DE LA SALLE UNIVERSITY

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Introduction to Graph Neural Networks

GRAPH BASED MACHINE LEARNING MODELS

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GRAPH NEURAL NETWORKS

Contents

What are Graphs?

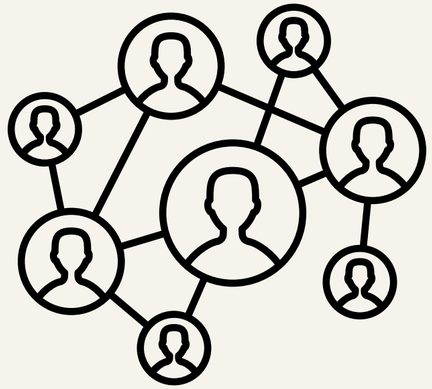
A **graph** has **nodes** and **edges**.

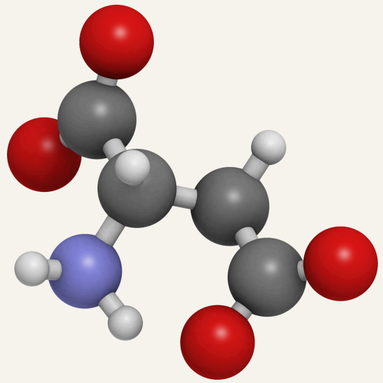
Represented as **G = (V, E)**, where:

- **V** set of nodes (vertices).
- **E** set of edges (connections).

Real-world examples of graphs:

- **Social networks**
- **Citation networks**
- **Molecular structures**



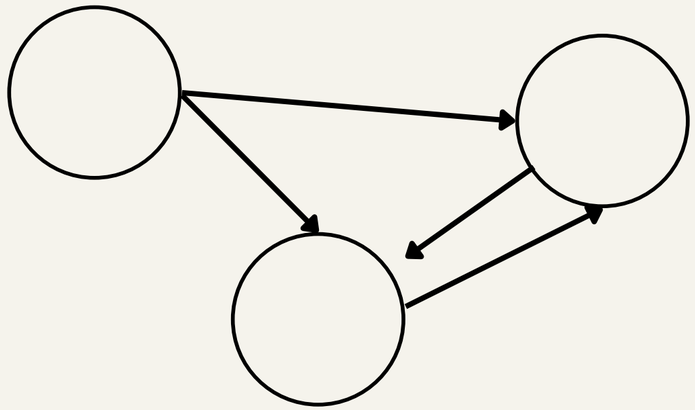


Types of Graphs

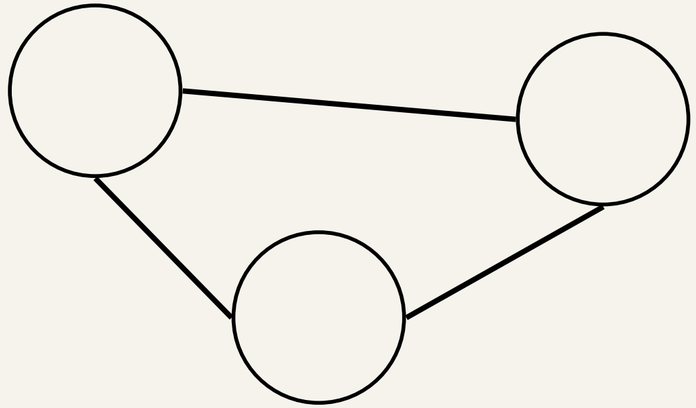
Directed vs. Undirected Graphs

- **Directed Graphs**: Edges have a direction (e.g., Twitter follows).
- **Undirected Graphs**: No direction in edges / 2 way (e.g., Facebook friendships).

