

Link Prediction on the Patent Citation Network

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Advanced Data
Mining



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Problem Definition

- Link prediction (LP) is cast as a binary classification problem
 - Does a link exist between any two pair of nodes?
- INPUT:** Adjacency list
- OUTPUT:** Ranked list of most likely edges

Motivation

- Generate citation recommendations on new patents
- LP on the Patent Citation Dataset is unprecedented
 - LP on large and temporal graphs is less well studied
- Compare the performance of SDNE to other classical network embedding methods on different graph types

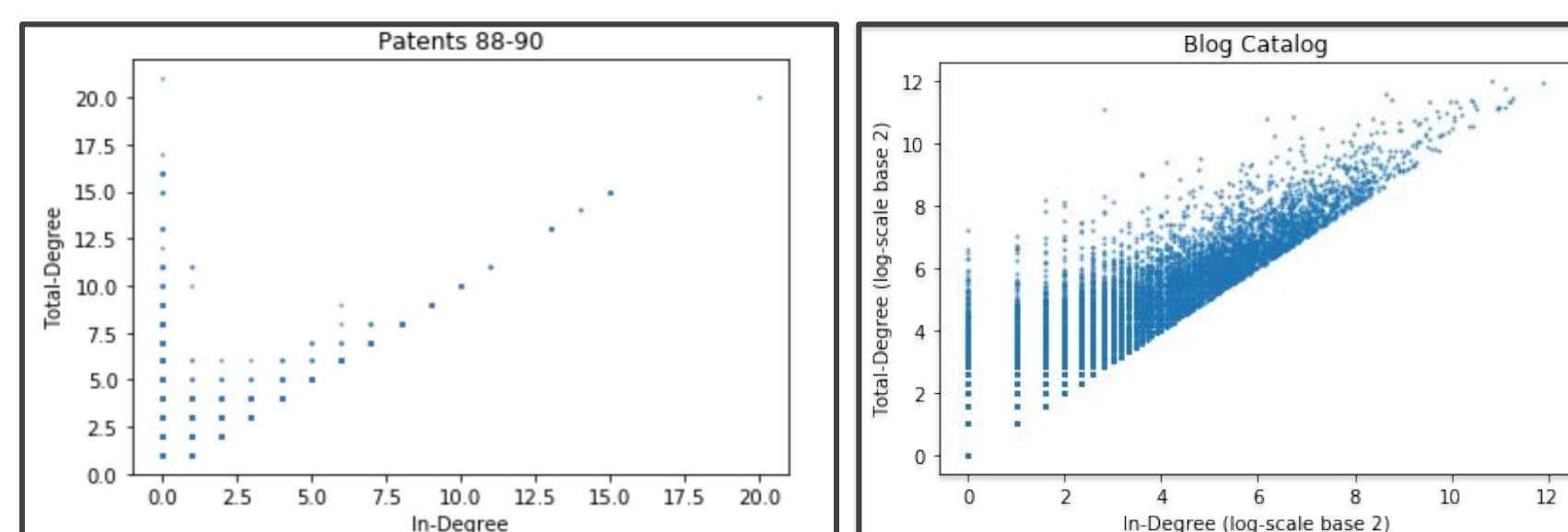
Datasets

Patent Citation Dataset

- 1988 - 1989 subgraph: 40K nodes, 30K edges
- 1990 - 1996 subgraph: 580K nodes, 1.2M edges
 - Yielded poor results because of size
- "Future" test set: 500 proceeding nodes with 2 or more outward edges, inward edges removed

Blog Catalog: 10K nodes, 300K edges

- Undirected graph



References

- Grover and Leskovec. [node2vec: Scalable Feature Learning for Networks](#). ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), 2016.
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- Wang et al. [Structural deep network embedding](#). In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining. ACM 2016, 1225–1234.
- Niwtanukul et al. [Using of Jaccard coefficient for keywords similarity](#). In Proceedings of the international multicongress of engineers and computer scientists 2013 (Vol. 1, No. 6, pp. 380-384).
- Lerer et al. (2019). [PyTorch-BigGraph: A Large-scale Graph Embedding System](#). arXiv preprint 2019, arXiv:1903.12287.

