Question 1

for directed graphs

By processing directed graphs, we can use the same algorithm as for undirected graphs, but we need to consider the direction of the edges. Thus, the random walk must be changed to take into account the direction of the edges. We just need to use outgoing edges to compute the transition probabilities. Additionnaly, the transition probability $\mathbb{P}(v_j|\phi(v_i))$, has to be limited to the set of nodes reachable from v_i via outgoing edges.

for weighted graphs

For weighted graphs, one can also modify the random walk: the probability of moving from v_i to v_j is proportional to the weight of the edge (v_i, v_j), such as:

$$\mathbb{P}(v_j|\phi(v_i)) = \frac{w(v_i, v_j)}{\sum_{v_k \in \text{outgoing neighbors}(v_i)} w(v_i, v_k)}.$$

Question 2

By examining the two embeddings X_1 and X_2, we notice that the second row of X_2 is identical to the second row of X_1, except with the opposite sign. Despite this sign difference, the overall structure and relative distances between nodes remain unchanged in both embeddings. This is because DeepWalk embeddings focus on capturing the relative positions and relationships between nodes, rather than assigning fixed coordinates. This invariance to transformations such as reflections—in this case, along the second dimension—ensures that the embeddings still encode the same structural information. Thus, both X_1 and X_2 are valid embeddings.

Question 3

In the architecture described in Task 10, there are two message-passing layers. Each message-passing layer aggregates information from the direct neighbors of a node. Consequently, after the second message-passing layer, each node incorporates information from its "neighbors of neighbors." This implies that the maximum distance between a node and the nodes contributing to the computation of $\hat{Y}_i$ in this GCN architecture is **2 edges**.

More generally, for an architecture with k message-passing layers, the maximum distance of nodes involved in the computation is k edges.

Question 4

(a)

To compute the matrix Z^1, let us first normalize the adjacency matrix. For K_4:

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

Thus,

$$\tilde{A} = A + I_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

Then, with $\tilde{D}ii = \sum_j \tilde{A}ij$, we have that

$$\tilde{D} = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} \quad \text{and therefore} \quad \tilde{D}^{-1/2} = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 \end{pmatrix}$$

Thus, the normalized adjacency matrix is

$$\begin{aligned} \hat{A} &= \tilde{D}^{-1/2}\ \tilde{A}\ \tilde{D}^{-1/2} \\ &= \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{pmatrix} \\ &= \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \end{pmatrix} \end{aligned}$$

Then, compute $Z_0 = \text{ReLU}(\hat{A}\ X\ W^0)$, with $X = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$, and $W^0 = \begin{pmatrix} -0.8 & 0.5 \end{pmatrix}$.

$$\hat{A}\ X = \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix},$$

so

$$\hat{A}\ X\ W^0 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} -0.8 & 0.5 \end{pmatrix} = \begin{pmatrix} -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \end{pmatrix}.$$

Finally we can compute,

$$Z_0 = \text{ReLU}(\hat{A}\ X\ W^0) = \text{ReLU}(\begin{pmatrix} -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \\ -0.8 & 0.5 \end{pmatrix}) = \begin{pmatrix} 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \end{pmatrix}$$

Thus, we obtain $Z_1 = \text{ReLU}(\hat{A}\ Z^0\ W^1)$, with $\hat{A}$ and Z^0 as defined previously, and $W^1 = \begin{pmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{pmatrix}$.

$$\hat{A}\ Z^0 = \begin{pmatrix} 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \end{pmatrix} \begin{pmatrix} 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \end{pmatrix} = \begin{pmatrix} 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \end{pmatrix}$$

Then,

$$\hat{A}\ Z^0\ W^1 = \begin{pmatrix} 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \\ 0 & 0.5 \end{pmatrix} \begin{pmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{pmatrix} = \begin{pmatrix} -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \end{pmatrix}$$

We thus obtain:

$$Z^1 = \text{ReLU}(\hat{A}\ Z^0\ W^1) = \text{ReLU}(\begin{pmatrix} -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \\ -0.2 & 0.3 & 0.25 \end{pmatrix}) = \begin{pmatrix} 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \\ 0 & 0.3 & 0.25 \end{pmatrix}$$

(b)

Let's do the same for S_4:

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

$$\tilde{A} = A + I_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

With $\tilde{D}ii = \sum_j \tilde{A}ij$, we have:

$$\tilde{D} = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \quad \text{and therefore} \quad \tilde{D}^{-1/2} = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1/\sqrt{2} \end{pmatrix}$$

