Relational/Graph Learning

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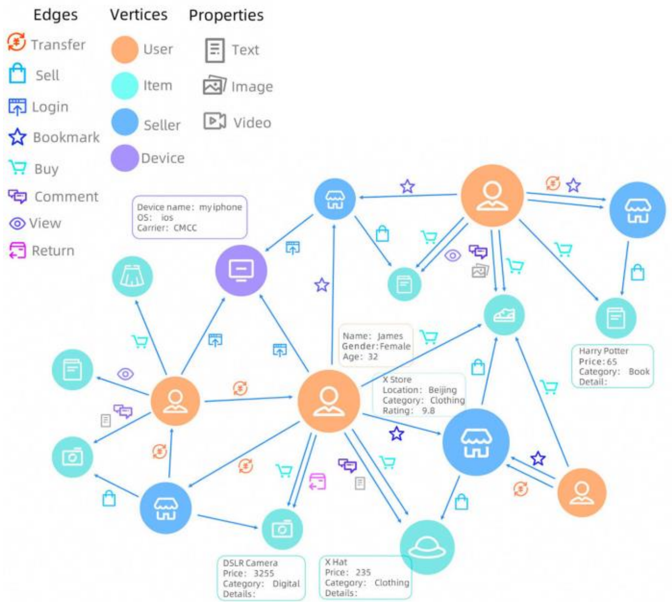
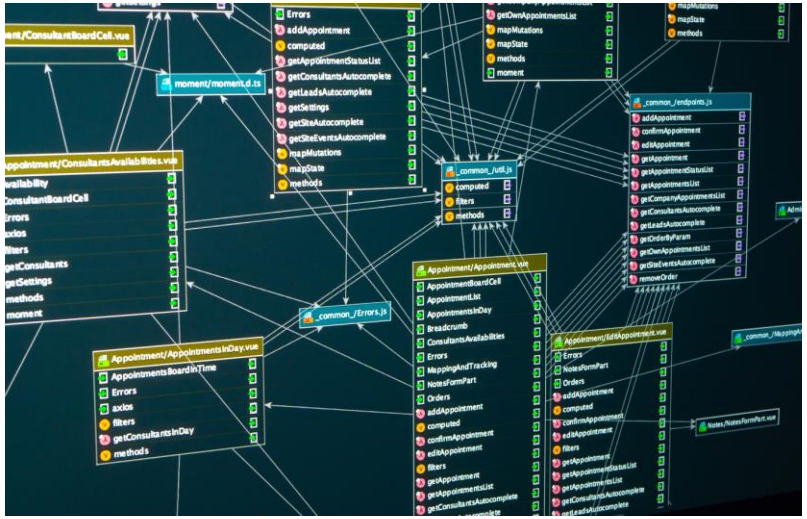
Relational/Graph Data are Everywhere

Social networks



E-commerce



Relational databases

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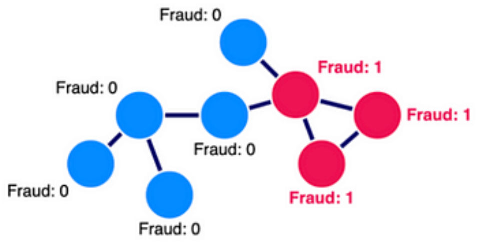
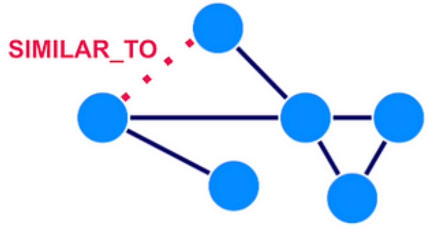
The Aim of Graph Learning

- Graph learning, machine learning on graphs, aims to learn complex relationships among nodes and the topological structure of graphs.



