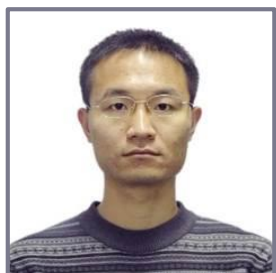




Asymmetric Transitivity Preserving Graph Embedding

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Tsinghua U Tsinghua U Simon Fraser U **Tsinghua U** Tsinghua U



Graph Embedding

Graph Data

Social Network

Citation/
Collaboration

Image/Video
Tag/Caption

Web Hyperlink

Etc.

Graph Data
Representation

Graph
Embedding

Application

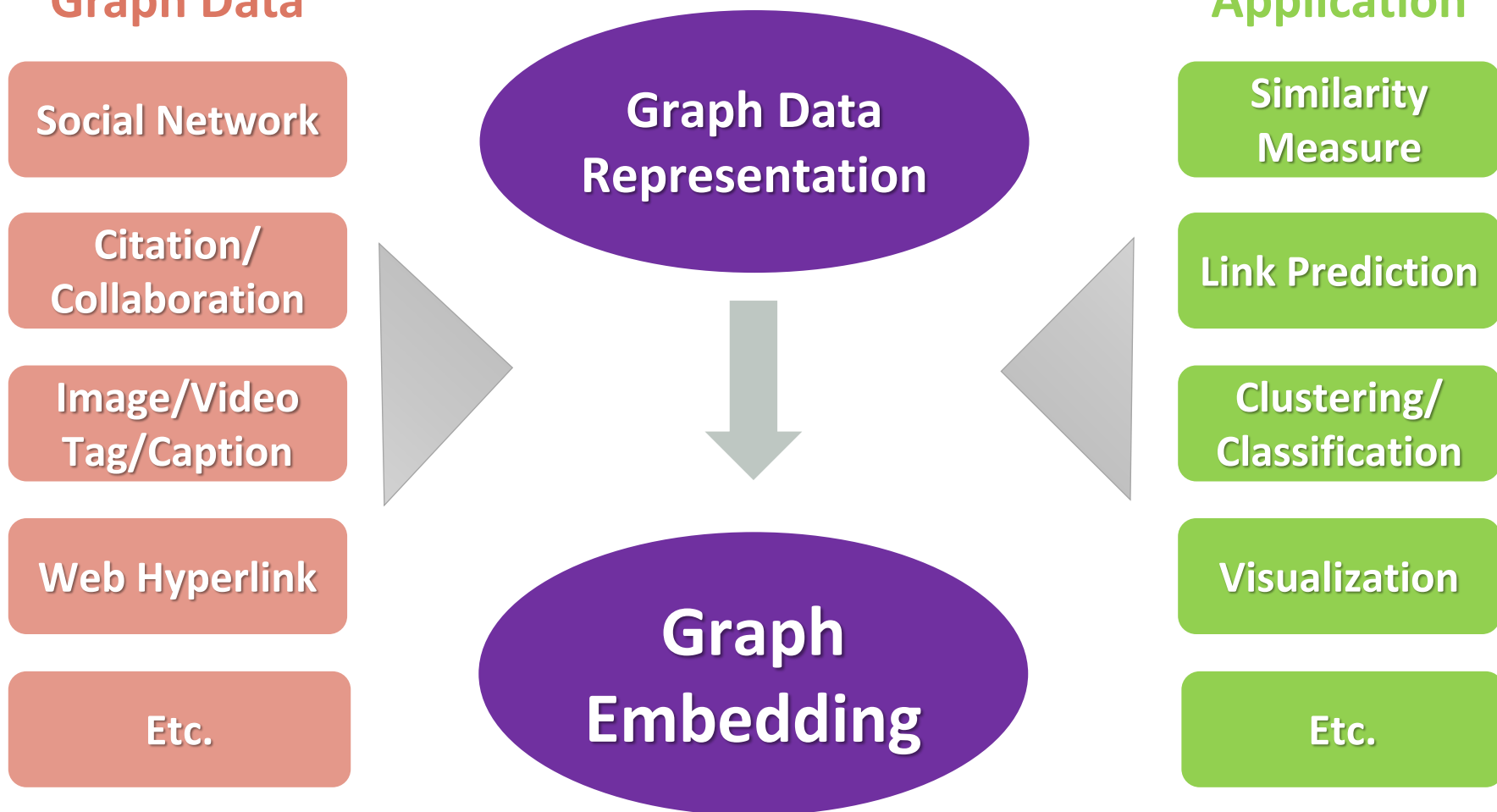
Similarity
Measure

Link Prediction

Clustering/
Classification

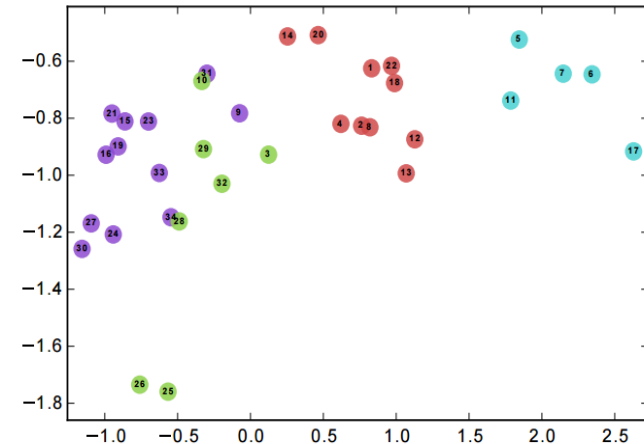
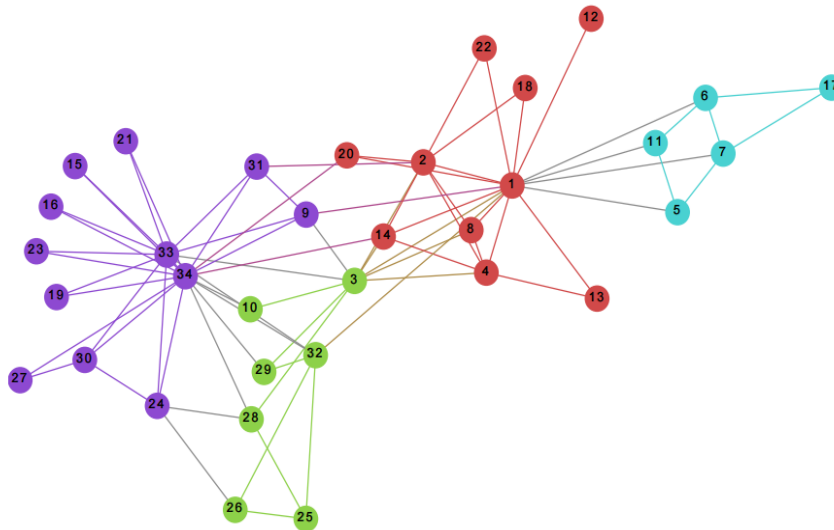
Visualization

Etc.



Graph Embedding

- **Graph Embedding:**



Input graph/network → Low dimensional space

□ Advantages:

- Fast computation of nodes similarity
