

Network Embedding: from Theoretical Understanding to System Design

Jiezhong Qiu

Tsinghua University

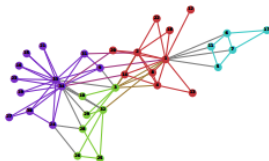
August 13, 2021

About Me

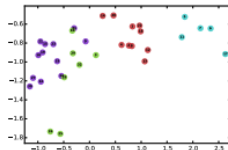
- A 6th year PhD student at Department of Computer Science and Technology of Tsinghua University, under the supervision of Prof. Jie Tang.
- My research interests include algorithm design for large-scale information networks and representation learning for graph-structured data.
- Nomination Award of the 2018 MSRA Fellowship and Nomination Award of the 2020 WAIC Youth Outstanding Paper.
- Google Scholar Citation 1,290.

What is Graph Representation Learning and Network Embedding?

- Network Embedding (NE)

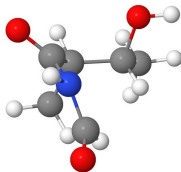


(a) Input: Karate Graph

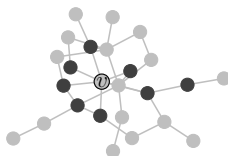


(b) Output: Representation

- Graph Neural Networks (GNN)

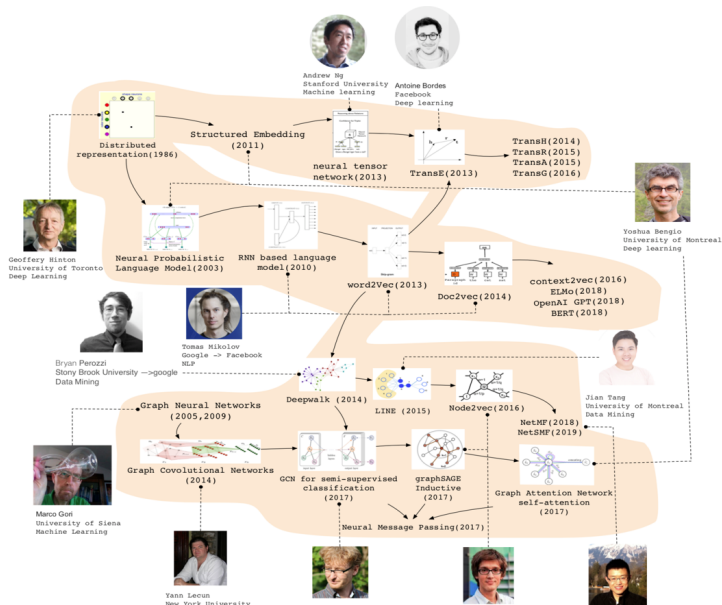


(a) A molecule



(b) An ego-network

History of Graph Representation Learning



About Today's Talk

Three Questions

- 1 Theory of Network Embedding.
 - 2 Sample complexity of Network embedding algorithms?
 - 3 Design better and scalable network embedding system.
- Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec (WSDM'18 most cited, Nomination Award of the 2020 WAIC Youth Outstanding Paper)
 - A Matrix Chernoff Bound for Markov Chains and Its Application to Co-occurrence Matrices (NeurIPS'20)
 - NetSMF: Large-Scale Network Embedding As Sparse Matrix Factorization (WWW '19); LightNE: A Lightweight Graph Processing System for Network Embedding (SIGMOD'21)

1 Network Embedding (NE)

- Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec
- A Matrix Chernoff Bound for Markov Chains and Its Application to Co-occurrence Matrices
- NetSMF: Network Embedding as Sparse Matrix Factorization
- LightNE: A Lightweight Graph Processing System for Network Embedding

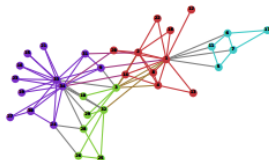
Motivation and Problem Formulation

Problem Formulation

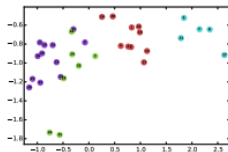
Give a network $G = (V, E)$, aim to learn a function $f : V \rightarrow \mathbb{R}^p$ to capture neighborhood similarity and community membership.

