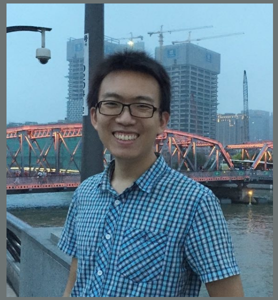
Link Prediction Based on Graph Neural Networks

Muhan Zhang and Yixin Chen, NeurIPS 2018



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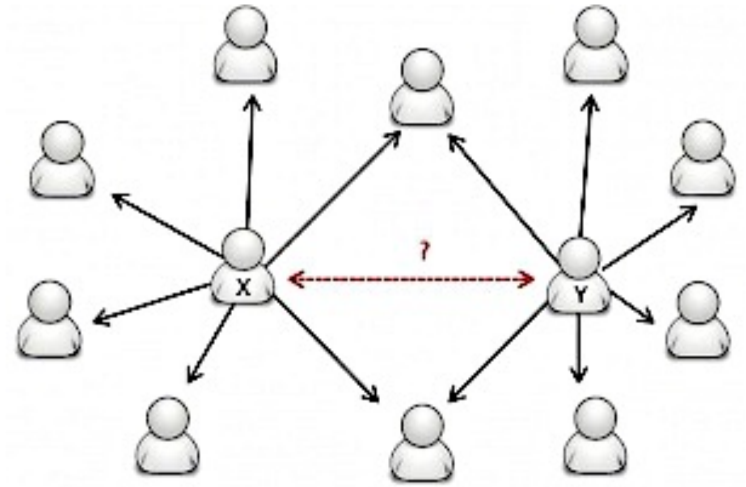
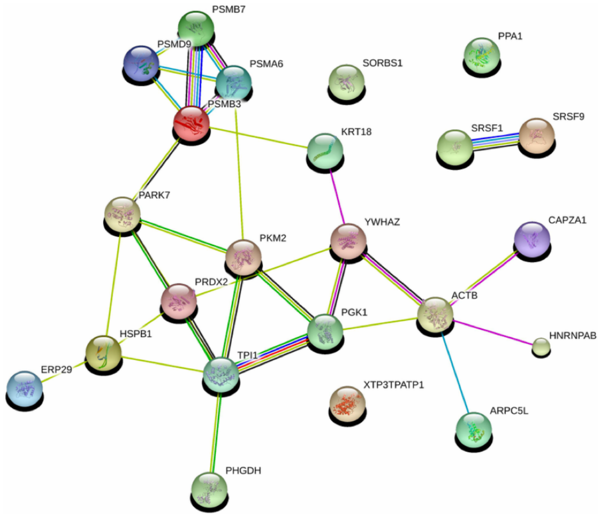
Link Prediction (LP) Problem

Given an incomplete network, predict whether two nodes are likely to have a link.

Applications:
- Friend recommendation in social networks
- Product recommendation in ecommerce
- Interaction prediction in biological networks
- Knowledge graph completion
- …



social network



Biological network

Figures from the Internet.

Heuristic Methods for LP

Calculate a proximity score for each pair of nodes.

Table 1: Popular Heuristics for Link Prediction

Name	Formula	Order
common neighbors	$\lvert\Gamma(x) \cap \Gamma(y)\rvert$	first
Jaccard	$\frac{\lvert\Gamma(x)\cap\Gamma(y)\rvert}{\lvert\Gamma(x)\cup\Gamma(y)\rvert}$	first
preferential attachment	$\lvert\Gamma(x)\rvert \cdot \lvert\Gamma(y)\rvert$	first
Adamic-Adar	$\sum_{z\in\Gamma(x)\cap\Gamma(y)} \frac{1}{\log \lvert\Gamma(z)\rvert}$	second
resource allocation	$\sum_{z\in\Gamma(x)\cap\Gamma(y)} \frac{1}{\lvert\Gamma(z)\rvert}$	second
Katz	$\sum_{l=1}^{\infty} \beta^l \lvert\text{path}(x,y) = l\rvert$	high
PageRank	$q_{xy} + q_{yx}$	high
SimRank	$\gamma \frac{\sum_{a\in\Gamma(x)}\sum_{b\in\Gamma(y)}\text{score}(a,b)}{\lvert\Gamma(x)\rvert\cdot\lvert\Gamma(y)\rvert}$	high
resistance distance	$\frac{1}{l^+_{xx}+l^+_{yy}-2l^+_{xy}}$	high

