Learning from Networks

Nodes and Graph Embedding

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November 13^{th}, 2024

Course Recap

Until now, we have seen how to compute interesting measures for a network or its nodes, e.g.:

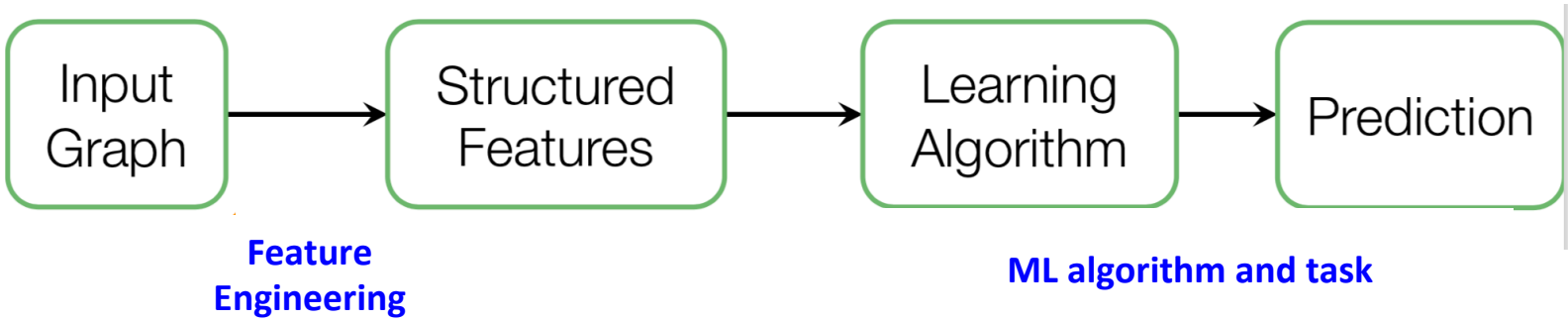
- centrality scores
- clustering coefficient
- graphlet/motifs score

Why?

- they provide useful information on the network (e.g., network motifs)
- they can be used as features in a vector representation of nodes/graphs to be used as input for a Machine Learning (ML) task

We are now going to focus on this second aspect.

The Traditional Framework for ML with Graphs



Given a graph:

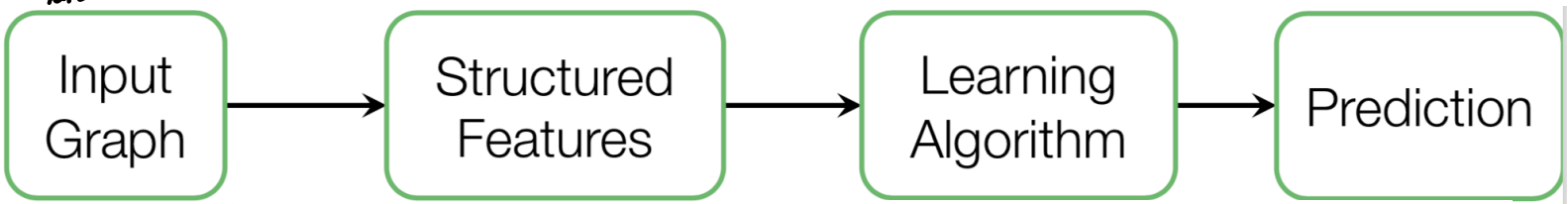
- extract nodel-level or graph-level features (*feature engineering*)
- learn a model that maps feature vectors to labels

1 per node

Note: feature engineering is required for every task/application!

Graph Representation Learning Framework

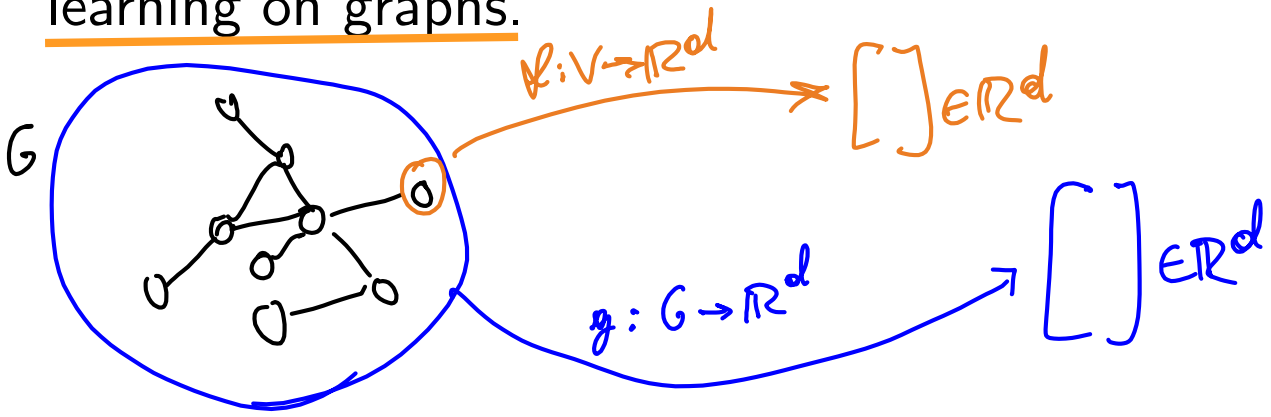
Representation learning: *automatically learn* the features to be used in the downstream prediction task



