NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization

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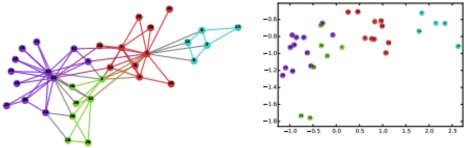
Motivation and Problem Formulation

Problem Formulation

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

Applications:

- link prediction
- community detection
- label classification



(a) Input: Karate Graph (b) Output: Representation

Figure 1: A toy example (Figure from DeepWalk).

Two Genres of Network Embedding Algorithm

- Local Context Methods:
  - LINE, DeepWalk, node2vec, metapath2vec.
  - Usually be formulated as a skip-gram-like problem, and optimized by SGD.
- Global Matrix Factorization Methods.
  - NetMF, GraRep, HOPE.
  - Leverage global statistics of the input networks.
  - Not necessarily a gradient-based optimization problem.
  - Usually requires explicit construction of the matrix to be factorized.

Notations

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

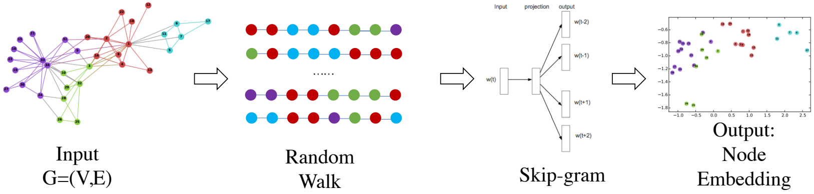
- Adjacency matrix $\boldsymbol{A} \in \mathbb{R}_{+}^{n \times n}$:

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

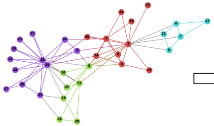
- Degree matrix $\boldsymbol{D} = \operatorname{diag}(d_1, \cdots, d_n)$, where d_i is the generalized degree of vertex i.
- Volume of the graph G: $\operatorname{vol}(G) = \sum_i \sum_j \boldsymbol{A}_{i,j}$.

Contents

DeepWalk and NetMF



DeepWalk and NetMF



Input
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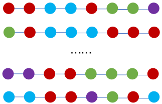
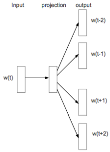
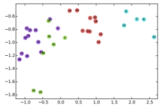


Random
Walk



Skip-gram



Output:
Node
Embedding

Levy & Goldberg (NIPS 14)

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

b Number of negative samples

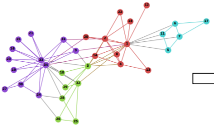
$\#(w,c)$ Co-occurrence of w and c

$\#(w)$ Occurrence of word w

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

$\#(c)$ Occurrence of context c

DeepWalk and NetMF



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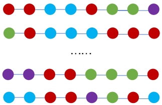

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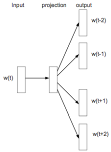

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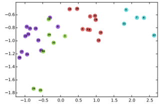

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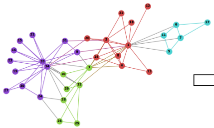

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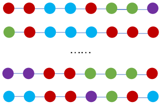

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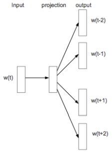
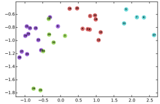


Skip-gram



Output:
Node
Embedding

Levy & Goldberg (NIPS 14)

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

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

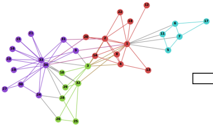
$\boldsymbol{A}$ Adjacency matrix

$\boldsymbol{D}$ Degree matrix

$\mathrm{vol}(G) = \sum_i \sum_j \boldsymbol{A}_{i,j}$

b Number of negative samples

DeepWalk and NetMF



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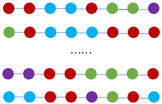

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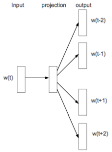

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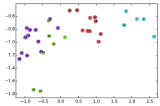

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$$\log\left(\frac{\#(w,c)\,|\mathcal{D}|}{b\#(w)\#(c)}\right)$$

Matrix
Factorization

Contents

Contents

Computation Challanges of NetMF

For small world networks,

$$\frac{\mathrm{vol}(G)}{b}\left(\frac{1}{T}\sum_{r=1}^{T}\underbrace{\left(\boldsymbol{D}^{-1}\boldsymbol{A}\right)^{r}}_{\text{matrix power}}\right)\boldsymbol{D}^{-1} \text{ is always a dense matrix .}$$

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Why?