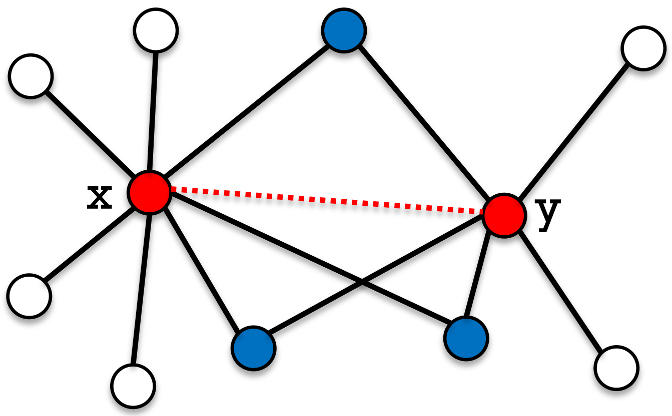
Notes: $\Gamma(x)$ denotes the neighbor set of vertex x. $\lvert\text{path}(x, y) = l\rvert$ counts the number of length-l paths between x and y. q_{xy} is the stationary distribution probability of y under the random walk from x with restart, see [10]. SimRank score is a recursive definition. l^+_{xy} is the (x, y) entry of the pseudoinverse of the graph's Laplacian matrix.

- Good performance
- Easy to calculate
- Interpretable
- No training required

First-Order Heuristics

Notations: $\Gamma(x)$ is the neighbor set of node x in the graph

- The common neighbors (CN) heuristic: $|\,\Gamma(x) \cap \Gamma(y)\,|$

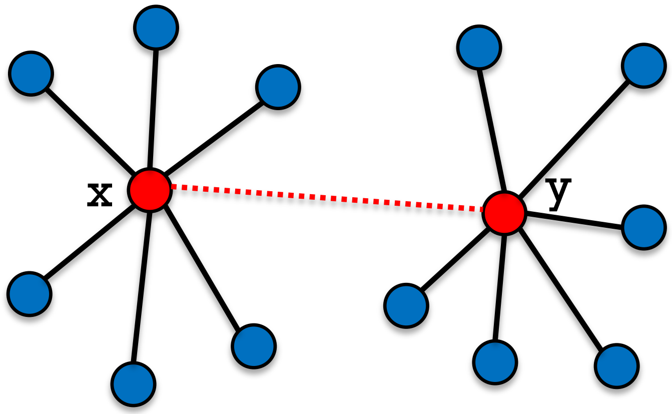


x and y are likely to have a link
if they have many common neighbors.

- First-order heuristic, need only 1-hop neighbors to compute.

First-Order Heuristics

- The preferential attachment (PA) heuristic: $|\Gamma(x)| \cdot |\Gamma(y)|$

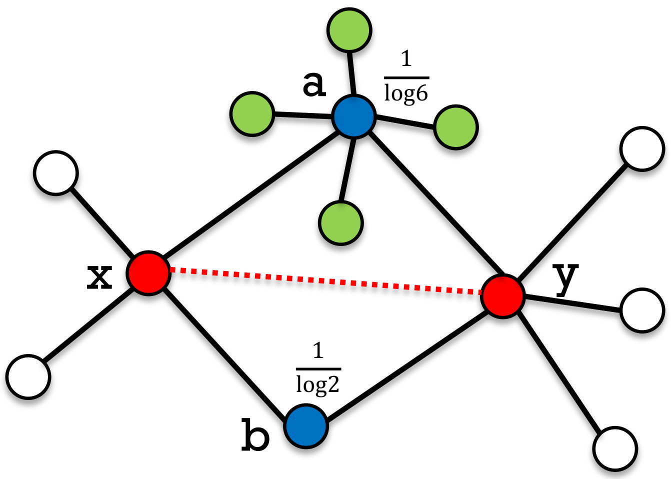


x prefers to connect to y if y is popular.

