Graph Neural Network

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Introduction

- Many objects can be understood in terms of their relationships with other entities and the connections between a set of objects can be inherently represented as a graph. Many types of data can be treated as graphs like social networks, citation networks and internet.
- But graphs are complex. They have arbitrary size and complex topological structure
- The task is to map nodes into an embedding space to encode network information and use it for many downstream predictions like node and graph classification

Objectives

We will be focusing mainly on:

- performing simple **node embedding** using a simple similarity criterion
- implementing a **Graph Convolutional Network (GCN)** to perform node-level and graph-level classification on benchmarking datasets

Node Embedding

- The goal is for nodes that have similar roles in the graph to be represented by similar vectors in the embedding space

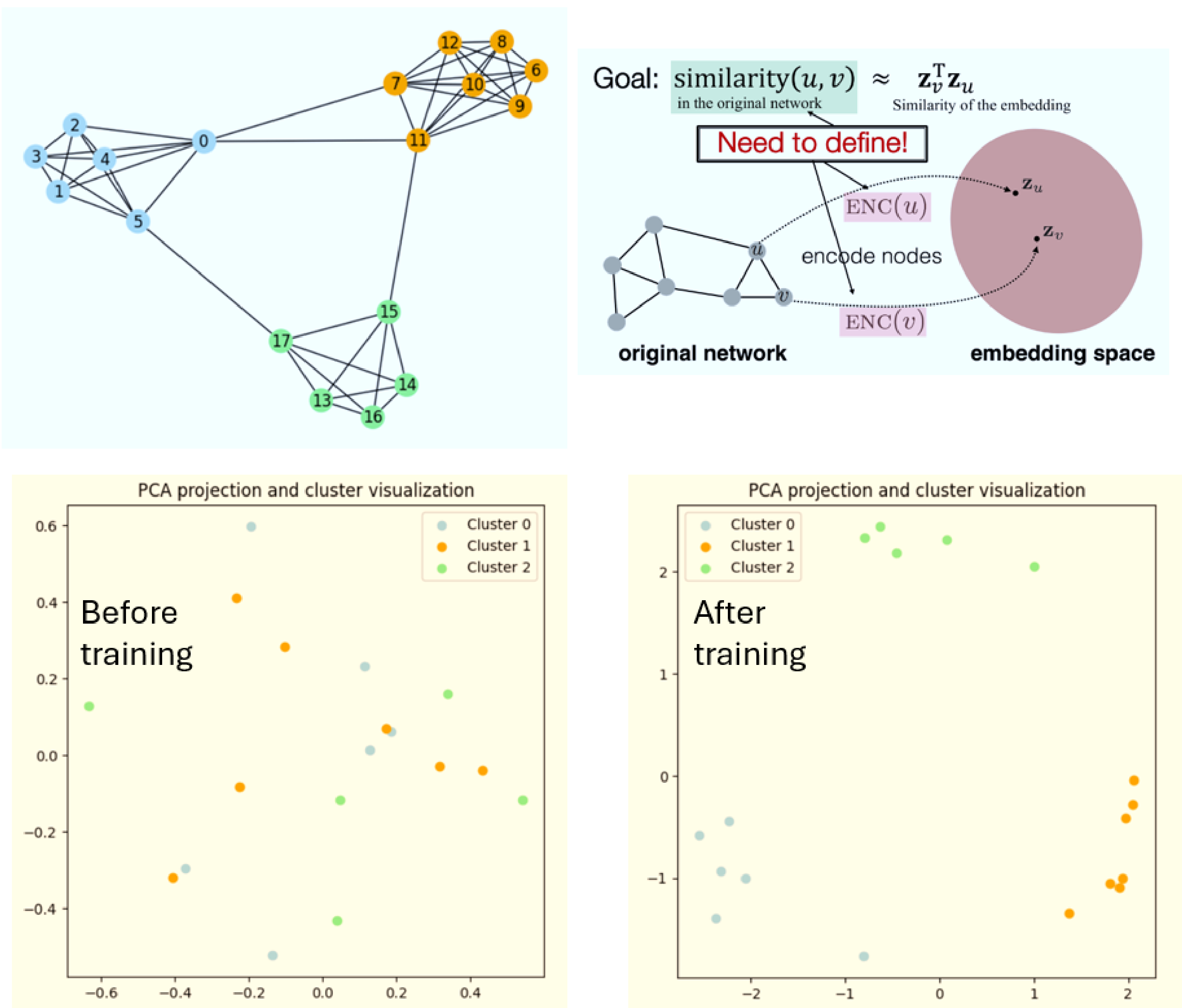

Figure 1. Training a node embedding to encode graph of 3 clusters (top left)

