



Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

图表示学习

Zhou Shen

School of Computer Science, Wuhan University

October 20, 2021



Outline

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

1 Word2Vec

2 DeepWalk

3 Node2Vec

4 Struc2Vec

5 LINE

6 SDNE



Word2Vec

One-Hot Encoding

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

1-of-N Encoding

apple = [1 0 0 0 0]

bag = [0 1 0 0 0]

cat = [0 0 1 0 0]

dog = [0 0 0 1 0]

elephant = [0 0 0 0 1]



Word2Vec

One-Word Context

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

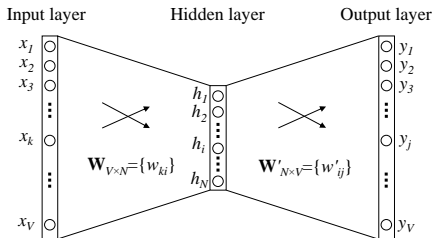


Figure 1: A simple CBOW model with only one word in the context

$$\mathbf{h} = \mathbf{W}^T \mathbf{x} = \mathbf{W}_{(k, \cdot)}^T := \mathbf{v}_{w_I}^T, u_j = \mathbf{v}'_{w_j} h \quad (1)$$

$$p(w_j | w_I) = y_j = \frac{\exp(u_j)}{\sum_{j'=1}^V \exp(u_{j'})} \quad (2)$$



Word2Vec

Objective Function

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

$$\begin{aligned}\max p(w_O \mid w_I) &= \max y_{j^*} \\ &= \max \log y_{j^*} \\ &= u_{j^*} - \log \sum_{j'=1}^V \exp(u_{j'}) := -E\end{aligned}\tag{3}$$

常用变形

$$\min E = -u_{j^*} + \log \sum_{j'=1}^V \exp(u_{j'})$$



Word2Vec

CBOW

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

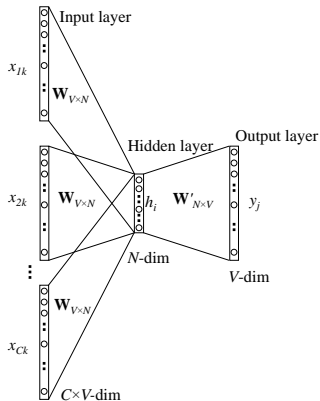


Figure 2: Continuous bag-of-words model

$$\mathbf{h} = \frac{1}{C}(\mathbf{v}_{w_1} + \mathbf{v}_{w_2} + \dots + \mathbf{v}_{w_C})^T$$

$$E = -\log p(w_O | w_{I,1}, \dots, w_{I,C})$$

$$= -u_{j^*} + \log \sum_{j'=1}^V \exp(u_{j'})$$



Word2Vec

Skip-Gram

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

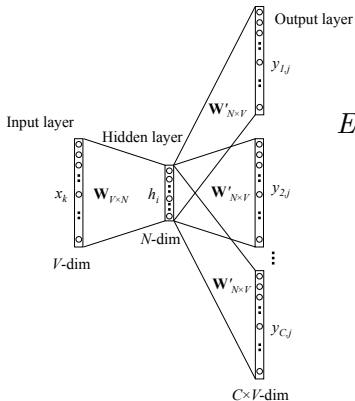


Figure 3: The skip-gram model.

$$\begin{aligned}
 E &= -\log p(w_{O,1}, w_{O,2}, \dots, w_{O,C} \mid w_I) \\
 &= -\log \prod_{c=1}^C \frac{\exp(u_{c,j_c^*})}{\sum_{j'=1}^V \exp(u_{j'})} \\
 &= -\sum_{c=1}^C u_{j_c^*} + C \cdot \log \sum_{j'=1}^V \exp(u_{j'})
 \end{aligned}$$



Word2Vec

Hierarchical Softmax

Graph
Embedding

S. Zhou

Word2Vec

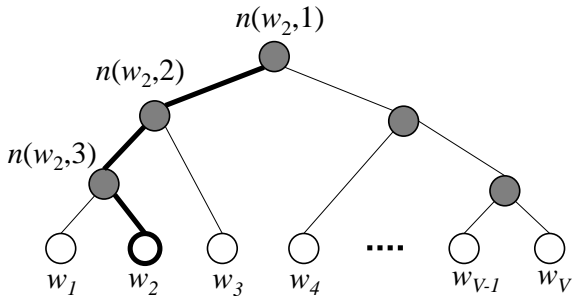
DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE



$$p(w = w_O) = \prod_{j=1}^{L(w)-1} \sigma \left([n(w, j+1) = \text{ch}(n(w, j))] \cdot \mathbf{v}'_{n(w, j)} {}^T \mathbf{h} \right)$$



