

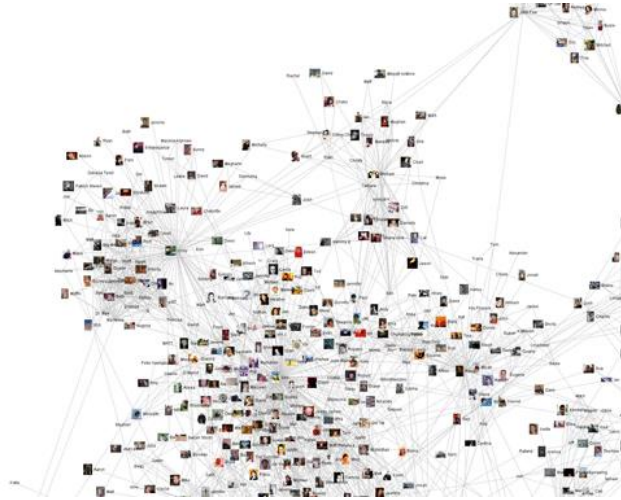
Representation Learning on Networks

Yuxiao Dong

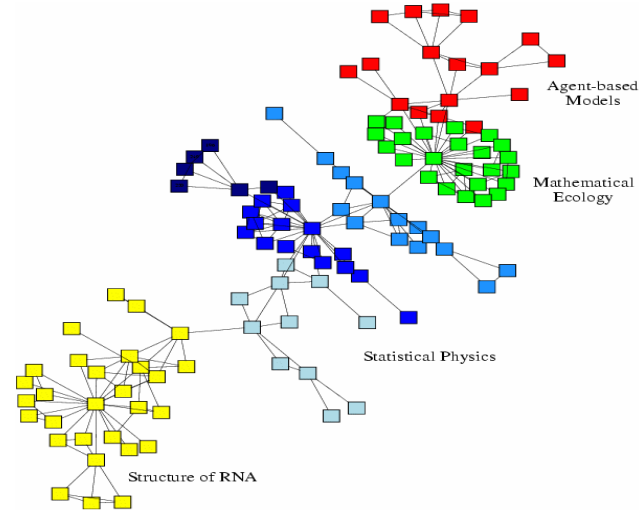
Microsoft Research, Redmond

Joint work with Jiezhong Qiu, Jie Zhang, Jie Tang (Tsinghua University)
Hao Ma (MSR & Facebook AI) and Kuansan Wang (MSR)