- Utilization of vector-based machine learning techniques
- Facilitating parallel computing

Existing graph embedding methods

❑ Existing work:

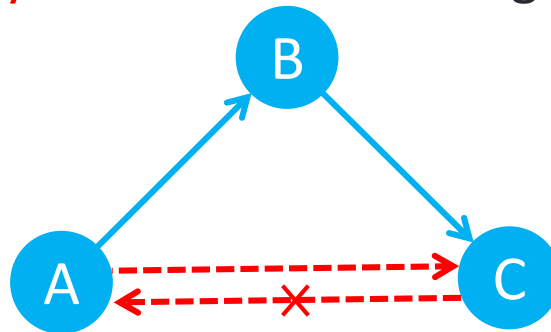
- ❑ LINE(Tang J, et al. WWW 2015): explicitly preserves first-order and second-order proximity
- ❑ DeepWalk(Perozzi B, et al. KDD 2014): random walk on graphs + SkipGram Model from NLP
- ❑ GraRep(Cao S, et al. CIKM 2015)
- ❑ SDNE(Daixin W, et al. KDD 2016)

❑ Most methods focus on undirected graph

Directed Graph

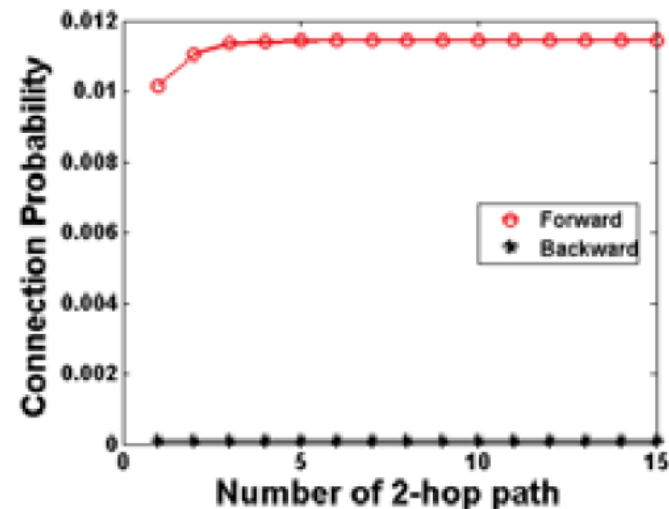
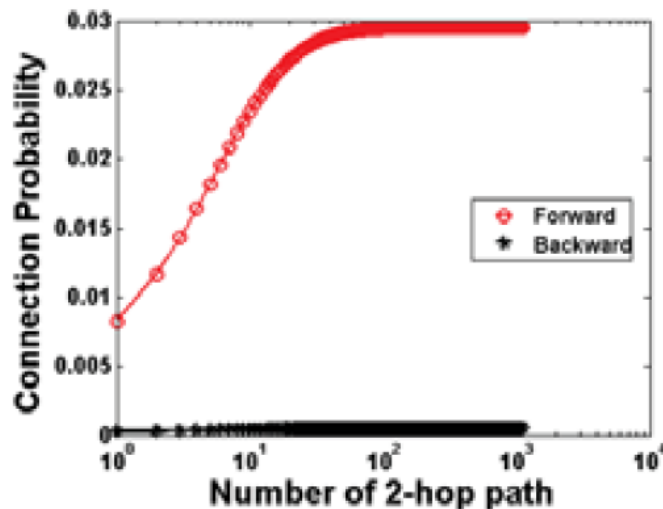
Critical property in directed graph: **Asymmetric Transitivity**

□ Transitivity is **Asymmetric** in directed graph:



□ Key in **graph inference**.

