A Broader Picture of Random-walk Based Graph Embedding

KDD'21

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Research papers

- [PARS14] DeepWalk: online learning of social representations
- [GL16] node2vec: scalable feature learning for networks
- ... (with many more items omitted)
- [CM20] InfiniteWalk: deep network embeddings as ...
- [ZLHK21] Node proximity is all you need: ...

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Surveys

- [HYL17] Representation learning on graphs: methods and applications
- ...
- [CAEHP$^+$20] Machine learning on graphs: a model and comprehensive taxonomy

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Difficult to compare existing methods and to design novel ones

Question: link prediction

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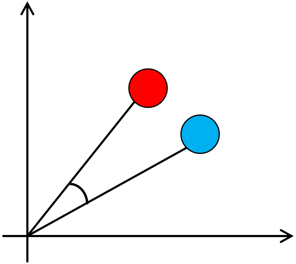
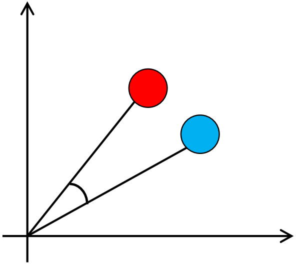


(a) Dot product
[OCP+16, WCZ16, ZCW+18]

Question: link prediction



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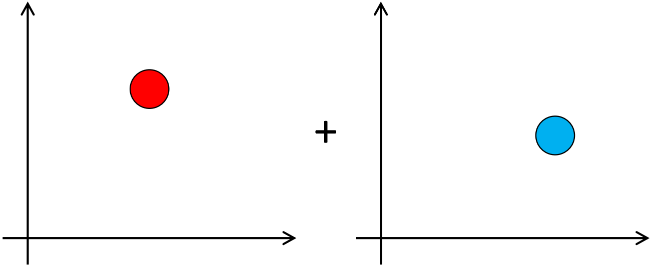

(b) Classification based on combined embeddings
[GL16, NLR+18, JDE+20]

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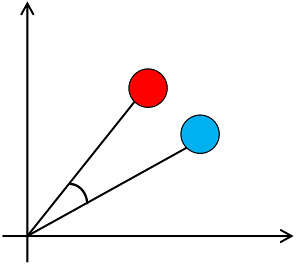

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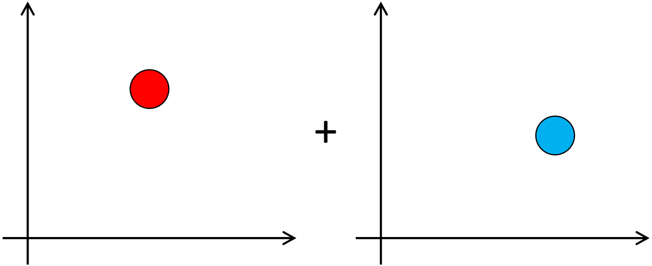
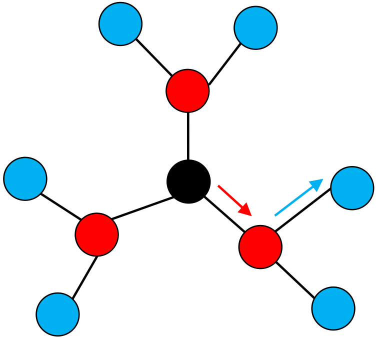


(b) Classification based on combined embeddings
[GL16, NLR+18, JDE+20]

How should embeddings be used for link prediction?

Question: multiscale



(a) Random-walks capture multiple structural scales [DYB10]

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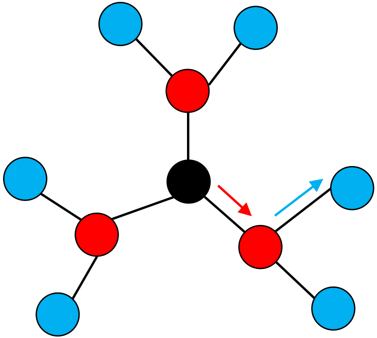