Word2Vec

Negative Sample

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

1. 词频计算

$$weight(w_i) = \frac{count(w_i)^{0.75}}{\sum_j^V count(w_j)^{0.75}}$$

2. 目标函数

$$E = -\log \sigma(\mathbf{v}'_{w_o} \mathbf{h}) - \sum_{w_j \in \mathcal{W}_{\text{neg}}} \log \sigma(-\mathbf{v}'_{w_j} \mathbf{h})$$



DeepWalk

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

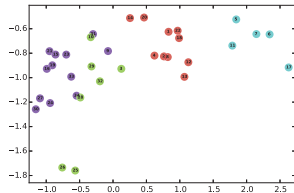
Struc2Vec

LINE

SDNE



(a) Input: Karate Graph



(b) Output: Representation

Definition

Problem Definition Let $G = (V, E)$, where V are the members of the network, and E be its edges. Our goal is to learn $X_E \in \mathcal{R}^{|V| \times d}$, where d is number of latent dimensions.



DeepWalk

Graph
Embedding

S. Zhou

Word2Vec

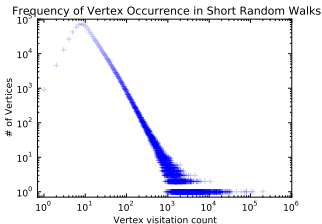
DeepWalk

Node2Vec

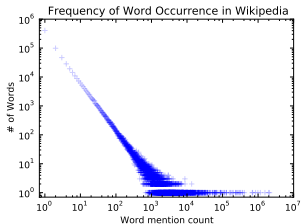
Struc2Vec

LINE

SDNE



(a) YouTube Social Graph



(b) Wikipedia Article Text

Connection

The power-law distribution of vertices appearing in the short random walks follows a power-law, much like the distribution of words in natural language.



DeepWalk

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

- 1 give a sequence of random walk from vertice i

$$\mathcal{W}_i^n = \{v_1, v_2, v_3, \dots, v_n\} \quad (4)$$

- 2 maximize the likelihood

$$\Pr(v_i \mid (\Phi(v_1), \Phi(v_2), \dots, \Phi(v_{i-1}))) \quad (5)$$

Mapping Function Φ

$\Phi : v \in V \mapsto \mathcal{R}^{|V| \times d}$ where d is the number of dimensions



DeepWalk

Disadvantages and Optimizations

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

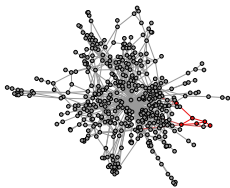
Node2Vec

Struc2Vec

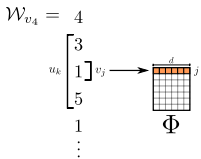
LINE

SDNE

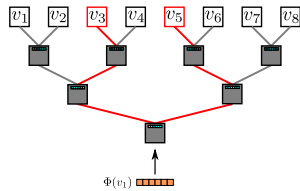
- As the walk length grows, computing this objective function becomes unfeasible.
- Restricts the order in which vertices appear



(a) Random walk generation.



(b) Representation mapping.



(c) Hierarchical Softmax.



DeepWalk

Algorithm

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE

Algorithm 1 DEEPWALK(G, w, d, γ, t)

Input: graph $G(V, E)$

 window size w

 embedding size d

 walks per vertex γ

 walk length t

Output: matrix of vertex representations $\Phi \in \mathbb{R}^{|V| \times d}$

1: Initialization: Sample Φ from $\mathcal{U}^{|V| \times d}$

2: Build a binary Tree T from V

3: **for** $i = 0$ to γ **do**

4: $\mathcal{O} = \text{Shuffle}(V)$

5: **for each** $v_i \in \mathcal{O}$ **do**

6: $\mathcal{W}_{v_i} = \text{RandomWalk}(G, v_i, t)$

7: $\text{SkipGram}(\Phi, \mathcal{W}_{v_i}, w)$

8: **end for**

9: **end for**

Corollary

$$\underset{\Phi}{\text{minimize}} -\log \Pr(\{v_{i-w}, \dots, v_{i-1}, v_{i+1}, \dots, v_{i+w}\} \mid \Phi(v_i))$$



Node2Vec

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE



Struc2Vec

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE



LINE

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE



SDNE

Graph
Embedding

S. Zhou

Word2Vec

DeepWalk

Node2Vec

Struc2Vec

LINE

SDNE