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JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2025

B.Tech-VI Semester (CSE/IT)

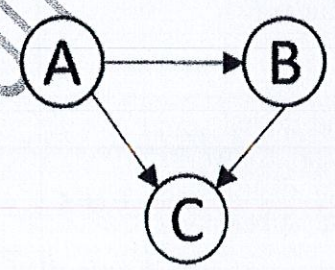
COURSE CODE (CREDITS): 25B1WCI641 (3) MAX. MARKS: 35

COURSE NAME: GRAPH NEURAL NETWORKS

COURSE INSTRUCTORS: Prof. Vivek Kumar Sehgal MAX. TIME: 2 Hours

Note: (a) All questions are compulsory.

(b)) Use of calculator is not allowed

<table>
<tr><th>Q.No</th><th>Question</th><th>CO</th><th>Marks</th></tr>
<tr><td>Q1</td><td>Consider a graph $G = (V, A, X)$, where A is the adjacency matrix and $X \in \mathbb{R}^{|V| \times m}$ is the node feature matrix. Define permutation invariance and permutatic equivariance for a graph function f. Prove that
$$f(A, X) = f(PAP^T, PX)$$
represents permutation invariance, and
$$Pf(A, X) = f(PAP^T, PX)$$
represents permutation equivariance, where P is a permutation matrix. Explain why Graph Neural Networks satisfy these properties.</td><td>CO-3</td><td>5</td></tr>
<tr><td>Q2</td><td>For a Graph Convolutional Network (GCN), the neighborhood aggregation update rule is given by
$h_v^{(k+1)} = \sigma\left(W_k \sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|} + B_k h_v^{(k)}\right)$ where $h_v^{(0)} = x_v$. Derive the matrix form
$$H^{(k+1)} = \sigma(\hat{A} H^{(k)} W_k + H^{(k)} B_k)$$
With $\hat{A} = D^{-1}A$ and explain the role of matrices A, D, W_k, and B_k.</td><td>CO-3,4</td><td>5</td></tr>
<tr><td>Q3</td><td>Consider the following graph of friendship request


<table>
<tr><th>NODE</th><th>Features</th></tr>
<tr><td>A</td><td>Vegetarian</td></tr>
<tr><td>B</td><td>Non-Vegetarian</td></tr>
<tr><td>C</td><td>Both</td></tr>
</table>
Classify the features of each friend after establing the friendship network using Graph Convolutional Neural Network (GCNN)</td><td>CO-3,4</td><td>5</td></tr>
</table>

Q4	For a Graph Attention Network (GAT), the attention coefficients are computed as $e_{vu} = a\left(W^{(l)}h_u^{(l-1)}, W^{(l)}h_v^{(l-1)}\right)$ and normalized using the softmax function: $\alpha_{vu} = \frac{\exp\,(e_{vu})}{\sum_{k\in N(v)}\ \exp\,(e_{vk})}$ The node embedding update rule is $h_v^{(l)} = \sigma\left(\sum_{u\in N(v)}\ \alpha_{vu} W^{(l)} h_u^{(l-1)}\right)$ Derive the above equations and explain the significance of learned attention weights α_{vu} in comparison with the fixed averaging used in GCNs.	CO-4,5	5
Q5	Consider a K-layer Graph Neural Network where the node embedding after layer l is given by $h_v^{(l)} = \sigma\left(\sum_{u\in N(v)}\ \frac{W^{(l)}h_u^{(l-1)}}{\lvert N(v)\rvert}\right)$ Explain the concept of receptive field in GNNs and prove that a K-layer GNN aggregates information from the K-hop neighborhood. Discuss the over-smoothing problem and explain how skip connections modify the update equation to $h_v^{(l)} = \sigma\left(\sum_{u\in N(v)} \frac{W^{(l)}h_u^{(l-1)}}{\lvert N(v)\rvert} + h_v^{(l-1)}\right)$ to alleviate over-smoothing.	CO-5	5
Q6	For a node classification task in a Graph Neural Network (GNN), suppose the node embeddings after L layers are $\left\{h_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}$ The prediction head is defined as $\hat{y}_v = W^{(H)}h_v^{(L)}$ where $W^{(H)} \in \mathbb{R}^{k\times d}$ Derive the cross-entropy loss function for N training nodes $\mathrm{CE}(y^{(i)}, \hat{y}^{(i)}) = -\sum_{j=1}^{K} y_j^{(i)} \log\left(\hat{y}_j^{(i)}\right)$ and hence show that the total loss becomes $\text{Loss} = \sum_{i=1}^{N}\ \mathrm{CE}\left(y^{(i)}, \hat{y}^{(i)}\right)$. Explain the significance of Softmax activation in multi-class node classification.	CO-5	5
Q7	Compare global mean pooling, global max pooling, and global sum pooling used for graph-level prediction in Graph Neural Networks (GNNs). Explain why global sum pooling may fail to distinguish structurally different graphs and discuss how a virtual super-node improves graph representation learning.	CO-5	5