Graph Neural Networks

Common Tasks

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Graph Neural Networks

- A Graph Neural Network (GNN) is a model that processes graph-structured data by taking in node features (embeddings) X and an adjacency matrix A as inputs.
- The GNN applies a series of K layers, where each layer updates the node embeddings to produce intermediate representations H_i.
- At the start, each column of X contains features specific to individual nodes.
- By the final layer, H_K represents each node along with contextual information from its neighbors.
- GNNs address three main types of tasks:
  1. **Graph-level tasks** – predictions for the entire graph
  2. **Node-level tasks** – predictions for individual nodes
  3. **Edge prediction tasks** – predictions about connections between nodes

Graph-level Tasks

In graph-level tasks, the model predicts labels or values that describe the entire graph.

- Examples:
  - Predicting the melting point of a molecule
  - Determining whether a molecule is toxic to humans

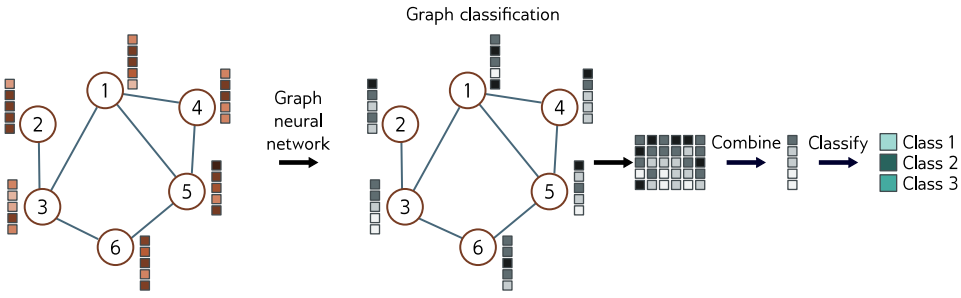
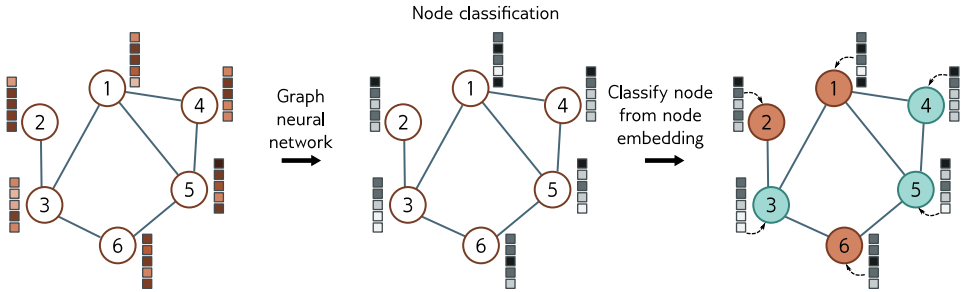


Image credit: Understanding Deep Learning

Node-level Tasks

In node-level tasks, the model predicts labels or values for each node within the graph.

- Example:
  - Classifying political books as left-leaning or right-leaning based on node features



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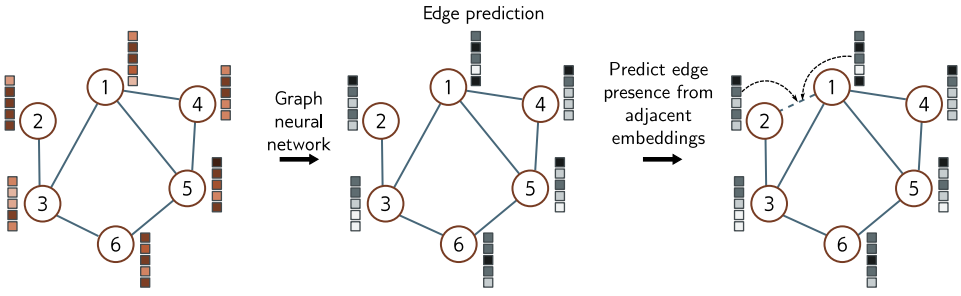
Edge Prediction Tasks

In edge prediction tasks, the model predicts whether an edge (relationship) should exist between two nodes n and m.

- Example:
  - In a social network, predicting if two people know each other and suggesting a connection if they do



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