

3 Question 1

Two nodes that are connected in the same K2 graph, will have a higher cosinus similarity since they share an edge, a relation, compared to two nodes that are not directly connected to each other, and therefore, less "linked" to each other.

4 Question 2

For the DeepWalk model, the time complexity is mainly controlled by the training time of the Skip-Gram model, which is equal to $O(|V|tw(d + d\log|V|))$ with the number of random walks, V the number of nodes, t the walk length, w the window size, and d the representation size. [1]

As for the spectral embedding technics using Laplacian L of size $n \times n$, the time complexity is equal to $O(n^3)$. [2]

5 Question 3

The self-loops have an important effect on the graphs. In fact, self-loops are enable to connect nodes to themselves in the graph. Without them, we would sum up all the feature vectors of all neighboring nodes except for the node itself. Therefore, if the self-loops are absent, it will affect the information propagation and the features of the node itself would disappear within the network layers. We would lose information about the node itself.

6 Question 4

Let's first compute $Z_{C_4}^0$ and $Z_{C_4}^0$ for the Cycle Graph C_4 :

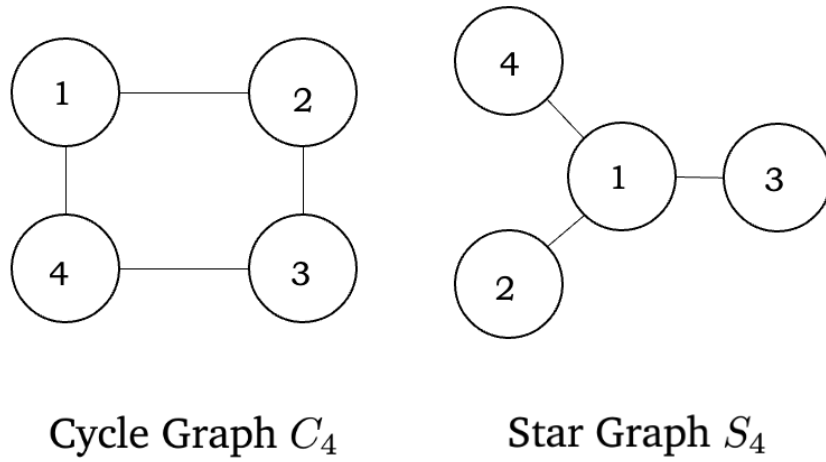


Figure 3: Graphs

$$\tilde{A}_{C_4} = A_{C_4} + I = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \quad (1)$$

$$\hat{A}_{C_4} = \tilde{D}_{C_4}^{-1/2} \tilde{A}_{C_4} \tilde{D}_{C_4}^{-1/2} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix} \quad (2)$$

Let's computer Z^0 :

$$\hat{A}_{C_4} X W^0 = \frac{1}{3} \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 0.5 & -0.2 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 3 \\ 3 \\ 3 \\ 3 \end{bmatrix} \begin{bmatrix} 0.5 & -0.2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 0.5 & -0.2 \end{bmatrix} = \begin{bmatrix} 0.5 & -0.2 \\ 0.5 & -0.2 \\ 0.5 & -0.2 \\ 0.5 & -0.2 \end{bmatrix} \quad (3)$$

$$Z_{C_4}^0 = f(\hat{A}_{C_4} X W^0) = \begin{bmatrix} 0.5 & 0 \\ 0.5 & 0 \\ 0.5 & 0 \\ 0.5 & 0 \end{bmatrix}$$

Let's compute Z^1 :

$$\hat{A}_{C_4} Z_{C_4}^0 W^1 = \frac{1}{3} \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0.5 & 0 \\ 0.5 & 0 \\ 0.5 & 0 \\ 0.5 & 0 \end{bmatrix} \begin{bmatrix} 0.3 & -0.4 & 0.8 & 0.5 \\ -1.1 & 0.6 & -0.1 & 0.7 \end{bmatrix} \quad (4)$$

