Mid-term Exam (Graph Neural Networks –Fall 2024)

Full Name:
Student ID:

1. (10pt) Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

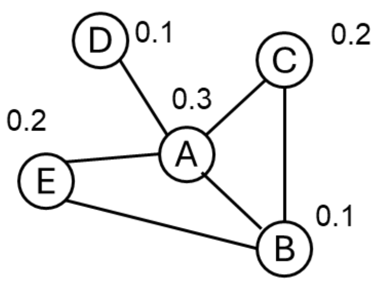
$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} -2 & 1 \\ -3 & -3 \\ -1 & 4 \\ 2 & 2 \\ 4 & 0 \end{bmatrix}$$

Assume that the hidden layer of an GCN model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left(A \cdot H^{(k-1)}\right),$$

where $H^{(k)}$ denotes the output at layer k, σ is a ReLU function $\mathrm{ReLU}(x) = \max(0, x)$. Calculate the output of the GCN model at layer $k = 1$.

2. (10pt) Consider an undirected graph G of five nodes A, B, C, D, and E given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $h_A^{(0)} = 0.3$). According to GraphSAGE model with an AGGREGATE is a MEAN function, the feature of a node i at layer k can be updated as:

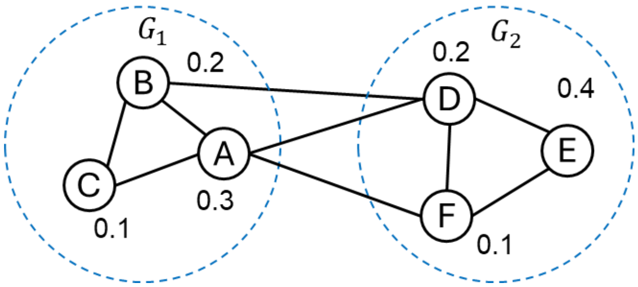


$$h_{N(i)}^{(k)} = \mathrm{AGGREGATE}\left(\left\{h_u^{(k-1)}, \forall u \in N(i)\right\}\right)$$
$$h_i^{(k)} = \mathrm{ReLU}\left(h_i^{(k-1)} || h_{N(i)}^{(k)}\right)$$

where || is a concatenation, $\mathrm{ReLU}(x) = \max(0, x)$, *N(i)* is the neighbour nodes of node *i*.

a) Calculate the feature of each node at $k = 1$.
b) Calculate a graph-level embedding h_G by using a 'Mean' global pooling when $k = 1$.

3. (10pt) Consider an undirected graph G of six nodes A, B, C, D, E and F given in the following figure. The graph G contains two cluster G_1 and G_2. Each node has initial features that are the numbers standing next to it. According to ClusterGCN model, the feature of a node i at layer k can be updated as:



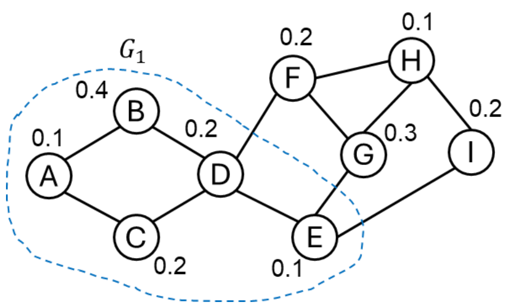
$$h_{N(i)}^{(k)} = \text{MEAN}\left(\left\{h_u^{(k-1)}, \forall u \in N(i), G_u = G_i\right\}\right)$$

$$h_i^{(k)} = \text{ReLU}\left(h_i^{(k-1)} || h_{N(i)}^{(k)}\right)$$

where || is a concatenation.

Calculate the output representations of all nodes at layer $k = 1$.

4. (10pt) Consider an undirected graph G of six nodes A, B, C, D, E and F given in the following figure. The graph G has subgraph sampling G_1. Each node has initial features that are the numbers standing next to it. According to GraphSAINT model, the feature of a node i at layer k can be updated as:



$$h_{N(i)}^{(k)} = \text{MEAN}\left(\left\{h_u^{(k-1)}, \forall u \in N(i), G_u = G_i\right\}\right)$$

$$h_i^{(k)} = \text{ReLU}\left(h_i^{(k-1)} || h_{N(i)}^{(k)}\right)$$

where || is a concatenation.

Calculate the output representations of all nodes at layer $k = 1$.

