SE125 Machine Learning

Graph Neural Networks

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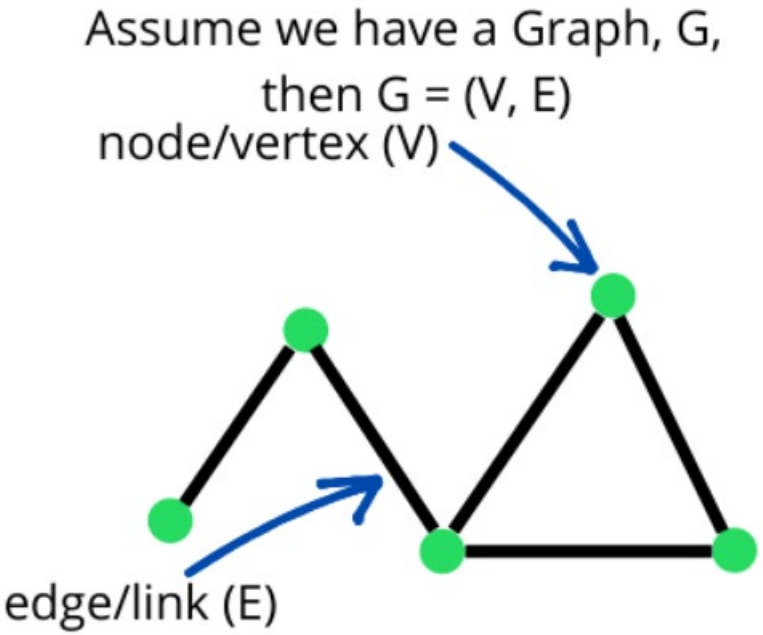
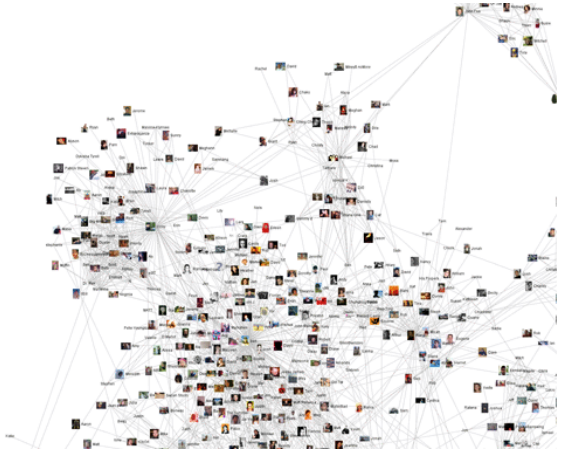
What is a Graph?

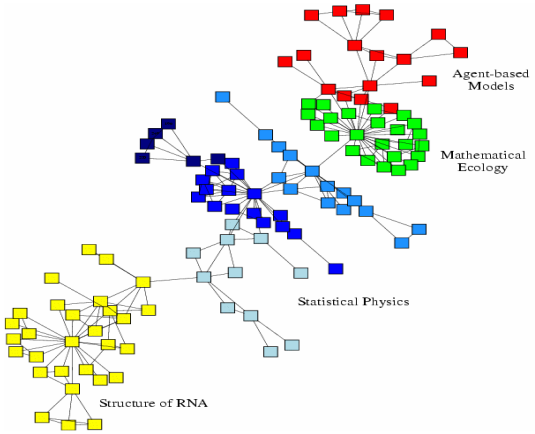
- Graphs are powerful data structures that model a set of objects and their relationships. These objects represent the nodes and the relationships represent edges.



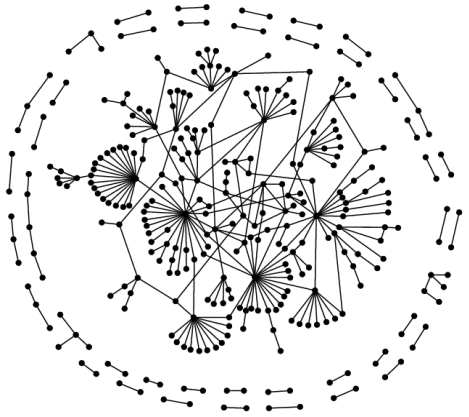
What is a Graph?