Applications:

- link prediction
- community detection
- label classification

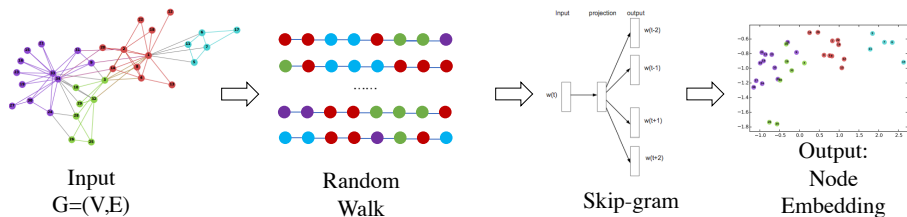


(a) Input: Karate Graph



(b) Output: Representation

DeepWalk and Three Questions We Want to Answer



Questions

- 1 Theory behind DeepWalk.
- 2 Sample complexity of DeepWalk?
- 3 Design better and more scalable network embedding systems.

Notations

Consider an undirected weighted graph $G = (V, E)$, where $|V| = n$ and $|E| = m$.

- Adjacency matrix $\mathbf{A} \in \mathbb{R}_+^{n \times n}$:

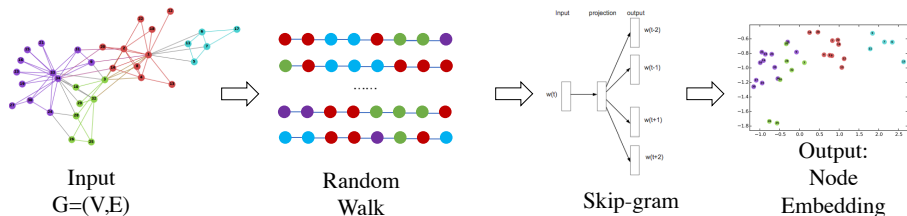
$$\mathbf{A}_{i,j} = \begin{cases} a_{i,j} > 0 & (i,j) \in E \\ 0 & (i,j) \notin E \end{cases}.$$

- Degree matrix $\mathbf{D} = \text{diag}(d_1, \dots, d_n)$, where d_i is the generalized degree of vertex i .
- Volume of the graph G : $\text{vol}(G) = \sum_i \sum_j \mathbf{A}_{i,j}$.

Assumption

$G = (V, E)$ is connected, undirected, and not bipartite, which makes $P(w) = \frac{d_w}{\text{vol}(G)}$ a unique stationary distribution.

DeepWalk: Random Walk on Graph + Skip-gram

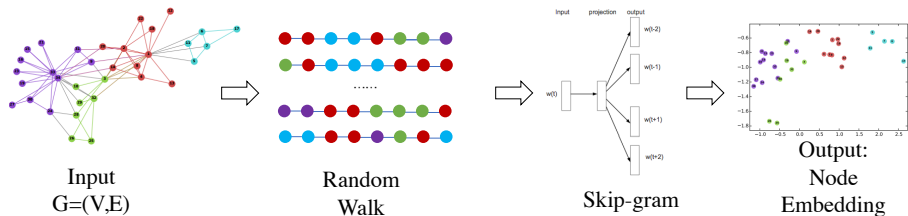


The objective of skip-gram model:

$$\mathcal{L}(\mathbf{X}, \mathbf{Y}) = |\mathcal{D}| \sum_w \sum_c \left(\frac{\#(w, c)}{|\mathcal{D}|} \log g(\mathbf{x}_w^\top \mathbf{y}_c) + b \frac{\#(w)}{|\mathcal{D}|} \frac{\#(c)}{|\mathcal{D}|} \log g(-\mathbf{x}_w^\top \mathbf{y}_c) \right).$$

$\#(w, c)$ indicates the number of times the pair (w, c) appears in a size- T sliding window.

Skip-gram as PMI Matrix Factorization



Levy & Goldberg (NIPS 14)

