0 \\ \frac{2+\sqrt{2}}{8} & 0 \end{bmatrix}$$

After the first layer, we can calculate :

$$\hat{A} \cdot Z^0 = \begin{bmatrix} \frac{7+9\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \end{bmatrix}$$

Then :

$$\hat{A} \cdot Z^0 \cdot W^1 = \begin{bmatrix} \frac{7+9\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \\ \frac{10+3\sqrt{2}}{32} & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{3}{10} & -\frac{2}{5} & \frac{4}{5} & \frac{1}{2} \\ -\frac{11}{10} & \frac{3}{5} & -\frac{1}{10} & \frac{7}{10} \end{bmatrix} = \begin{bmatrix} \frac{3(7+9\sqrt{2})}{320} & -\frac{7+9\sqrt{2}}{16\times 5} & \frac{7+9\sqrt{2}}{40} & \frac{7+9\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & -\frac{10+3\sqrt{2}}{16\times 5} & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & -\frac{10+3\sqrt{2}}{16\times 5} & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & -\frac{10+3\sqrt{2}}{16\times 5} & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \end{bmatrix}$$

In the end :

$$Z^1 = ReLU(\hat{A} \cdot Z^0 \cdot W^1) = \begin{bmatrix} \frac{3(7+9\sqrt{2})}{320} & 0 & \frac{7+9\sqrt{2}}{40} & \frac{7+9\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & 0 & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & 0 & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \\ \frac{30+9\sqrt{2}}{320} & 0 & \frac{10+3\sqrt{2}}{40} & \frac{10+3\sqrt{2}}{64} \end{bmatrix}$$

4.2 Cycle graph C_4

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

$$\tilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix} = \frac{\sqrt{3}}{3} I_4$$

Hence :

$$\hat{A} = \tilde{D}^{-\frac{1}{2}} \cdot \tilde{A} \cdot \tilde{D}^{-\frac{1}{2}} = \frac{1}{3}\tilde{A} = \frac{1}{3}\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$$

$$\frac{1}{3}\tilde{A} \cdot X \cdot W^0 = \frac{1}{3}\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \\ \frac{1}{2} & -\frac{1}{5} \end{bmatrix} = \frac{1}{3}\begin{bmatrix} \frac{3}{2} & -\frac{3}{5} \\ \frac{3}{2} & -\frac{3}{5} \\ \frac{3}{2} & -\frac{3}{5} \\ \frac{3}{2} & -\frac{3}{5} \end{bmatrix}$$

We can deduce :

$$Z^0 = ReLU(\hat{A} \cdot X \cdot W^0) = \begin{bmatrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \end{bmatrix}$$

Then in the second layer, we have :

$$\hat{A} \cdot Z^0 = \frac{1}{3}\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \end{bmatrix}$$

Then :

$$\hat{A} \cdot Z^0 \cdot W^1 = \begin{bmatrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{3}{10} & -\frac{2}{5} & \frac{4}{5} & \frac{1}{2} \\ -\frac{11}{10} & \frac{3}{5} & -\frac{1}{10} & \frac{7}{10} \end{bmatrix} = \begin{bmatrix} \frac{3}{20} & -\frac{1}{5} & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & -\frac{1}{5} & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & -\frac{1}{5} & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & -\frac{1}{5} & \frac{2}{5} & \frac{1}{4} \end{bmatrix}$$

Finally we get :

$$Z^1 = ReLU(\hat{A} \cdot Z^0 \cdot W^1) = \begin{bmatrix} \frac{3}{20} & 0 & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & 0 & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & 0 & \frac{2}{5} & \frac{1}{4} \\ \frac{3}{20} & 0 & \frac{2}{5} & \frac{1}{4} \end{bmatrix}$$

We see for both representations of Z^1 that the second column is null, which mean that the hidden states in relation with the information of the second node is not taken into account. Furthermore, we see that for the first Z^1, the nodes $2, 3, 4$ have the same hidden states (it seems normal knowing they have the same distribution with the same node). For the second, as expected all the nodes have the same hidden states because all the nodes are commutable.

References

[1] Michael I. Jordan Donghui Yan, Ling Huang. Fast approximate spectral clusterings. 2009.

[2] Yifan Hu Steven Skiena Haochen Chen, Bryan Perozzi. Harp: Hierarchical representation learning for networks. 2017.