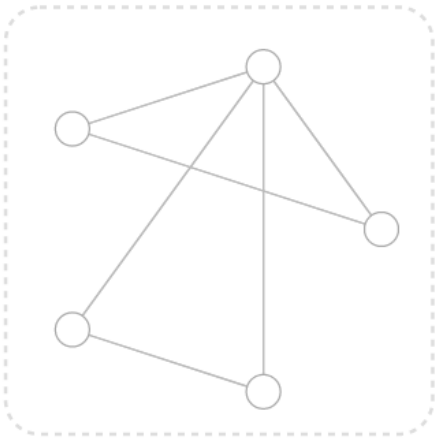
GNN

A Gentle Introduction to Graph Neural Networks (2021) 35

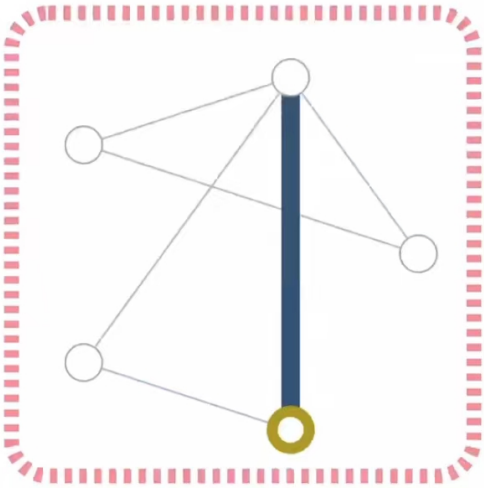
Graph structured data



V Vertex (or node) attributes
e.g., node identity, number of neighbors

E Edge (or link) attributes and directions
e.g., edge identity, edge weight

U Global (or master node) attributes
e.g., number of nodes, longest path

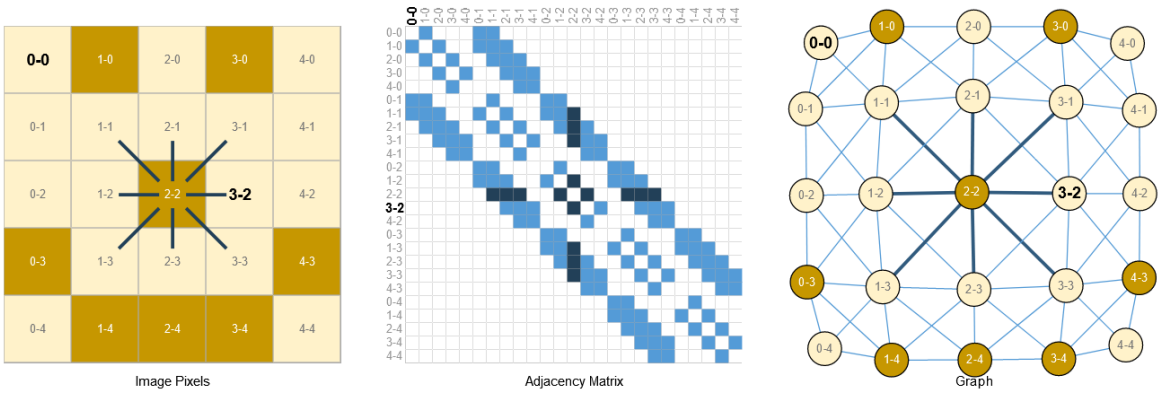


Vertex (or node) embedding

Edge (or link) attributes and embedding