Directed



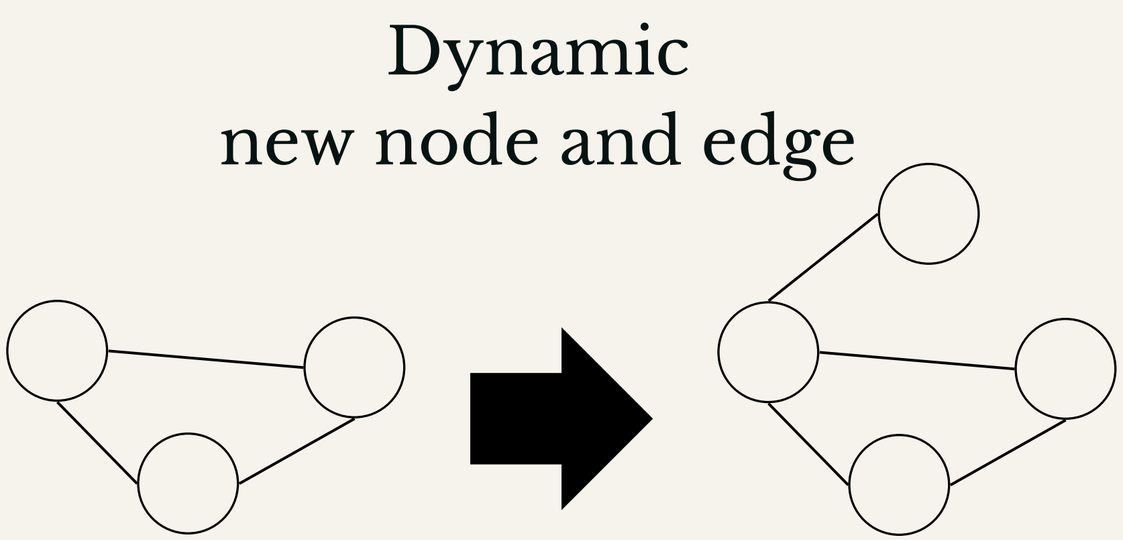
Undirected



Types of Graphs

Static vs. Dynamic Graphs

- **Static Graphs:** Fixed structure (e.g., molecular graphs).
- **Dynamic Graphs:** Evolve over time (e.g., social networks, traffic networks).

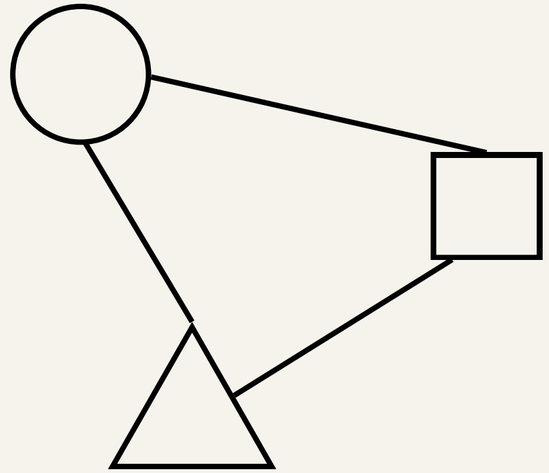


Types of Graphs

Homogeneous vs. Heterogeneous

- **Homogeneous Graphs:** Only one type of node and edge (e.g., social networks).
- **Heterogeneous Graphs:** Multiple node and edge types (e.g., knowledge graphs).

Heterogenous graph

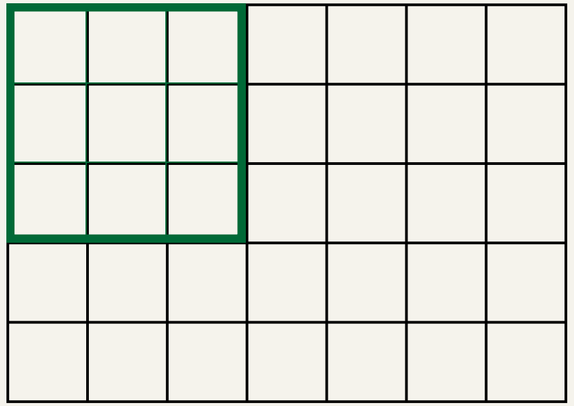


Limitations of Traditional Neural Networks on Graph Data

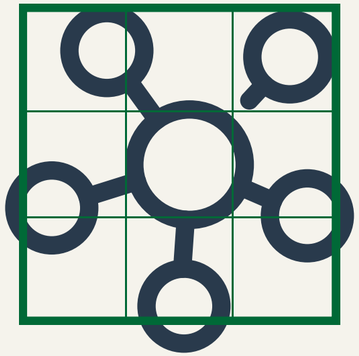
Graphs have **irregular structures** with **varying numbers of neighbors** per node. This means that **we cannot** use standard convolutional operations.

Many machine learning algorithms rely on Euclidean distances, which do not apply well to graphs since edges can use different metrics.

CNN used for grid data



CNN cannot be used for graph data



Core Concepts of Graph Neural Networks (GNNs)

GNNs learn node representations from **graph-structured data.**

Key Concept: Message Passing Mechanism

- Nodes **aggregate information** from their neighbors.
- This process **updates node embeddings** iteratively.

