Supervised vs Unsupervised

The supervised learner doesn't know much



The unsupervised learner knows what it is doing



Supervised learning tasks with networks

Node classification

Given a network (e.g. friendship network) and some labels (e.g. political party). Can we predict the labels of a node from the labels of their neighbours?

Graph classification

Given many networks (e.g. ego-networks, brain networks) and outcomes (e.g. political party, mental disorders). Can we predict the outcomes from the topology of the network?

Link prediction

Given a network (e.g. friendship network) and optionally some metadata (e.g. political party).
 Can we predict which links we are missing (or will be created)?



Does this link exist?



Does this link exist?

- 1. Model Validation
- Observe part of the adjacency matrix (fit model)
- Predict held out entries (cross validation)



Does this link exist?

- 1. Model Validation
- 2. De-noising / network reconstruction
- Real-world data are noisy / contain errors



Does this link exist?

- 1. Model Validation
- 2. De-noising / network reconstruction
- 3. Predict missing links
- Observed edges are assumed correct
- Predict which unobserved edges exist



Does this link exist?

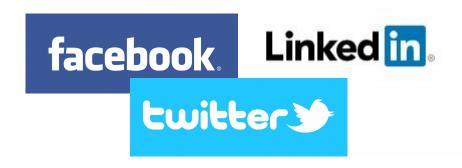
- 1. Model Validation
- 2. De-noising / network reconstruction
- 3. Predict missing links
- 4. Predict future links
- Observe the adjacency matrix at time (t)
- Predict edges in time (t+1)



Does this link exist?

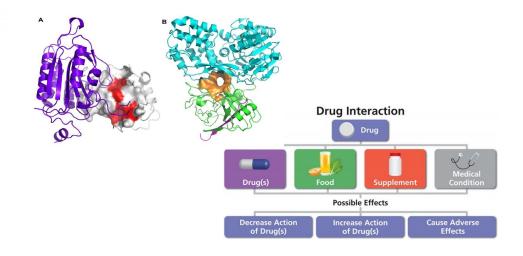
- 1. Model Validation
- 2. De-noising / network reconstruction
- 3. Predict missing links
- 4. Predict future links

Applications



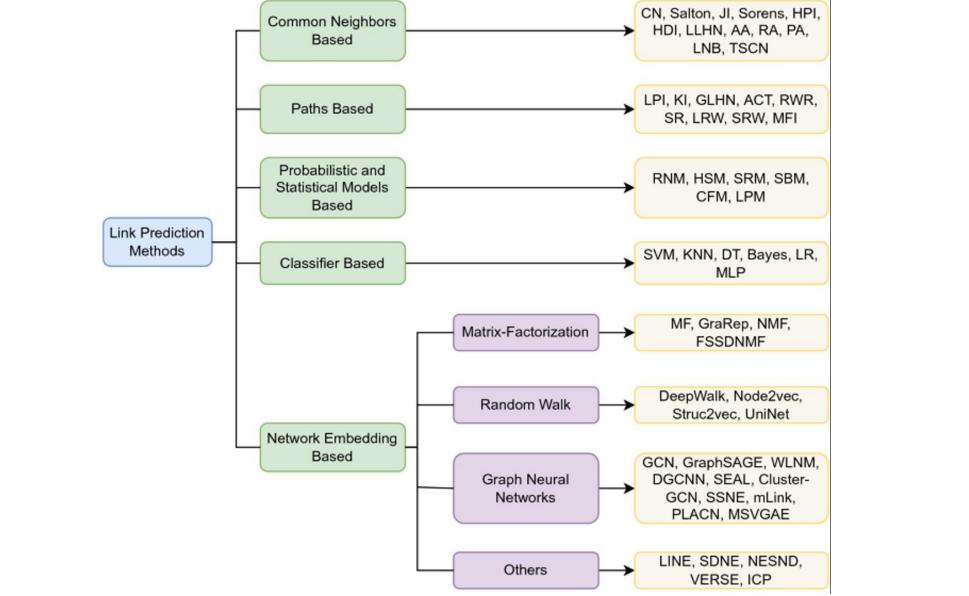
Suggesting social and professional connections