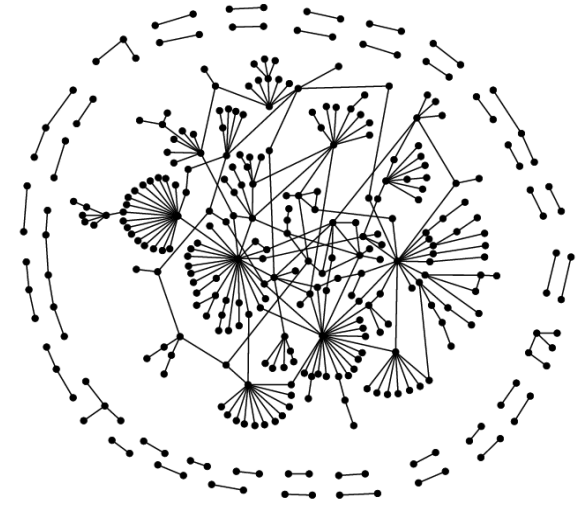
Networks



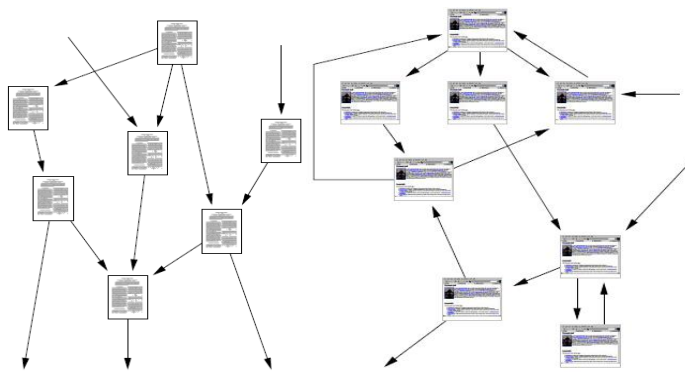
Social networks



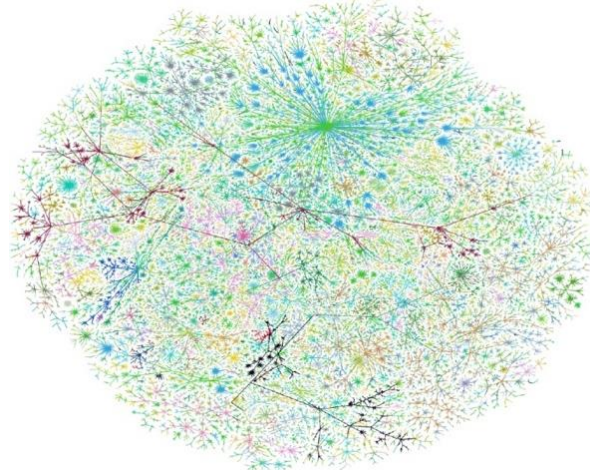
Economic networks



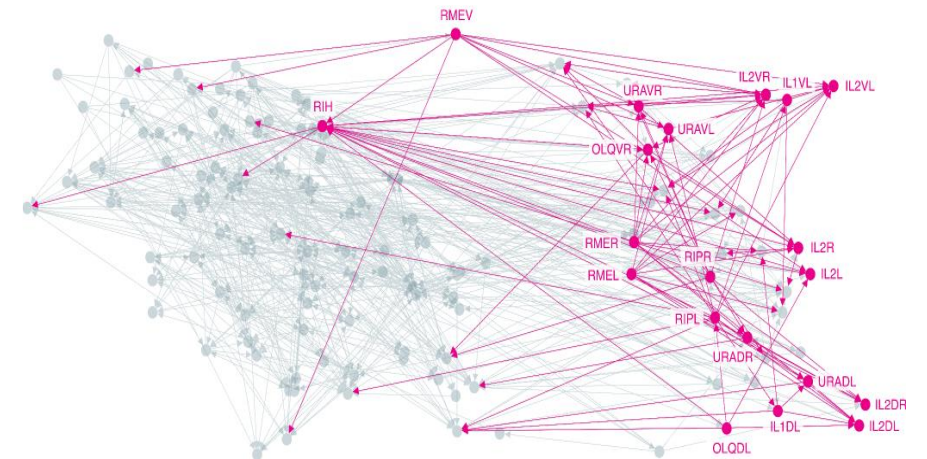
Biomedical networks



Information networks

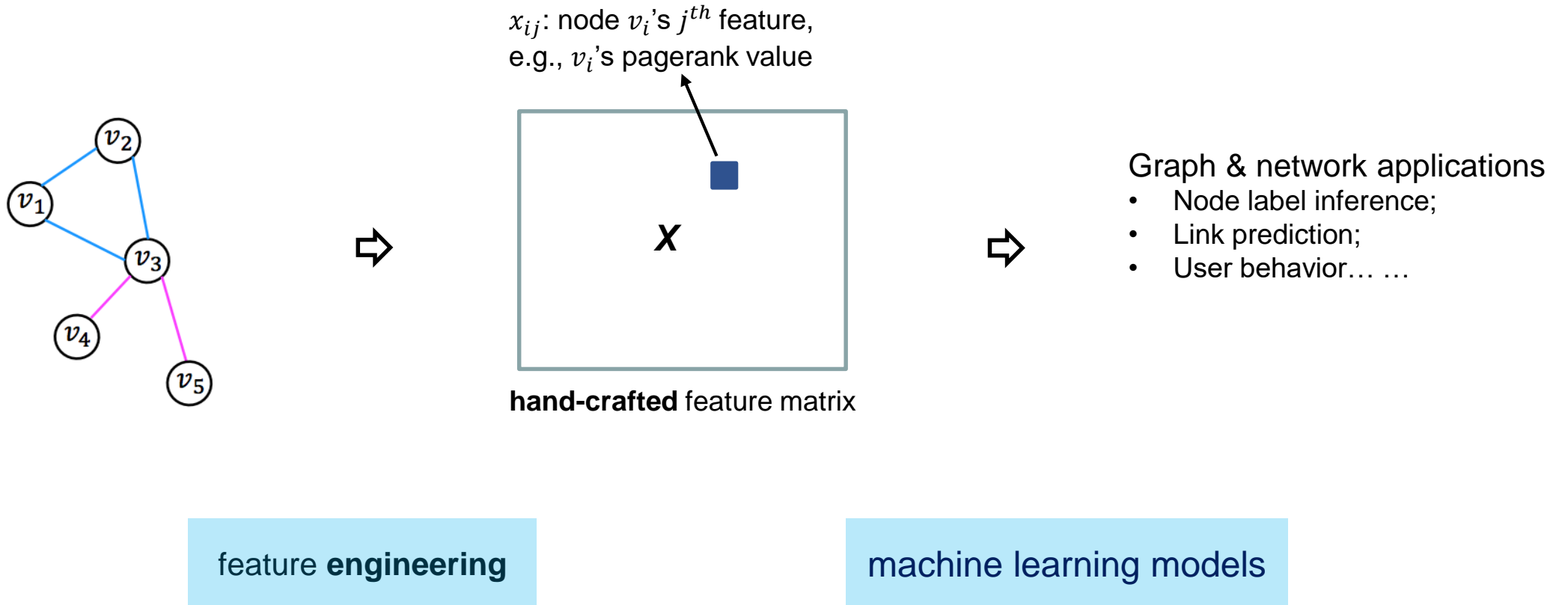


Internet

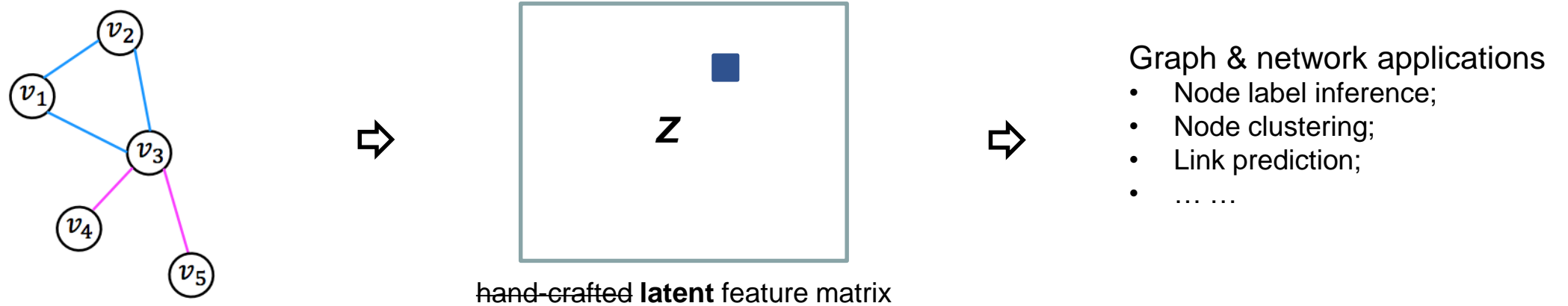


Networks of neurons

The Network & Graph Mining Paradigm



Representation Learning for Networks

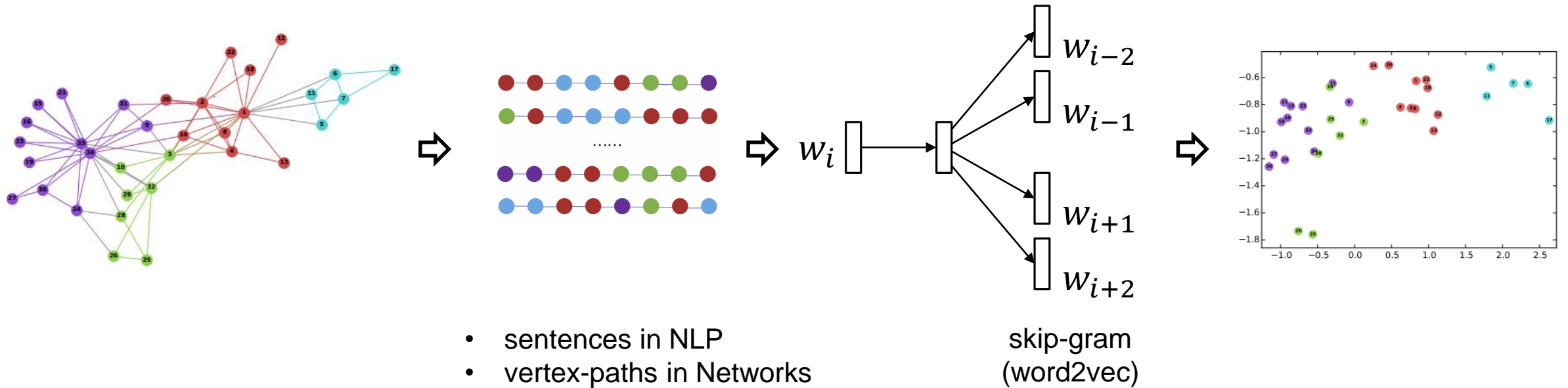


Feature engineering **learning**

machine learning models

- Input: a network $G = (V, E)$
- Output: $Z \in R^{|V| \times k}$, $k \ll |V|$, k -dim vector Z_v for each node v .

Network Embedding: Random Walk + Skip-Gram



Random Walk Strategies

- Random Walk
 - DeepWalk (walk length > 1)
 - LINE (walk length = 1)
- Biased Random Walk
 - 2nd order Random Walk
 - **node2vec**
 - Metapath guided Random Walk
 - **metapath2vec**

Application: Embedding Heterogeneous Academic Graph

225,572,477
Papers

244,499,947
Authors

664,891
Topics

4,397
Conferences

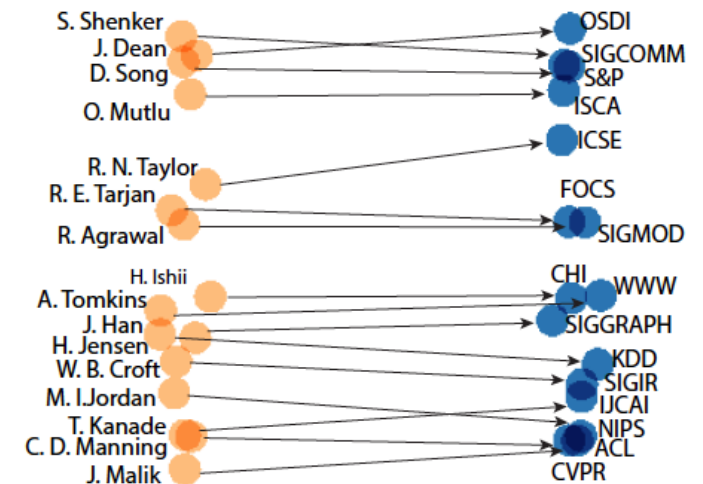
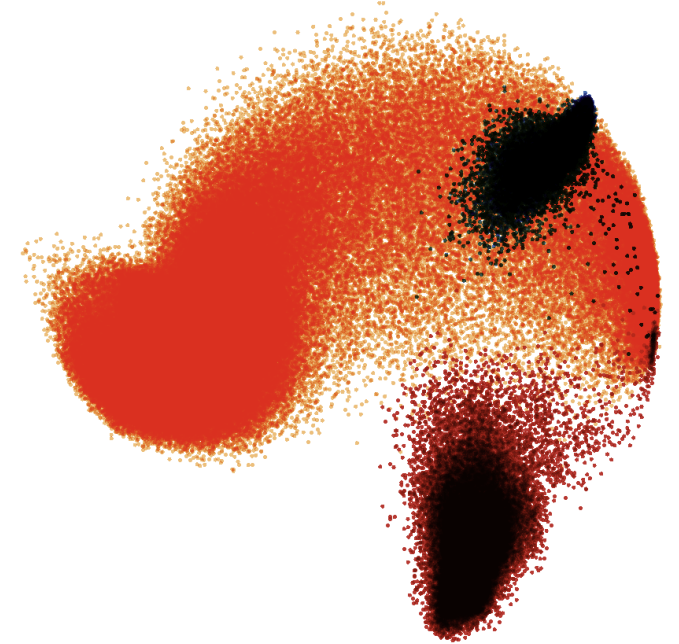
48,758
Journals

25,554
Institutions

Microsoft Academic Graph



metapath2vec



- <https://academic.microsoft.com/>
- <https://www.openacademic.ai/oag/>
- metapath2vec: scalable representation learning for heterogeneous networks. In *KDD* 2017.

Application 1: Related Venues

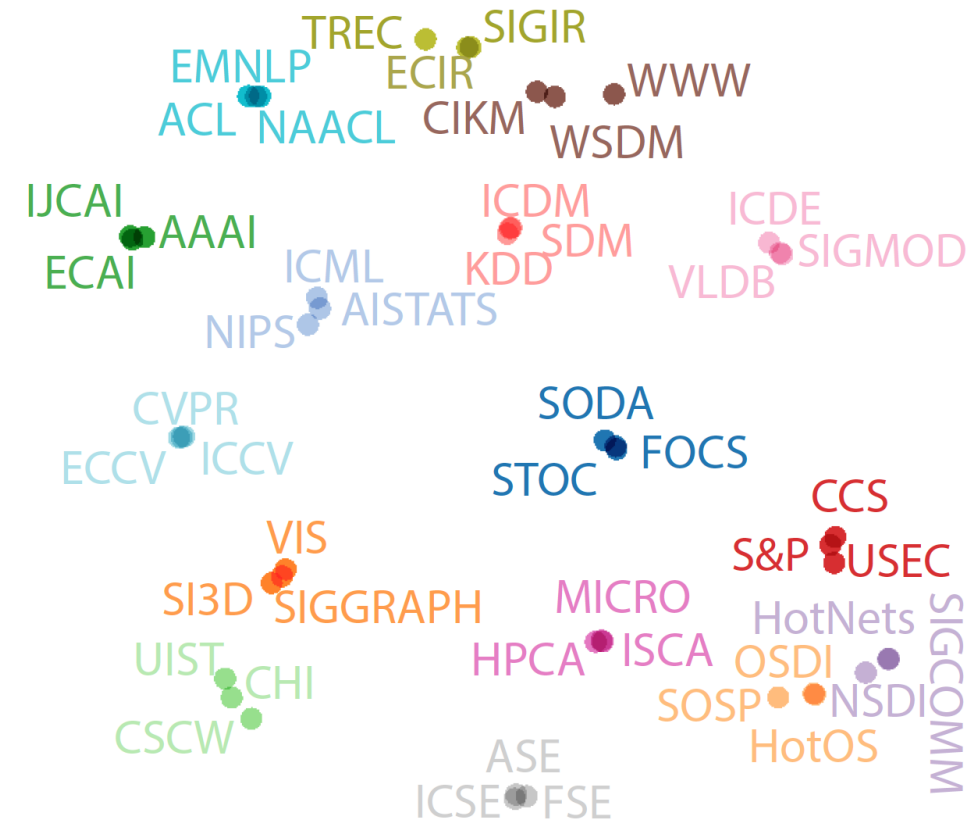
Science

Science, also widely referred to as Science Magazine, is the peer-reviewed academic journal of the American Association for the Advancement of Science (AAAS) and one of the world's top academic journals. It was first published in 1880, is currently circulated weekly and has a subscriber base of around 130,000. Because institutional subscriptions and online access serve a larger audience, its estimated readership is 570,400 people.