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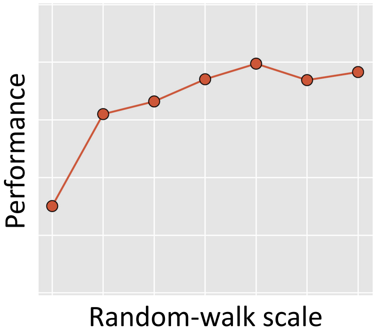

(b) Embedding performance [GL16] insensitve to random-walk scales

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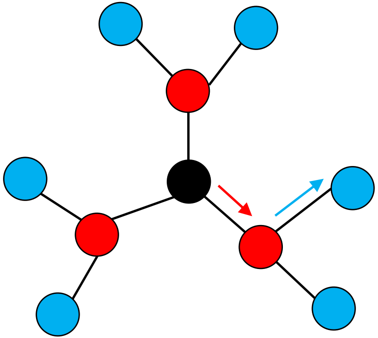

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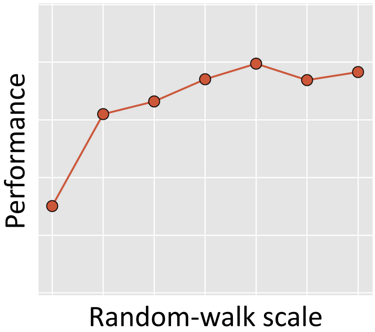

(b) Embedding performance [GL16] insensitve to random-walk scales

How do embeddings capture different structural scales?

Our analytical framework

random-walk process + similarity metric + embedding algorithm

Our analytical framework

	random-walk process	similarity metric	embedding algorithm
DeepWalk	standard	PMI	sampling

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Our analytical framework

	random-walk process	similarity metric	embedding algorithm
DeepWalk	standard	PMI	sampling
node2vec	*biased*	PMI	sampling
Multiscale	standard	*autocovariance*	*factorization*
...	...	...	...

Random-walk process

M: transition matrix

π, Π: stationary distribution

Random-walk process

M: transition matrix

π, Π: stationary distribution

Process

Random-walk based embedding methods

Standard

DeepWalk, LINE
Multiscale, NetMF
NetSMF, InfiniteWalk

Non-standard

node2vec, APP
NetMF, NERD

Similarity metric

PMI[1]: $R = \log(\Pi M^{\tau}) - \log(\pi\pi^{T})$

[1] [LG14] Levy and Goldberg. Neural word embedding as implicit matrix factorization. NeurIPS'14.

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PMI[1]: $R = \log(\Pi M^\tau) - \log(\pi\pi^T)$ Autocovariance[2]: $R = \Pi M^\tau - \pi\pi^T$

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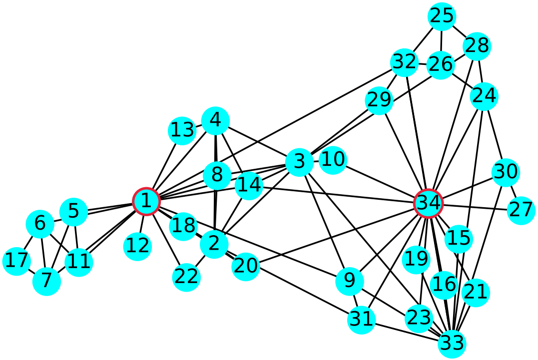