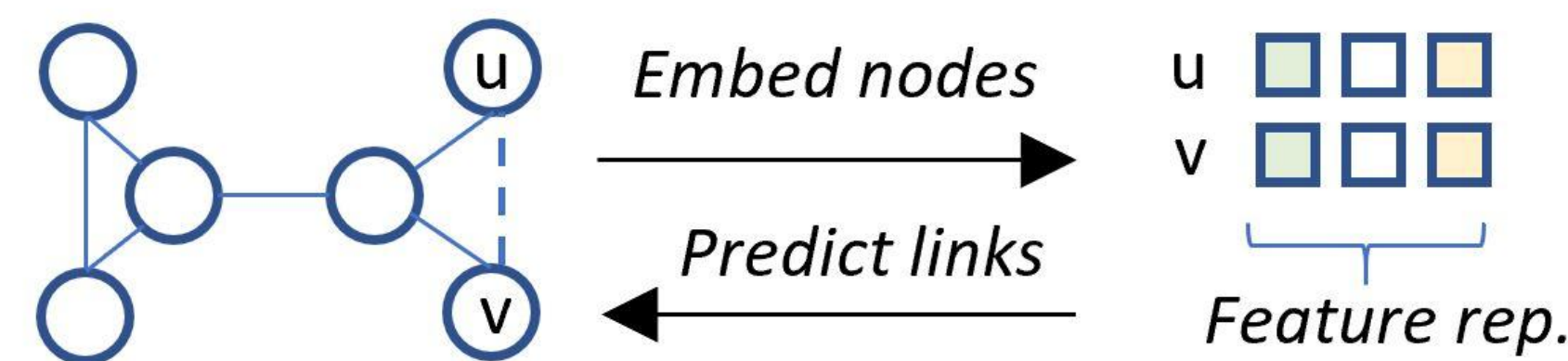
Our Approach

Data Partitioning

- Sub-graphs are divided into training and test sets
- 15% of the links in the sub-graph are hidden from the training set

Link Prediction from Node Embeddings

- Methods embed similar nodes close together
- Use node embeddings to predict hidden links



Approach 1: SDNE

Nodes embedded by optimizing weighted loss from:

- Supervised "first-order proximity"
 - Influenced by Laplacian Eigenmaps
 - Captures pairwise similarities i.e. common neighbors
- Unsupervised autoencoder "second-order proximity"
 - Mimics Graph Convolutional Network
 - Captures global structure i.e. role in network
- High unsupervised weight should help in sparse graphs

Approach 2: node2vec

- Focused on learning low-dimensional representation learning
- Node embeddings generated through random walk approach
- Random walks can be biased
 - Uses unbiased in this work

Approach 3: Jaccard Coefficient

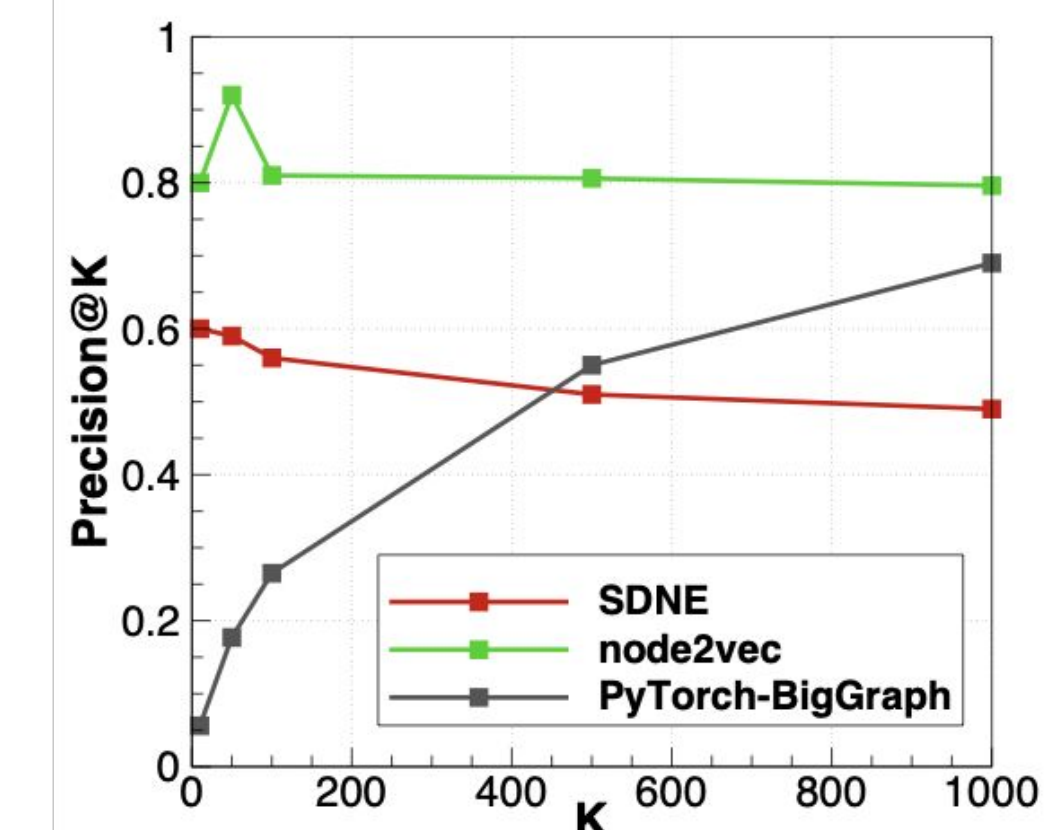
- Predicts whether two nodes share a relationship, in this case a link, based on the intersection over union of their neighborhoods
- No learning involved, but very expensive at inference time