Node Embedding Task: map *nodes* into an embedding space, tipicamente $\mathbb{R}^d$

Graph Embedding Task: map *graphs* into an embedding space

Goal: *efficient* and *task-independent* feature learning for machine learning on graphs.



Motivation

Node Embedding Task: map nodes into an embedding space

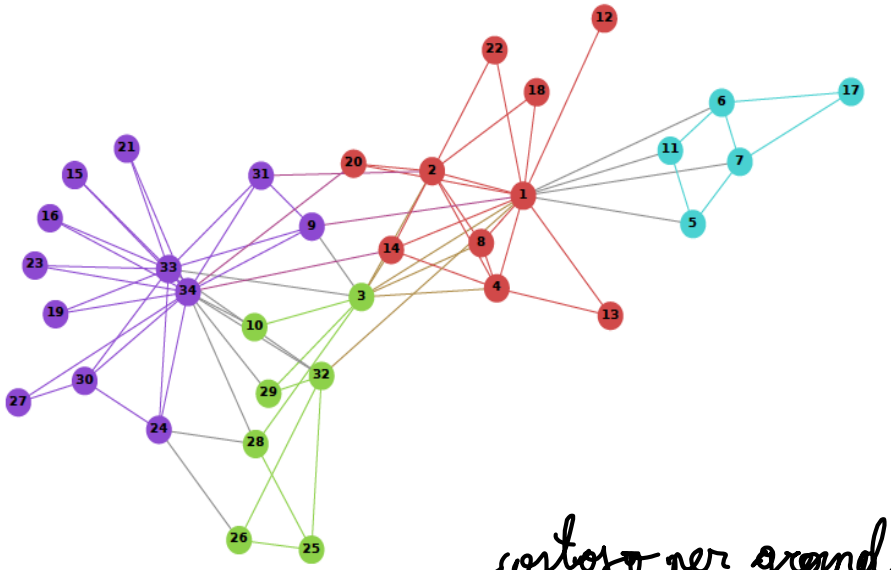
Why?

- the similarity of embeddings indicates the similarity in the network
- encode the network information
- can be used for many downstream task predictions