$$= \frac{1}{3} \begin{bmatrix} 1.5 & 0 \\ 1.5 & 0 \\ 1.5 & 0 \\ 1.5 & 0 \end{bmatrix} \begin{bmatrix} 0.3 & -0.4 & 0.8 & 0.5 \\ -1.1 & 0.6 & -0.1 & 0.7 \end{bmatrix} \\ = \begin{bmatrix} 0.45 & -0.6 & 1.2 & 0.75 \\ 0.45 & -0.6 & 1.2 & 0.75 \\ 0.45 & -0.6 & 1.2 & 0.75 \\ 0.45 & -0.6 & 1.2 & 0.75 \end{bmatrix} \quad (5)$$

$$Z_{C_4}^1 = f(\hat{A}_{C_4} Z_{C_4}^0 W^1) = \begin{bmatrix} 0.45 & 0 & 1.2 & 0.75 \\ 0.45 & 0 & 1.2 & 0.75 \\ 0.45 & 0 & 1.2 & 0.75 \\ 0.45 & 0 & 1.2 & 0.75 \end{bmatrix}$$

Let's first compute $Z_{S_4}^0$ and $Z_{S_4}^1$ for the Star Graph S_4 :

$$\tilde{A}_{S_4} = A_{S_4} + I = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \quad (6)$$

$$\hat{A}_{S_4} = \tilde{D}_{S_4}^{-1/2} \tilde{A}_{S_4} \tilde{D}_{S_4}^{-1/2} = \begin{bmatrix} \frac{1}{\sqrt{4}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{4}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 0 & 0 \\ \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} & 0 \\ \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2\sqrt{2}} \end{bmatrix} \quad (7)$$

Let's compute $Z_{S_4}^0$:

$$\hat{A}_{S_4} X W^0 = \begin{bmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 0 & 0 \\ \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} & 0 \\ \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} [0.5 \quad -0.2] = \begin{bmatrix} 1.311 \\ 0.707 \\ 0.707 \\ 0.707 \end{bmatrix} [0.5 \quad -0.2] = \begin{bmatrix} 0.655 & -0.2621 \\ 0.353 & -0.1414 \\ 0.353 & -0.1414 \\ 0.353 & -0.1414 \end{bmatrix} \quad (8)$$

$$Z_{S_4}^0 = f(\hat{A}_{S_4} X W^0) = \begin{bmatrix} 0.655 & 0 \\ 0.353 & 0 \\ 0.353 & 0 \\ 0.353 & 0 \end{bmatrix}$$

Let's compute $Z_{S_4}^1$:

$$\begin{aligned} \hat{A}_{S_4} Z_{S_4}^0 W^1 &= \begin{bmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & 0 & 0 \\ \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} & 0 \\ \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0.655 & 0 \\ 0.353 & 0 \\ 0.353 & 0 \\ 0.353 & 0 \end{bmatrix} \begin{bmatrix} 0.3 & -0.4 & 0.8 & 0.5 \\ -1.1 & 0.6 & -0.1 & 0.7 \end{bmatrix} \\ &= \begin{bmatrix} 0.2625 & -0.35 & 0.7 & 0.4375 \\ 0.3 & -0.4 & 0.8 & 0.5 \\ 0.3 & -0.4 & 0.8 & 0.5 \\ 0.3 & -0.4 & 0.8 & 0.5 \end{bmatrix} \end{aligned} \quad (9)$$

$$Z_{S_4}^1 = f(\hat{A}_{S_4} Z_{S_4}^0 W^1) = \begin{bmatrix} 0.2625 & 0 & 0.7 & 0.4375 \\ 0.3 & 0 & 0.8 & 0.5 \\ 0.3 & 0 & 0.8 & 0.5 \\ 0.3 & 0 & 0.8 & 0.5 \end{bmatrix}$$

We observe that the node embeddings represented by $Z^1 S_4$ lines are identical for all nodes except node 1. This is logic considering that node 1 in the star graph holds a unique position due to its 3 degrees. The embeddings denoted by $Z^1 C_4$ lines, reflecting the cyclic graph, exhibit complete similarity, since all the nodes in this graph have the exact same features.

References

- [1] Bryan Perozzi Steven Skiena Haochen Chen, Yifan Hu. Harp: Hierarchical representation learning for networks. 2017.
- [2] Huang L. Jordan M.I. Yan, D. Fast approximate spectral clustering. page 907–916, 2009.