Approach 4: PyTorch BigGraph

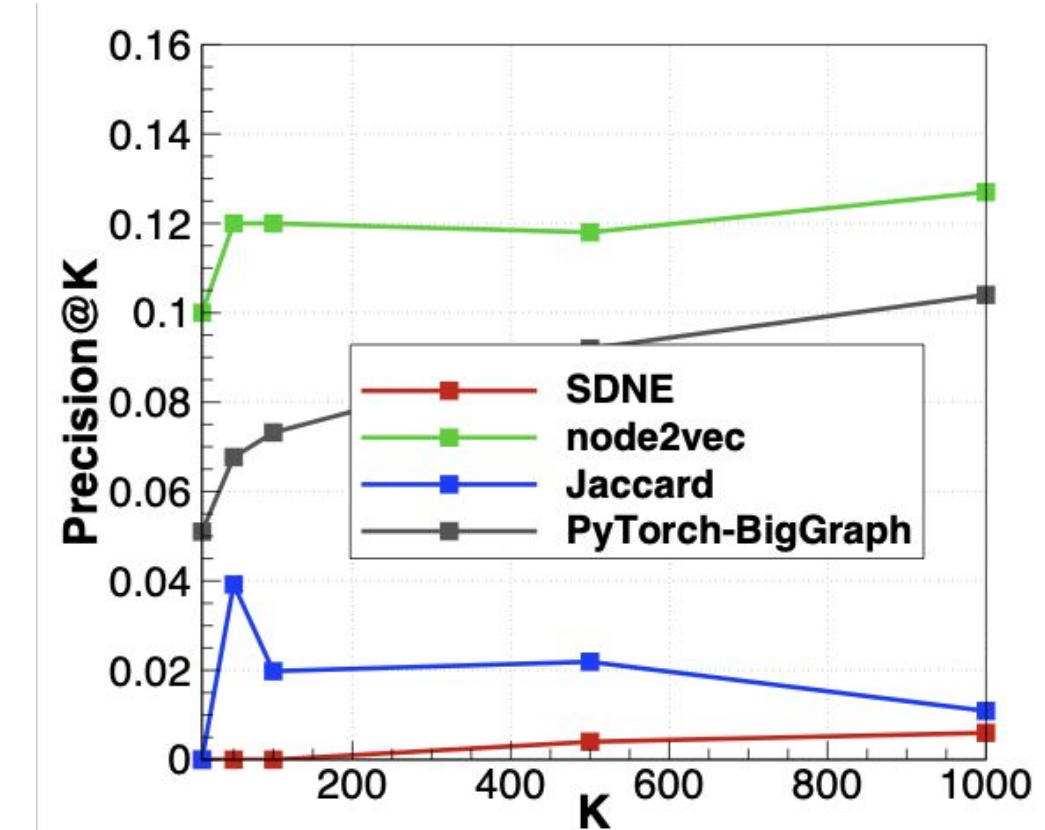
- Learns node embedding by minimizing distance between adjacent nodes
- Gains efficiency by augmenting negative sampling with uniform samples used as negatives

