Graph Neural Network Lecture 3



Overview

Introduction to GCNs

2 Mathematical Formulation

What is a Graph Convolutional Network (GCN)?

- A type of Graph Neural Network (GNN) designed for graph-structured data.
- Extends the concept of convolutional neural networks (CNNs) to graphs.
- Captures local graph structure and node features.

Why GCNs?

- **Graph-Structured Data**: Many real-world problems involve graphs (e.g., social networks, molecular structures).
- Node-Level Tasks: Node classification, link prediction.
- Graph-Level Tasks: Graph classification, clustering.

The GCN layer is defined as:

$$H^{(l+1)} = \sigma \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$$

- $\tilde{A} = A + I$: Adjacency matrix with self-loops.
- \tilde{D} : Degree matrix of \tilde{A} .
- $H^{(l)}$: Node features at layer l.
- $W^{(l)}$: Learnable weight matrix.
- σ : Activation function (e.g., ReLU).

Intuition Behind GCN

- Normalization: $\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$ ensures normalized aggregation.
- **Feature Propagation**: Each node aggregates features from its neighbors.
- Nonlinearity: Activation function introduces nonlinearity.