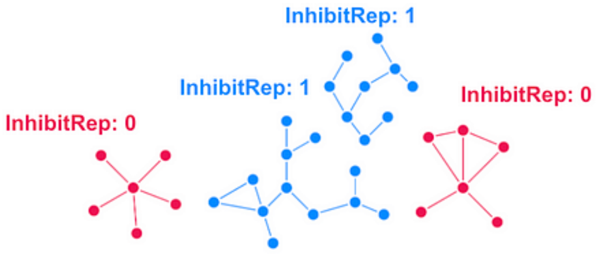
Node Property Prediction

Predict a discrete or continuous node property, called **node classification** and **node regression** respectively.



Link Prediction

Predict if a relationship should exist between two nodes. Often a binary classification task, but can sometimes include more link types or continuous properties.



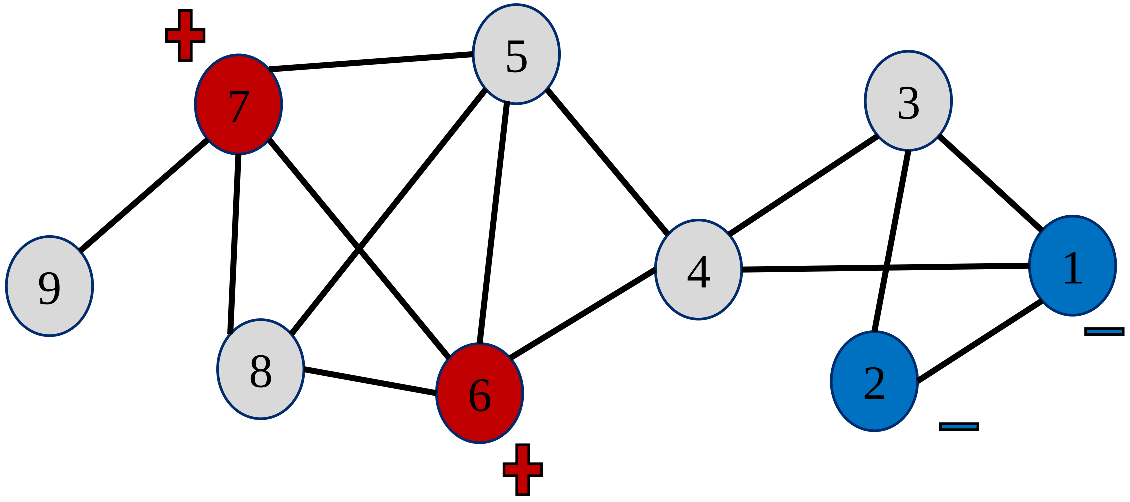
Graph Property Prediction

Predict a discrete or continuous property of a graph or subgraph.

https://medium.com/towards-data-science/graph-machine-learning-an-overview-c996e53fab90

A Graph Node Classification Example

- **Objective**: Exploit the structural information within a graph to enhance the prediction of node attributes or labels.

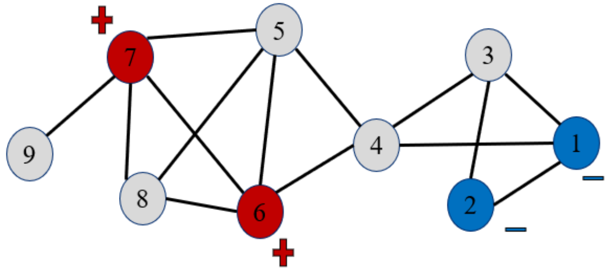


Given the graph structure with some labeled nodes (i.e., 1, 2, 6, 7 are labeled), predict the labels for the remaining nodes.