Example: Zachary's Karate Club

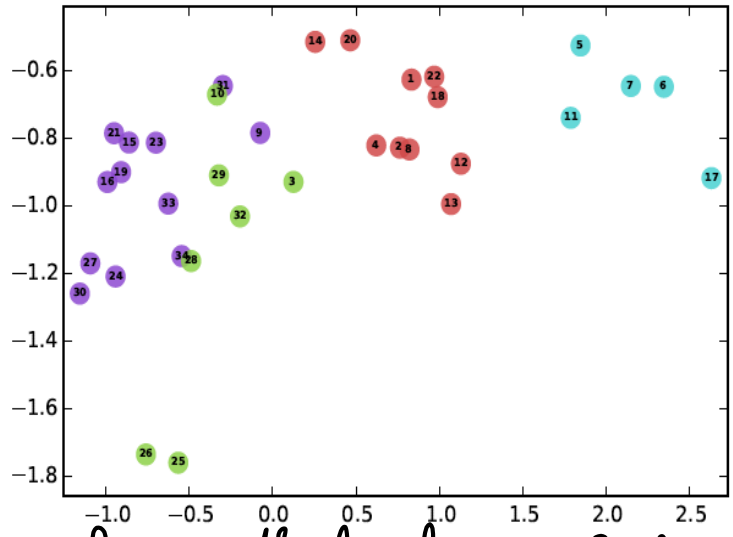
$G = (V, E)$

Input



embedding di nodi di V in $\mathbb{R}^2$

Output

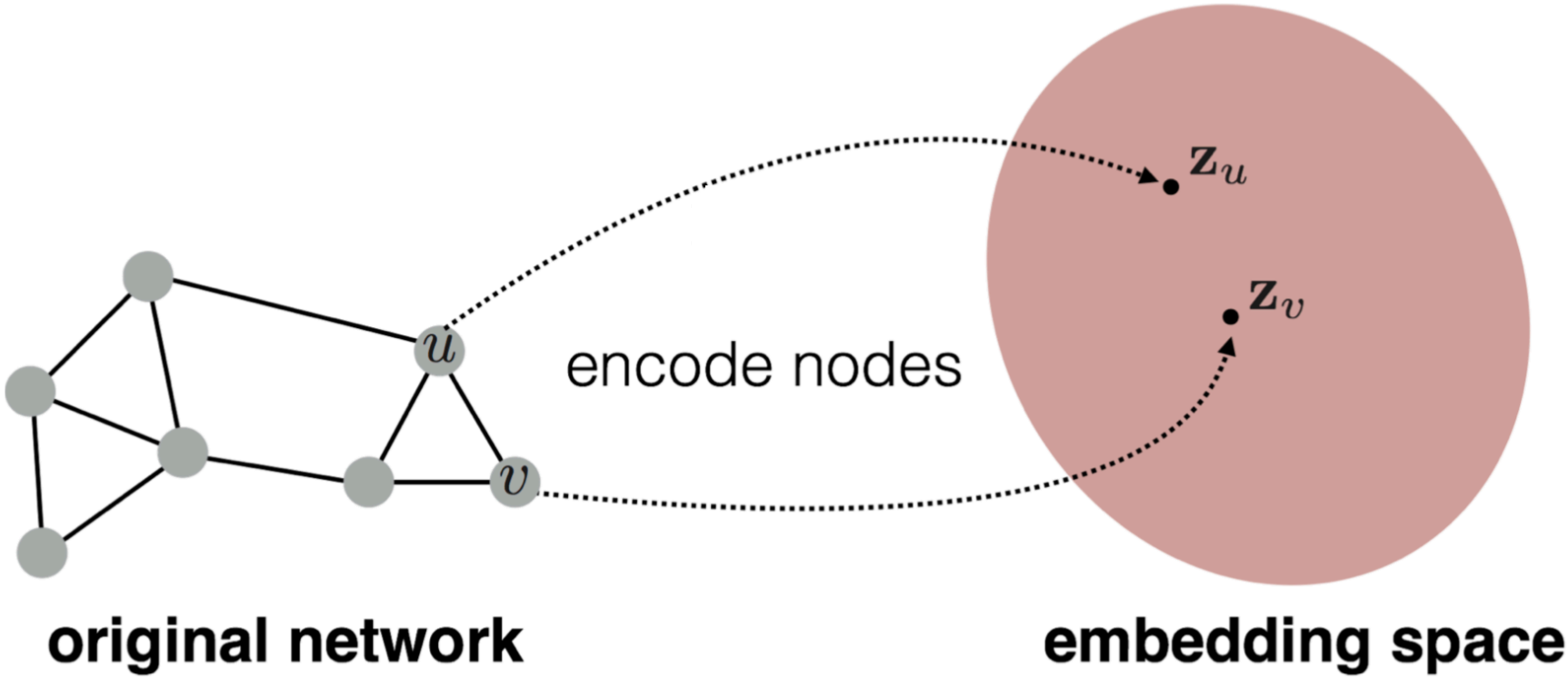


costoso per grandi grafi ⇒ piuttosto facile cluster se embedding

Colors: labels from clustering on the network (not available in input to the embedding method)

Node Embedding: General Framework

Given a graph $G = (V, E)$, we want to embed its nodes so that the similarity in the embedding space approximates the similarity in the graph.