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

b Number of negative samples

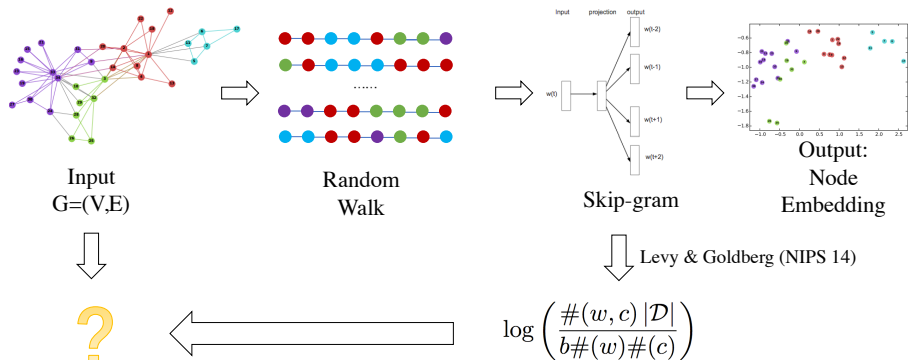
$\#(w, c)$ Co-occurrence of w and c

$\#(w)$ Occurrence of word w

$|\mathcal{D}|$ Total number of word-context pairs

$\#(c)$ Occurrence of context c

PMI Matrix of Random Walks on a Graph



b Number of negative samples
 $\#(w, c)$ Co-occurrence of w and c
 $|\mathcal{D}|$ Total number of word-context pairs
 $\#(w)$ Occurrence of word w
 $\#(c)$ Occurrence of context c

Our Results

Denote $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$, which is the transition probability matrix. Also note that we want to analyze $\frac{\#(w,c)|\mathcal{D}|}{\#(w) \cdot \#(c)} = \frac{\frac{\#(w,c)}{|\mathcal{D}|}}{\frac{\#(w)}{|\mathcal{D}|} \cdot \frac{\#(c)}{|\mathcal{D}|}}$

Theorem

When the length of random walk $L \rightarrow \infty$, we have

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

Consequently, $\frac{\#(w)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_w}{\text{vol}(G)}$ and $\frac{\#(c)}{|\mathcal{D}|} \xrightarrow{p} \frac{d_c}{\text{vol}(G)}$, as $L \rightarrow \infty$.

Theorem

For DeepWalk, when the length of random walk $L \rightarrow \infty$,

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

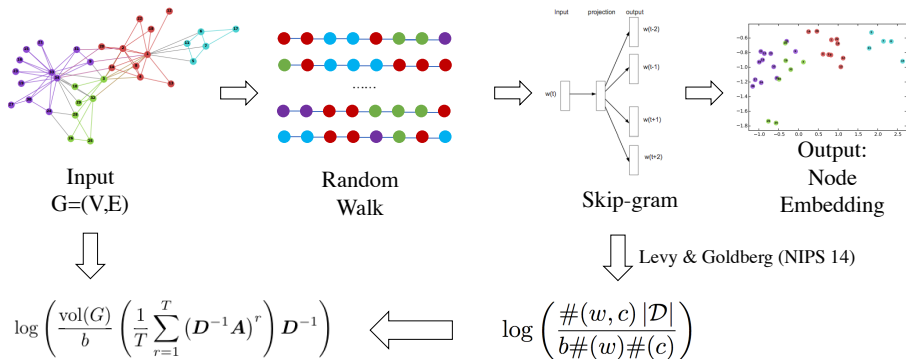
Theorem

DeepWalk is asymptotically and implicitly factorizing

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

Detailed proof

DeepWalk as Matrix Factorization



\mathbf{A} Adjacency matrix $\text{vol}(G) = \sum_i \sum_j \mathbf{A}_{i,j}$
 \mathbf{D} Degree matrix b Number of negative samples

Summary

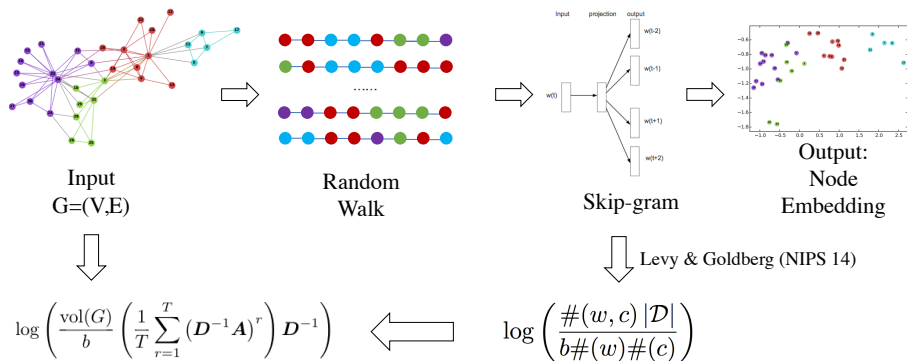
Table 1: The matrices that are implicitly approximated and factorized by DeepWalk, LINE, PTE, and node2vec.