Outline

- **Shallow Methods**
  - Weighted-vote relational neighbor
  - Label Propagation
- Deep Learning Methods

Recap: Traditional Non-Graph Learning Methods

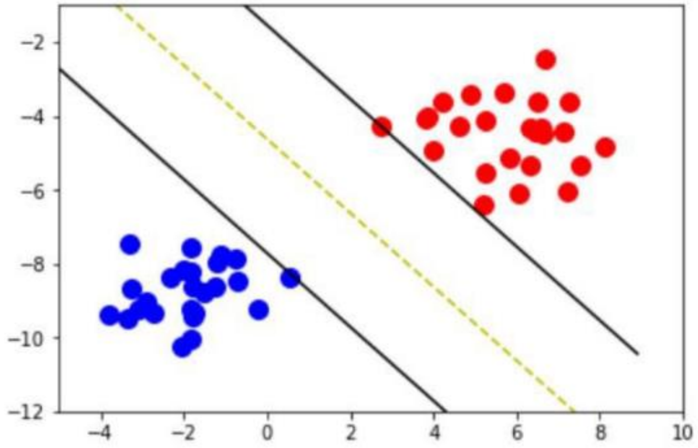


Node features (by edge)

$$u_1 = [0, 1, 1, 1, 0, 0, 0, 0, 0]$$
$$u_2 = [1, 0, 1, 0, 0, 0, 0, 0, 0]$$
$$\vdots$$

Node labels

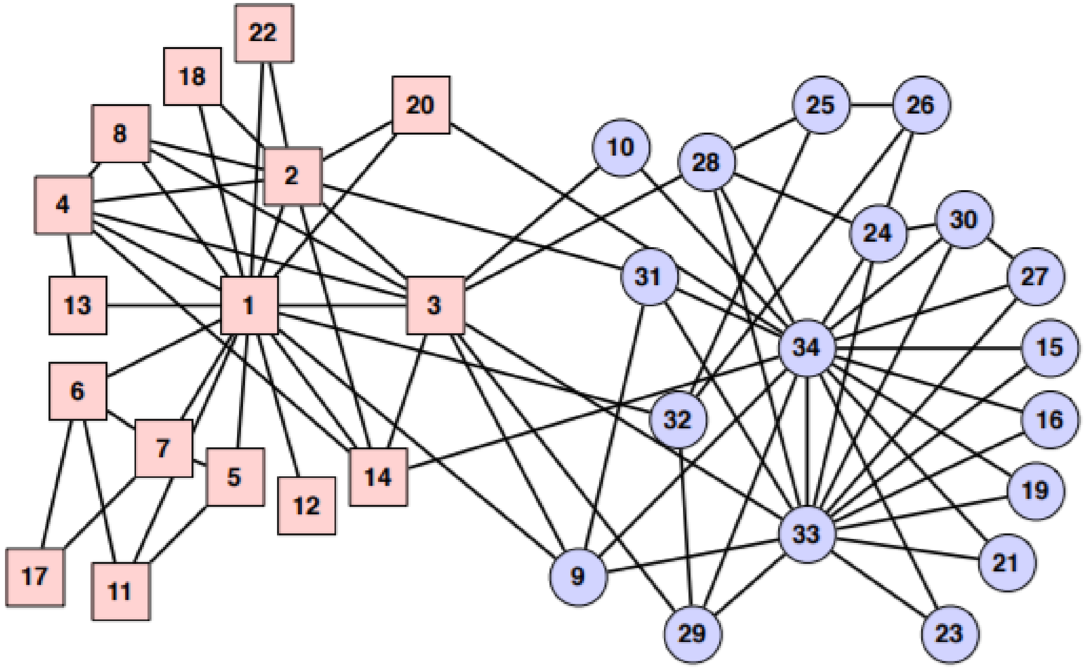
$$y_1 = 0$$
$$y_2 = 0$$
$$y_6 = 1$$
$$y_7 = 1$$



Common classifiers: (like linear classifiers and SVMs)

How To Use Graph Information Effectively?