Website links: sciencemag.org, en.wikipedia.org

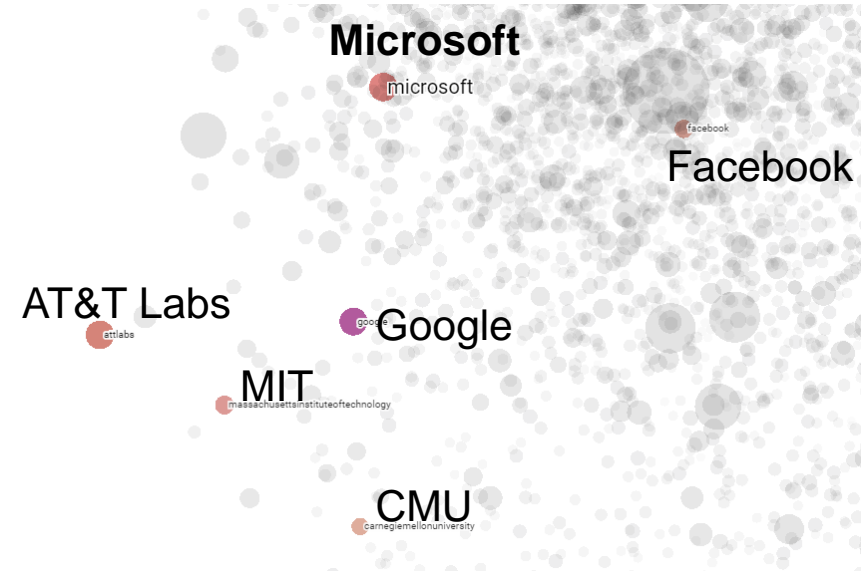
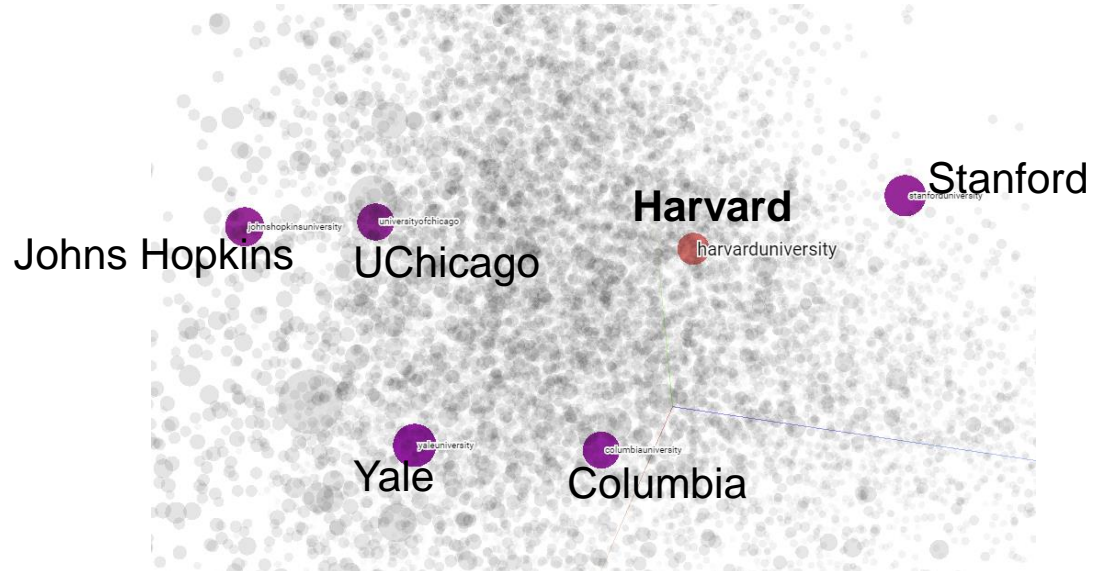
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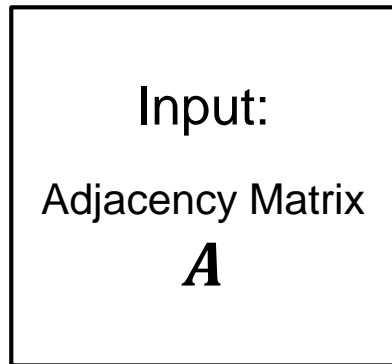
- <https://academic.microsoft.com/>
- <https://www.openacademic.ai/oag/>
- metapath2vec: scalable representation learning for heterogeneous networks. In *KDD* 2017.

Application 2: Similarity Search (Institution)

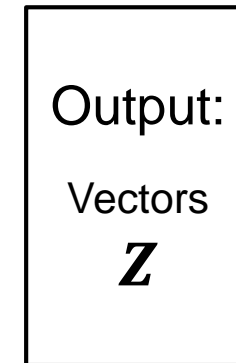


- <https://academic.microsoft.com/>
- <https://www.openacademic.ai/oag/>
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Network Embedding



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Unifying DeepWalk, LINE, PTE, & node2vec as Matrix Factorization

- DeepWalk $\log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$
- LINE $\log \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} \mathbf{A} \mathbf{D}^{-1} \right)$
- PTE $\log \left(\begin{bmatrix} \alpha \text{vol}(G_{\text{ww}}) (\mathbf{D}_{\text{row}}^{\text{ww}})^{-1} \mathbf{A}_{\text{ww}} (\mathbf{D}_{\text{col}}^{\text{ww}})^{-1} \\ \beta \text{vol}(G_{\text{dw}}) (\mathbf{D}_{\text{row}}^{\text{dw}})^{-1} \mathbf{A}_{\text{dw}} (\mathbf{D}_{\text{col}}^{\text{dw}})^{-1} \\ \gamma \text{vol}(G_{\text{lw}}) (\mathbf{D}_{\text{row}}^{\text{lw}})^{-1} \mathbf{A}_{\text{lw}} (\mathbf{D}_{\text{col}}^{\text{lw}})^{-1} \end{bmatrix} \right) - \log b$
- node2vec $\log \left(\frac{\frac{1}{2T} \sum_{r=1}^T (\sum_u \mathbf{X}_{w,u} \mathbf{P}_{c,w,u}^r + \sum_u \mathbf{X}_{c,u} \mathbf{P}_{w,c,u}^r)}{b (\sum_u \mathbf{X}_{w,u}) (\sum_u \mathbf{X}_{c,u})} \right)$

\mathbf{A} Adjacency matrix

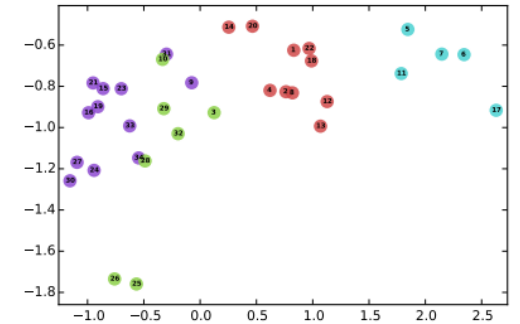
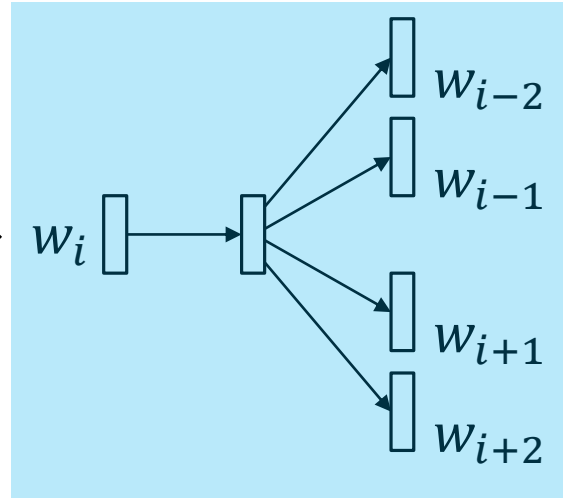
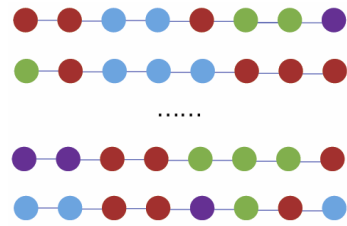
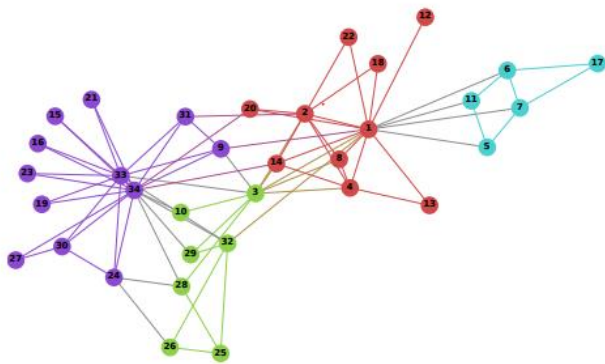
\mathbf{D} Degree matrix

$$\text{vol}(G) = \sum_i \sum_j A_{ij}$$

b : #negative samples

T : context window size

Understanding Random Walk + Skip Gram



$G = (V, E)$

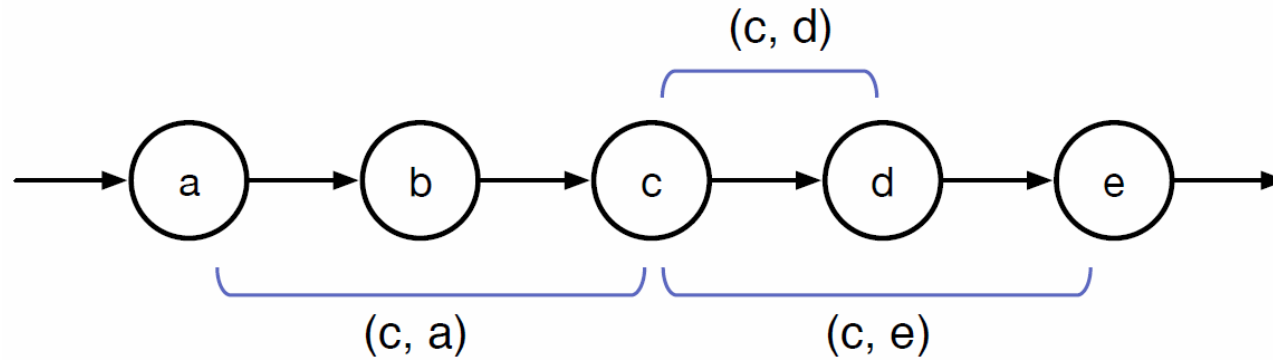
- Adjacency matrix A
- Degree matrix D
- Volume of G : $vol(G)$

?

$$\log\left(\frac{\#(w, c)|\mathcal{D}|}{b\#(w)\#(c)}\right)$$

- (w, c) : co-occurrence of w & c
- $\#(w)$: occurrence of node w
- $\#(c)$: occurrence of context c
- \mathcal{D} : node-context pair (w, c) multi-set
- $|\mathcal{D}|$: number of node-context pairs