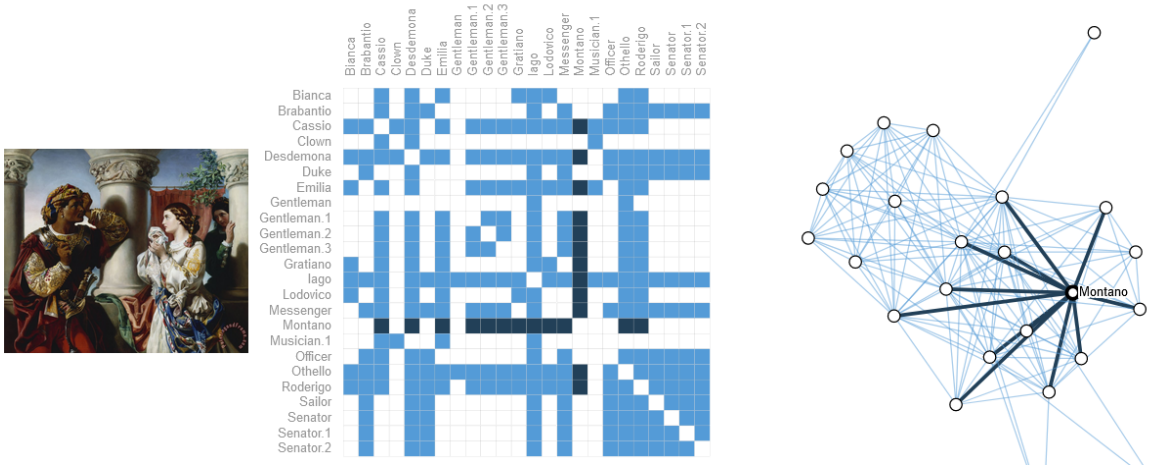
Global (or master node) embedding

Images as graphs



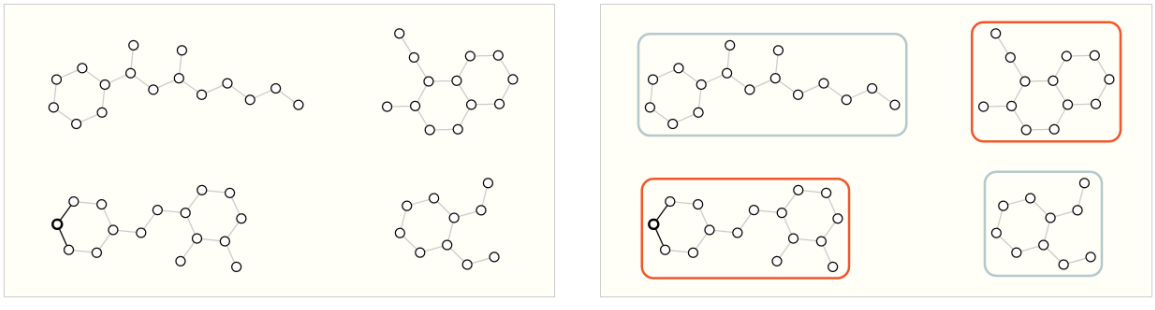
Click on an image pixel to toggle its value, and see how the graph representation changes.

Social networks as graphs



There are three general types of prediction tasks on graphs: graph-level, node-level, and edge-level.

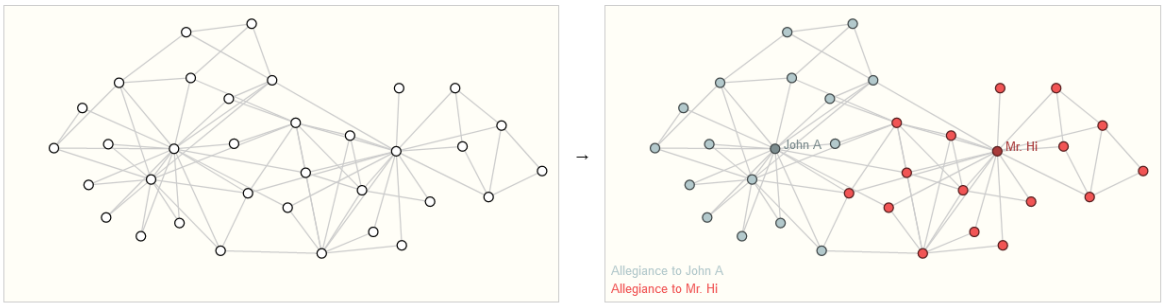
Graph-level task



Input: graphs

Output: labels for each graph, (e.g., "does the graph contain two rings?")