- In small world networks, each pair of vertices (i, j) can reach each other in a small number of hops.
- Make the corresponding matrix entry a positive value.

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Why?

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- Make the corresponding matrix entry a positive value.

Idea

- Sparse matrix is easier to handle.
- Can we achieve a matrix sparse but ‘good enough’ matrix.

Observation

Definition

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

$$\boldsymbol{L} = \boldsymbol{D} - \sum_{r=1}^{T} \alpha_r \boldsymbol{D} \left(\boldsymbol{D}^{-1}\boldsymbol{A}\right)^r \tag{1}$$

is a T-degree random-walk matrix polynomial.

Observation

For $\alpha_1 = \cdots = \alpha_T = \frac{1}{T}$:

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

Random-walk Matrix Polynomial Sparsification

Theorem

[CCL[+]15] For random-walk matrix polynomial $\boldsymbol{L} = \boldsymbol{D} - \sum_{r=1}^{T} \alpha_r \boldsymbol{D} \left(\boldsymbol{D}^{-1} \boldsymbol{A} \right)^r$, one can construct, in time $O(T^2 m \epsilon^{-2} \log^2 n)$, a $(1+\epsilon)$-spectral sparsifier, $\widetilde{\boldsymbol{L}}$, with $O(n \log n \epsilon^{-2})$ non-zeros. For unweighted graphs, the time complexity can be reduced to $O(T^2 m \epsilon^{-2} \log n)$.

NetSMF—Algorithm

The proposed NetSMF algorithm consists of three steps:

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

$$\operatorname{trunc\_log}^{\circ}\left(\frac{\operatorname{vol}(G)}{b}\boldsymbol{D}^{-1}(\boldsymbol{D}-\widetilde{\boldsymbol{L}})\boldsymbol{D}^{-1}\right)$$

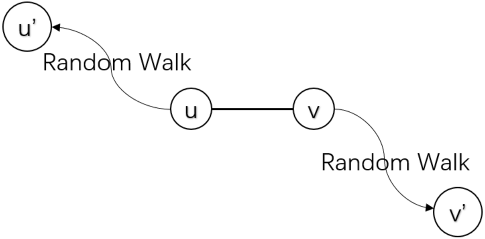
- Truncated randomized singular value decomposition.

Detailed Algorithm

Algorithm Details

PathSampling:

- Sample an edge (u, v) from edge set.
- Start very short random walk from u and arrive u'.
- Start very short random walk from v and arrive v'.
- Record vertex pair (u', v').



Randomized SVD:

- Project origin matrix to low dimensional space by Gaussian random matrix.
- Deal with the projected small matrix.

NetSMF — System Design

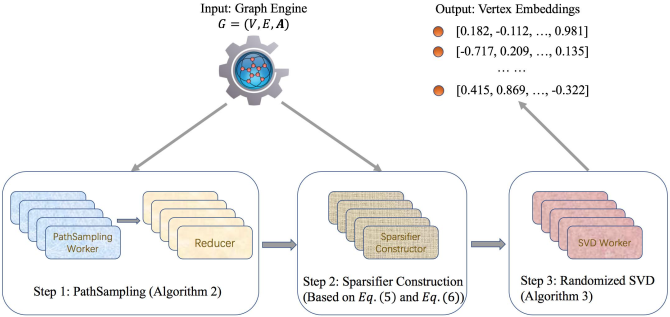


Figure 2: The System Design of NetSMF.

Contents

Setup

Label Classification:

- BlogCatelog, PPI, Flickr, YouTube, OAG.
- Logistic Regression
- NetSMF ($T = 10$), NetMF ($T = 10$), DeepWalk, LINE.