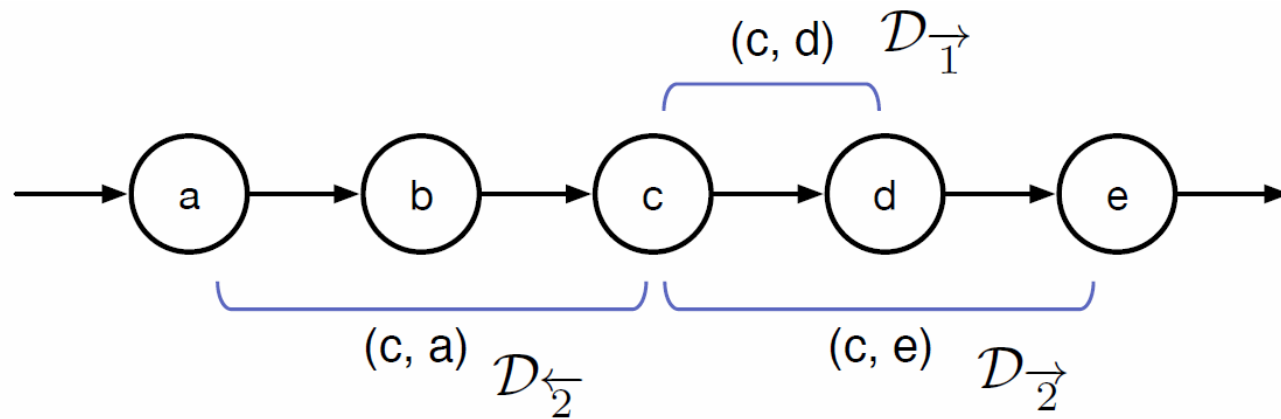
Understanding Random Walk + Skip Gram



$$\log\left(\frac{\#(w, c)|\mathcal{D}|}{b\#(w)\#(c)}\right)$$

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Understanding Random Walk + Skip Gram



$$\log\left(\frac{\#(w, c)|\mathcal{D}|}{b\#(w)\#(c)}\right)$$

- (w, c) : co-occurrence of w & c
- (w) : occurrence of node w
- (c) : occurrence of context c
- \mathcal{D} : node-context pair (w, c) multi-set
- $|\mathcal{D}|$: number of node-context pairs

- Partition the multiset \mathcal{D} into several sub-multisets according to the way in which each node and its context appear in a random walk node sequence.
- More formally, for $r = 1, 2, \dots, T$, we define

$$\mathcal{D}_{\vec{r}} = \{(w, c) : (w, c) \in \mathcal{D}, w = w_j^n, c = w_{j+r}^n\}$$

$$\mathcal{D}_{\overleftarrow{r}} = \{(w, c) : (w, c) \in \mathcal{D}, w = w_{j+r}^n, c = w_j^n\}$$

Distinguish direction and distance

Understanding Random Walk + Skip Gram

$$\log \left(\frac{\#(w, c) |\mathcal{D}|}{b \#(w) \cdot \#(c)} \right) = \log \left(\frac{\frac{\#(w, c)}{|\mathcal{D}|}}{b \frac{\#(w)}{|\mathcal{D}|} \frac{\#(c)}{|\mathcal{D}|}} \right)$$

the length of random walk $L \rightarrow \infty$

- (w, c) : co-occurrence of w & c
- \mathcal{D} : (w, c) multi-set

$$\frac{\#(w, c)}{|\mathcal{D}|} = \frac{1}{2T} \sum_{r=1}^T \left(\frac{\#(w, c)_{\vec{r}}}{|\mathcal{D}_{\vec{r}}|} + \frac{\#(w, c)_{\leftarrow r}}{|\mathcal{D}_{\leftarrow r}|} \right)$$

$$\frac{\#(w, c)_{\vec{r}}}{|\mathcal{D}_{\vec{r}}|} \xrightarrow{p} \frac{d_w}{\text{vol}(G)} (\mathbf{P}^r)_{w,c}$$

$$\frac{\#(w, c)_{\leftarrow r}}{|\mathcal{D}_{\leftarrow r}|} \xrightarrow{p} \frac{d_c}{\text{vol}(G)} (\mathbf{P}^r)_{c,w}$$

$$\frac{\#(w, c)}{|\mathcal{D}|} \xrightarrow{p} \frac{1}{2T} \sum_{r=1}^T \left(\frac{d_w}{\text{vol}(G)} (\mathbf{P}^r)_{w,c} + \frac{d_c}{\text{vol}(G)} (\mathbf{P}^r)_{c,w} \right)$$

$$\mathbf{P} = \mathbf{D}^{-1} \mathbf{A}$$

$$\frac{\#(w)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_w}{\text{vol}(G)}$$

$$\frac{\#(c)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_c}{\text{vol}(G)}$$

Understanding Random Walk + Skip Gram

$$\log \left(\frac{\#(w, c) |\mathcal{D}|}{b \#(w) \cdot \#(c)} \right) = \log \left(\frac{\frac{\#(w, c)}{|\mathcal{D}|}}{b \frac{\#(w)}{|\mathcal{D}|} \frac{\#(c)}{|\mathcal{D}|}} \right)$$

the length of random walk $L \rightarrow \infty$

$$\frac{\#(w, c)}{|\mathcal{D}|} \xrightarrow{p} \frac{1}{2T} \sum_{r=1}^T \left(\frac{d_w}{\text{vol}(G)} (P^r)_{w,c} + \frac{d_c}{\text{vol}(G)} (P^r)_{c,w} \right)$$

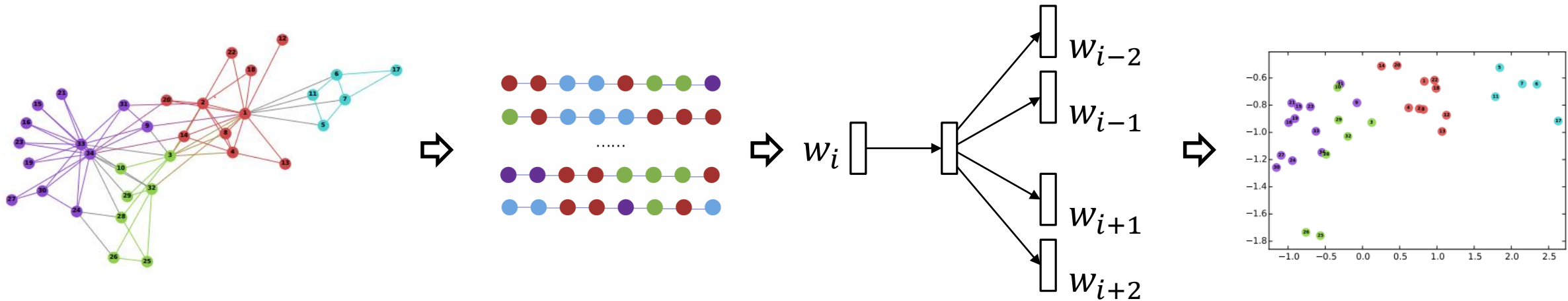
$$\frac{\#(w)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_w}{\text{vol}(G)} \qquad \frac{\#(c)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_c}{\text{vol}(G)}$$

$P = D^{-1}A$

$$\frac{\#(w, c) |\mathcal{D}|}{\#(w) \cdot \#(c)} = \frac{\frac{\#(w, c)}{|\mathcal{D}|}}{\frac{\#(w)}{|\mathcal{D}|} \cdot \frac{\#(c)}{|\mathcal{D}|}} \xrightarrow{p} \frac{\frac{1}{2T} \sum_{r=1}^T \left(\frac{d_w}{\text{vol}(G)} (P^r)_{w,c} + \frac{d_c}{\text{vol}(G)} (P^r)_{c,w} \right)}{\frac{d_w}{\text{vol}(G)} \cdot \frac{d_c}{\text{vol}(G)}}$$

$$= \text{vol}(G) \left(\frac{1}{T} \sum_{r=1}^T P^r \right) D^{-1}.$$

Understanding Random Walk + Skip Gram



DeepWalk is asymptotically and implicitly factorizing

$$\log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

\mathbf{A} Adjacency matrix

\mathbf{D} Degree matrix

$$\text{vol}(G) = \sum_i \sum_j A_{ij}$$

b : #negative samples

T : context window size

Unifying DeepWalk, LINE, PTE, & node2vec as Matrix Factorization

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- LINE $\log \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} \mathbf{A} \mathbf{D}^{-1} \right)$
- PTE $\log \left(\left[\begin{array}{c} \alpha \text{vol}(G_{\text{ww}}) (\mathbf{D}_{\text{row}}^{\text{ww}})^{-1} \mathbf{A}_{\text{ww}} (\mathbf{D}_{\text{col}}^{\text{ww}})^{-1} \\ \beta \text{vol}(G_{\text{dw}}) (\mathbf{D}_{\text{row}}^{\text{dw}})^{-1} \mathbf{A}_{\text{dw}} (\mathbf{D}_{\text{col}}^{\text{dw}})^{-1} \\ \gamma \text{vol}(G_{\text{lw}}) (\mathbf{D}_{\text{row}}^{\text{lw}})^{-1} \mathbf{A}_{\text{lw}} (\mathbf{D}_{\text{col}}^{\text{lw}})^{-1} \end{array} \right] \right) - \log b$
- node2vec $\log \left(\frac{\frac{1}{2T} \sum_{r=1}^T (\sum_u \mathbf{X}_{w,u} \mathbf{P}_{c,w,u}^r + \sum_u \mathbf{X}_{c,u} \mathbf{P}_{w,c,u}^r)}{b (\sum_u \mathbf{X}_{w,u}) (\sum_u \mathbf{X}_{c,u})} \right)$

NetMF: explicitly factorizing the DeepWalk matrix



DeepWalk is asymptotically and implicitly factorizing

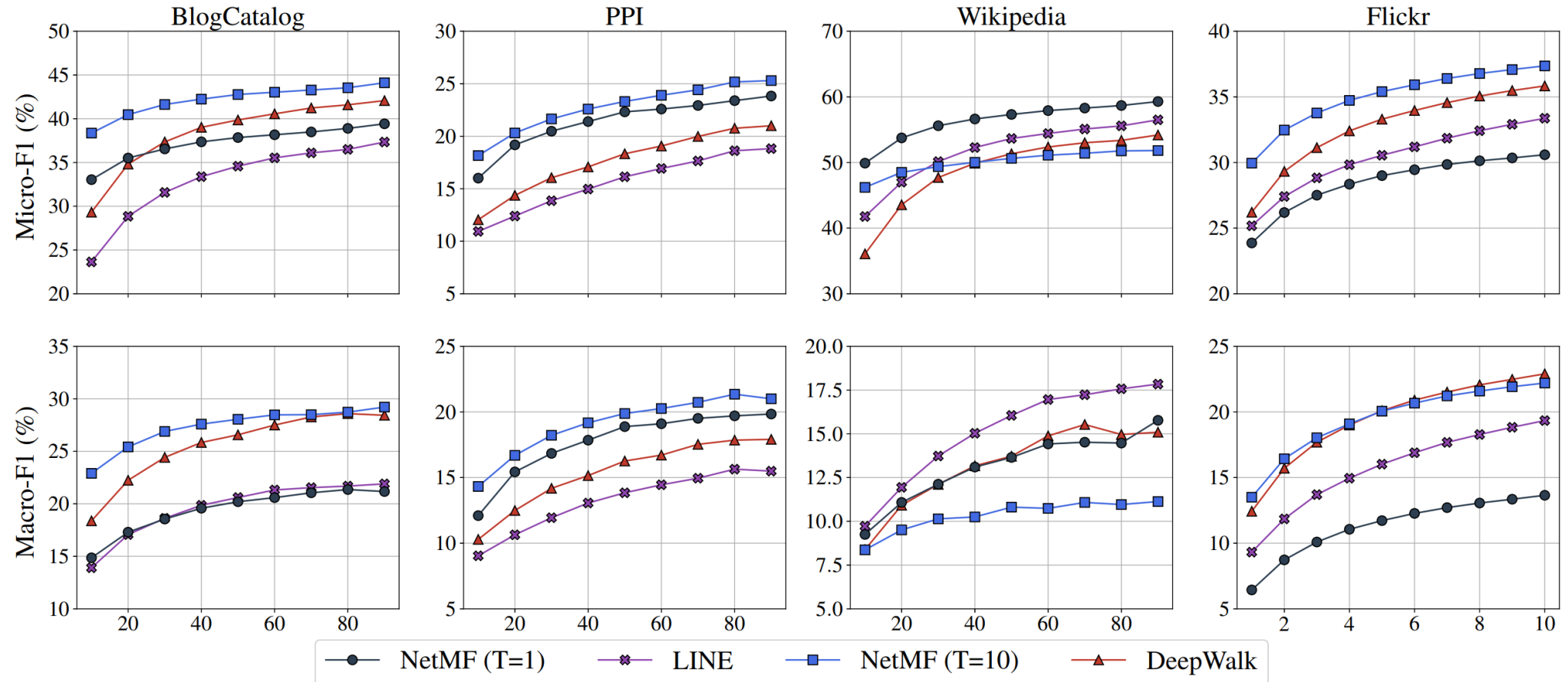
$$\log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