□ Data Validation: Tencent Weibo and Twitter



□ **Asymmetric transitivity** is important!

Asymmetric Transitivity \rightarrow Graph Embedding

- ❑ Challenge: incorporate asymmetric transitivity in graph embedding
- ❑ Problem: metric space is **symmetric**

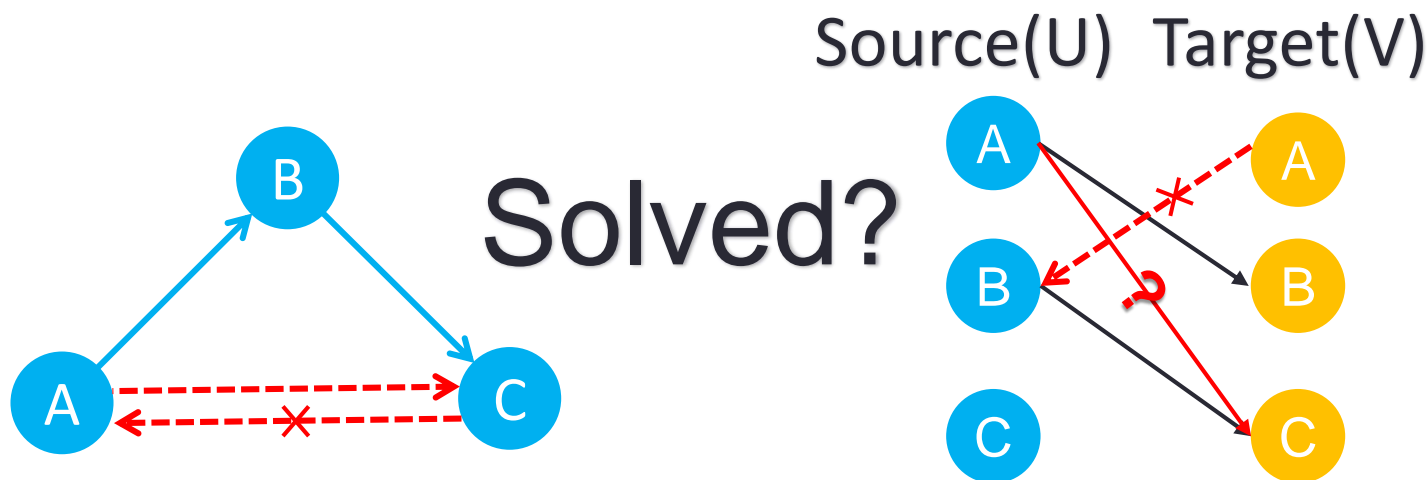
asymmetric transitivity

metric space



Asymmetric Transitivity → Graph Embedding

- **Directed graph embedding:** use **two vectors** to represent each node
 - LINE(Tang J, et al. WWW 2015): second-order proximity is directed
 - PPE(Song H H, et al. SIGCOMM 2009): using sub-block of the proximity matrix



- **Asymmetric: YES; Transitive: NO!**

Similarity metric with asymmetric transitivity

- Asymmetric transitivity:

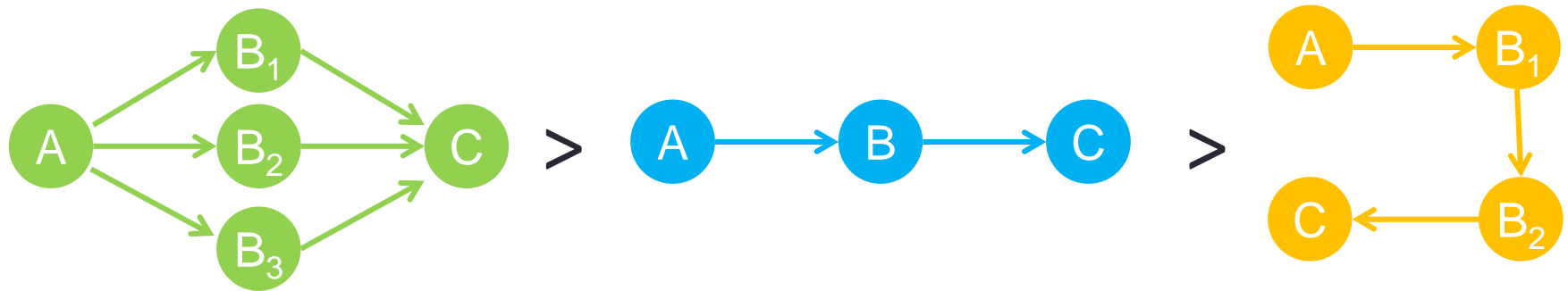
- Asymmetry: **not symmetric** in directed graph

