Graph Neural Networks

Code: CS32127CS	Course Type: Elective	Semester: I
Evolution Scheme (TA-MSE-ESE): 20-30-100	Total Marks: 150	L-T-P (Credits): 3-0-0 (3)

Pre-Requisites: Linear Algebra, Probability & Statistics, Introductory Graph Theory.

Course Objective: To enable students to understand and apply graph neural networks for real-world problem-solving and creative ideas for new architectureson graph data.

Course Outcomes: At the end of the course, the student will be able to

CO-1	Construct graph representations for real-world data and apply spectral tools and classical graph algorithms to analyze structural properties.
CO-2	Explain the message-passing framework and compare GCN, GAT, GraphSAGE, and GIN architectures in terms of design choices and expressive power.
CO-3	Understanding Deep Graph Neural Networks and Optimization Challenges.
CO-4	Design and develop a GNN-based end-to-end solution for a domain problem such as drug discovery, fraud detection, or recommender systems and other application areas.

Course Articulation Matrix:

PO	PEO-1	PEO-2	PEO-3	PEO-4	PEO-5
CO-1	3	1	1	1	1
CO-2	3	2	1	2	2
CO-3	3	2	1	1	3
CO-4	3	3	3	2	3

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Unit-1: Foundation Graph Theory and Graph Learning: Graph types: directed, undirected, bipartite, heterogeneous, dynamic. Graph representations: adjacency matrix, adjacency list. Graph Laplacian and spectral properties. Overview of important graph analytics tasks such as node classification, community detection, and link prediction etc. Node embedding techniques – DeepWalk, Node2Vec, Skip-Gram.

Unit-2: Message Passing & Core GNN Architectures: Message-passing neural networks (MPNN): aggregate, combine, readout. Graph Convolutional Network (GCN), GraphSAGE: inductive learning & neighbourhood sampling strategies, Graph Attention Network (GAT): attention coefficients, multi-head, Graph Isomorphism Network (GIN).

Unit-3: Deep GNNs and Optimization ChallengesTraining Bottlenecks: Over-smoothing (information loss in deep layers), vanishing gradients, and over-squashing. Architectural Solutions: Residual/Skip connections, and other techniques.

Unit-4: Applications in:Social networks, Recommendation systems, Fraud detection, Drug discovery. Graph embeddings, Hybrid GNN architectures, Overview of PyTorch Geometric (PyG) and Deep Graph Library (DGL).

Learning Resources:

Text Books:

1. William L. Hamilton, Graph Representation Learning, Morgan & Claypool Publishers, 2020.ISBN: 9781681739632
2. Ma & Tang, Deep Learning on Graphs, Cambridge University Press, 2021. ISBN: 978-1108831741.

Reference Books and Resources:

1. Goodfellow, Bengio, Courville, Deep Learning, MIT Press, 2016.ISBN: 978-0262035613
2. CS224W: Machine Learning with Graphs — Stanford University (free online lectures, slides, assignments).
3. PyTorch Geometric Documentation (official, for lab/implementation reference).