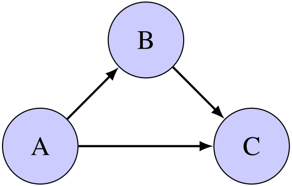
# Graph Neural Network
# Lecture 1

# Overview

# 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.

# Key Components of GNNs

**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.

**Key Idea:**

- Nodes aggregate information from their neighbors.
- Enables nodes to learn representations based on local graph structure.

**Process:**

- Each node receives messages (feature vectors) from its neighbors.
- Messages are combined using a differentiable function (e.g., sum, mean, max).
- The aggregated message is used to update the node's state.

**Mathematical Formulation:**

$$h_v^{(l+1)} = \text{UPDATE}\left(h_v^{(l)}, \text{AGGREGATE}\left(\{h_u^{(l)} \mid u \in \mathcal{N}(v)\}\right)\right)$$

Where:

- $h_v^{(l)}$: Embedding of node $v$ at layer
- $\mathcal{N}(v)$: Neighbors of node $v$.

**Key Idea:**

- Transform node features into a low-dimensional vector space.
- Captures structural and feature-based information.

**Process:**

- Each node starts with an initial feature vector.
- Through message passing, embeddings are refined over multiple layers.
- Final embeddings encode both local and global graph context.

**Mathematical Formulation:**

$$h_v^{(l)} = \sigma\left(W^{(l)} \cdot \text{AGGREGATE}\left(\{h_u^{(l-1)} \mid u \in \mathcal{N}(v)\}\right)\right)$$

Where:

- $W^{(l)}$: Learnable weight matrix at layer $l$.
- $\sigma$: Non-linear activation function (e.g., ReLU).

**Key Idea:**

- Pool node embeddings to form a graph-level representation.
- Enables tasks like graph classification or regression.

**Process:**

- Combine embeddings of all nodes in the graph.
- Common pooling methods: sum, mean, max, or attention-based.
- The resulting vector represents the entire graph.

**Mathematical Formulation:**

$$h_G = \text{POOL}\left(\{h_v^{(L)} \mid v \in V\}\right)$$

Where:

- $h_G$: Graph-level embedding.
- $h_v^{(L)}$: Final embedding of node $v$ at layer $L$.
- $V$: Set of all nodes in the graph.

## 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).

- 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.

# Architecture Overview

- 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.

Graph Neural Networks (GNNs) are used in various structured data problems. These tasks are categorized into:

- Node-Level Tasks
- Edge-Level Tasks
- Graph-Level Tasks
- Dynamic and Spatio-Temporal Graph Tasks
- Other Applications

# Node-Level Tasks

- **Node Classification**: Predicting categories of nodes (e.g., detecting fake accounts in social networks).
- **Node Clustering / Community Detection**: Identifying closely connected groups (e.g., social media groups).
- **Anomaly Detection**: Detecting unusual nodes (e.g., fraud detection in financial transactions).

## Edge-Level Tasks

- **Link Prediction**: Predicting missing or future connections (e.g., friend recommendations on Facebook).
- **Edge Classification**: Classifying relationships between nodes (e.g., type of citation between research papers).

# Graph-Level Tasks

- **Graph Classification**: Predicting the category of an entire graph (e.g., drug discovery by classifying molecular structures).
- **Graph Similarity / Matching**: Comparing graphs (e.g., plagiarism detection in research papers).
- **Graph Regression**: Predicting numerical properties of a graph (e.g., estimating molecular solubility).

# Dynamic and Spatio-Temporal Graph Tasks

- **Dynamic Graph Learning**: Learning from evolving graphs (e.g., predicting social network interactions over time).
- **Spatio-Temporal Forecasting**: Using spatial and temporal dependencies (e.g., traffic prediction in road networks).

# Other Applications

- **Recommendation Systems**: Using graph-based collaborative filtering (e.g., movie recommendations on Netflix).
- **Knowledge Graph Completion**: Predicting missing relations in knowledge graphs (e.g., completing facts in Wikidata).
- **Computer Vision with GNNs**: Using scene graphs for object detection.
- **NLP with Graphs**: Enhancing text representation (e.g., citation graphs for text classification).
- **Robotics and Control Systems**: Path planning and robot perception using scene graphs.

**Advantages:**

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

**Challenges:**

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

# 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.