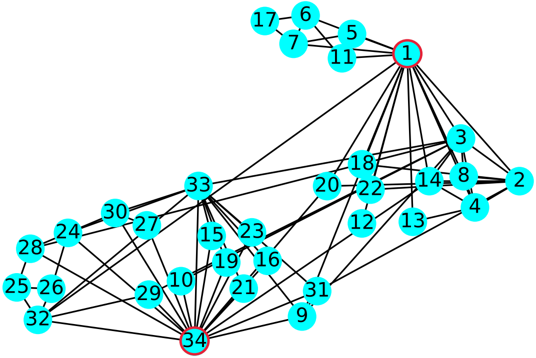

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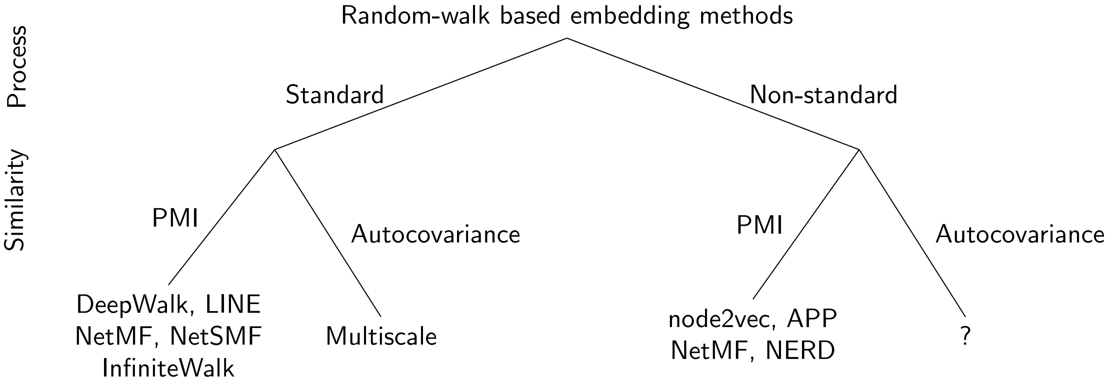

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Embedding algorithm

Explicit: Factorization (SVD)

$$\min \|UU^T - R\|_F^2$$

Implicit: Sampling (SGD)

$$\max \sum_{u,v} \log \Pr((u,v) \in \mathcal{D} | \mathbf{u}_u, \mathbf{v}_v)$$

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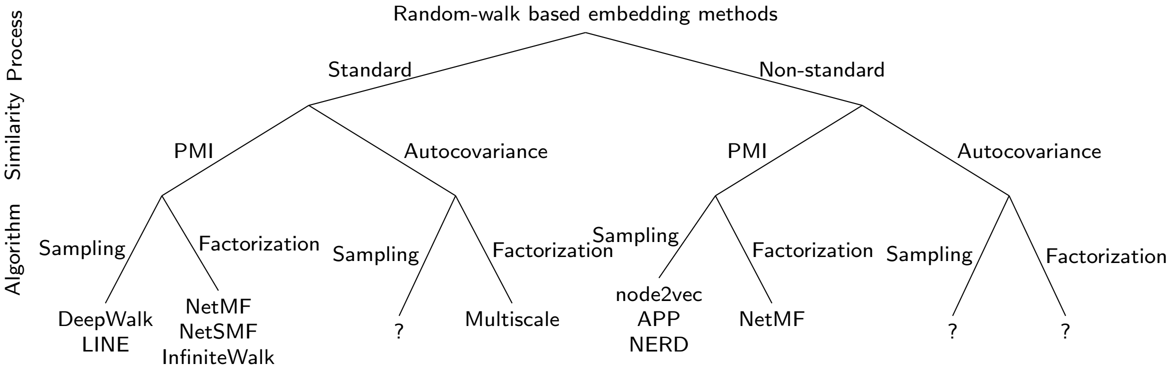

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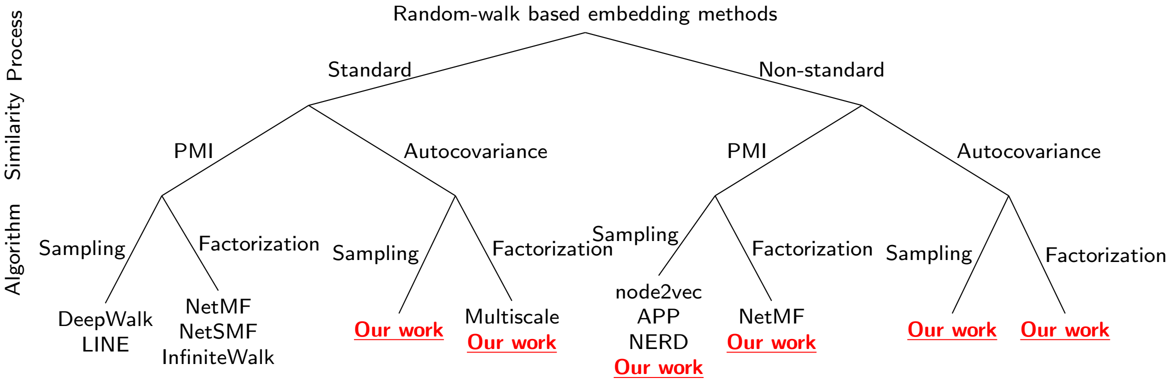