5. (10pt) Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

$$A = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} -2 & 0 \\ 2 & -2 \\ 2 & 4 \\ -2 & 2 \\ 4 & 3 \end{bmatrix}$$

Assume that the output of an JK network model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \max\left(\sigma\left(\tilde{A} \cdot H^{(0)}\right), \sigma\left(\tilde{A} \cdot H^{(1)}\right), \ldots, \sigma\left(\tilde{A} \cdot H^{(k)}\right)\right)$$

where $H^{(k)}$ denotes the output at layer k, $\tilde{A}$ is the normalized matrix ($\tilde{A} = D^{-1}A$), σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.

a) Calculate $\tilde{A}$.

b) Calculate the output representations at layer $k = 2$.

6. (15pt) Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} 3 \\ -2 \\ 2 \\ 4 \\ 3 \end{bmatrix}$$

Assume that the output of an GCNII model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left[\left((1-\beta)I_n\right) \cdot \left((1-\alpha)\tilde{A} \cdot H^{(k-1)} + \alpha H^{(0)}\right)\right]$$

where $H^{(k)}$ denotes the output at layer $k, \tilde{A}$ is the normalized matrix ($\tilde{A} = D^{-1}A$), I_n is the identity matrix, $\alpha = \beta = 0.5$, σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.

a) Calculate $\tilde{A}$.

b) Calculate the output representations at layer $k = 1$.

7. (10pt) Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

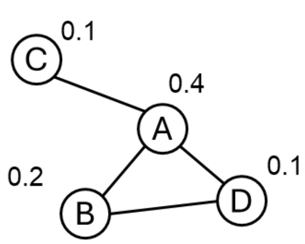
$$A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} 0 & -2 \\ -1 & 3 \\ 4 & -2 \\ 0 & -5 \end{bmatrix}$$

Assume that the hidden layer of an DeepGCNs model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left(A \cdot H^{(k-1)}\right) + H^{(k-1)},$$

where $H^{(k)}$ denotes the output at layer k, σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.
Calculate the output of the GCN model at layer $k = 2$.

8. (15pt) Consider an undirected graph G of four nodes A, B, C, and D given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $h_A^{(0)} = 0.4$). According to GAT model, the weight matrix W is randomly initialized as [0.5]. The feature of node 'i' at layer (k) can be updated as:



$$h_i^{(k)} = \sigma\left(\sum_{m \in N(i)} \alpha_{im} W h_m\right)$$

Where $\alpha_{im} = \frac{e_{im}}{\sum_{k \in N(i)} e_{ik}}$ and

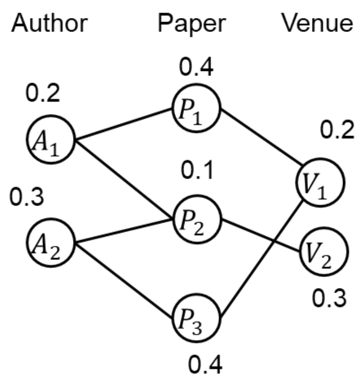
$$e_{im} = \sigma\left(\text{MEAN}(Wh_i, Wh_m)\right)$$

σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.

a) Calculate the attention coefficients e_{AB}, e_{AC}, and e_{AD}

b) Calculate the feature of node ‘A’ at $k = 1$.

9. (10pt) Consider a heterogeneous graph given in the following figure. There are three types of nodes in the academic network: Author (A), Paper (P), and Venue (V). Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node ‘A_1’ is $h_{A_1}^{(0)} = 0.2$). According to HAN model, the weight matrix W is randomly initialized as [0.5]. The feature of node ‘i’ at layer (k) can be updated as:



$$h_i^{(k)} = \sigma\left(\sum_{m\in N(i)} \alpha_{im}^{\Phi} W h_m\right)$$

Where $\alpha_{im}^{\Phi} = \frac{e_{im}^{\Phi}}{\sum_{k\in N^{\Phi}(i)} e_{ik}^{\Phi}}$ and

$$e_{im}^{\Phi} = \sigma\left(\text{MEAN}\left(Wh_i^{\Phi}, Wh_m^{\Phi}\right)\right)$$

σ is a ReLU function $\text{ReLU}(x) = \max(0, x)$.

a) List all the meta-path PAP and PVP. Calculate the attention coefficients of each meta-path PAP and PVP.

b) Calculate the feature of node ‘P_1’ at $k = 1$.