the NetMF algorithm

1. Construction
2. Factorization

$$\mathbf{S} = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

Results

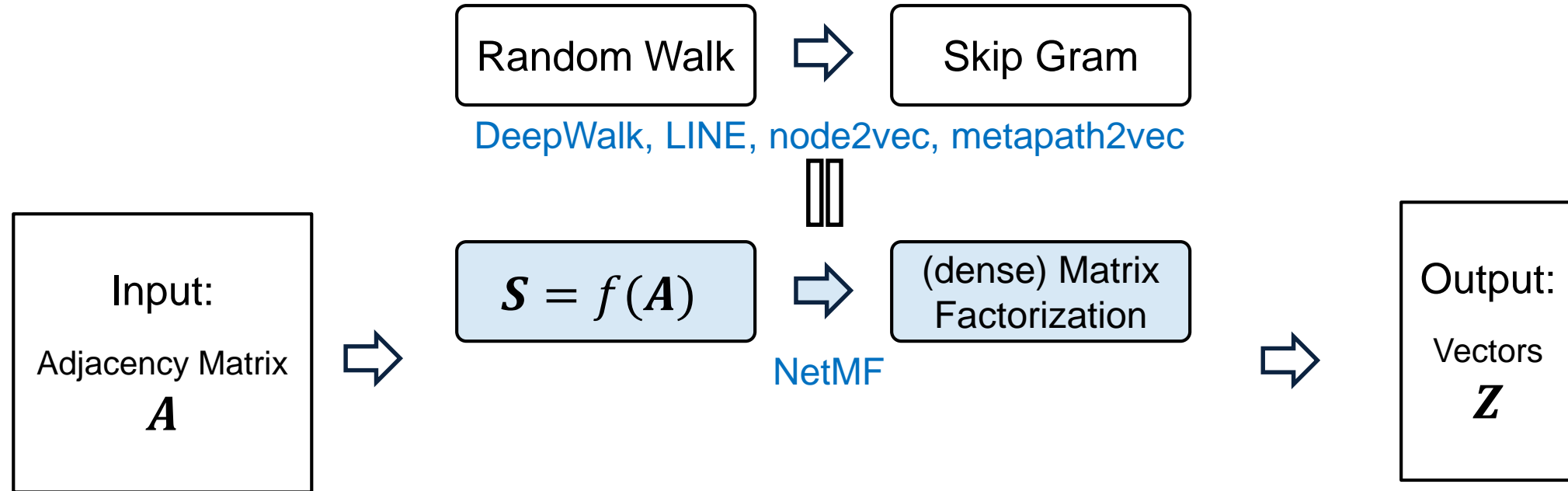


- Predictive performance on varying the ratio of training data;
- The x-axis represents the ratio of labeled data (%)

Results

Explicit matrix factorization (NetMF) offers performance gains over implicit matrix factorization (DeepWalk & LINE)

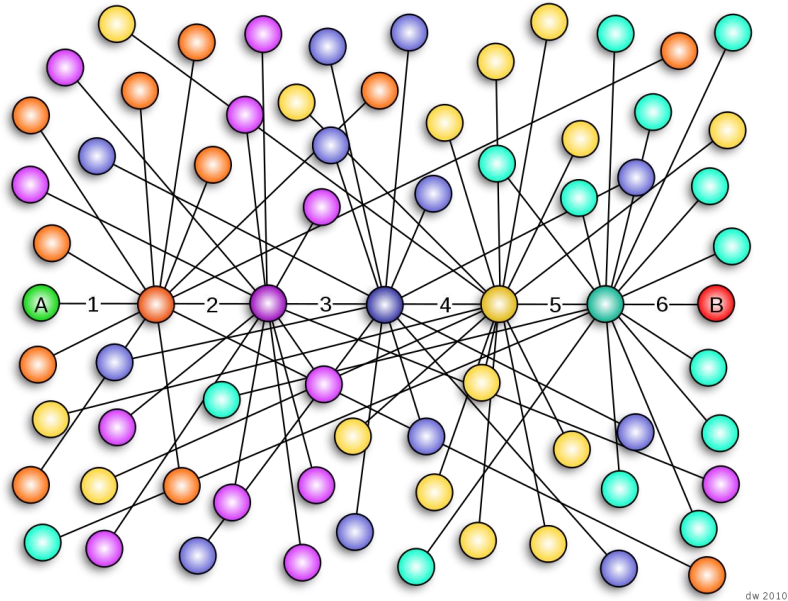
Network Embedding



Incorporate network structures A into the similarity matrix S , and then factorize S

$$f(A) = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (D^{-1} A)^r \right) D^{-1} \right)$$

Challenges



$$\Rightarrow \mathbf{S} = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (D^{-1} A)^r \right) D^{-1} \right) \text{dense}$$

NetMF is not practical for very large networks

NetMF

How can we solve this issue?

1. Construction
2. Factorization

$$\mathbf{S} = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

NetSMF--Sparse

How can we solve this issue?

1. **Sparse Construction**
2. **Sparse Factorization**

$$\mathbf{S} = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

Sparsify S

For random-walk matrix polynomial $L = D - \sum_{r=1}^T \alpha_r D (D^{-1} A)^r$

where $\sum_{r=1}^T \alpha_r = 1$ and α_r non-negative

One can construct a $(1 + \epsilon)$ -spectral sparsifier \tilde{L} with $O(n \log n \epsilon^{-2})$ non-zeros

in time $O(T^2 m \epsilon^{-2} \log^2 n)$

$O(T^2 m \epsilon^{-2} \log n)$ for undirected graphs

Suppose $G = (V, E, A)$ and $\tilde{G} = (V, \tilde{E}, \tilde{A})$ are two weighted undirected networks. Let $L = D_G - A$ and $\tilde{L} = D_{\tilde{G}} - \tilde{A}$ be their Laplacian matrices, respectively. We define G and \tilde{G} are $(1 + \epsilon)$ -spectrally similar if

$$\forall \mathbf{x} \in \mathbb{R}^n, (1 - \epsilon) \cdot \mathbf{x}^\top \tilde{L} \mathbf{x} \leq \mathbf{x}^\top L \mathbf{x} \leq (1 + \epsilon) \cdot \mathbf{x}^\top \tilde{L} \mathbf{x}.$$

- Dehua Cheng, Yu Cheng, Yan Liu, Richard Peng, and Shang-Hua Teng, Efficient Sampling for Gaussian Graphical Models via Spectral Sparsification, COLT 2015.
- Dehua Cheng, Yu Cheng, Yan Liu, Richard Peng, and Shang-Hua Teng. Spectral sparsification of random-walk matrix polynomials. arXiv:1502.03496.

Sparsify \mathbf{S}

For random-walk matrix polynomial $\mathbf{L} = \mathbf{D} - \sum_{r=1}^T \alpha_r \mathbf{D} (\mathbf{D}^{-1} \mathbf{A})^r$

where $\sum_{r=1}^T \alpha_r = 1$ and α_r non-negative

One can construct a $(1 + \epsilon)$ -spectral sparsifier $\tilde{\mathbf{L}}$ with $O(n \log n \epsilon^{-2})$ non-zeros

in time $O(T^2 m \epsilon^{-2} \log^2 n)$

$$\mathbf{S} = \log^{\circ} \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right)$$

$$\alpha_1 = \dots = \alpha_T = \frac{1}{T} \quad \Rightarrow \quad = \log^{\circ} \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} (\mathbf{D} - \mathbf{L}) \mathbf{D}^{-1} \right)$$

$$\approx \log^{\circ} \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} (\mathbf{D} - \tilde{\mathbf{L}}) \mathbf{D}^{-1} \right)$$

NetSMF --- Sparse

- ▶ Construct a random walk matrix polynomial sparsifier, $\tilde{\mathbf{L}}$
- ▶ Construct a NetMF matrix sparsifier.

$$\text{trunc_log}^\circ \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} (\mathbf{D} - \tilde{\mathbf{L}}) \mathbf{D}^{-1} \right)$$

- ▶ Factorize the constructed *sparse* matrix

	Time	Space
Step 1	$O(MT \log n)$ for weighted networks $O(MT)$ for unweighted networks	$O(M + n + m)$
Step 2	$O(M)$	$O(M + n)$
Step 3	$O(Md + nd^2 + d^3)$	$O(M + nd)$

NetSMF---bounded approximation error

$$\begin{aligned}
 & \log^\circ \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (\mathbf{D}^{-1} \mathbf{A})^r \right) \mathbf{D}^{-1} \right) \\
 &= \log^\circ \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} (\mathbf{D} - \mathbf{L}) \mathbf{D}^{-1} \right) \longrightarrow \mathbf{M} \\
 &\approx \log^\circ \left(\frac{\text{vol}(G)}{b} \mathbf{D}^{-1} (\mathbf{D} - \tilde{\mathbf{L}}) \mathbf{D}^{-1} \right) \longrightarrow \tilde{\mathbf{M}}
 \end{aligned}$$