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

1 Network Embedding (NE)

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- A Matrix Chernoff Bound for Markov Chains and Its Application to Co-occurrence Matrices
- NetSMF: Network Embedding as Sparse Matrix Factorization
- LightNE: A Lightweight Graph Processing System for Network Embedding

Q2: Sample Complexity of DeepWalk



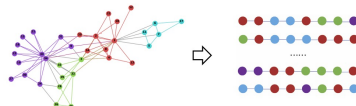
Question

- NetMF studies the convergence of co-occurrence matrices of random walk on graphs in the limit ($L \rightarrow \infty$).
- How about the convergence rate?

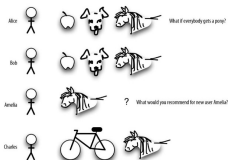
Applications of Co-occurrence Matrices

counts	i	like	enjoy	deep	learning	NLP	flying	.
i	0	2	1	0	0	0	0	0
like	2	0	0	1	0	1	0	0
enjoy	1	0	0	0	0	0	1	0
deep	0	1	0	0	1	0	0	0
learning	0	0	0	1	0	0	0	1
NLP	0	1	0	0	0	0	0	1
flying	0	0	1	0	0	0	0	1
.	0	0	0	0	1	1	1	0

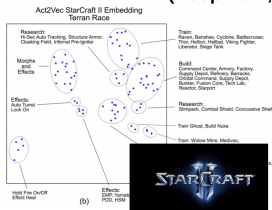
NLP
(LDA, Word2vec, Glove)



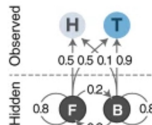
Graph Learning
(DeepWalk, node2vec, metapath2vec)



Recommendation System
(Pin2Vec, Item2vec)



Reinforcement Learning
(Act2Vec)



Hidden Markov Models
(Emission Co-occurrence)

Question:

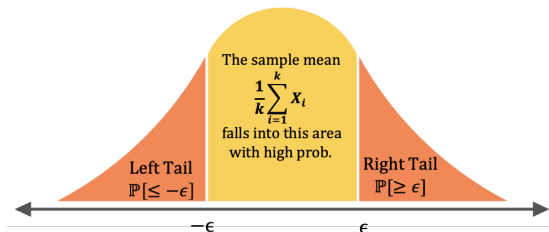
What is the #samples required to estimate a good co-occurrence matrix?

Chernoff Bound

Theorem

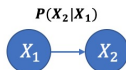
If X_1, \dots, X_k are k independent zero-mean scalar-valued random variables with $|X_i| \leq 1$. Then for $\epsilon \in (0, 1)$:

$$\mathbb{P} \left[\left| \frac{1}{k} \sum_{i=1}^k X_i \right| \geq \epsilon \right] \leq 2 \exp(-k\epsilon^2/4).$$

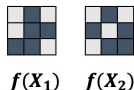


Our Matrix Chernoff Bound for Markov Chains

Independence
Markov Dependence



Scalar-valued
Random Variables
Matrix-valued
Random Variables

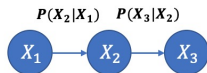


Sample Mean Matrix

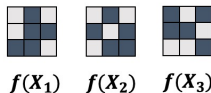
$$\frac{1}{2}(f(X_1) + f(X_2))$$

Our Matrix Chernoff Bound for Markov Chains

~~Independence~~
Markov Dependence



~~Scalar-valued~~
~~Random Variables~~
Matrix-valued
Random Variables

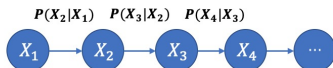


Sample Mean Matrix

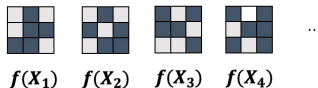
$$\frac{1}{3}(f(X_1) + f(X_2) + f(X_3))$$

Our Matrix Chernoff Bound for Markov Chains

Independence
Markov Dependence

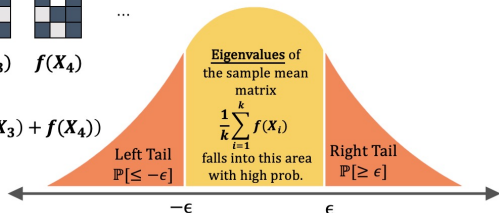


Scalar-valued
Random Variables
Matrix-valued
Random Variables



Sample Mean Matrix

$$\frac{1}{4} (f(X_1) + f(X_2) + f(X_3) + f(X_4))$$



Comparison to Previous Results

We want bound the tail probability of extreme eigenvalues:

$$\mathbb{P} \left[\lambda_{\min} \left(\frac{1}{k} \sum_{i=1}^k f(X_i) \right) \right] \text{ and } \mathbb{P} \left[\lambda_{\max} \left(\frac{1}{k} \sum_{i=1}^k f(X_i) \right) \right].$$