Table 1: 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

Experimental Results

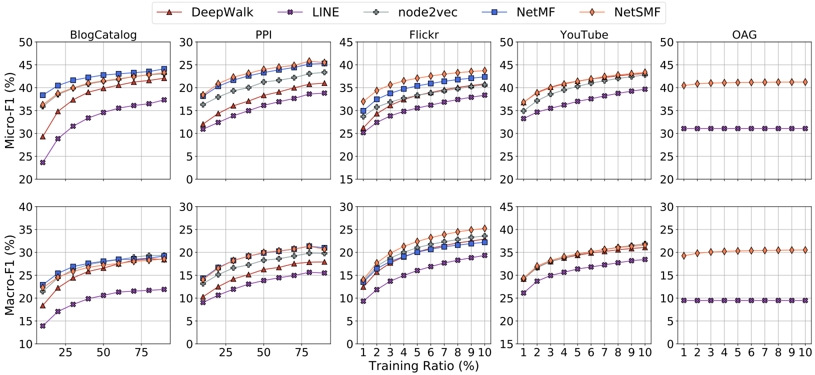


Figure 3: Predictive performance on varying the ratio of training data. The x-axis represents the ratio of labeled data (%), and the y-axis in the top and bottom rows denote the Micro-F1 and Macro-F1 scores respectively.

Running Time

Table 2: Running Time

	LINE	**DeepWalk**	**node2vec**	**NetMF**	**NetSMF**
BlogCatalog	40 mins	12 mins	56 mins	2 mins	13 mins
PPI	41 mins	4 mins	4 mins	16 secs	10 secs
Flickr	42 mins	2.2 hours	21 hours	2 hours	48 mins
YouTube	46 mins	1 day	4 days	$\times$	4.1 hours
OAG	2.6 hours	–	–	$\times$	24 hours

Conclusion and Future Work

We propose NetSMF, a scalable, efficient, and effective network embedding algorithm.

Future Work

- A distributed-memory implementation.
- Extension to directed, dynamic, heterogeneous graphs.

Thanks.

- Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec (WSDM '18)
- NetSMF: Network Embedding as Sparse Matrix Factorization (WebConf '19)

Code for NetMF available at `github.com/xptree/NetMF`
Code for NetSMF available at `github.com/xptree/NetSMF`
Q&A

On the Large-dimensionality Assumption of [LG14]

Recall the objective of skip-gram model:

$$\min_{\boldsymbol{X},\boldsymbol{Y}} \mathcal{L}(\boldsymbol{X},\boldsymbol{Y})$$

where

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

Theorem

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

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

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

Back

NetSMF — Approximation Error

Denote $\boldsymbol{M} = \boldsymbol{D}^{-1}\left(\boldsymbol{D} - \boldsymbol{L}\right)\boldsymbol{D}^{-1}$ in

$$\operatorname{trunc\_log}^{\circ}\left(\frac{\operatorname{vol}(G)}{b}\boldsymbol{D}^{-1}(\boldsymbol{D} - \widetilde{\boldsymbol{L}})\boldsymbol{D}^{-1}\right),$$

and $\widetilde{\boldsymbol{M}}$ to be its sparsifier the we constructed.

Theorem

The singular value of $\widetilde{\boldsymbol{M}} - \boldsymbol{M}$ satisfies

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

Theorem

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

$$\left\|\operatorname{trunc\_log}^{\circ}\left(\frac{\operatorname{vol}(G)}{b}\widetilde{\boldsymbol{M}}\right) - \operatorname{trunc\_log}^{\circ}\left(\frac{\operatorname{vol}(G)}{b}\boldsymbol{M}\right)\right\|_F \leq \frac{4\epsilon\operatorname{vol}(G)}{b\sqrt{d_{\min}}}\sqrt{\sum_{i=1}^{n}\frac{1}{d_i}}.$$

Spectrally Similar

Definition

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

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

Algorithm 1: NetSMF

Input : A social network $G = (V, E, \boldsymbol{A})$ which we want to learn network embedding; The number of non-zeros M in the sparsifier; The dimension of embedding d.

Output: An embedding matrix of size $n \times d$, each row corresponding to a vertex.