- First-order heuristic, only involves 1-hop neighbors.

Second-Order Heuristics

- The Adamic-Adar (AA) heuristic: $\sum_{z\in\Gamma(x)\cap\Gamma(y)} \frac{1}{\log|\Gamma(z)|}$



Weighted common neighbors;

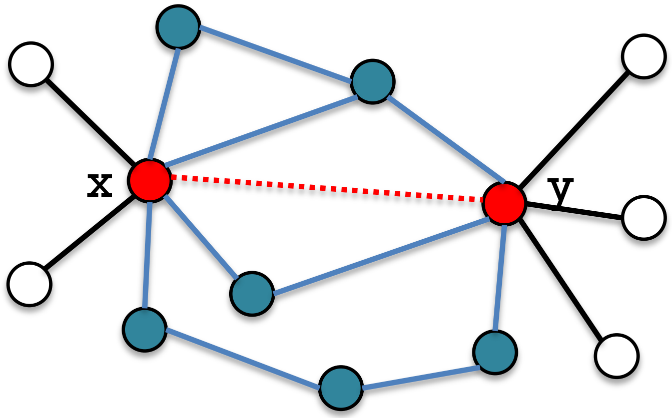
Popular common neighbors contribute less.

- Second-order heuristic. Involves 2-hop neighbors of x and y.

- First-order and second-order heuristics can be calculated from local subgraphs around links.

High-Order Heuristics

- The Katz index heuristic: $\sum_{l=1}^{\infty} \beta^l |\text{walks}(x, y) = l|$



Sum all walks between x and y; each walk discounted by β^l.

$\beta < 1$ is the discount factor

l is the length of a walk

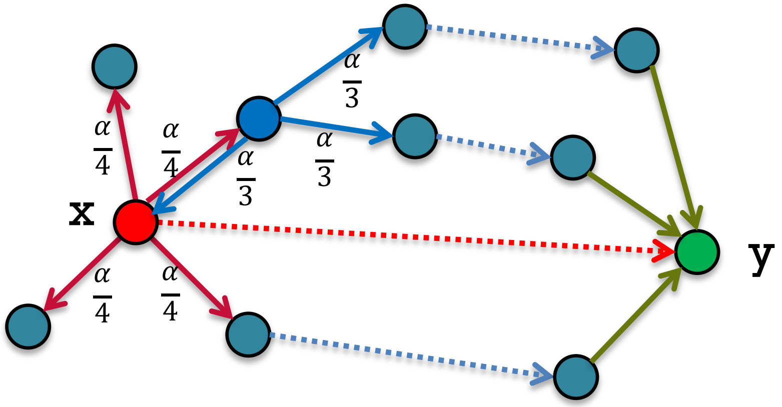
Longer walks contribute less.

- High-order heuristic
- Need to search the entire network.

High-Order Heuristics

- The Rooted PageRank heuristic:

  Let π_x be the stationary distribution of a random walker starting from x who randomly moves to one of its current neighbors with probability α or returns to x with probability $1-\alpha$.



Use $[\pi_x]_y$ as the likelihood of link (x,y).