Comparison	X	f	Tail Prob.
Chernoff'52	i.i.d scalars	identity	$\exp(-\Omega(k\epsilon^2))$
Tropp'12	i.i.d $d \times d$ matrices	identity	$d \exp(-\Omega(k\epsilon^2))$
CLLM'12	random walk on a regular Markov chain with spectral expansion λ	$[N] \rightarrow \mathcal{C}$	$\exp(-\Omega(k(1-\lambda)\epsilon^2))$
GLSS'18	random walk on an undirected regular graph with 2nd eigenvalue λ	$[N] \rightarrow \mathcal{C}^{d \times d}$	$d \exp(-\Omega(k(1-\lambda)\epsilon^2))$
Ours	random walk on a regular Markov chain with spectral expansion λ	$[N] \rightarrow \mathcal{C}^{d \times d}$	$d \exp(-\Omega(k(1-\lambda)\epsilon^2))$

Matrix Chernoff Bound for Ergodic Markov Chains

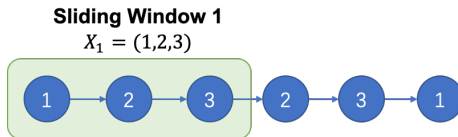
Theorem

Let \mathbf{P} be an ergodic Markov chain with state space $[N]$, stationary distribution π and spectral norm λ . Let $f : [N] \rightarrow \mathbb{R}^{d \times d}$ be a function such that (1) $\forall v \in [N]$, $f(v)$ is symmetric and $\|f(v)\|_2 \leq 1$; (2) $\sum_{v \in [N]} \pi_v f(v) = 0$. Let (v_1, \dots, v_k) denote a k -step random walk on \mathbf{P} starting from a distribution ϕ on $[N]$. Then given $\epsilon \in (0, 1)$,

$$\mathbb{P} \left[\lambda_{\max} \left(\frac{1}{k} \sum_{j=1}^k f(v_j) \right) \geq \epsilon \right] \leq \|\phi\|_{\pi} d^2 \exp \left(-(\epsilon^2(1 - \lambda)k/72) \right)$$

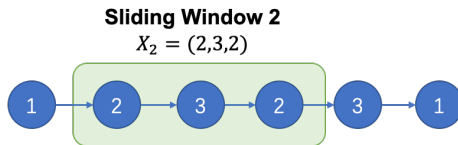
$$\mathbb{P} \left[\lambda_{\min} \left(\frac{1}{k} \sum_{j=1}^k f(v_j) \right) \leq -\epsilon \right] \leq \|\phi\|_{\pi} d^2 \exp \left(-(\epsilon^2(1 - \lambda)k/72) \right).$$

Co-occurrence Matrix of Sequential Data



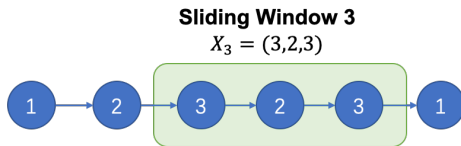
$$C = \frac{1}{4} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Co-occurrence Matrix of Sequential Data



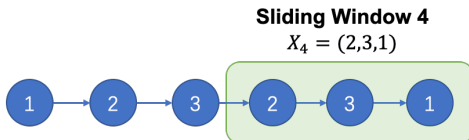
$$\mathbf{c} = \frac{1}{2} \left[\frac{1}{4} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right]$$

Co-occurrence Matrix of Sequential Data



$$\mathbf{C} = \frac{1}{3} \left[\frac{1}{4} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 2 \end{pmatrix} \right]$$

Co-occurrence Matrix of Sequential Data



$$\begin{aligned} C &= \frac{1}{4} \left[\frac{1}{4} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 2 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right] \\ &= \frac{1}{4} (f(X_1) + f(X_2) + f(X_3) + f(X_4)) \end{aligned}$$

Observations

- Co-occurrence matrix can be written as sample mean $C = \frac{1}{k} \sum_{i=1}^k f(X_i)$.
- If the input sequence is a Markov Chain, then sliding window X_i is also a Markov Chain.