Node Embedding: Encoder-Decoder Framework

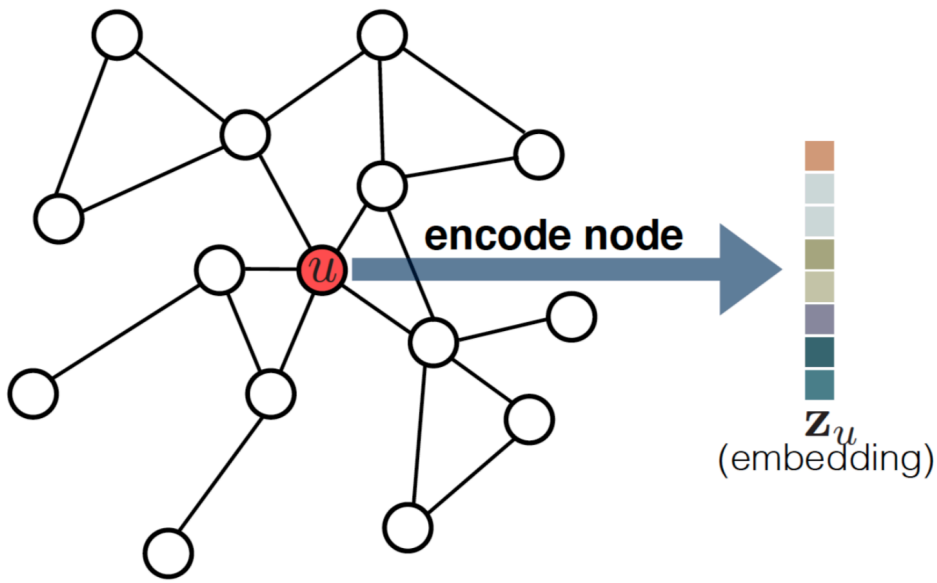
Overall Idea:

- *encoder*: maps nodes to their embeddings
- *similarity function*: defines the similarity of pairs of nodes in the (original) network
- *decoder*: maps embeddings to the (estimated) similarity score
- **optimize the parameters of the encoder so that the similarity of two nodes in the network is approximated by their embeddings**

Encoder-Decoder Components: Encoder

$ENC : V \rightarrow \mathbb{R}^d$

Given $v \in V$, ENC generates the embedding $ENC(v) = \mathbf{z}_v$ of node v

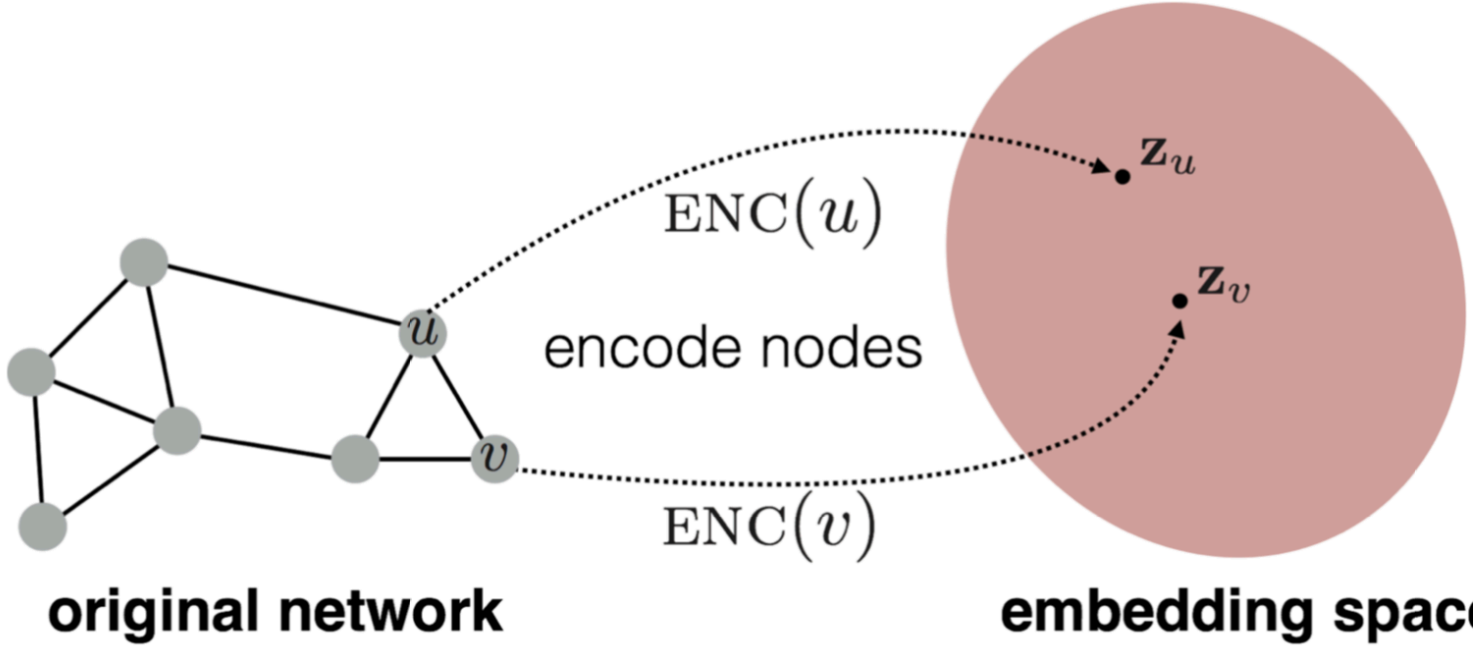


The encoder ENC depends on several parameters that are trained/optimized during the *learning* phase.