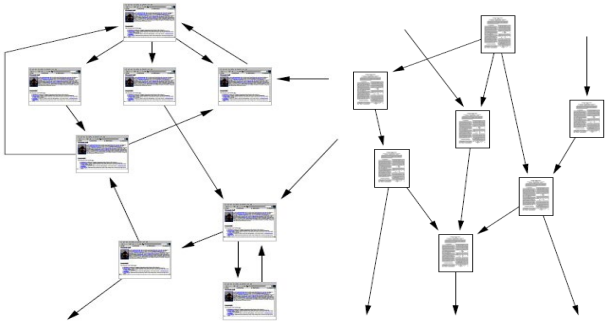
Social networks



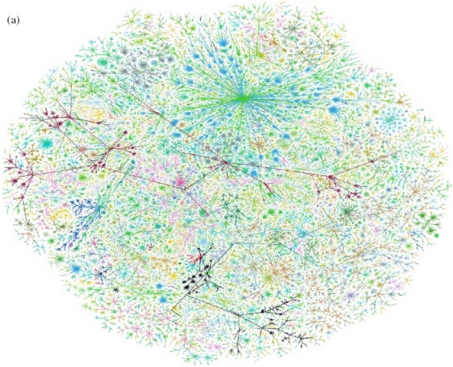
Economic networks



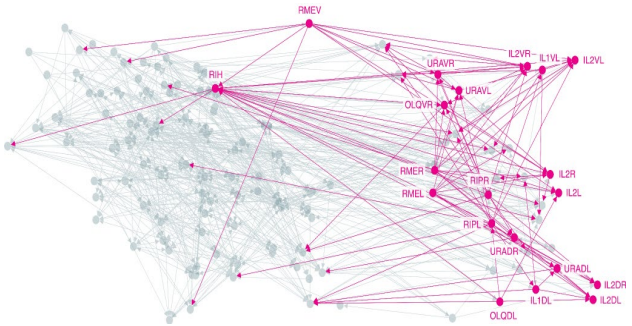
Biomedical networks



Information networks:
Web & citations



Internet



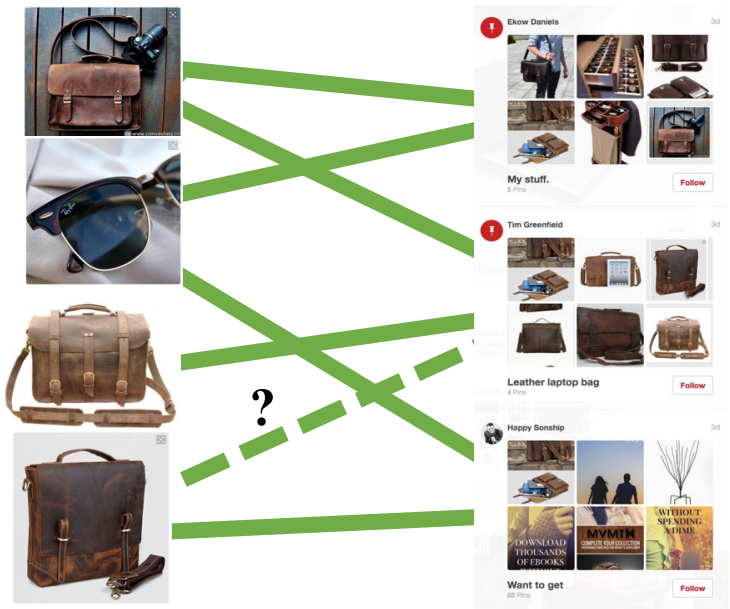
Networks of neurons

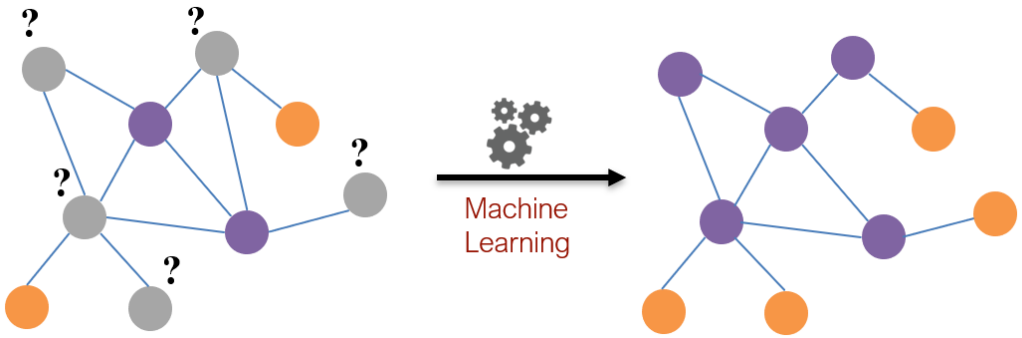
What is Graph Neural Network (GNN)?