Convergence Rate of Co-occurrence Matrices

Theorem (Convergence Rate of Co-occurrence Matrices)

Let \mathbf{P} be a regular Markov chain with state space $[n]$, stationary distribution π and mixing time τ . Let (v_1, \dots, v_L) denote a L -step random walk on \mathbf{P} starting from a distribution ϕ on $[n]$. Given step weight coefficients $(\alpha_1, \dots, \alpha_T)$ s.t. $\sum_{r=1}^T |\alpha_r| = 1$, and $\epsilon \in (0, 1)$, the probability that the co-occurrence matrix \mathbf{C} deviates from its asymptotic expectation $\mathbb{AE}[\mathbf{C}]$ (in 2-norm) is bounded by:

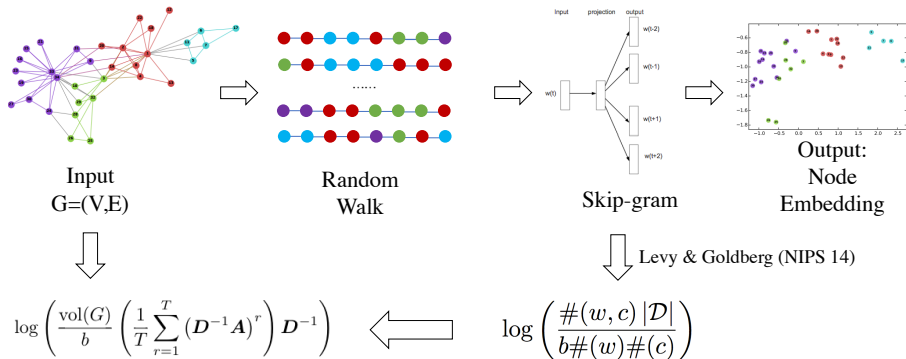
$$\mathbb{P} [\|\mathbf{C} - \mathbb{AE}[\mathbf{C}]\|_2 \geq \epsilon] \leq 2 (\tau + T) \|\phi\|_{\pi} n^2 \exp \left(-\frac{\epsilon^2 (L - T)}{576 (\tau + T)} \right).$$

Roughly, one needs $L = O(\tau(\log n + \log \tau)/\epsilon^2)$ samples to guarantee good estimation to the co-occurrence matrix.

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Q3: How to Design Better NE Systems



A Adjacency matrix $\text{vol}(G) = \sum_i \sum_j A_{i,j}$
 D Degree matrix b Number of negative samples

- DeepWalk: SGD on $O(|V|d)$ parameters.
- NetMF: the matrix is dense.

Random-walk Matrix Polynomial Sparsification

Theorem ([CCL⁺15])

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, in time $O(T^2 m \epsilon^{-2} \log^2 n)$, a $(1 + \epsilon)$ -spectral sparsifier, $\tilde{\mathbf{L}}$, with $O(n \log n \epsilon^{-2})$ non-zeros. For unweighted graphs, the time complexity can be reduced to $O(T^2 m \epsilon^{-2} \log n)$.

Definition

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

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

Setting $\alpha_1 = \dots = \alpha_T = \frac{1}{T}$ in $\mathbf{L} = \mathbf{D} - \sum_{r=1}^T \alpha_r \mathbf{D} (\mathbf{D}^{-1} \mathbf{A})^r$, we can observe the tight connection between random walk matrix polynomial and NetMF:

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

Idea

Rewrite the NetMF matrix in terms of random walk matrix polynomial \mathbf{L} , and further approximate \mathbf{L} with $\tilde{\mathbf{L}}$.

NetSMF—Algorithm

The proposed NetSMF algorithm consists of three steps:

- Construct a random walk matrix polynomial sparsifier, $\tilde{\mathbf{L}}$, by calling algorithm proposed in [CCL⁺15].
- Construct a NetMF matrix sparsifier.

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

- Truncated randomized singular value decomposition.

Detailed Algorithm

Experiments

Label Classification:

- BlogCatalog, PPI, Flickr, YouTube, OAG.
- Logistic Regression
- DeepWalk, LINE, node2vec, NetMF¹ ($T = 10$), NetSMF² ($T = 10$).

Table 2: Statistics of Datasets.