Experimental Results

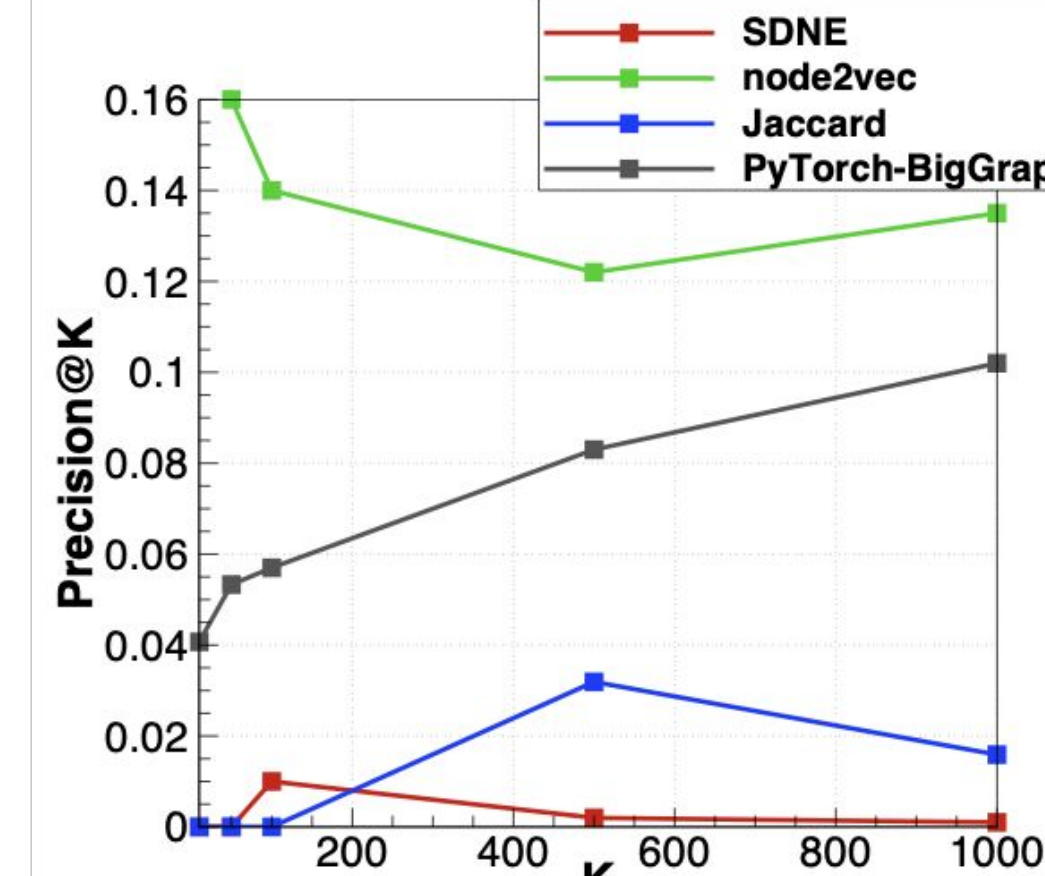
Blog Catalog



1988-1989 Baseline



1988-1999 Future



(Figures report Link Prediction precision@k)

- SDNE Parameters:
 - Embedding size: 100¹, 40²
 - Hidden layer size: 1000¹, 400²
 - Supervised loss wt: 1
 - Unsupervised loss wt: 100
- node2vec Parameters:
 - Embedding dimension: 128
 - RW length: 80
 - 10 RW per source

SDNE vs. Node2vec:

- node2vec: Much more computationally efficient than SDNE
- node2vec: Performs better than SDNE, particularly on sparse graph
- node2vec: Prediction on future is better than baseline

Jaccard Observation:

- Worst asymptotic complexity

BigGraph Observation:

- Performance increases with k.
- Highly scalable

Conclusions

- LP can work well on temporal graphs. However, sparse graphs makes LP difficult
- RW methods do disproportionately better than nn in this situation
- Scalability is challenging for all methods studied, Pytorch handles best
- Future directions: link prediction on more dense temporal graphs