- GNN is a technique in deep learning that extends existing neural networks for processing data on graphs.
  - Using neural networks, nodes in a GNN structure add information gathered from neighboring nodes. The last layer then combines all this added information and outputs either a prediction or classification

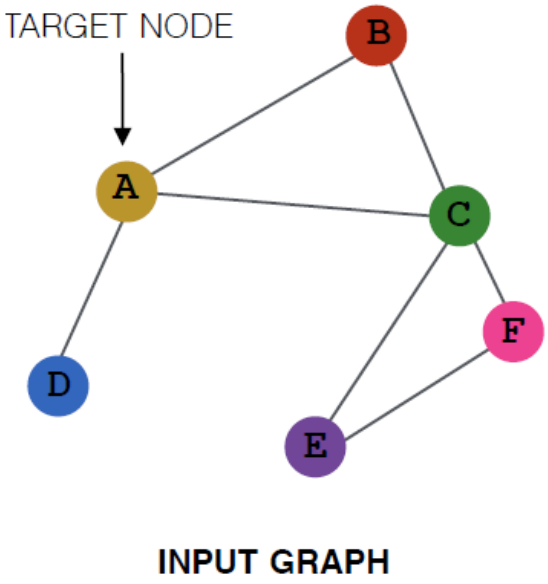
GNN Outputs

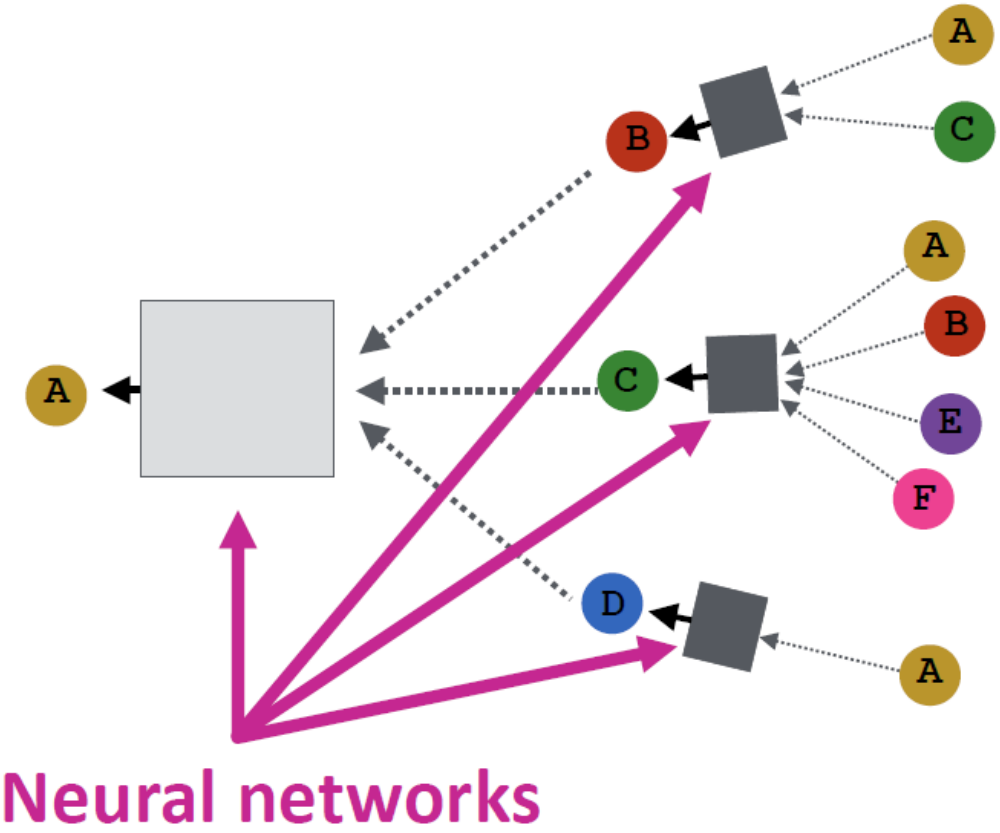
- Node classification
- Link prediction
- Graph classification





