Graph Neural Network
Lecture

Overview

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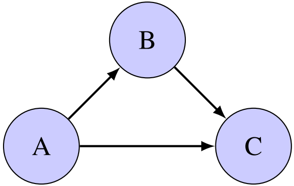
What Are Graph Neural Networks?

- GNNs are a type of deep learning model designed for graph-structured data
- Graphs consist of:
  - Nodes (Vertices): Represent entities (e.g., people in a social network).
  - Edges/Links: Represent relationships or interactions (e.g., friendships).



- GNNs leverage the structure of graphs to learn meaningful representations.

Message Passing:

Nodes aggregate information from neighbors.

Node Embeddings

Transform features into a low-dimensional vector space.

Graph Aggregation:

Pool node embeddings to form a graph-level representation.

Why Use GNNs?

- Graph data is everywhere in real-world applications.
- Traditional neural networks struggle with non-Euclidean data.
- GNNs enable learning directly on graph structures, capturing both:
  - Node features.
  - Topological relationships (connectivity).

Examples of Graph Data

- Social networks: Users as nodes, friendships as edges.
- Molecular graphs: Atoms as nodes, chemical bonds as edges.
- Knowledge graphs: Entities as nodes, relationships as edges.
- Transportation networks: Locations as nodes, roads as edges.

- General structure:
  - **Input:** Graph data (nodes, edges, and features).
  - **Hidden layers:** Message passing and aggregation.
  - **Output:** Node embeddings, edge predictions, or graph-level classifications.
- Iterative information exchange across graph layers.
- Key insight: Combining node features with graph topology.

GNN Workflow

1. Initialize node features (e.g., feature vectors).
2. Perform message passing for multiple layers.
3. Aggregate and update node embeddings.
4. Apply task-specific layers (e.g., classification or regression).

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- **Social Networks:** Friend recommendation, community detection.
- **Knowledge Graphs:** Entity linking, relation prediction.
- **Drug Discovery:** Molecular property prediction.
- **Transportation:** Traffic forecasting, route optimization.

Advantages and Challenges

Advantages:

- Captures graph topology.
- Flexible and powerful.
- Handles irregular data.

Challenges:

- Computationally expensive.
- Scalability to large graphs.
- Over-smoothing in deep GNNs.

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Summary

- Graph Neural Networks generalize deep learning to graph-structured data.
- Applications span diverse domains such as social networks, biology, and recommendation systems.
- Ongoing research addresses scalability and optimization challenges.