Three main types of Message Passing in GNNs:

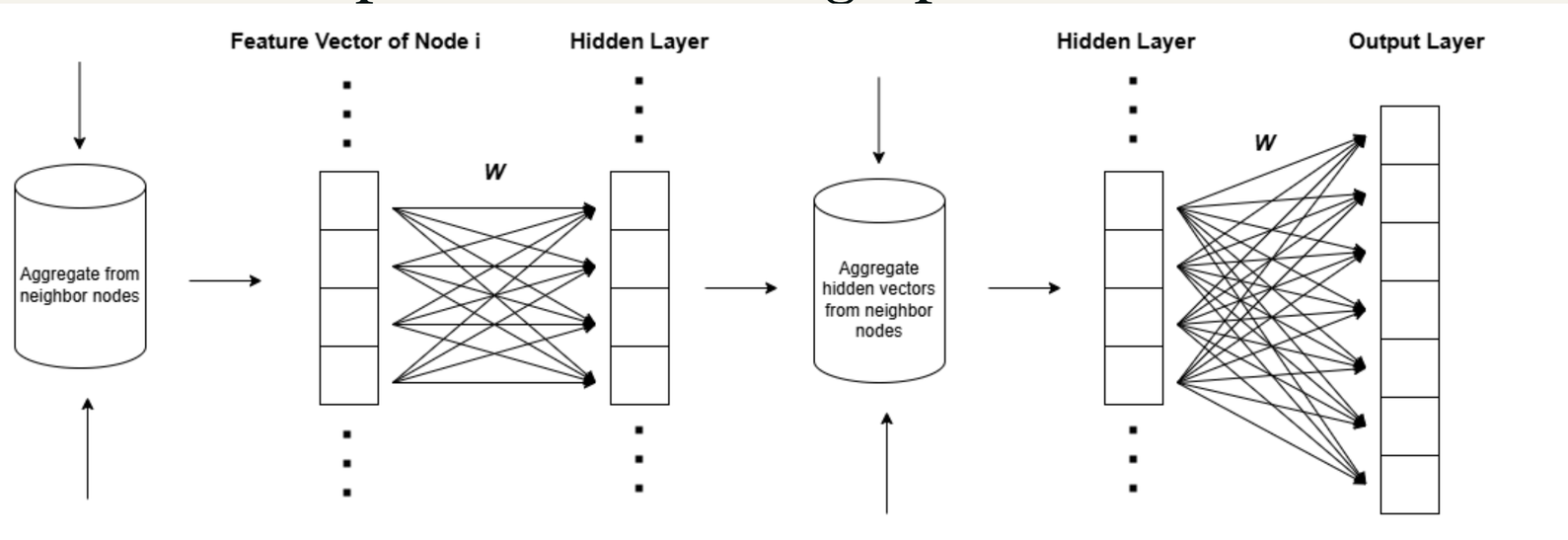
- **Convolutional GNNs** (e.g., GCN – Graph Convolutional Networks).
- **Attentional GNNs** (e.g., GAT – Graph Attention Networks).
- **General Message Passing GNNs**

GRAPH NEURAL NETWORKS

Message Passing Mechanism in Graph Neural Networks

Steps of message passing:

- **Aggregate**: A node gathers information from its neighboring nodes.
- **Update**: The node updates its own representation based on the aggregated information.
- **Repeat**: This process continues for multiple layers, allowing information to spread across the graph.



GNN Architectures

Graph Convolutional Network

- Uses graph convolution operations

Graph Attention Network

- Allows a node to focus on more relevant neighbors during aggregation.

GraphSAGE (Sample and Aggregate)

- Uses sampling to efficiently aggregate information from neighbors.

Expected Outputs

Node-Level Predictions (e.g., classification, regression)

- Example: Predicting if a user is friendly.

Edge-Level Predictions (e.g., link prediction, relationship strength estimation)

- Example: Predicting future friendships or interactions.

Graph-Level Predictions (e.g., entire graph classification)

- Example: Predicting if a social network is conservative or democratic.

Some Applications of GNN

- Social Network Analysis
- Recommendation Systems
- **Fraud Detection & Cybersecurity**

Python Notebook Exercise

bit.ly/3Dttvaa

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The End

THANK YOU FOR LISTENING