- Transitivity:

- More directed paths, larger similarity

- Shorter paths, larger similarity

- Compare A → C similarity:



High-order Proximity!
(E.g. Katz, Rooted PageRank)

High-Order Proximity

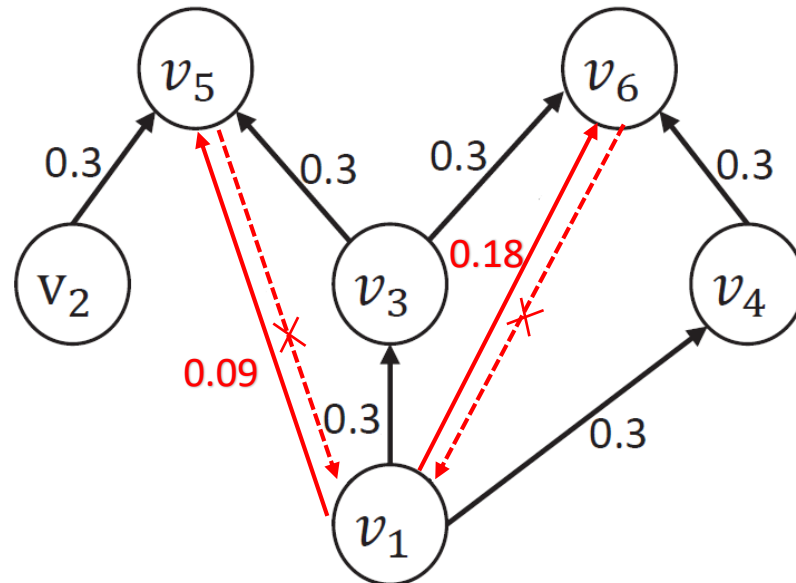
□ Solution: directly model transitivity using **high-order proximity**

□ Example: Katz Index

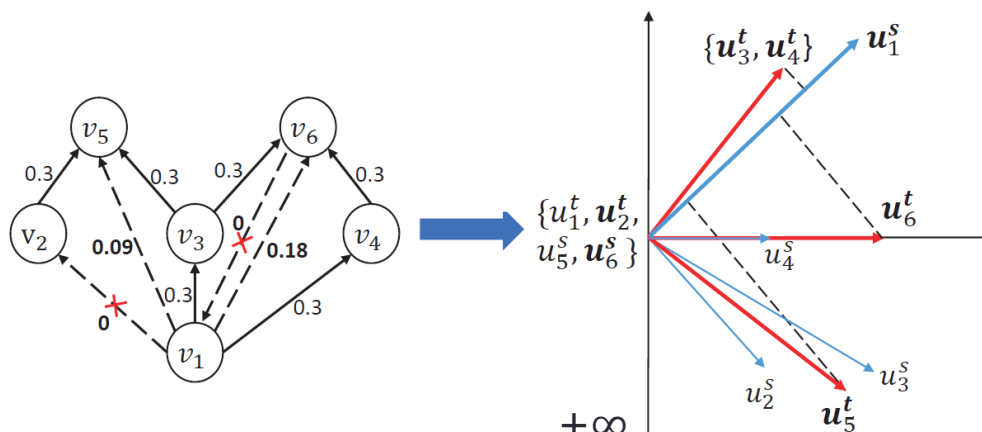
□ A : adjacency matrix, β : decaying constant

$$\mathbf{S}^{Katz} = \sum_{l=1}^{+\infty} (\beta \cdot A)^l$$

□ Example: when $\beta = 1$



Preserve high-order proximity embedding



Naive Solution: **SVD**?

$$\mathbf{S}^{Katz} = \sum_{l=1}^{+\infty} (\beta \cdot A)^l$$

$$\boxed{\mathbf{S}^{Katz}} = \boxed{\mathbf{U}^s} \times \boxed{\mathbf{U}^t}$$

□ Time and space complexity: $O(N^3)$, N : node number

High-Order Proximity: a general form

□ Katz Index:

$$\mathbf{S}^{Katz} = \sum_{l=1}^{+\infty} (\beta \cdot \mathbf{A})^l = (\mathbf{I} - \beta \cdot \mathbf{A})^{-1} \cdot (\beta \cdot \mathbf{A})$$

□ General Form

$$\mathbf{M}_g^{-1} \cdot \mathbf{M}_l$$

where $\mathbf{M}_g, \mathbf{M}_l$ are polynomial of adjacency matrix or its variants