Datasets

	$\lvert\mathcal{V}\rvert$	$\lvert\mathcal{E}\rvert$	labels
BlogCatalog	10,312	333,983	interests
Airport	3,158	18,606	countries/continents
Wiki-words	4,777	92,157	tags
PoliticalBlogs	1,222	16,717	ideologies

Downstream tasks

- Node classification (Micro/Macro-F1)
- Link prediction (precision@k)
- Community detection (NMI)

Embedding dimension = 128

Comparing similarity metrics: node classification

PMI: $R = \log(\Pi M^{\tau}) - \log(\pi\pi^{T})$ Autocovariance: $R = \Pi M^{\tau} - \pi\pi^{T}$

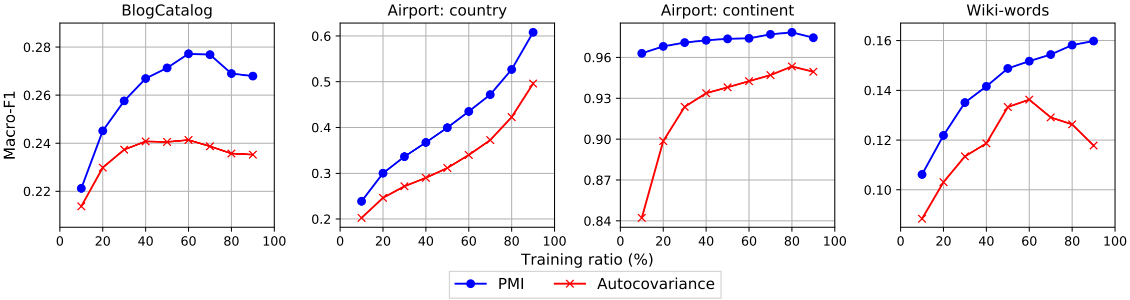

Figure: PMI consistently outperforms autocovariance in node classification.

Comparing similarity metrics: link prediction

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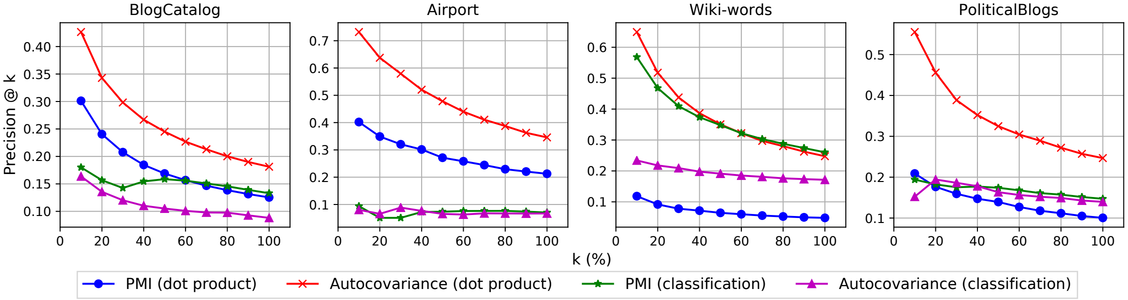

Figure: Autocovariance with dot product ranking consistently outperforms PMI (with either ranking scheme) in link prediction.

Understanding the difference

predicted degree $\propto$ embedding norm $\|\mathbf{u}\|$

Understanding the difference

$$\text{predicted degree} \propto \text{embedding norm } \|\mathbf{u}\| \propto \begin{cases} \text{actual degree} & \text{for autocov.} \\ \text{constant} & \text{for PMI} \end{cases}$$

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Autocovariance captures heterogeneous degree distribution in graphs!