- We chose to define the similiarity between two nodes u and v as the scalar product between their respective embedding vectors as follows: $similarity(u, v) \approx z_v^T z_u$

GCN

- The goal is to generalize convolutions beyond simple lattices Leverage node features like images.
- In GCNs, each node aggregates information from its neighbors to update its own feature representation. This process is called message passing
- The aggregation involves summing, averaging, or applying a neural network layer to combine the features of neighboring nodes
- Every node defines a computation graph based on its neighborhood
- We use a list of convolution layers (GCNConv) in a GCN to allow the network to learn multi-hop neighborhood information and extract hierarchical features from the graph. A single GCN layer aggregates information only from immediate neighbors (1-hop). Multiple layers allow information to propagate further across the graph

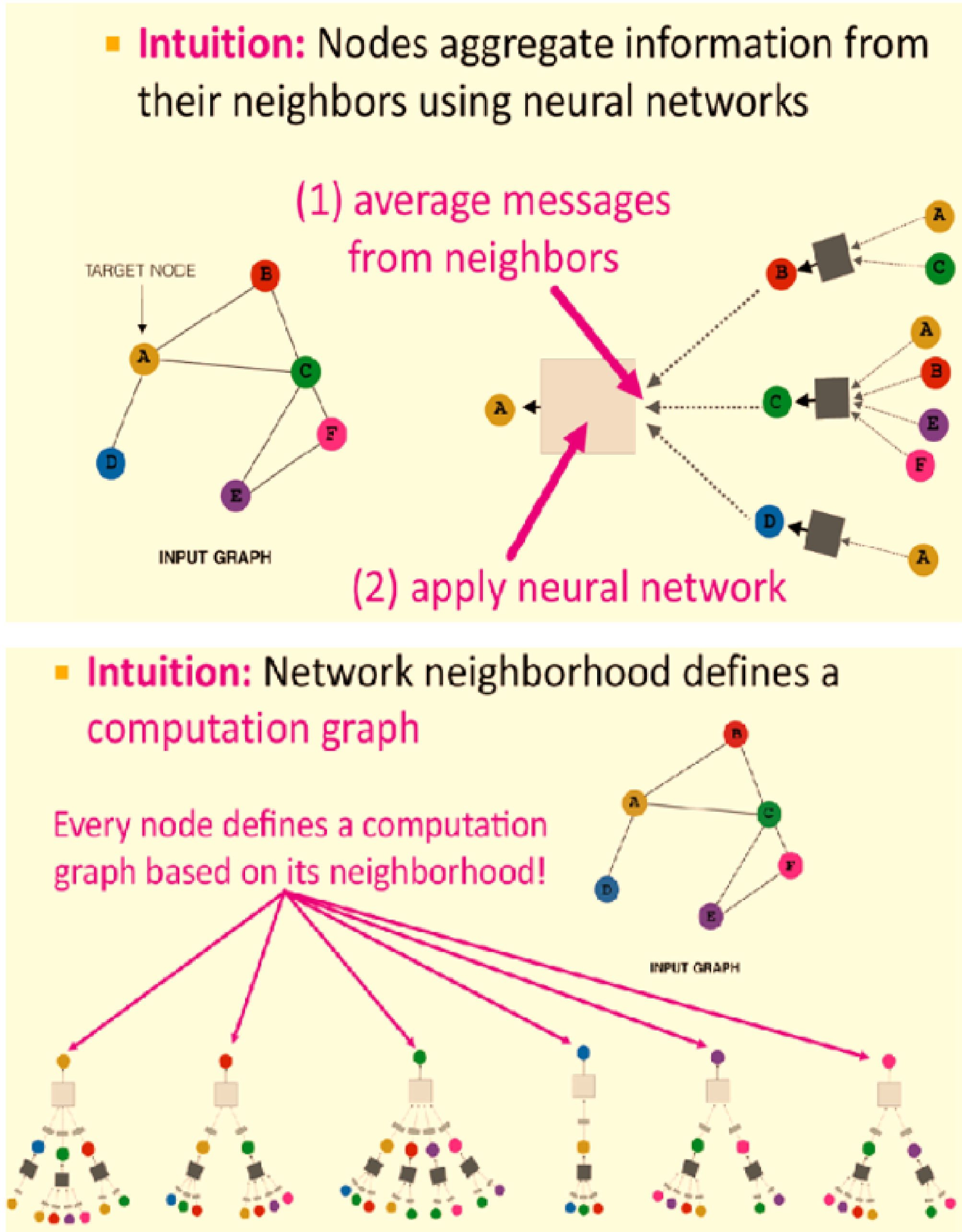

Figure 2. Neighborhood infomration aggregation from computation graph

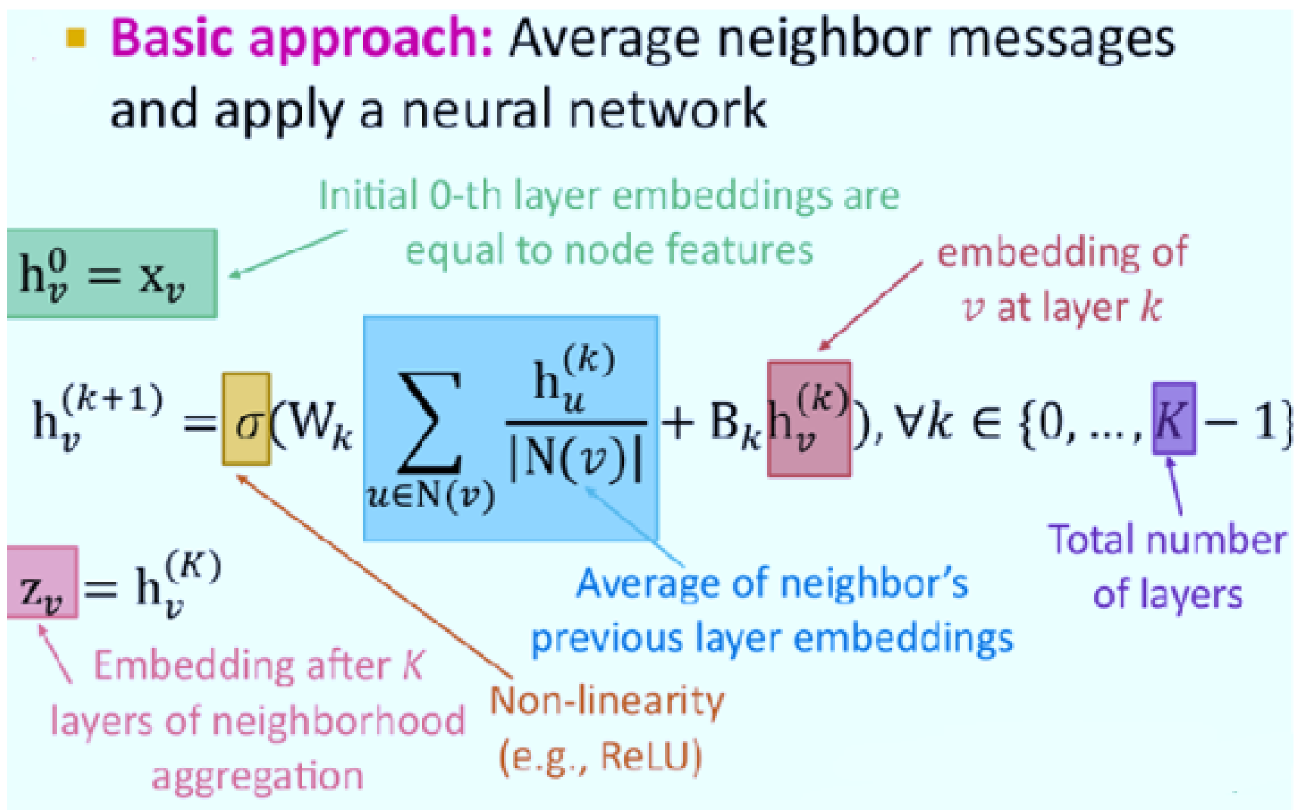

Figure 3. Neural network on the neighbor messages

Node and Graph prediction

Dataset: **ogbn-arxiv**, derived from the arXiv academic paper repository and designed for link prediction tasks

Accuracy	Training	Validation	Test
Node	53.85%	54.23%	54.24%

Table 1. Nodes prediction results

Dataset: **ogbg-molhiv**, used for molecular property prediction tasks

AUROC	Training	Validation	Test
Graph	67.69%	62.38%	61.41%

Table 2. Graph prediction results

References

[1] Jure Leskovec.
Cs224w: Machine learning with graphs https://web.stanford.edu/class/cs224w/, 2024.