Theorem

The singular value of $\tilde{\mathbf{M}} - \mathbf{M}$ satisfies

$$\sigma_i(\tilde{\mathbf{M}} - \mathbf{M}) \leq \frac{4\epsilon}{\sqrt{d_i d_{\min}}}, \forall i \in [n].$$

Theorem

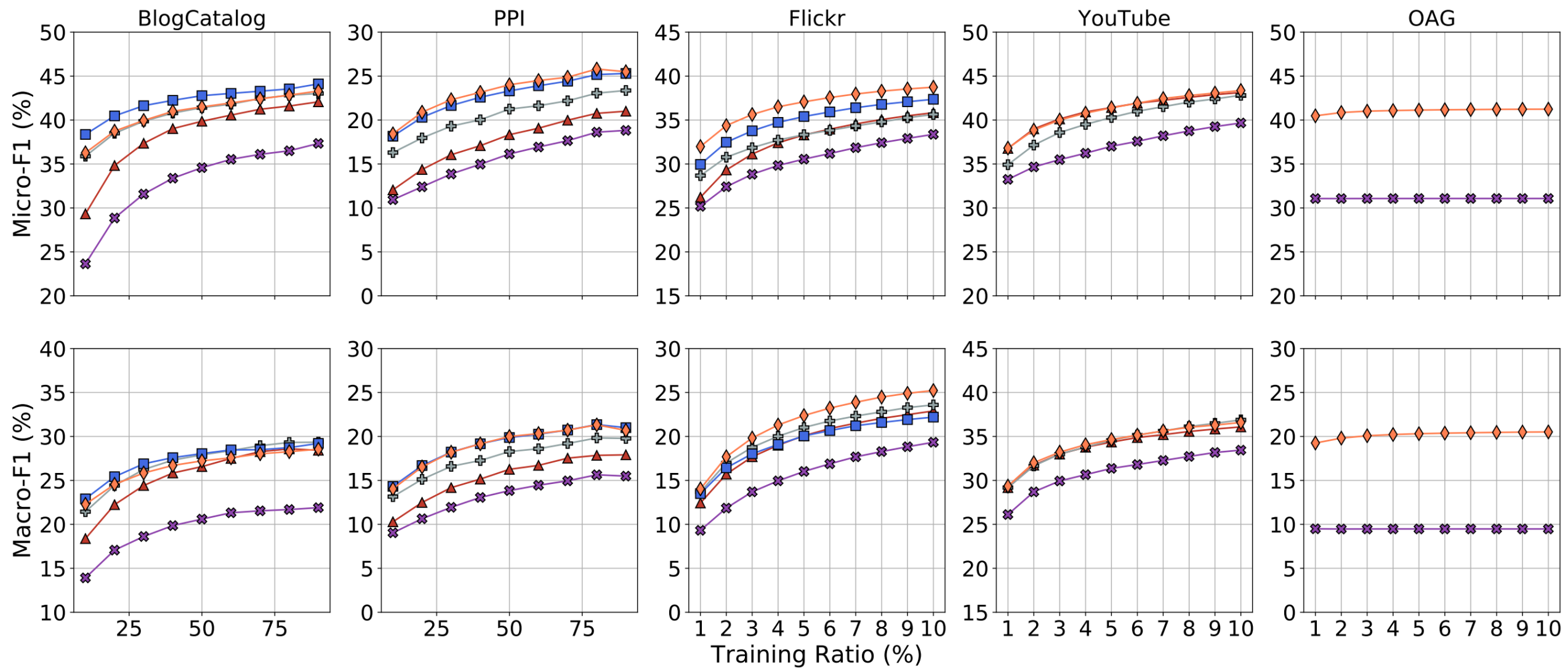
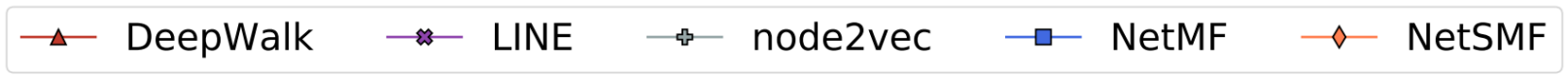
Let $\|\cdot\|_F$ be the matrix Frobenius norm. Then

$$\left\| \text{trunc_log}^\circ \left(\frac{\text{vol}(G)}{b} \tilde{\mathbf{M}} \right) - \text{trunc_log}^\circ \left(\frac{\text{vol}(G)}{b} \mathbf{M} \right) \right\|_F \leq \frac{4\epsilon \text{vol}(G)}{b\sqrt{d_{\min}}} \sqrt{\sum_{i=1}^n \frac{1}{d_i}}.$$

Dataset	BlogCatalog	PPI	Flickr	You Tube	OAG
$ V $	10,312	3,890	80,513	1,138,499	67,768,244
$ E $	333,983	76,584	5,899,882	2,990,443	895,368,962
#labels	39	50	195	47	19

#non-zeros

~4.5 Quadrillion → 45 Billion



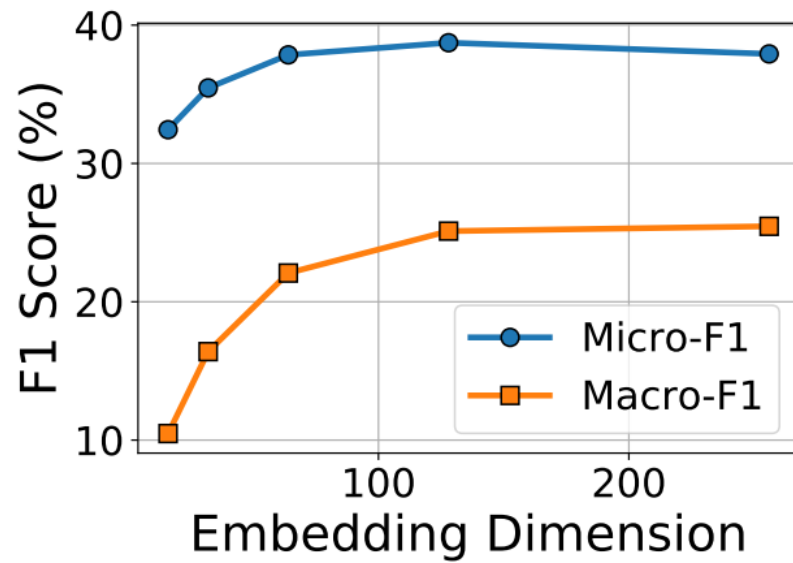
Effectiveness:

- (sparse MF)NetSMF \approx (explicit MF)NetMF $>$ (implicit MF) DeepWalk/LINE

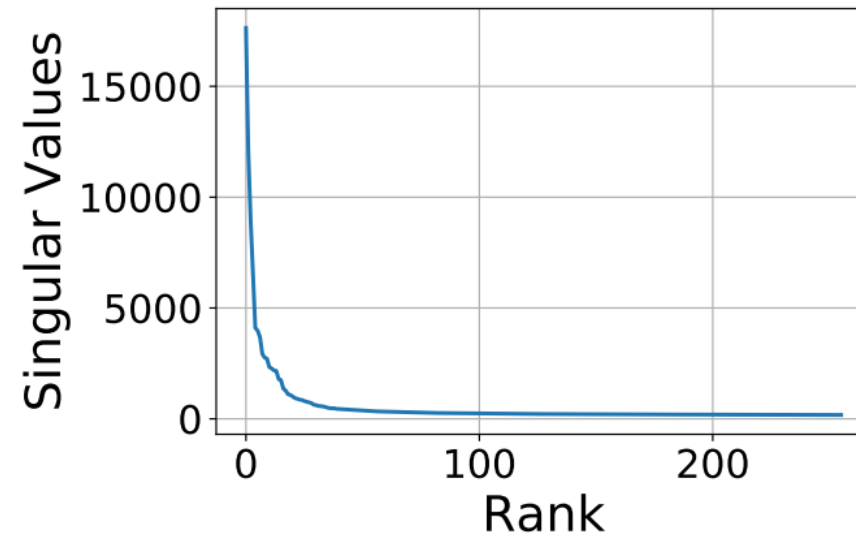
Efficiency:

- Sparse MF can handle billion-scale network embedding

Embedding Dimension?

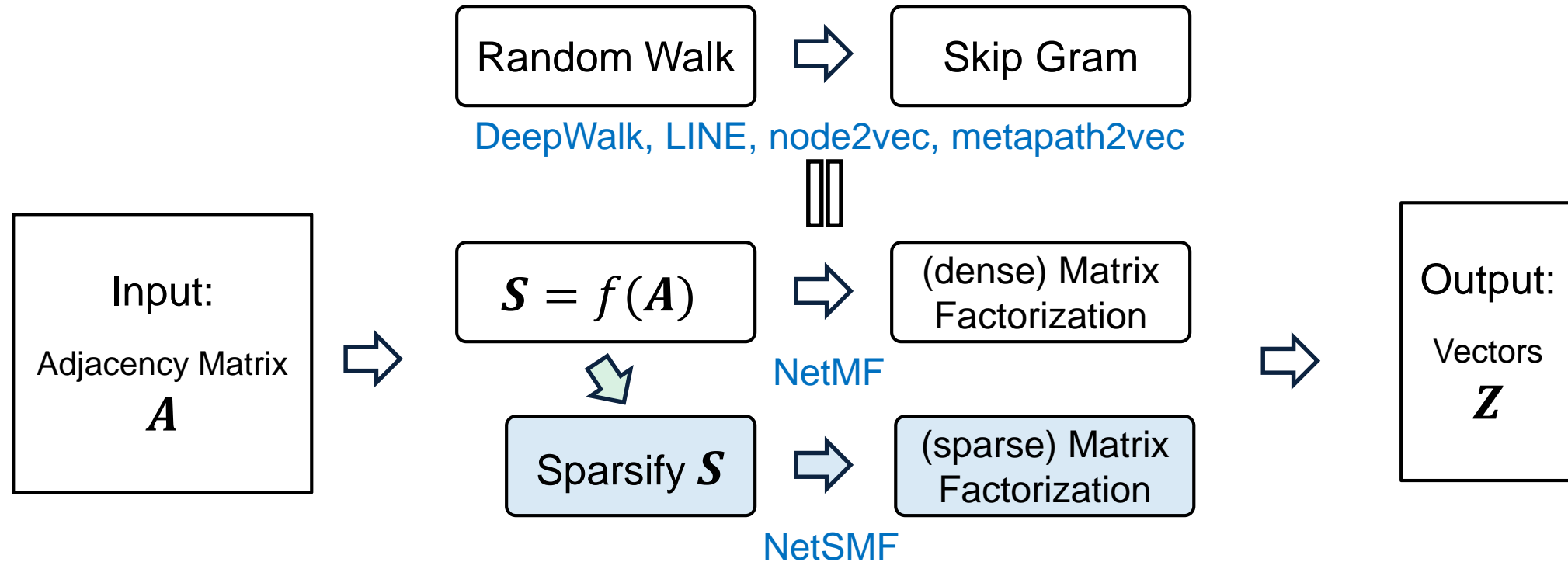


(a)