$\widetilde{G} \leftarrow (V, \emptyset, \widetilde{\boldsymbol{A}} = \boldsymbol{0})$

`/* Create an empty network with` $E = \emptyset$ `and` $\widetilde{\boldsymbol{A}} = 0$. `*/`

for $i \leftarrow 1$ **to** M **do**

  Uniformly pick an edge $e = (u, v) \in E$

  Uniformly pick an integer $r \in [T]$

  $u', v', Z \leftarrow$ `PathSampling(e, r)`

  Add an edge $\left(u', v', \frac{2rm}{MZ}\right)$ to $\widetilde{G}$

  `/* Parallel edges will be merged into one edge, with their weights summed up together. */`

end

Compute $\widetilde{\boldsymbol{L}}$ to be the unnormalized graph Laplacian of $\widetilde{G}$

Compute $\widetilde{\boldsymbol{M}} = \boldsymbol{D}^{-1}\left(\boldsymbol{D} - \widetilde{\boldsymbol{L}}\right)\boldsymbol{D}^{-1}$

$\boldsymbol{U}_d, \boldsymbol{\Sigma}_d, \boldsymbol{V}_d \leftarrow$ `RandomizedSVD`$\left(\mathrm{trunc\_log}^{\circ}\left(\frac{\mathrm{vol}(G)}{b}\widetilde{\boldsymbol{M}}\right), d\right)$

return $\boldsymbol{U}_d\sqrt{\boldsymbol{\Sigma}_d}$ as network embeddings

Back

NetSMF—Algorithm

Algorithm 2: PathSampling algorithm as described in [CCL+15].

Procedure `PathSampling`($e = (u, v)$, r)
  Uniformly pick an integer $k \in [r]$
  Perform $(k-1)$-step random walk from u to u_0
  Perform $(r-k)$-step random walk from v to u_r
  Keep track of $Z(\boldsymbol{p}) = \sum_{i=1}^{r} \frac{2}{\boldsymbol{A}_{u_{i-1}, u_i}}$ along the length-r path $\boldsymbol{p}$ between u_0 and u_r
  return $u_0, u_r, Z(\boldsymbol{p})$

Back

Randomized SVD

Algorithm 3: Randomized SVD on NetMF Matrix Sparsifier

Procedure `RandomizedSVD(`$\boldsymbol{A}$, d`)`
- Sampling Gaussian random matrix $\boldsymbol{O}$ // $\boldsymbol{O} \in \mathbb{R}^{n\times d}$
- Compute sample matrix $\boldsymbol{Y} = \boldsymbol{A}^\top \boldsymbol{O} = \boldsymbol{A}\boldsymbol{O}$ // $\boldsymbol{Y} \in \mathbb{R}^{n\times d}$
- Orthonormalize $\boldsymbol{Y}$
- Compute $\boldsymbol{B} = \boldsymbol{A}\boldsymbol{Y}$ // $\boldsymbol{B} \in \mathbb{R}^{n\times d}$
- Sample another Gaussian random matrix $\boldsymbol{P}$ // $\boldsymbol{P} \in \mathbb{R}^{d\times d}$
- Compute sample matrix of $\boldsymbol{Z} = \boldsymbol{B}\boldsymbol{P}$ // $\boldsymbol{Z} \in \mathbb{R}^{n\times d}$
- Orthonormalize $\boldsymbol{Z}$
- Compute $\boldsymbol{C} = \boldsymbol{Z}^\top \boldsymbol{B}$ // $\boldsymbol{C} \in \mathbb{R}^{d\times d}$
- Run Jacobi SVD on $\boldsymbol{C} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top$
- **return** $\boldsymbol{Z}\boldsymbol{U}$, $\boldsymbol{\Sigma}$, $\boldsymbol{Y}\boldsymbol{V}$

/* Result matrices are of shape $n \times d, d \times d, n \times d$ resp. */

Time and Space Complexity

Table 3: Time and Space Complexity of NetSMF.

	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	$O(Md+nd^2+d^3)$	$O(M+nd)$

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).

Omer Levy and Yoav Goldberg, *Neural word embedding as implicit matrix factorization*, Advances in neural information processing systems, 2014, pp. 2177–2185.