Encoder-Decoder Components: Similarity Function

We consider pairwise similarity functions: $S : V \times V \to \mathbb{R}$

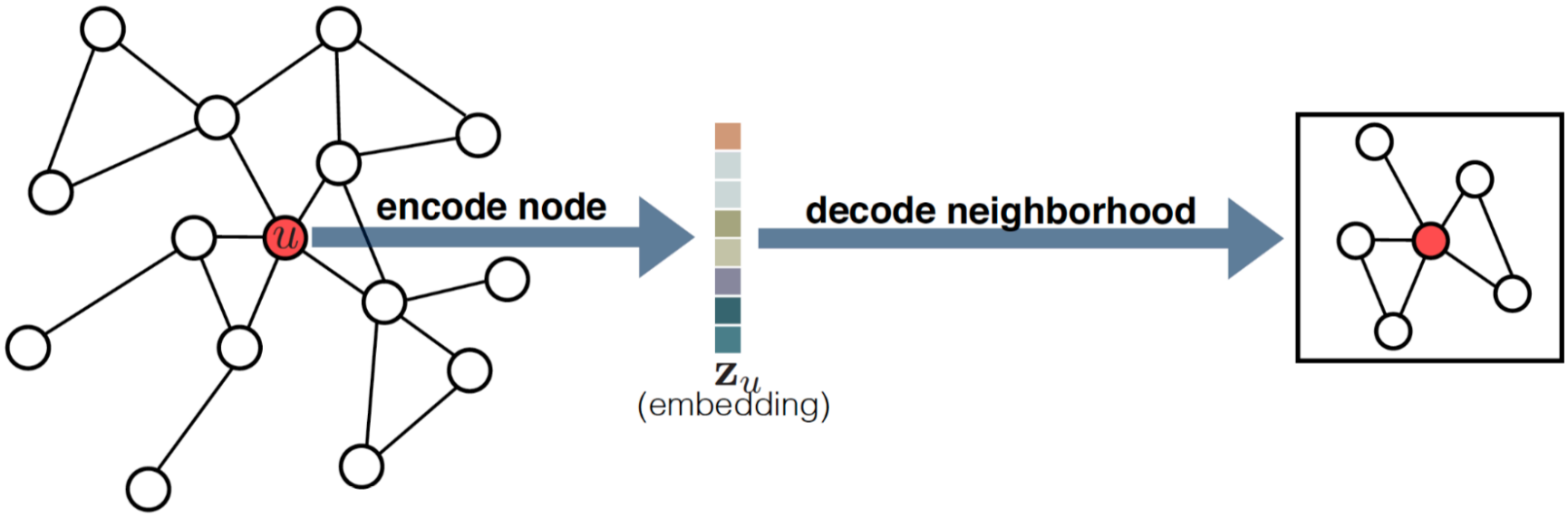
Given u and v in V, $S(u, v)$ measures the similarity between u and v in G