(b)

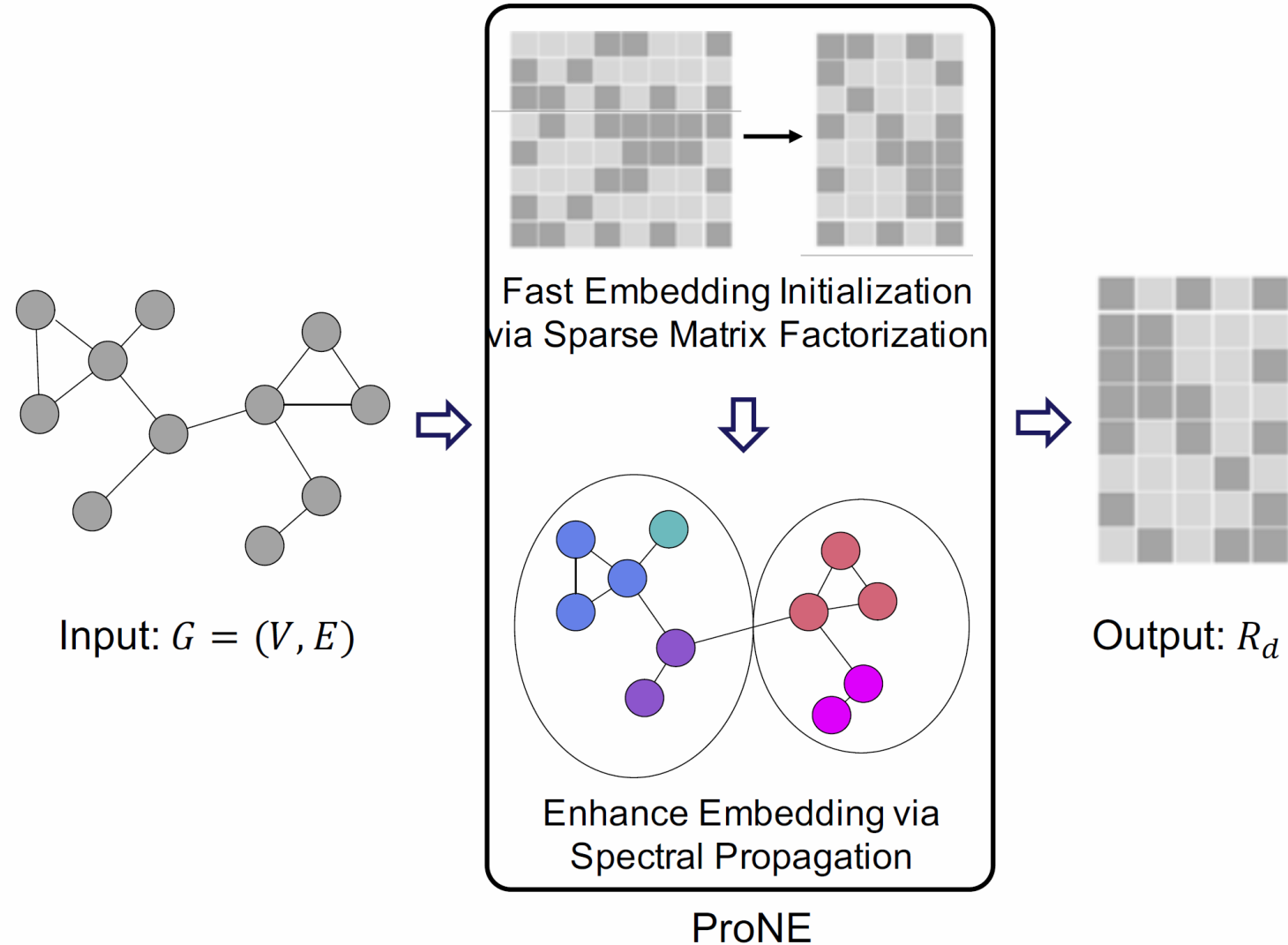
Network Embedding



Incorporate network structures A into the similarity matrix S , and then factorize S

$$f(A) = \log \left(\frac{\text{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^T (D^{-1} A)^r \right) D^{-1} \right)$$

ProNE: More fast & scalable network embedding



Embedding enhancement via spectral propagation

$$R_d \leftarrow D^{-1}A(I_n - \tilde{L}) R_d$$

$\tilde{L} = Ug(\Lambda)U^T$ is the spectral filter of $L = I_n - D^{-1}A$

$D^{-1}A(I_n - \tilde{L})$ is $D^{-1}A$ modulated by the filter in the spectrum

The idea of **Graph Neural Networks**

Performance

<i>Dataset</i>	20 Threads			1 Thread
	<i>DeepWalk</i>	<i>LINE</i>	<i>node2vec</i>	<i>ProNE</i>
<i>PPI</i>	272	70	828	3
<i>Wiki</i>	494	87	939	6
<i>BlogCatalog</i>	1,231	185	3,533	21
<i>DBLP</i>	3,825	1,204	4,749	24
<i>Youtube</i>	68,272	5,890	>5days	627

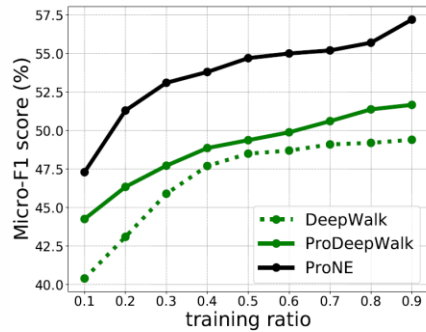
19hours
98mins
10mins

Dataset	training ratio	0.01	0.03	0.05	0.07	0.09
DBLP	DeepWalk	49.3	55.0	57.1	57.9	58.4
	LINE	48.7	52.6	53.5	54.1	54.5
	node2vec	48.9	55.1	57.0	58.0	58.4
	GraRep	50.5	52.6	53.2	53.5	53.8
	HOPE	52.2	55.0	55.9	56.3	56.6
	ProNE (SMF)	50.8	54.9	56.1	56.7	57.0
Youtube	ProNE	48.8	56.2	58.0	58.8	59.2
	($\pm\sigma$)	(± 1.0)	(± 0.5)	(± 0.2)	(± 0.2)	(± 0.1)
	DeepWalk	38.0	40.1	41.3	42.1	42.8
	LINE	33.2	35.5	37.0	38.2	39.3
	ProNE (SMF)	36.5	40.2	41.2	41.7	42.1
	ProNE	38.2	41.4	42.3	42.9	43.3
	($\pm\sigma$)	(± 0.8)	(± 0.3)	(± 0.2)	(± 0.2)	(± 0.2)

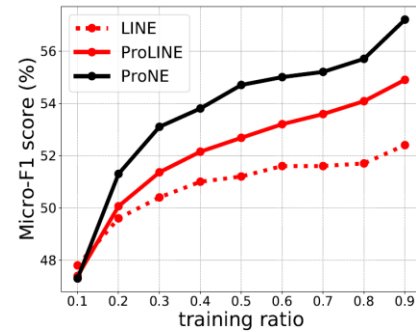
**ProNE offers 10-400X speedups
(1 thread vs 20 threads)**

**ProNE embeds 100,000,000 nodes by 1 thread:
29 hours with performance superiority**

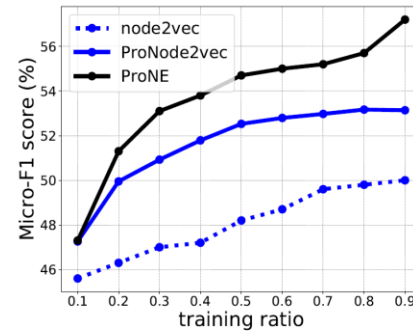
A general embedding enhancement framework



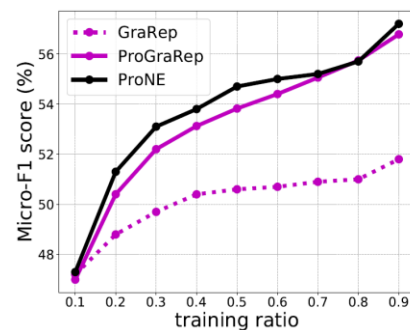
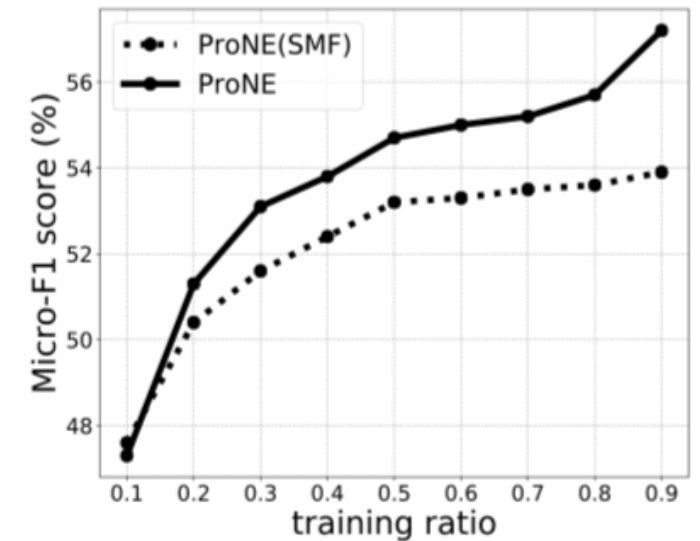
(a) ProDeepWalk



