Romain AMÉDÉE
romain.amedee@telecom-sudparis.eu

Lab session # 5
ALTEGRAD 2023

12/05/23

1 Question 1

A graph is composed of M connected components, each of which are K_2 complete graphs. The Deepalk algorithm generates embeddings of the node (in this case 2M since there are M connected components with 2 nodes each) that reflect the local structure around these nodes. Since all connected components are K_2, the random walks starting from every node will all consist in the entire connected component the starting node belongs to.

Therefore, we can expect a very similar, if not identical, embedding for two nodes that belong to the same connected component (every random walk that contains one of the nodes also contains the other). This would result in a cosine similarity very close to, if not equal to, one.

On the other hand, two nodes from different connected components are expected to have very different embeddings since every random walk with one of the nodes is certain not to contain the other node. This would result in a cosine similarity very close to, if not equal to, zero.

2 Question 2

According to [1] the time complexity of the DeepWalk algorithm is :

$$\mathcal{O}(\gamma|V|tw(d + dlog|V|))$$

where :

- γ is the number of random walks
- t is the length of the walks
- d is the representation size
- w is the window size

According to [2] the time complexity of the spectral embedding thechnique is : $\mathcal{O}(n^3)$ with n the number of data points.

3 Question 3

The absence of self-loops means that the node's own information is not taken into account when computing its hidden state. The hidden state update in a single layer only depends on the information of neighbor nodes. This might lead to information loss, especially for nodes with low degrees, as their influence on their neighbors would be limited. Adding self-loops allows the node's own information to be propagated through hidden states, therefore capturing more aspects of its local structure.
In a two-layer GNN without self-loops, the hidden state of a node in the second layer is influenced only by the aggregated information from its neighbors in the first layer.

4 Question 4

4.1 Star graph

Let us study the following graph S_4 :

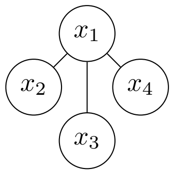

Figure 1: S_4 graph

It's adjacency matrix is as follows :

$$A_{S_4} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Let us normalize this matrix to obtain $\hat{A} = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$, with :

$\tilde{A} = A + I = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$ and $\tilde{D} = diag(\sum_j \tilde{A}_{ij}) = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$

We then have : $\tilde{D}^{-\frac{1}{2}} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$

Finnaly we have :

$$\hat{A} = \begin{pmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

Let us consider $X = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$. We will now compute Z^0 and Z^1 for the GNN architecture used in the lab.

We have :

$$Z^0 = ReLu(\hat{A}XW^0) = ReLu\left(\begin{pmatrix} \frac{1+\sqrt{18}}{8} & -0.2 \times \frac{1+\sqrt{18}}{8} \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & -0.2 \times \frac{1+\sqrt{2}}{4\sqrt{2}} \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & -0.2 \times \frac{1+\sqrt{2}}{4\sqrt{2}} \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & -0.2 \times \frac{1+\sqrt{2}}{4\sqrt{2}} \end{pmatrix}\right) = \begin{pmatrix} \frac{1+\sqrt{18}}{8} & 0 \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & 0 \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & 0 \\ \frac{1+\sqrt{2}}{4\sqrt{2}} & 0 \end{pmatrix}$$

Then :

$$Z^1 = ReLu(\hat{A}Z^0W^1) = ReLu\left(\begin{pmatrix} 0.3 \times \frac{7+9\sqrt{2}}{32} & -0.4 \times \frac{7+9\sqrt{2}}{32} & 0.8 \times \frac{7+9\sqrt{2}}{32} & 0.5 \times \frac{7+9\sqrt{2}}{32} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & -0.4 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & -0.4 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & -0.4 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \end{pmatrix}\right)$$

Finally :

$$Z^1 = \begin{pmatrix} 0.3 \times \frac{7+9\sqrt{2}}{32} & 0 & 0.8 \times \frac{7+9\sqrt{2}}{32} & 0.5 \times \frac{7+9\sqrt{2}}{32} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0 & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0 & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \\ 0.3 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0 & 0.8 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} & 0.5 \times \frac{3+5\sqrt{2}}{16\sqrt{2}} \end{pmatrix}$$

Here we notice that the first line of Z^1 is different from the 3 next lines. This can be explained by the difference of the environment of node 1 (x_1 on Figure 1) and the structure around x_2, x_3 and x_4 which have the same neighbor x_1.

4.2 Cycle graph

Let us study the following graph C_4 :

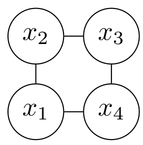

Figure 2: C_4 graph

It's adjacency matrix is as follows :

$$A_{C_4} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Let us normalize this matrix to obtain $\hat{A} = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$, with :

$$\tilde{A} = A + I = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix} \text{ and } \tilde{D} = diag(\textstyle\sum_j \tilde{A}_{ij}) = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

We then have : $\tilde{D}^{-\frac{1}{2}} = \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} \end{pmatrix}$

Finnaly we have :

$$\hat{A} = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

Let us consider $X = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$. We will now compute Z^0 and Z^1 for the GNN architecture used in the lab.

We have :

$$Z^0 = ReLu(\hat{A}_{C_4} X W^0) = ReLu\left(\begin{pmatrix} 1/2 & -0.2 \\ 1/2 & -0.2 \\ 1/2 & -0.2 \\ 1/2 & -0.2 \end{pmatrix}\right) = \begin{pmatrix} 1/2 & 0 \\ 1/2 & 0 \\ 1/2 & 0 \\ 1/2 & 0 \end{pmatrix}$$

Then :

$$Z^1 = ReLu(\hat{A}Z^0W^1) = ReLu\left(\begin{pmatrix} 0.15 & -0.2 & 0.4 & 0.25 \\ 0.15 & -0.2 & 0.4 & 0.25 \\ 0.15 & -0.2 & 0.4 & 0.25 \\ 0.15 & -0.2 & 0.4 & 0.25 \end{pmatrix}\right)$$

Finally :

$$\boxed{Z^1 = \begin{pmatrix} 0.15 & 0 & 0.4 & 0.25 \\ 0.15 & 0 & 0.4 & 0.25 \\ 0.15 & 0 & 0.4 & 0.25 \\ 0.15 & 0 & 0.4 & 0.25 \end{pmatrix}}$$

All four lines are identical. This can be explained by the fact that the vector X with only ones was given as input and the four nodes of the cycle graph have the exact same environment with two edges each. Each line represents one of the n

References

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

[2] Mu Li, Xiao Chen, James Kwok, and Bao-Liang Lu. Time and space efficient spectral clustering via column sampling. pages 2297–2304, 06 2011.