Usually $S(u, v)$ is represented by a matrix S with $S_{u,v} = S(u, v)$

Encoder-Decoder Components: Decoder

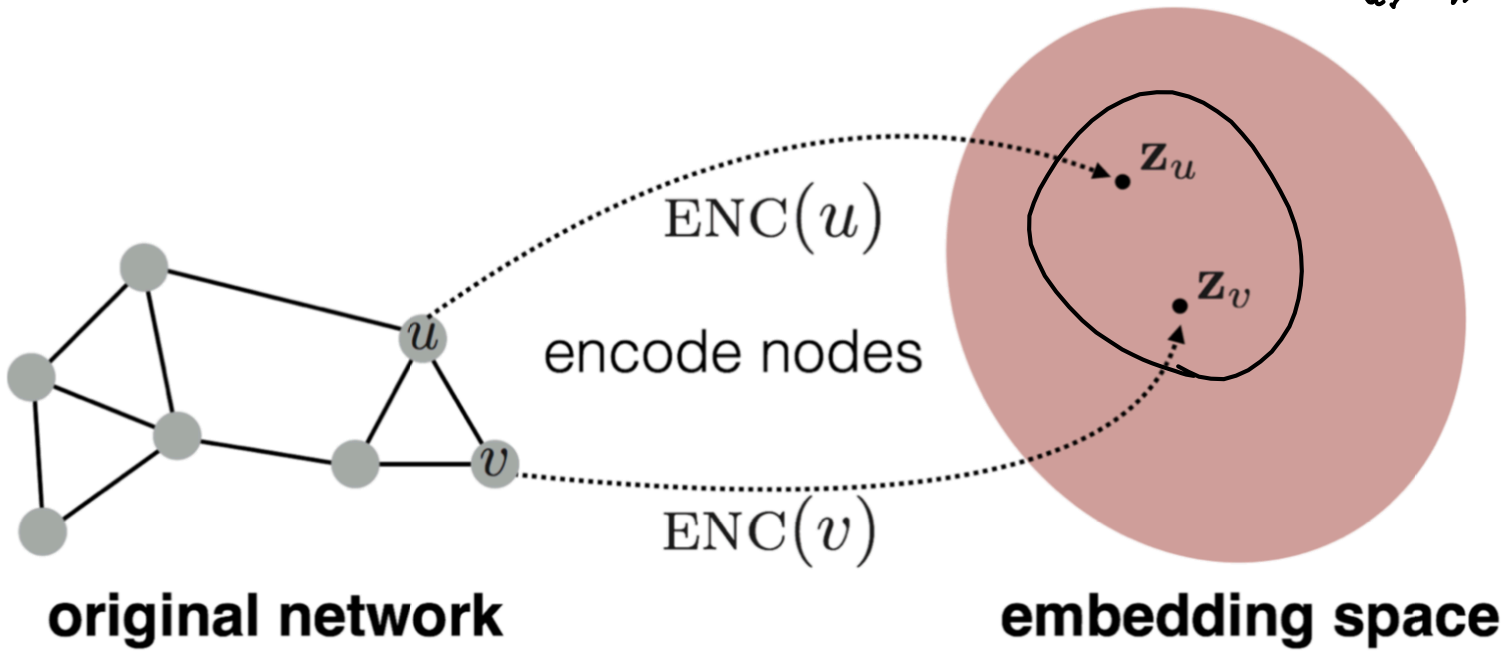
In general: a function that, given a *set of node embeddings*, computes a (user specified) *graph statistic*.



Encoder-Decoder Components: Decoder (continue)

We focus on commonly used *pairwise decoders*:
$DEC : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$.

$DEC(\vec{z}_u, \vec{z}_v) \approx s(u,v)$



Given embeddings of $\mathbf{z}_u$ and $\mathbf{z}_v$ of u and v in V, it reconstructs the similarity of nodes u and v in G.

Usually DEC has no trainable parameters.

Loss Function

Given nodes $u, v \in V$, the loss function is:

$$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v))$$

$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v))$ measures the discrepancy between the *decoded* similarity value $DEC(\mathbf{z}_u, \mathbf{z}_v)$ and the *true* similarity $S(u, v)$.

Overall Goal: optimize the parameters of ENC so that each pair $u, v \in V$:

$$DEC(\mathbf{z}_u, \mathbf{z}_v) = DEC(ENC(u), ENC(v)) \approx S(u, v)$$

$\approx$: captured by $\ell(DEC(ENC(u), ENC(v)), S(u, v))$

Encoder-Decoder Framework

In practice: set *ENC* parameters to minimize the *empirical loss*:

$$\mathcal{L} = \sum_{u,v \in V \times V} \ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u,v))$$

niente media come in ML
⇓
con notazione più facile

Sometimes: a set $\mathcal{D}$ of training pairs of nodes is used

$$\mathcal{L} = \sum_{u,v \in \mathcal{D}} \ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u,v))$$