General Formulation for High-Order Proximity measurements

Proximity Measurement	\mathbf{M}_g	\mathbf{M}_l
Katz	$\mathbf{I} - \beta \cdot \mathbf{A}$	$\beta \cdot \mathbf{A}$
Personalized Pagerank	$\mathbf{I} - \alpha \mathbf{P}$	$(1 - \alpha) \cdot \mathbf{I}$
Common neighbors	\mathbf{I}	\mathbf{A}^2
Adamic-Adar	\mathbf{I}	$\mathbf{A} \cdot \mathbf{D} \cdot \mathbf{A}$

The Power of General Form

$$\min_{U_s, U_t} \|S - U_s \cdot U_t^T\|_F^2$$

$$S = M_g^{-1} \cdot M_l$$

Generalized SVD (Singular Value Decomposition) theorem

If we have the singular value decomposition of the general formulation

$$\mathbf{M}_g^{-1} \cdot \mathbf{M}_l = \mathbf{V}^s \Sigma \mathbf{V}^{t\top}$$

where \mathbf{V}^t and \mathbf{V}^s are two orthogonal matrices,

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_N)$$

Then, there exists a nonsingular matrix \mathbf{X} and two diagonal matrices, i.e. Σ^l and Σ^g , satisfying that

$$\mathbf{V}^{t\top} \mathbf{M}_l^\top \mathbf{X} = \Sigma^l \quad \mathbf{V}^{s\top} \mathbf{M}_g^\top \mathbf{X} = \Sigma^g$$

, where

$$\Sigma^l = \text{diag}(\sigma_1^l, \sigma_2^l, \dots, \sigma_N^l) \quad \sigma_1^l \geq \sigma_2^l \geq \dots \geq \sigma_K^l \geq 0$$

$$\Sigma^g = \text{diag}(\sigma_1^g, \sigma_2^g, \dots, \sigma_N^g) \quad 0 \leq \sigma_1^g \leq \sigma_2^g \leq \dots \leq \sigma_K^g$$

$$\forall i \quad \sigma_i^{l2} + \sigma_i^{g2} = 1$$

The Power of General Form

$$\min_{U_s, U_t} \|S - U_s \cdot U_t^T\|_F^2$$

$$S = M_g^{-1} \cdot M_l$$

- Generalized SVD: decompose S **without** actually calculating it
- JDGSVD: Time Complexity

$$O(K^2 L \cdot m)$$

The diagram shows the time complexity $O(K^2 L \cdot m)$ at the top. Three arrows point downwards from this expression to three terms: 'Embedding Dimension (constant)', 'Iteration (constant)', and 'Edge number'. This indicates that the complexity is linear with respect to the edge number, while the other two terms are constants.

- **Linear complexity** w.r.t. the volume of data (i.e. edge number)

--> **Scalable** algorithm, suitable for **large-scale** data

Theoretical Guarantee

□ Approximation Error Upper Bound:

THEOREM 2. *Given the proximity matrix, \mathbf{S} , of a directed graph, and the embedding vectors, \mathbf{U}^s and \mathbf{U}^t , learned by HOPPE. Then the approximation error is*

$$\|\mathbf{S} - \mathbf{U}^s \cdot \mathbf{U}^t\|_F^2 = \sum_{i=K+1}^N \sigma_i^2$$

, and the relative approximation error is:

$$\frac{\|\mathbf{S} - \mathbf{U}^s \cdot \mathbf{U}^t\|_F^2}{\|\mathbf{S}\|_F^2} = \frac{\sum_{i=K+1}^N \sigma_i^2}{\sum_{i=1}^N \sigma_i^2} \quad (22)$$

where $\{\sigma_i\}$ are the singular values of \mathbf{S} in descend order.

HOPE: HIGH-ORDER PROXIMITY PRESERVED EMBEDDING

HOPE: High-Order Proximity preserved Embedding

Algorithm framework:

Algorithm 1 High-order Proximity preserved Embedding

Require: adjacency matrix \mathbf{A} , embedding dimension K , parameters of high-order proximity measurement θ .

Ensure: embedding source vectors \mathbf{U}^s and target vectors \mathbf{U}^t .

- 1: calculate \mathbf{M}_g and \mathbf{M}_l .
 - 2: perform JDGSVD with \mathbf{M}_g and \mathbf{M}_l , and obtain the generalized singular values $\{\sigma_1^l, \dots, \sigma_K^l\}$ and $\{\sigma_1^g, \dots, \sigma_K^g\}$, and the corresponding singular vectors, $\{\mathbf{v}_1^s, \dots, \mathbf{v}_K^s\}$ and $\{\mathbf{v}_1^t, \dots, \mathbf{v}_K^t\}$.
 - 3: calculate singular values $\{\sigma_1, \dots, \sigma_K\}$ according to Equation (21).
 - 4: calculate embedding matrices \mathbf{U}^s and \mathbf{U}^t according to Equation (19) and (20).
-

Experiment Setting: Datasets

Datasets:

- ❑ Synthetic (Syn): generate using Forest Fire Model
- ❑ Cora¹: citation network of academic papers
- ❑ SN-Twitter²: Twitter Social Network
- ❑ SN-TWeibo³: Tencent Weibo Social Network

Statistics of datasets. $|V|$ denotes the number of vertexes and $|E|$ denotes the number of edges.