- Observation: Linked nodes tend to have similar labels



The karate club with ground truth

The Key Idea Is "Collective Classification"

- Definition: Perform collaborative classification of unlabeled nodes in a partially labeled network using techniques such as label propagation or approximate inference [1]. Two typical methods:
  - Weighted-vote relational neighbor
  - Label propagation

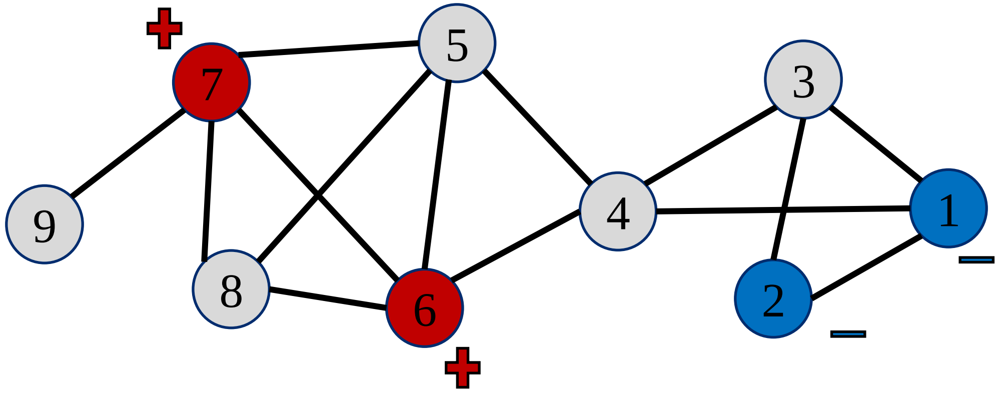
[1] Sen, Prithviraj, et al. "Collective classification in network data." *AI magazine* 29.3 (2008): 93-93.

Weighted-vote Relational Neighbor (wvRN)

- The labels of unlabeled node v_i are determined by a weighted vote among their neighbors $\mathcal{N}(v_i)$.

$$P(y_i = 1|\mathcal{N}(v_i)) = \frac{1}{|\mathcal{N}(v_i)|} \sum_{v_j \in \mathcal{N}(v_i)} P(y_j = 1|\mathcal{N}(v_j))$$

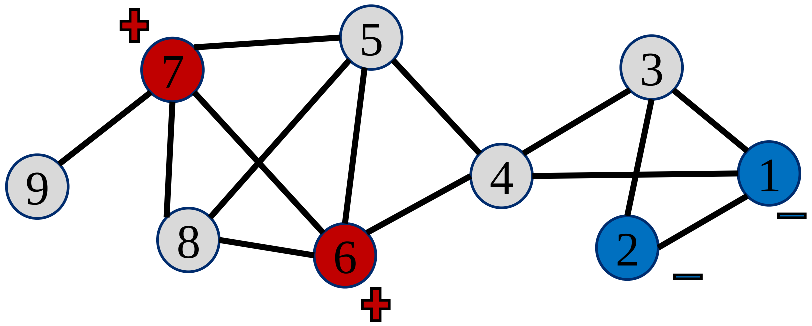
y_i is the label of node v_i



Macskassy, Sofus A., and Foster Provost. "A simple relational classifier." In Proceedings of the second workshop on multi-relational data mining (MRDM-2003) at KDD, pp. 64-76. 2003.

Weighted-vote Relational Neighbor (wvRN)

- The key idea
  1. Keep the labels of labeled nodes fixed.
  2. Recalculate probabilities iteratively based on neighbors' labels until convergence.



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An Example of wvRN

- Initialization of unlabeled nodes

$$P(y_i = 1|\mathcal{N}(v_i)) = 0.5$$

  - For node v_3, $\mathcal{N}(v_3) = \{1, 2, 4\}$

$$P(y_1 = 1|\mathcal{N}(v_1)) = 0$$
$$P(y_2 = 1|\mathcal{N}(v_2)) = 0$$
$$P(y_4 = 1|\mathcal{N}(v_4)) = 0.5$$
$$P(y_3 = 1|\mathcal{N}(v_3)) = 1/3(0 + 0 + 0.5) = 0.17$$