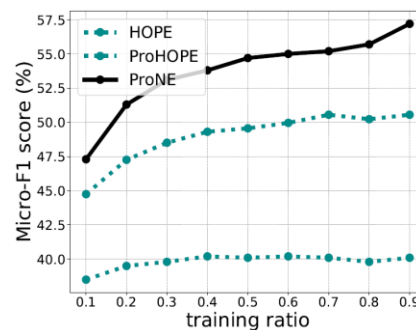
(b) ProLINE



(c) ProNode2vec

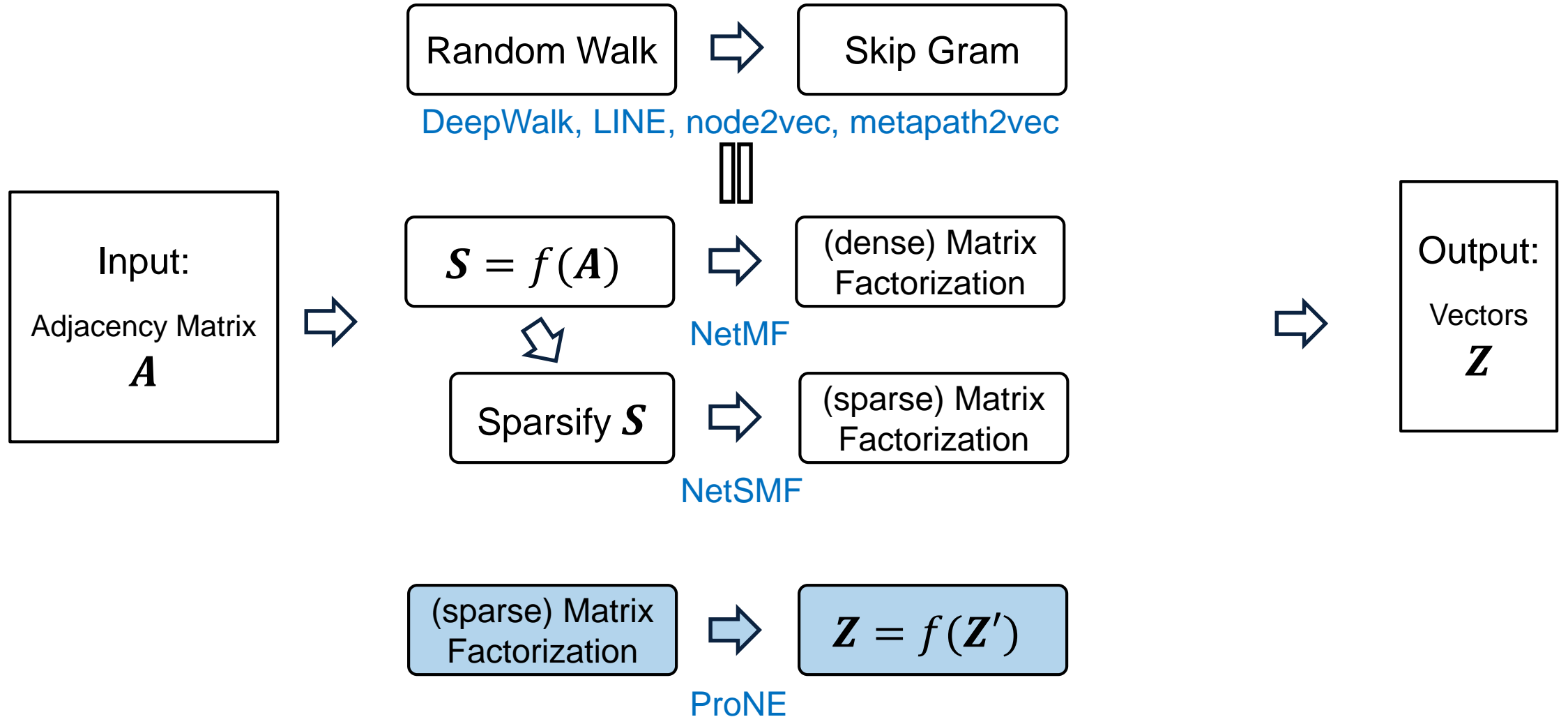


(d) ProGraRep



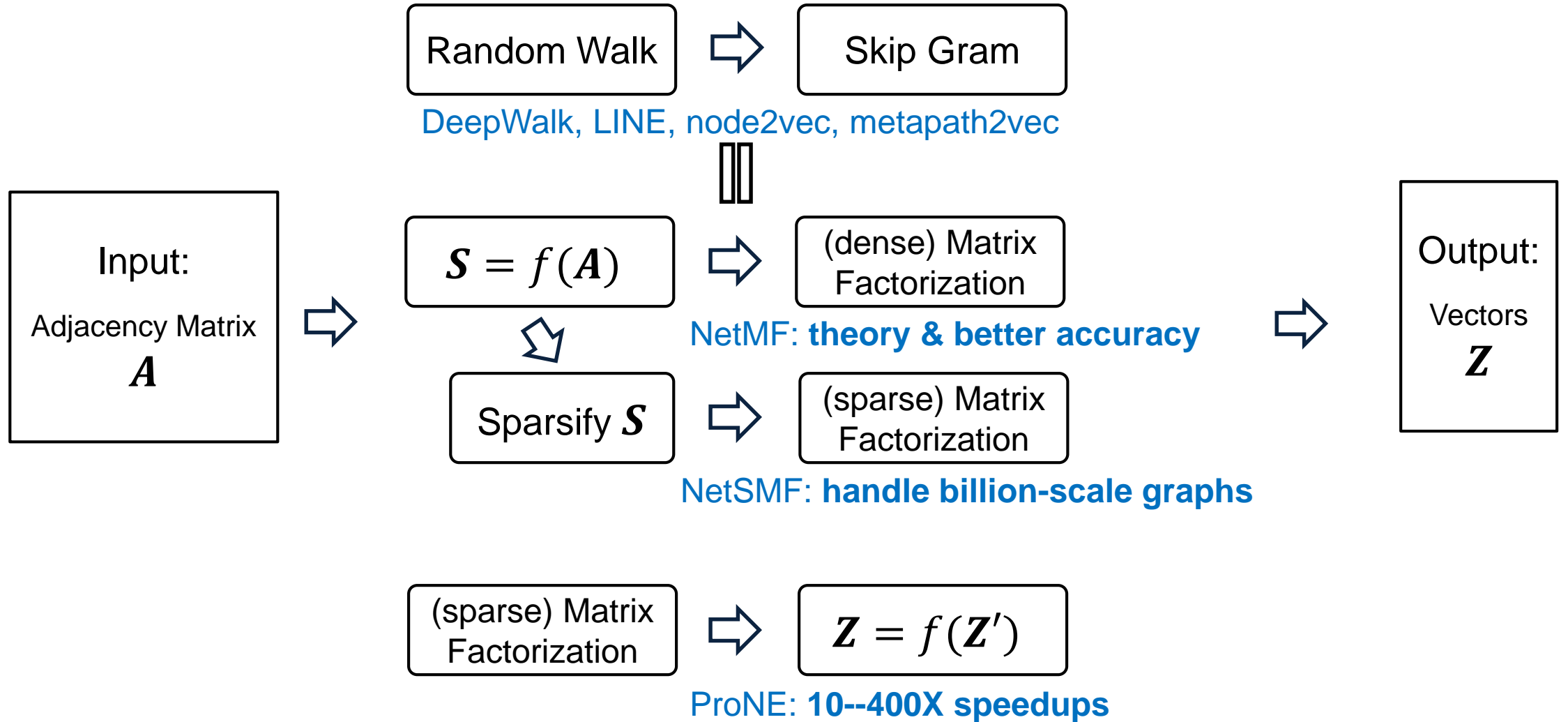
(e) ProHOPE

Network Embedding



Factorize A , and then incorporate network structures via spectral propagation

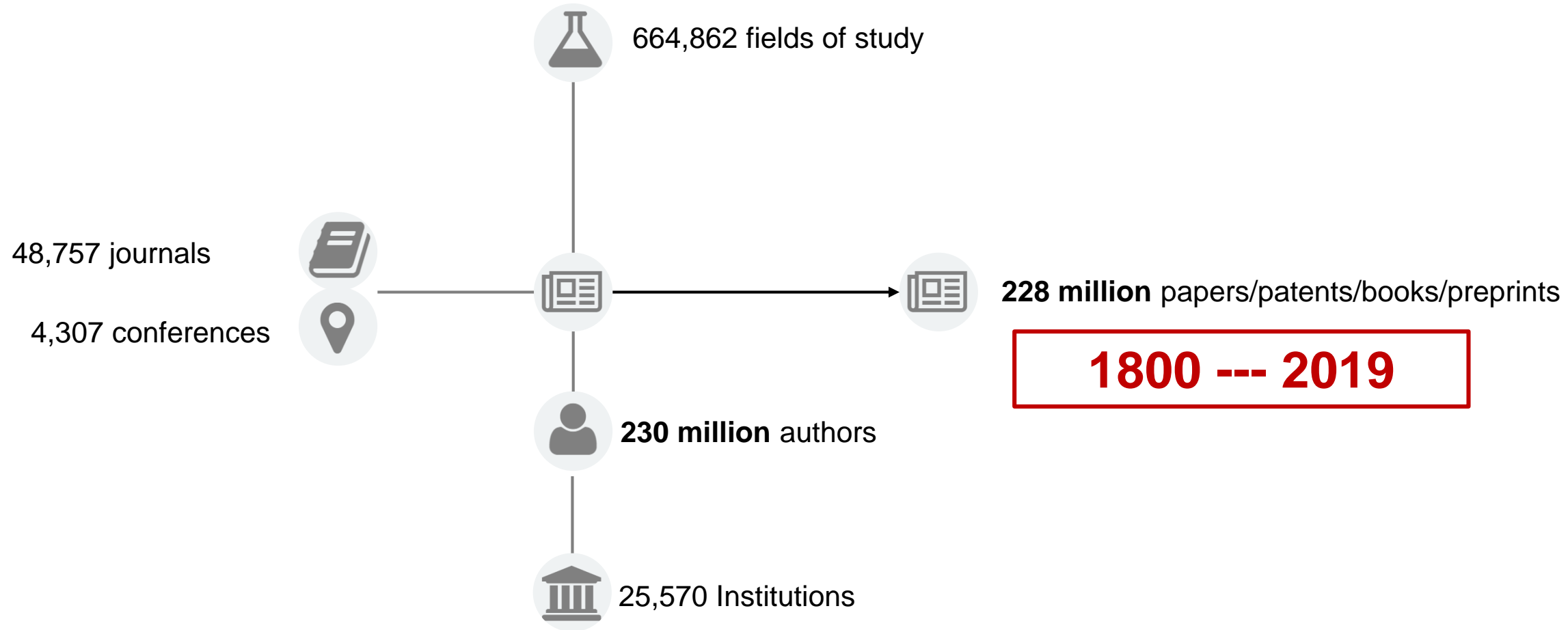
Network Embedding



References

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Microsoft Academic Graph



<https://academic.microsoft.com> as of Sep. 2019

The graph data is open!

Thank you!

Papers & data & code available at [https://ericdongyx.github.io/
ericdongyx@gmail.com](https://ericdongyx.github.io/ericdongyx@gmail.com)

Joint work with Jiezhong Qiu, Jie Zhang, Jie Tang (Tsinghua University)
Hao Ma (MSR & Facebook AI) and Kuansan Wang (MSR)