	Syn	Cora	SN-Twitter	SN-TWeibo
$ V $	10,000	23166	465,017	1,944,589
$ E $	144,555	91500	834,797	50,655,143

¹http://konect.uni-koblenz.de/networks/subelj_cora

²http://konect.uni-koblenz.de/networks/munmun_twitter_social

³<http://www.kddcup2012.org/c/kddcup2012-track1/data>

Experiment Setting: Task

- ❑ Approximation accuracy
 - ❑ **High-order proximity approximation:** how well can embedded vectors approximate high-order proximity
- ❑ Reconstruction
 - ❑ **Graph Reconstruction:** how well can embedded vectors reconstruct training sets
- ❑ Inference:
 - ❑ **Link Prediction:** how well can embedded vectors predict missing edges
 - ❑ **Vertex Recommendation:** how well can embedded vectors recommend vertices for each node

Experiment Setting: Baseline

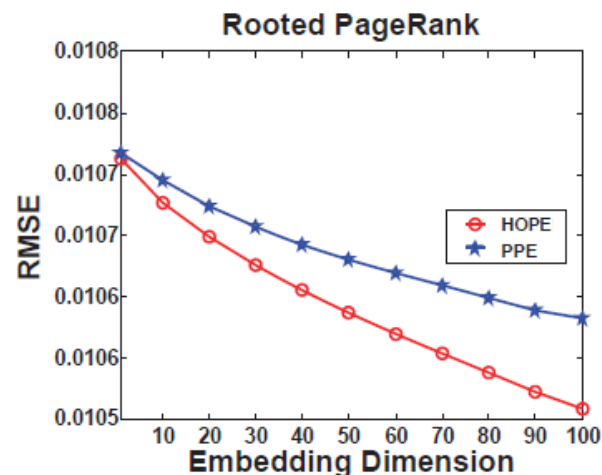
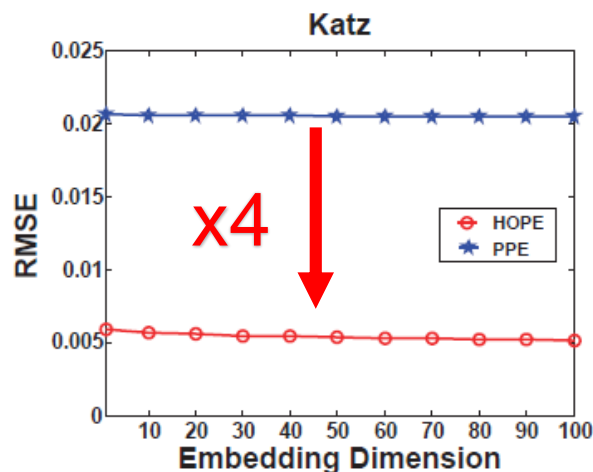
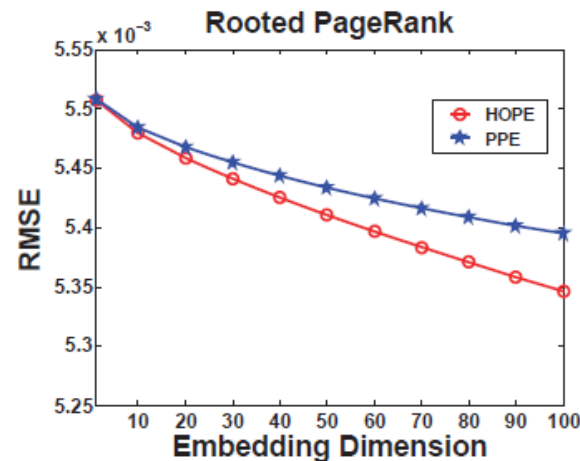
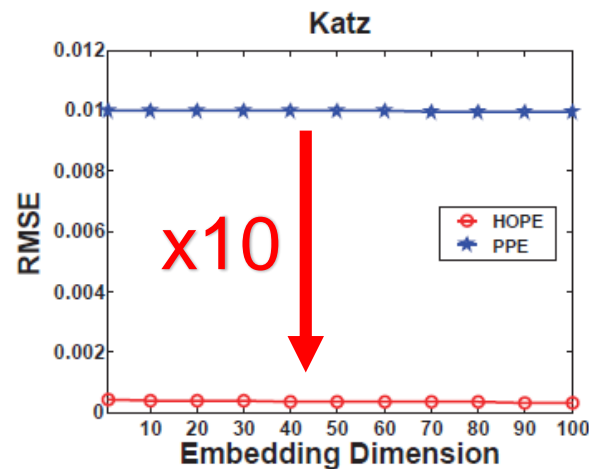
□ Graph embedding

- **PPE**: approximate high-order proximity by selecting landmarks and using sub-block of the proximity matrix
- **LINE**: preserves first-order and second-order proximity, called LINE1 and LINE2 respectively
- **DeepWalk**: random walk on graphs + SkipGram Model

□ Task Specific:

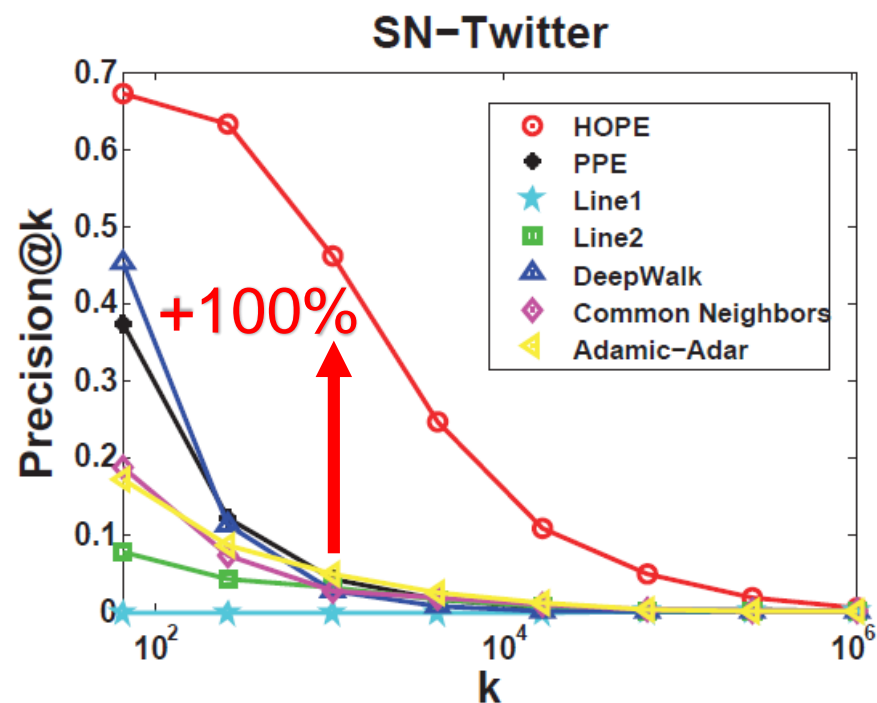
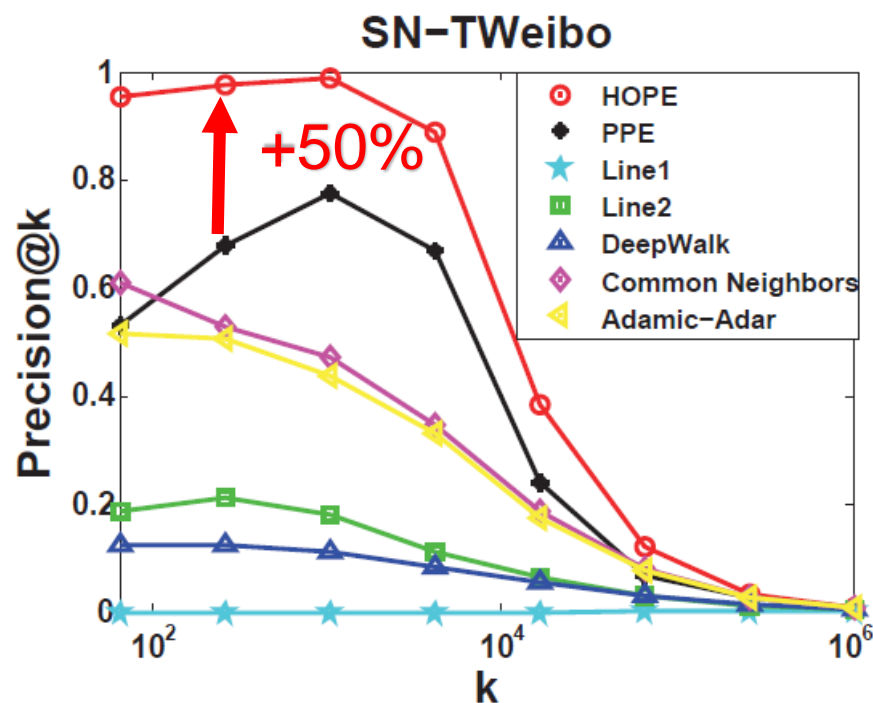
- **Common Neighbors**: used for link prediction and vertex recommendation task
- **Adamic-Adar**: used for link prediction and vertex recommendation task

Experiment result: high-order Proximity Approximation



Conclusion: HOPE achieves **much smaller RMSE** error
 -> generalized SVD achieves a **good approximation**