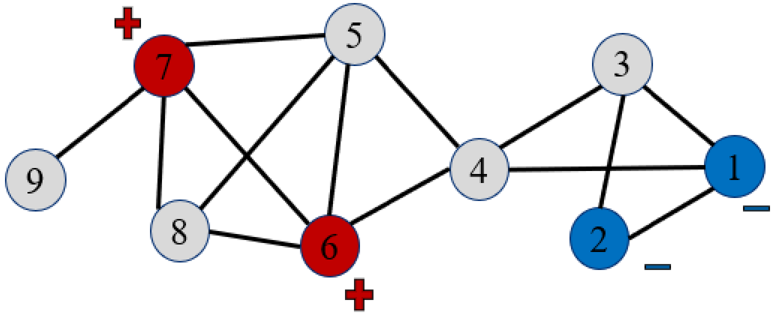
  - For node v_4, $\mathcal{N}(v_4) = \{1, 3, 5, 6\}$

$$P(y_4 = 1|\mathcal{N}(v_4)) = \frac{1}{4}(0 + 0.17 + 0.5 + 1) = 0.42$$

  - For node v_5, $\mathcal{N}(v_5) = \{4, 6, 7, 8\}$

$$P(y_5 = 1|\mathcal{N}(v_5)) = \frac{1}{4}(0.42 + 1 + 1 + 0.5) = 0.73$$

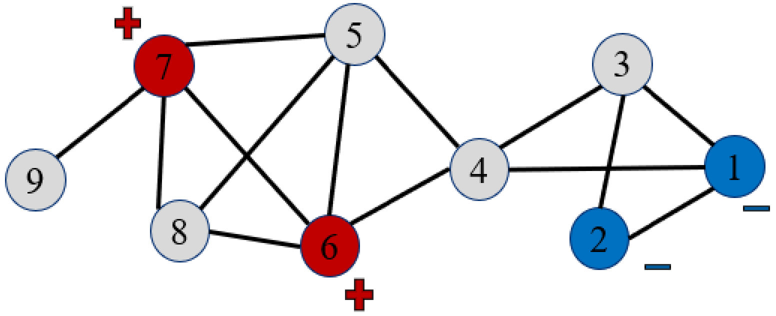
…



$$\mathbf{p}^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0.17 \\ 0.42 \\ 0.73 \\ 1 \\ 1 \\ 0.91 \\ 1.00 \end{bmatrix}$$

Iteration Results

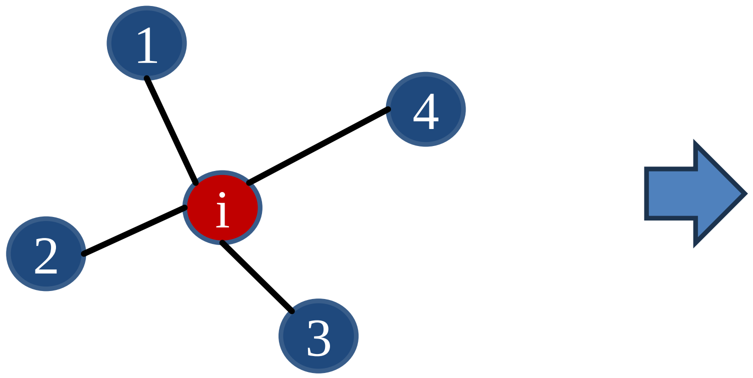
- Converge after 5 iterations
  - Nodes 5, 8, 9: + ($P(v_i) > 0.5$)
  - Node 3: - ($P(v_i) < 0.5$)
  - Node 4 is around $P(v_i) = 0.5$



