

1 Question 1

If we have a graph G such that each connected component is a complete K_2 graph, then the cosine similarities of the embeddings of the nodes fall under one of the 2 following cases:

- Nodes are in the same component, in which case we obtain embeddings that are nearly co-linear and same direction, i.e. high cosine similarity (around one).
- Nodes are in different components, in which case the embeddings are nearly orthogonal i.e. small cosine similarity.

2 Question 2

The 2 embeddings can be rewritten as

$$X_1 = \begin{bmatrix} x_1 & -x_1 \end{bmatrix} \text{ and } X_2 = \begin{bmatrix} x_1 & x_1 \end{bmatrix}$$

This means information contains in each embeddings is x_1 , so they are equally informative.

3 Question 3

GNN contains more than one message passing layer to gather information on higher order neighbours and they don't contain a very large number to not gather information on all the graph, which would be the same for all nodes thus not discriminant.

4 Question 4

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W_0 = torch.tensor([[0.5, -0.2]])
W_1 = torch.tensor([[0.3, -0.4, 0.8, 0.5], [-1.1, 0.6, -0.1, 0.7]])
A = torch.tensor([[0, 1, 0, 0], [1, 0, 1, 0], [0, 1, 0, 1], [0, 0, 1, 0]])
Atld = A + torch.eye(4)
D2 = torch.diag(Atld.sum(axis=-1)**-0.5)
Adj = D2 @ Atld @ D2
X = torch.ones((4, 1))
Z_0 = torch.relu(Adj @ X @ W_0)
Z_1 = torch.relu(Adj @ Z_0 @ W_1)
```

Figure 1: Computing matrix Z^1

Computation gives

$$Z^1 = \begin{bmatrix} 0.1339 & 0 & 0.3572 & 0.2232 \\ 0.1631 & 0 & 0.4350 & 0.2719 \\ 0.1631 & 0 & 0.4350 & 0.2719 \\ 0.1339 & 0 & 0.3572 & 0.2232 \end{bmatrix} =: \begin{bmatrix} a \\ b \\ b \\ a \end{bmatrix}$$

The 2nd coordinate is the same among nodes thus irrelevant. More interestingly, extremal nodes embeddings are the same and middle nodes embeddings are the same. This is due to symmetry of the graph we study.

References