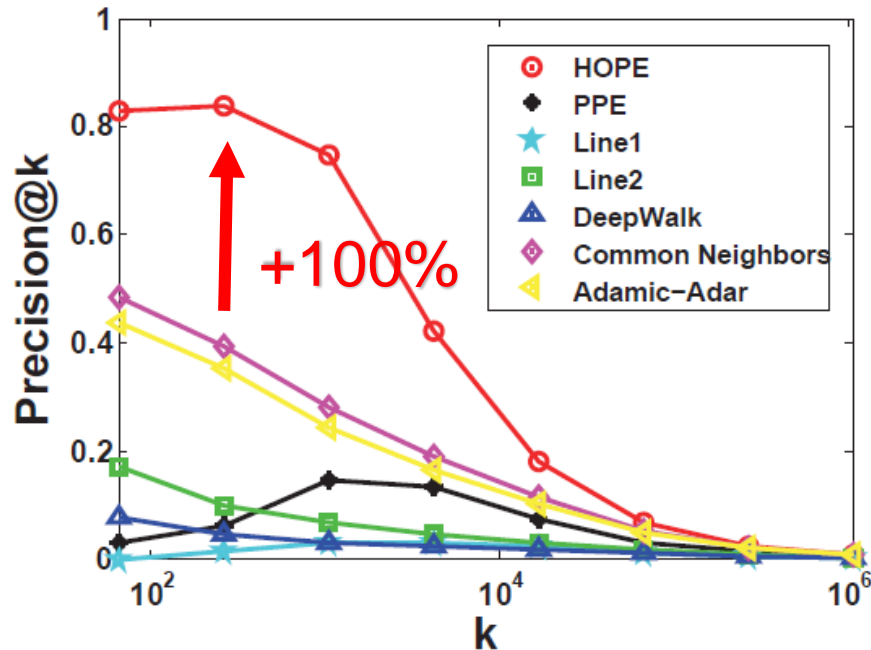
Experiment result: Graph Reconstruction



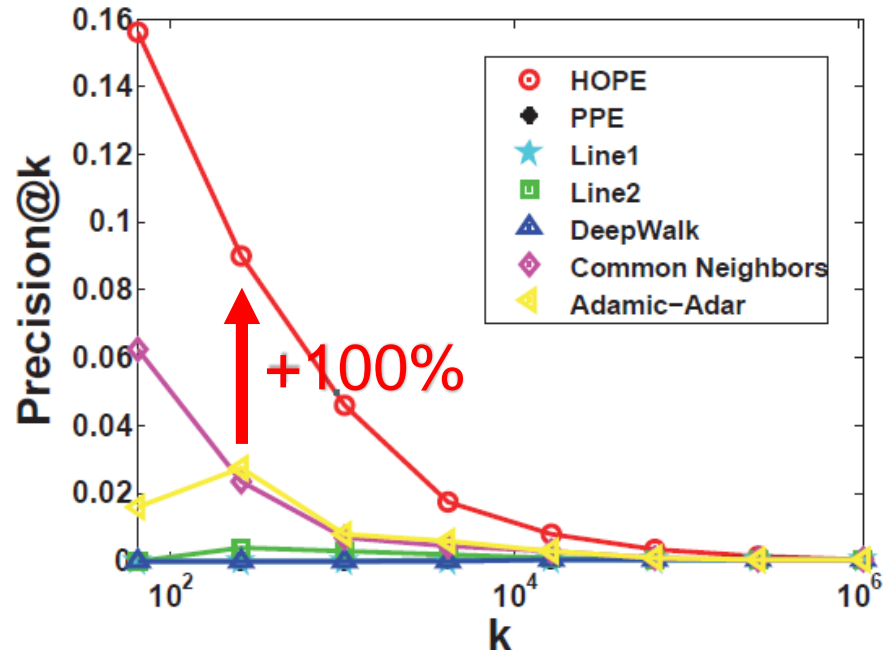
Conclusion: HOPE successfully capture the information of **training sets**

Experiment result: Link Prediction

SN-TWeibo



SN-Twitter



Conclusion: HOPE has good **inference** ability

-> based on **asymmetric transitivity**

Experiment result: Vertex Recommendation

+88% improvement

+81% improvement

Method	SN-TWebio			SN-Twitter		
	MAP@10	MAP@50	MAP@100	MAP@10	MAP@50	MAP@100
HOPE	0.2295	0.1869	0.169	0.1000	0.0881	0.0766
PPE	0.0928	0.0845	0.077	0.0061	0.0077	0.0081
LINE1	0	0	0.005	0.0209	0.0221	0.0221
LINE2	0.051	0.051	0.048	0.0044	0.0043	0.0035
DeepWalk	0.0635	0.0583	0.004	0.0006	0.0008	0.001
Common Neighbors	0.1217	0.1031	0.155	0.0394	0.0379	0.0369
Adamic-Adar	0.1173	0.0990	0.156	0.0455	0.0442	0.0423

Conclusion: HOPE significantly outperforms **all state-of-the-art baselines** on **all these experiments**

Conclusion

- ❑ Directed graph embedding:
 - ❑ **High-order Proximity \rightarrow Asymmetric Transitivity**
- ❑ Derivation of a **general form** for high-order proximities, and solution with **generalized SVD**
 - ❑ Covering multiple commonly used high order proximity
 - ❑ **Time complexity linear** w.r.t. graph size
 - ❑ **Theoretically guaranteed** accuracy.
- ❑ Extensive experiments on several datasets
 - ❑ Outperforming all baselines in various applications.
 - ❑ **x4/x10** smaller approximation error for Katz
 - ❑ **+50% improvement** in reconstruction and inference

Thanks!

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