"Shallow" Encoding

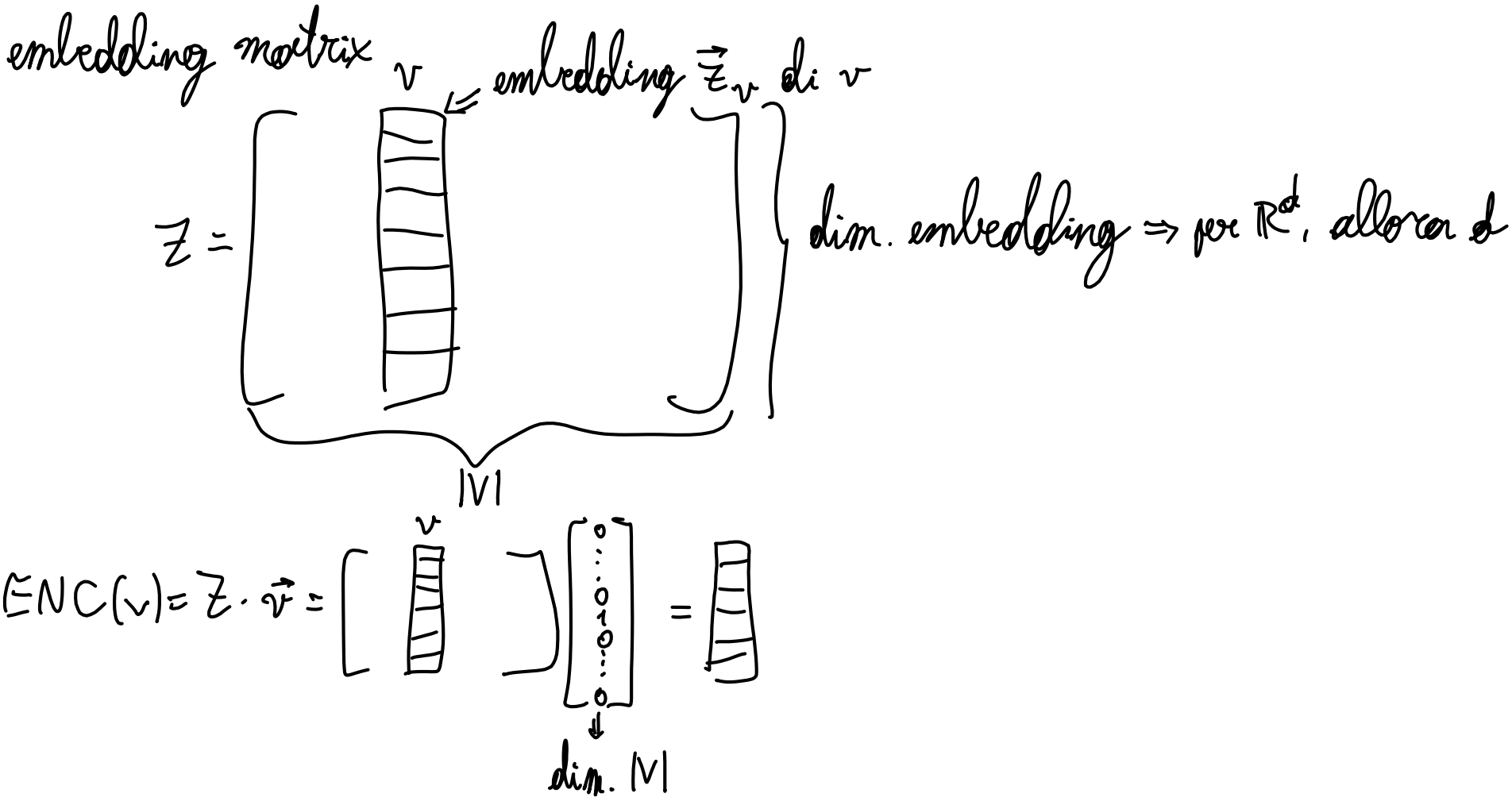
We now consider the simplest type of encoder: ENC is a look-up function

$$ENC(v) = \mathbf{z}_v = \mathbf{Z} \times \mathbf{v}$$

where

- $\mathbf{Z} \in \mathbb{R}^{d \times |V|}$: matrix where each column is a node embedding
- $\mathbf{v} \in \{0,1\}^{|V|}$: indicator vector, all 0's except a single 1 indicating node v

"Shallow" Encoding (continue)



"Shallow" Encoding: Notes

We directly optimize the embedding of each node

Parameters? All entries of $\mathbf{Z}$

Note: with "shallow" embeddings we are learning a *representation* (vector in $\mathbb{R}^d$) for each node $v \in V$, but we are not learning a *function* to obtain the representation of a node $v \in V$.

It is *unsupervised/self-supervised* way of learning node embeddings:

- we are not using node labels
- we are not using node features

These embeddings are *task independent*: they are not trained for a specific task but can be used for *any* task.

"Shallow" Encoding: Methods

Several methods to obtain "shallow" embeddings have been proposed.

Key difference: *definition of node similarity* $S(u, v)$

Question: when are two nodes u and v similar?

When they:

- are directly connected?
- have a similar neighborhood?
- ?

Adjacency-based Similarity Embeddings

Let A be adjacency matrix of G.