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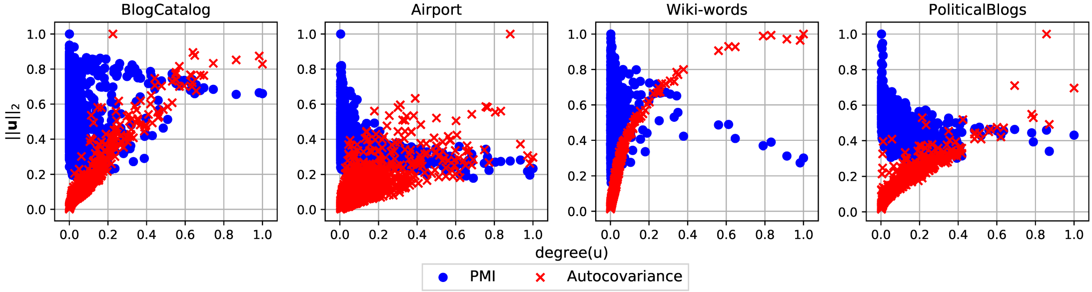

Figure: Autocovariance embedding norms correlate with actual degrees, but not PMI.

Understanding the difference

$$\text{predicted degree} \propto \text{embedding norm } \|\mathbf{u}\| \propto \begin{cases} \text{actual degree} & \text{for autocov.} \\ \text{constant} & \text{for PMI} \end{cases}$$

(a) PMI (b) Autocovariance

Figure: Autocovariance predicts more edges connecting to the hubs than PMI.

Multiscale

PMI: $R = \log(\Pi M^{\tau}) - \log(\pi\pi^{T})$ Autocovariance: $R = \Pi M^{\tau} - \pi\pi^{T}$

Multiscale

PMI: $\widetilde{R} = \log(\Pi \frac{1}{\tau} \sum_{t=1}^{\tau} M^t) - \log(\pi\pi^T)$

Autocovariance: $R = \Pi M^{\tau} - \pi\pi^T$

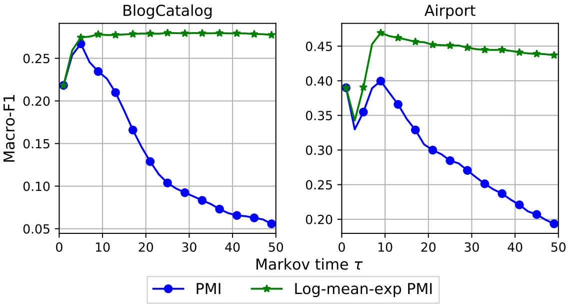

Figure: Node classification performance for PMI can be improved by smooth-averaging across multiple Markov times.

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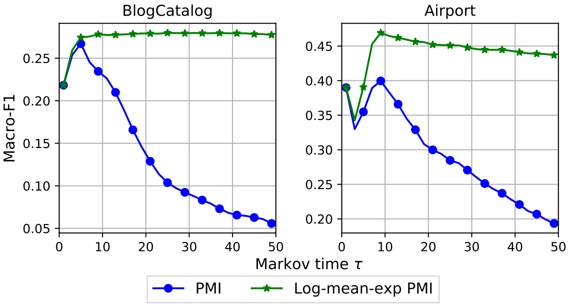

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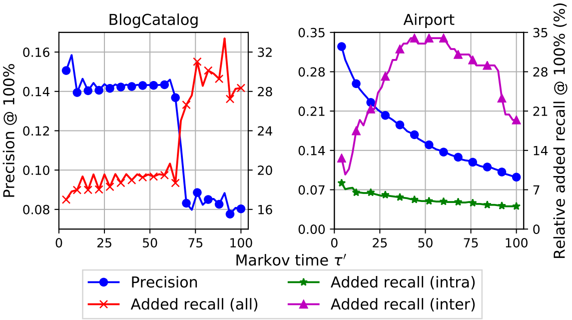

Figure: Prediction of edges of specific structural scales can be improved with different Markov times for autocovariance.

Problems:

1. How can one compare existing methods and to advance the SOTA?
2. How should embeddings be used for link prediction?
3. How do embeddings capture different structural scales?

Contributions:

1. A unified view of different processes, similarities, and algorithms.
2. Autocovariance embedding is significantly better for link prediction.
3. Ways to exploit multiscale similarity for optimized performance.

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