

GRAPH BASED LEARNING

Code: CS33322CS	Course Type: Core	Semester: III
Evolution Scheme (TA-MSE-ESE): 20-30-100	Total Marks: 150	L-T-P (Credits): 3-0-0 (3)

Pre-Requisites: Graph Theory, Machine Learning, Deep Learning

Course Objective: This course explores the representation of data as graphs and the development of machine learning algorithms to analyze these structures. It covers classical methods, spectral analysis, and the latest in Graph Neural Networks (GNNs).

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

CO-1	Understand the necessary mathematical bridge between linear algebra and graph topology.
CO-2	Understand the Traditional Graph-Based Algorithms, to form the backbone of semi-supervised learning on graphs.
CO-3	Understand the core of modern GBL, focusing on the message-passing paradigm.
CO-4	Understand to focus on scalability, robustness, and real-world deployment.

Course Articulation Matrix:

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

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Unit-1: Spectral Foundations & Representation

Graph Algebra: Review of Adjacency, Degree, and Incidence matrices. The Laplacian Family: Unnormalized (L), Symmetric Normalized, and Random Walk Laplacians. Spectral Graph Theory: Eigenvalue decomposition, the Fiedler vector for graph partitioning, and the Cheeger inequality. Signal Processing on Graphs: Graph Fourier Transform (GFT), Graph Filters, and the concept of "smoothness" on a graph.

Unit-2: Shallow Embeddings & Semi-Supervised Learning

Label Propagation: Gaussian Random Fields, Harmonic functions, and the Min-cut problem. Random

Walk Methods: Personalized PageRank (PPR), SimRank, and hitting/commute times. Skip-gram based Embeddings: Detailed study of DeepWalk, Node2Vec, and LINE (Second-order proximity). Matrix Factorization: Relationships between DeepWalk and NetMF; GraRep.

Unit-3: Deep Learning on Graphs (The GNN Era)

Message Passing Paradigm: Aggregate, Update, and Readout functions; Permutation Invariance and Equivariance. Neighborhood Aggregation: GCN (Graph Convolutional Networks): First-order spectral approximations. GraphSAGE: Inductive learning via neighbor sampling and pooling. GAT (Graph Attention Networks): Self-attention mechanisms on edge importance. Theoretical Limits: The Weisfeiler-Lehman (WL) Test and the expressive power of GNNs (Graph Isomorphism Networks - GIN).

Unit-4: Advanced Architectures & Scalability

Scalability Techniques: Graph Partitioning (METIS), Node Sampling, and Layer Sampling (FastGCN, L-GCN). Specialized Graphs: * Heterogeneous GNNs: Learning with multiple node/edge types (Metapaths). Temporal/Dynamic Graphs: Using RNNs/LSTMs with GNNs for evolving structures. Trustworthy GBL: Explainability in GNNs (GNNExplainer), robustness against adversarial attacks, and privacy-preserving graph learning. Case Studies: Recommendation systems (Pinterest/Uber-style), Drug Discovery (Molecular Graphs), and Traffic Prediction.

Learning Resources:

Textbooks:

1. Graph Representation Learning" by William L. Hamilton (Pre-print available online).
2. Deep Learning on Graphs" by Yao Ma and Jiliang Tang.
3. IIT Madras NPTEL Course on "Social Networks" and "Deep Learning" (Supplementary).