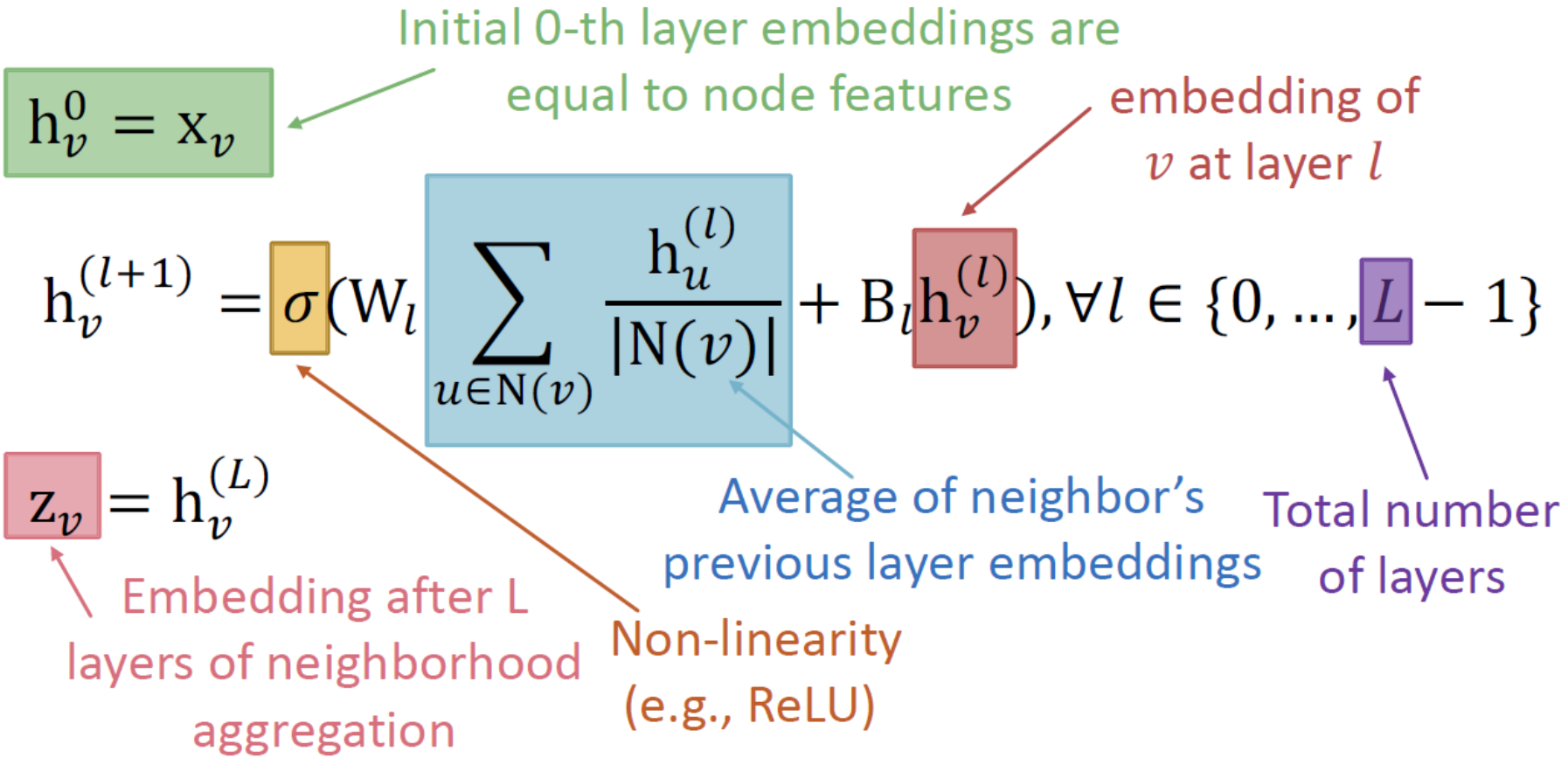
Graph Neural Networks





Graph Neural Networks

- **Basic approach:** Average neighbor messages and apply a neural network



Graph Convolutional Networks

Basic Neighborhood Aggregation

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right)$$

VS.

GCN Neighborhood Aggregation

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v) \cup v} \frac{\mathbf{h}_u^{k-1}}{\sqrt{|N(u)||N(v)|}}\right)$$

same matrix for self and neighbor embeddings

per-neighbor normalization

Graph Convolutional Networks

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v) \cup v} \frac{\mathbf{h}_u^{k-1}}{\sqrt{|N(u)||N(v)|}}\right)$$

Matrix Form:

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

$$\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$$

$$\mathbf{D}_{ii} = \sum_j \mathbf{A}_{i,j}$$