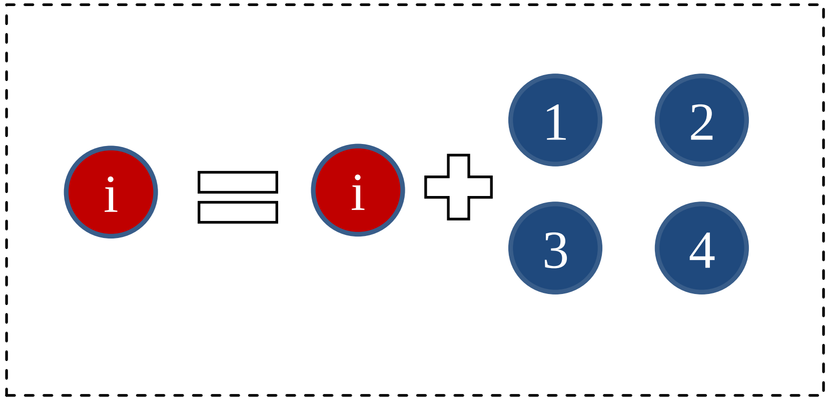
$$\mathbf{p}^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0.17 \\ 0.42 \\ 0.73 \\ 1 \\ 1 \\ 0.91 \\ 1.00 \end{bmatrix}, \mathbf{p}^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0.14 \\ 0.47 \\ 0.85 \\ 1 \\ 1 \\ 0.95 \\ 1.00 \end{bmatrix}, \mathbf{p}^{(3)} = \begin{bmatrix} 0 \\ 0 \\ 0.16 \\ 0.50 \\ 0.86 \\ 1 \\ 1 \\ 0.95 \\ 1.00 \end{bmatrix}, \mathbf{p}^{(4)} = \begin{bmatrix} 0 \\ 0 \\ 0.17 \\ 0.51 \\ 0.87 \\ 1 \\ 1 \\ 0.96 \\ 1.00 \end{bmatrix}, \mathbf{p}^{(5)} = \begin{bmatrix} 0 \\ 0 \\ 0.17 \\ 0.51 \\ 0.87 \\ 1 \\ 1 \\ 0.96 \\ 1.00 \end{bmatrix}.$$

Label Propagation (Consistency Method)

- Intuition
  1. Each node iteratively spreads its label to neighbors.
  2. Each node partly keeps its initial label information.



Given graph and label information



The process of label propagation

- Zhou D, Bousquet O, Lal T N, et al. Learning with local and global consistency[C] //Advances in neural information processing systems. 2004: 321-328.

Symbol Notations

- **G**: Input network structure
- **F**: Classification result matrix on nodes

$$F_{n\times c} = \begin{bmatrix} F_{11} & F_{12} & \cdots & F_{1c} \\ \cdots & \cdots & \cdots\cdot & \cdots\cdot \\ F_{n1} & F_{n2} & \cdots & F_{nc} \end{bmatrix} \quad \text{by labeling } v_i \text{ as } y_i = \operatorname{argmax}_{j\le c} F_{ij}$$

- **Y**: Initial labels of nodes

$$Y_{ij} = \begin{cases} 1, & \text{if } v_i \text{ is labeled as } y_i = j \\ 0, & \text{otherwise} \end{cases}$$

Consistency Method

- Symmetric normalization of G:

$$S = D^{-\frac{1}{2}} G D^{-\frac{1}{2}}$$

  where $D_{ii} = \sum_j G_{ij}$ is the degree matrix of the network.

- Iterate $F(t+1) = \alpha S F(t) + (1-\alpha) Y$ until converge

- Let F^* represent the limit of the sequence $\{F(t)\}$. The final classification result is:

$$y_i = \arg\max_{j \leq c} F^*_{ij}$$

The Closed-Form Solution of the Consistency Method

- Through the iterative equation, we obtain:

$$F(t) = (\alpha S)^{t-1}Y + (1-\alpha)\sum_{i=0}^{t-1}(\alpha S)^i Y.$$

Since $0 < \alpha < 1$ and the $\boxed{\text{eigenvalues of } S \text{ in [-1, 1]}}$

The advantage of normalization

- As $\lim_{t\to\infty}(\alpha S)^{t-1} = 0,$ and $\lim_{t\to\infty}\sum_{i=0}^{t-1}(\alpha S)^i = (I-\alpha S)^{-1}$, we get:

$$F^* = \lim_{t\to\infty} F(t) = (1-\alpha)(I-\alpha S)^{-1}Y$$

Thanks for your time.
QA.