We thus obtain the normalized adjacency matrix:

$$\begin{aligned} \hat{A} &= \tilde{D}^{-1/2}\ \tilde{A}\ \tilde{D}^{-1/2} \\ &= \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1/\sqrt{2} \end{pmatrix} \\ &= \begin{pmatrix} 0.25 & 0.3536 & 0.3536 & 0.3536 \\ 0.3536 & 0.5 & 0 & 0 \\ 0.3536 & 0 & 0.5 & 0 \\ 0.3536 & 0 & 0 & 0.5 \end{pmatrix} \end{aligned}$$

Then, $Z_0 = \text{ReLU}(\hat{A}\ X\ W^0)$, where $X = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$ and $W^0 = \begin{pmatrix} -0.8 & 0.5 \end{pmatrix}$.

$$\hat{A}\ X = \begin{pmatrix} 0.25 & 0.3536 & 0.3536 & 0.3536 \\ 0.3536 & 0.5 & 0 & 0 \\ 0.3536 & 0 & 0.5 & 0 \\ 0.3536 & 0 & 0 & 0.5 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1.3108 \\ 0.8536 \\ 0.8536 \\ 0.8536 \end{pmatrix}$$

Then,

$$\hat{A}\ X\ W^0 = \begin{pmatrix} 1.3108 \\ 0.8536 \\ 0.8536 \\ 0.8536 \end{pmatrix} \begin{pmatrix} -0.8 & 0.5 \end{pmatrix} = \begin{pmatrix} -1.0486 & 0.6554 \\ -0.6829 & 0.4268 \\ -0.6829 & 0.4268 \\ -0.6829 & 0.4268 \end{pmatrix}$$

Finally,

$$Z_0 = \text{ReLU}(\hat{A}\ X\ W^0) = \text{ReLU}(\begin{pmatrix} -1.0486 & 0.6554 \\ -0.6829 & 0.4268 \\ -0.6829 & 0.4268 \\ -0.6829 & 0.4268 \end{pmatrix}) = \begin{pmatrix} 0 & 0.6554 \\ 0 & 0.4268 \\ 0 & 0.4268 \\ 0 & 0.4268 \end{pmatrix}$$

Finally, we compute $Z_1 = \text{ReLU}(\hat{A}\ Z^0\ W^1)$, with $\hat{A}$ and Z^0 as defined previously, and $W^1 = \begin{pmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{pmatrix}$

$$\hat{A}\ Z^0 = \begin{pmatrix} 0.25 & 0.3536 & 0.3536 & 0.3536 \\ 0.3536 & 0.5 & 0 & 0 \\ 0.3536 & 0 & 0.5 & 0 \\ 0.3536 & 0 & 0 & 0.5 \end{pmatrix} \begin{pmatrix} 0 & 0.6554 \\ 0 & 0.4268 \\ 0 & 0.4268 \\ 0 & 0.4268 \end{pmatrix} = \begin{pmatrix} 0 & 0.5056 \\ 0 & 0.4518 \\ 0 & 0.4518 \\ 0 & 0.4518 \end{pmatrix}$$

Then,

$$\hat{A}\ Z^0\ W^1 = \begin{pmatrix} 0 & 0.5056 \\ 0 & 0.4518 \\ 0 & 0.4518 \\ 0 & 0.4518 \end{pmatrix} \begin{pmatrix} 0.1 & 0.3 & -0.05 \\ -0.4 & 0.6 & 0.5 \end{pmatrix} = \begin{pmatrix} -0.2022 & 0.3034 & 0.2528 \\ -0.1807 & 0.2711 & 0.2259 \\ -0.1807 & 0.2711 & 0.2259 \\ -0.1807 & 0.2711 & 0.2259 \end{pmatrix}$$

So finally, we obtain:

$$Z^1 = \mathrm{ReLU}(\hat{A}\ Z^0\ W^1) = \mathrm{ReLU}(\begin{pmatrix} -0.2022 & 0.3034 & 0.2528 \\ -0.1807 & 0.2711 & 0.2259 \\ -0.1807 & 0.2711 & 0.2259 \\ -0.1807 & 0.2711 & 0.2259 \end{pmatrix}) = \begin{pmatrix} 0 & 0.3034 & 0.2528 \\ 0 & 0.2711 & 0.2259 \\ 0 & 0.2711 & 0.2259 \\ 0 & 0.2711 & 0.2259 \end{pmatrix}.$$