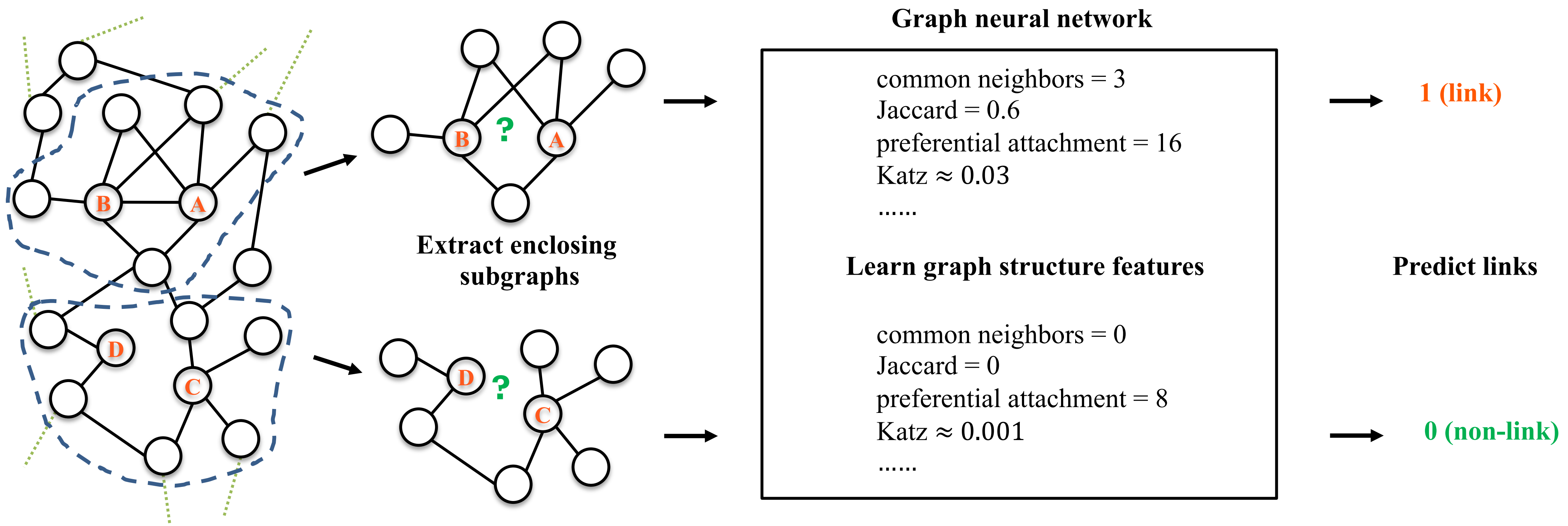
- High-order heuristic

- Need to know the entire network and iterate until convergence.

Drawbacks of Heuristic Methods

- Handcrafted graph structure features, not general.
- Have strong assumptions on link formation mechanisms.
- Only work well on certain networks.
- In our paper, we proposed **SEAL**:
    1. Automatically learn general graph structure features.
    2. No assumption on network properties at all.
    3. New state-of-the-art link prediction performance based on a graph neural network.

Proposed SEAL Framework



- Learn "heuristics" instead of using predefined ones.
- All first-order and second-order heuristics can be learned from local enclosing subgraphs.
- How about high-order heuristics?

A γ-decaying Heuristic Theory

Definition ***(γ-decaying heuristic)*** *A γ-decaying heuristic for (x, y) has the following form:*

$$\mathcal{H}(x,y) = \eta \sum_{l=1}^{\infty} \gamma^{l} f(x,y,l),$$

Main results:

1. A wide range of high-order heuristics can be unified into a γ-decaying heuristic framework, including Katz index, rooted PageRank, SimRank etc. => They intrinsically have the same form!
2. Under mild assumptions, all γ-decaying heuristics can be well approximated from local enclosing subgraphs. => We don't need the entire network to learn them!
3. The approximation error decreases exponentially with the subgraph size. => A small subgraph is enough!

Poster #121 Thurs 10:45 AM -- 12:45 PM @ Room 210 & 230 AB