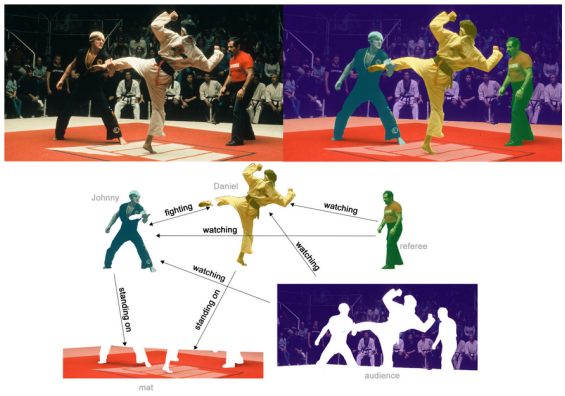
Node-level task

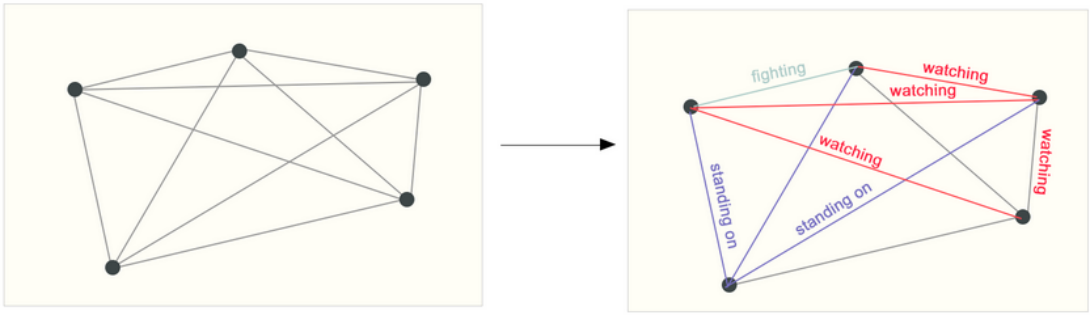


Input: graph with unlabled nodes

Output: graph node labels

Edge-level task





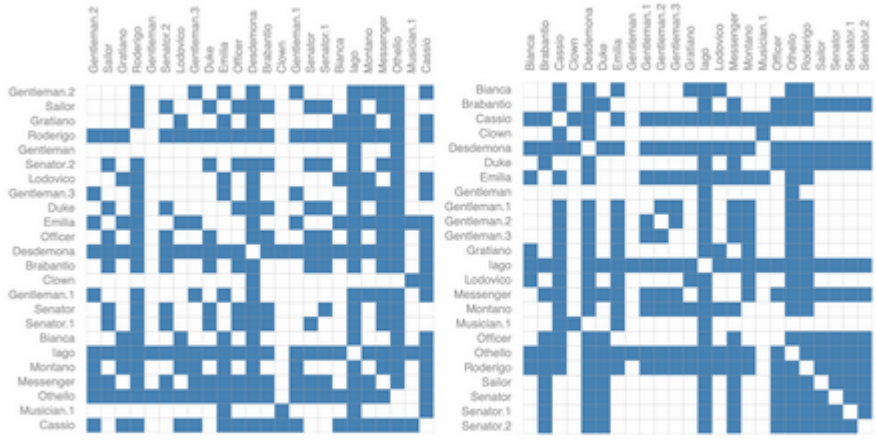
Input: fully connected graph, unlabeled edges

Output: labels for edges

The challenges of using graphs in machine learning

connectivity: adjacency matrix; sparse adjacency matrix → adjacency list

permutation invariant: adjacency matrices that encode the same connectivity should produce the same result in a deep neural network

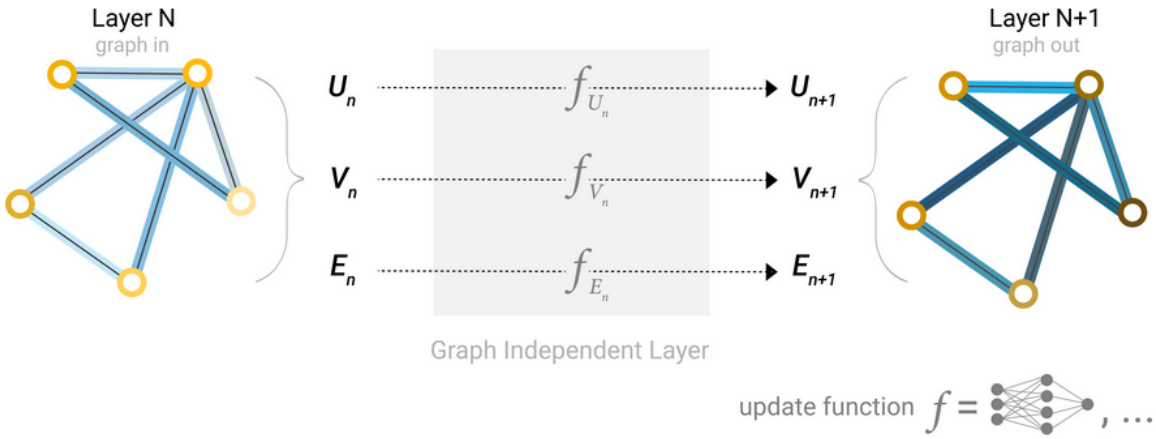


Two adjacency matrices representing the same graph.