Dataset	BlogCatalog	PPI	Flickr	YouTube	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

¹Qiu et al. Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec. WSDM'18

²Qiu et al. NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization. WWW'19

Experimental Results

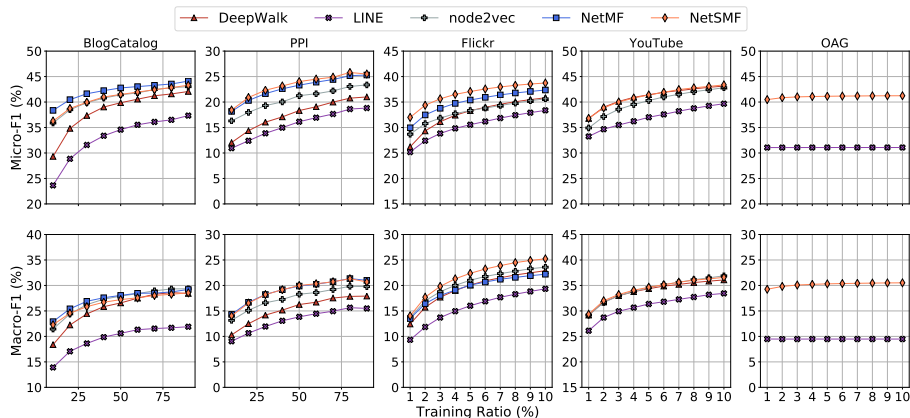
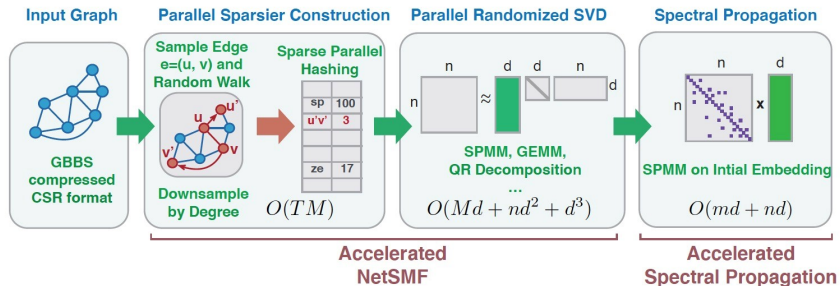


Figure 1: Predictive performance on varying the ratio of training data. The x-axis represents the ratio of labeled data (%), and the y-axis in the top and bottom rows denote the Micro-F1 and Macro-F1 scores respectively.

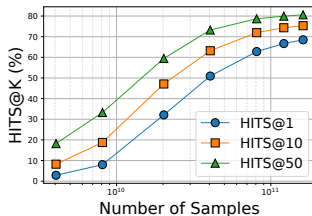
Q3: Even More Scalable?



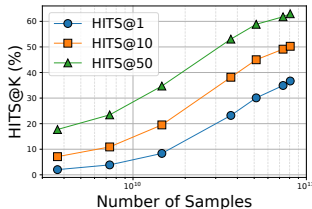
- Scalable: Embed graphs with 1B edges within 1.5 hours.
- Lightweight: Occupy hardware costs below 100 dollars measured by cloud rent to process 1B to 100B edges.
- Accurate: Achieve the highest accuracy in downstream tasks under the same time budget and similar resources.

LightNE on Very Large Graphs!

	ClueWeb	Hyperlink2014
$ V $	978,408,098	1,724,573,718
$ E $	74,744,358,622	124,141,874,032



(a) ClueWeb-Sym



(b) Hyperlink2014-Sym

Figure 2: HITS@K ($K = 1, 10, 50$) of LightNE w.r.t. the number of samples.

None of the existing network embedding systems can handle such large graphs in a single machine!

Thanks.

www.jiezhongqiu.com

- Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec (WSDM'18 most cited)
- A Matrix Chernoff Bound for Markov Chains and Its Application to Co-occurrence Matrices (NeurIPS'20)
- NetSMF: Large-Scale Network Embedding As Sparse Matrix Factorization (WWW '19)
- LightNE: A Lightweight Graph Processing System for Network Embedding (SIGMOD '21)

Q&A

1 Network Embedding (NE)

- Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec
- A Matrix Chernoff Bound for Markov Chains and Its Application to Co-occurrence Matrices
- NetSMF: Network Embedding as Sparse Matrix Factorization
- LightNE: A Lightweight Graph Processing System for Network Embedding

References I



Dehua Cheng, Yu Cheng, Yan Liu, Richard Peng, and Shang-Hua Teng, *Spectral sparsification of random-walk matrix polynomials*, arXiv preprint arXiv:1502.03496 (2015).