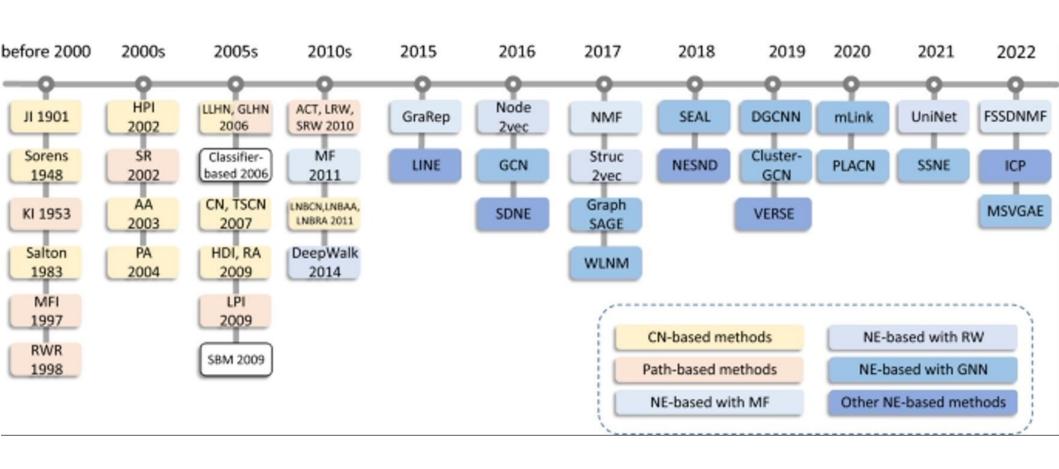
Predicting biological interactions





Recommending products and services





Link Prediction on Complex Networks: An Experimental Survey; Wu, Song, Ge, and Ge (2022)

Predicting missing links

Goal: Rank all non-edges according to how likely they are to exist

Assessed using measures such as accuracy, F1, AUC...

Local heuristics (common-neighbors approach)

Based on similarity of node connections

$$\Gamma(x) \leftarrow \text{neighbours of x}$$
 $k_x \leftarrow \text{degree of x}$

Similar neighbours

Common neighbours

$$s_{xy}^{\text{CN}} = |\Gamma(x) \cap \Gamma(y)|,$$

As matrix multiplication?

$$\Gamma(x) \leftarrow \text{neighbours of } x$$

Similar neighbours

Jaccard similarity

$$s_{xy}^{\text{Jaccard}} = \frac{|\Gamma(x) \cap \Gamma(y)|}{|\Gamma(x) \cup \Gamma(y)|}$$

$$\Gamma(x) \leftarrow \text{neighbours of } x$$

Similar neighbours

Cosine similarity

$$s_{xy}^{\text{Salton}} = \frac{|I'(x) \cap I'(y)|}{\sqrt{k_x \times k_y}}$$

$$k_x \leftarrow \text{degree of x}$$

$$\Gamma(x) \leftarrow \text{neighbours of x}$$

 $\Gamma(y)$ CN

BCD ABC **ABC ABC** CD

BC

 $\Gamma(x)$

ABC

ABC

CDE

Common Neighbours ignores degrees

Jaccard and Cosine provide similar rankings

2 0.5

0.33

Jaccard

0.2

0.66

0.25









Cosine

0.81

0.66

0.33

Other local heuristics

Adamic-Adar

Resource Allocation

$$s_{xy}^{AA} = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{1}{\log k_z} \qquad s_{xy}^{RA} = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{1}{k_z}$$

Preferential Attachment

$$s_{xy}^{\text{PA}} = k_x \times k_y$$

 $\Gamma(y)$

DE

DEFGH

 $\Gamma(x)$

ABCDEF

ABCDEF

Jaccard

Cosine

Jaccard and Cosine do not always provide the same ranking!

CN

Jaccard is biased towards nodes with similar degree

ABCDEF	DE	2

 $\Gamma(y)$

DEFGH

 $\Gamma(x)$

ABCDEF

Jaccard and Cosine do not always provide the same ranking!

Jaccard

0.38

0.33

CN

3

Cosine

0.55

0.58

Jaccard is biased towards nodes with similar degree

Other approaches

Global

heuristics: Similar to local heuristics, but considering longer path lengths

Model

Assign probability (or "likelihood") of edge existence

based: On Thursday: SBM