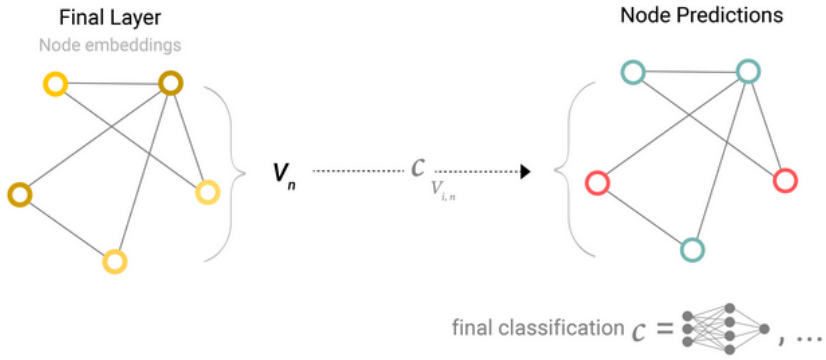
Graph Neural Networks

A GNN is an optimizable transformation on all attributes of the graph (nodes, edges, global-context) that preserves graph symmetries (permutation invariances).

“graph-in, graph-out”



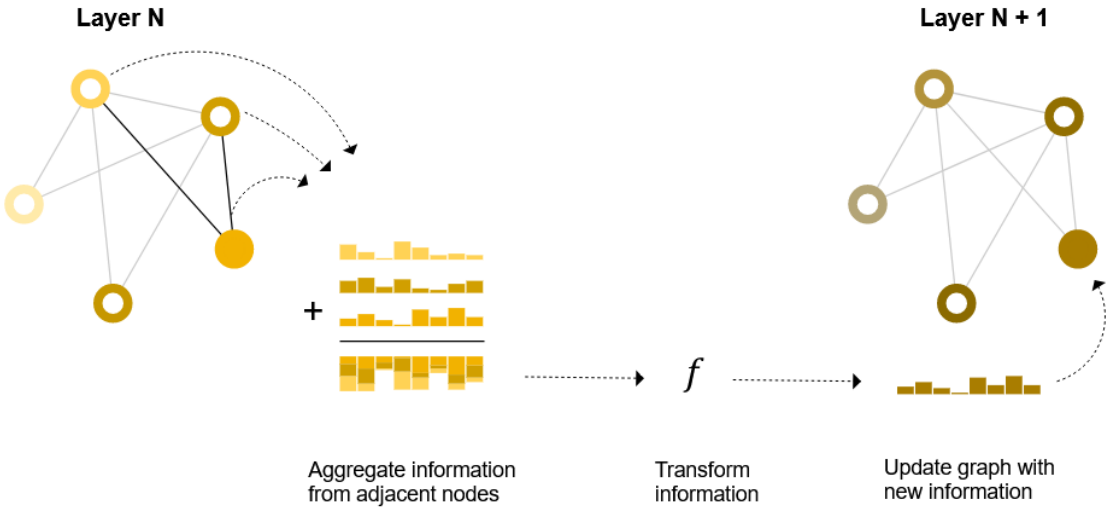
GNN Predictions by Pooling Information



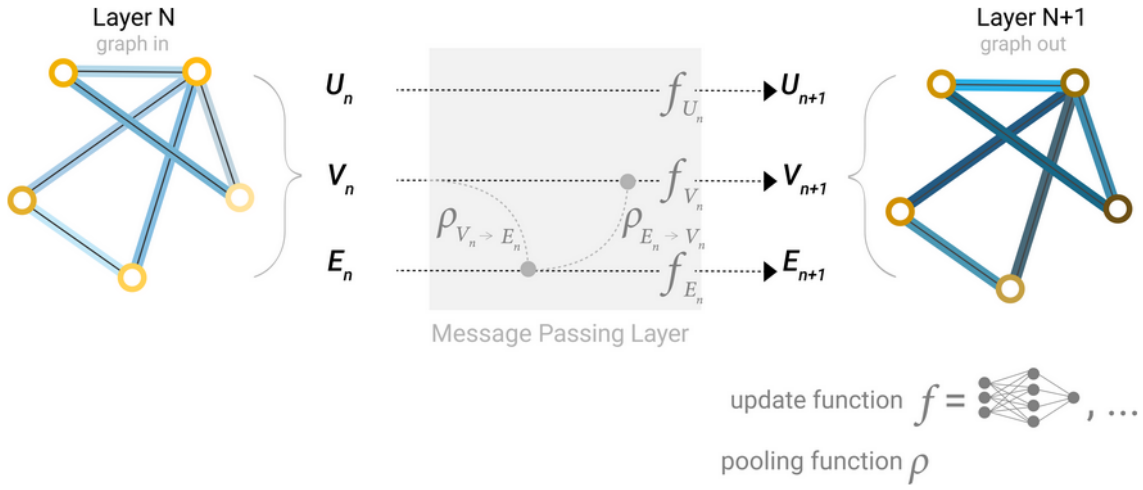
To make predictions on nodes:

- If we have node information, apply a linear classifier for each node embedding.
- If we have edge information but no node information, we do this by pooling: gather each of the embeddings of the edges connected to the nodes and aggregate them.

Passing messages between parts of the graph



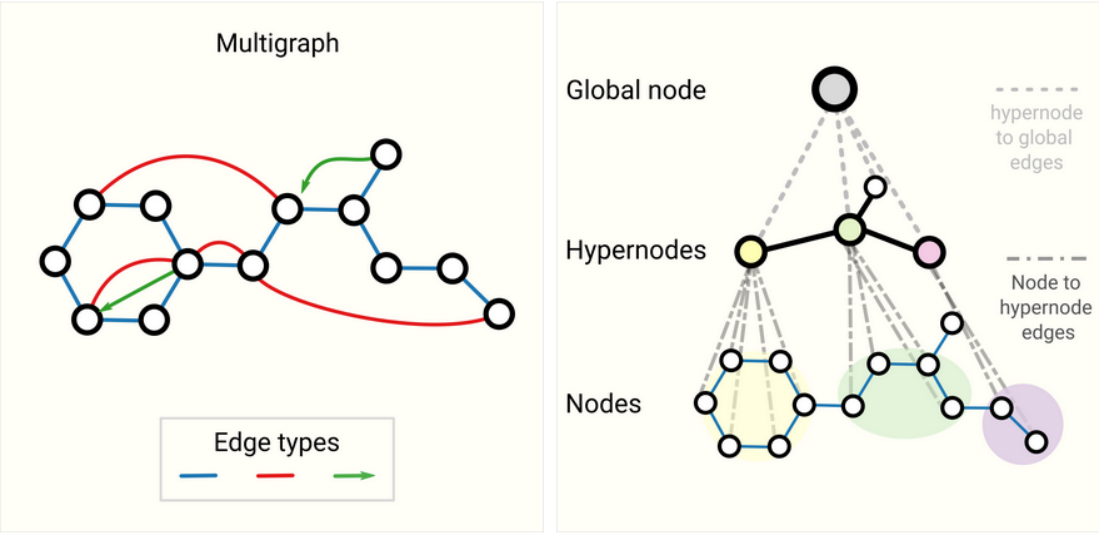
Learning edge representations



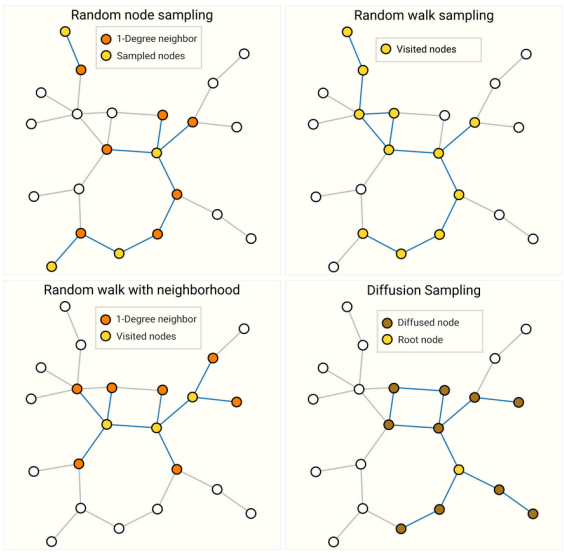
Adding global representations

Use the global representation of a graph (U) which is sometimes called a **master node** or context vector. It is connected to all other nodes and edges in the network, and can act as a bridge between them to pass information, building up a representation for the graph as a whole.

Other types of graphs (multigraphs, hypergraphs, hypernodes, hierarchical graphs)



Sampling Graphs and Batching in GNNs


Random node sampling
1-Degree neighbor
Sampled nodes
Random walk sampling
Visited nodes
Random walk with neighborhood
1-Degree neighbor
Visited nodes
Diffusion Sampling
Diffused node
Root node