Similarity: $S(u, v) = A_{u,v}$ = $\begin{cases} 1 \text{ if } (u,v) \in E \\ 0 \text{ otherwise} \end{cases}$

Encoder: shallow encoder $ENC(v) = \mathbf{Z} \times \mathbf{v} = \mathbf{z}_v$

Decoder: $DEC(\mathbf{z}_u, \mathbf{z}_v) = \mathbf{z}_u^T \mathbf{z}_v$ ⇒ praticamente sempre usato per shallow

Loss function: squared-loss

$$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v)) = \left(\mathbf{z}_u^T \mathbf{z}_v - A_{u,v}\right)^2$$

Adjacency-based Similarity Embeddings (continue)

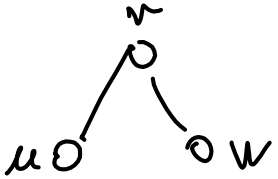
Empirical loss:

$$\mathcal{L} = \sum_{u,v \in V \times V} \ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u,v)) = \sum_{u,v \in V \times V} \left(\mathbf{z}_u^T \mathbf{z}_v - A_{u,v} \right)^2$$

Therefore the embeddings $\mathbf{z}_v$ for each $v \in V$ are given by the solution $\mathbf{Z}^*$ to

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \sum_{u,v \in V \times V} \left(\mathbf{z}_u^T \mathbf{z}_v - A_{u,v} \right)^2$$

Example



embedding in $\mathbb{R}^2 \Rightarrow \vec{z}_u = \begin{bmatrix} z_u^1 \\ z_u^2 \end{bmatrix}, \vec{z}_v, \vec{z}_w$

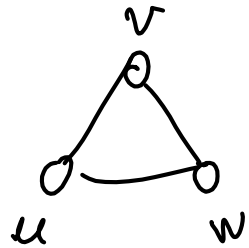
$\Downarrow$

adjacency matrix $A = \begin{array}{c} \\ u \\ v \\ w \end{array} \begin{array}{c} \begin{array}{ccc} u & v & w \end{array} \\ \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \end{array}$ $\Rightarrow$ goal: $\vec{z}_u^T \cdot \vec{z}_v \approx A_{u,v}$, $\vec{z}_v \cdot \vec{z}_w \approx 1$, $\vec{z}_w \cdot \vec{z}_u \approx 0$

$\Downarrow$

misurato da squared-loss

$\vec{z}_u = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\vec{z}_v = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $\vec{z}_w = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ $\Rightarrow$ così, $\mathcal{L} = 0 \Rightarrow$ sol. ottimale

G: 

$\Rightarrow$ $A = \begin{array}{c} \\ u \\ v \\ w \end{array} \begin{array}{c} \begin{array}{ccc} u & v & w \end{array} \\ \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \end{array}$

Embedding in $\mathbb{R}^2$ $\Rightarrow$ $\vec{z}_u = \vec{z}_v = \vec{z}_w = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

HW:

dato $G=(V,E)$ con $|E|=m$. $\exists$ embedding in $\mathbb{R}^m$ tale che $\mathcal{L}=0$?

Computing Adjacency-based Similarity Embeddings

We want to compute

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \sum_{u,v \in V \times V} \left(\mathbf{z}_u^T \mathbf{z}_v - A_{u,v} \right)^2$$

How do we compute $\mathbf{Z}^*$?

$\operatorname{argmin}_Z \|Z^T Z - A\|_F$

FROBENIUS FORM: $\|X\|_F = \sum_{i,j} X_{ij}^2$

Two ways:

- matrix decompositions (e.g., SVD): do not scale
- general optimization methods: ...

Gradient Descent (GD)

General approach for *minimizing* a differentiable convex function $f(\mathbf{z})$

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a differentiable function

Definition

The *gradient* $\nabla f(\mathbf{z})$ of f at $\mathbf{z} = (z_1, \ldots, z_d)$ is

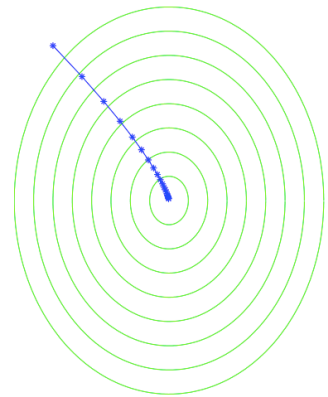
$$\nabla f(\mathbf{z}) = \left(\frac{\partial f(\mathbf{z})}{\partial z_1}, \ldots, \frac{\partial f(\mathbf{z})}{\partial z_d} \right)$$

Intuition: the gradient points in the direction of the greatest rate of increase of f around $\mathbf{z}$

Let $\eta \in \mathbb{R}, \eta > 0$ be a parameter.

GD algorithm:

$\mathbf{z} \leftarrow$ random vector in $\mathbb{R}^d$;
while *not converged* **do**
  $\mathbf{z} \leftarrow \mathbf{z} - \eta \nabla f(\mathbf{z})$;
return $\mathbf{z}$;



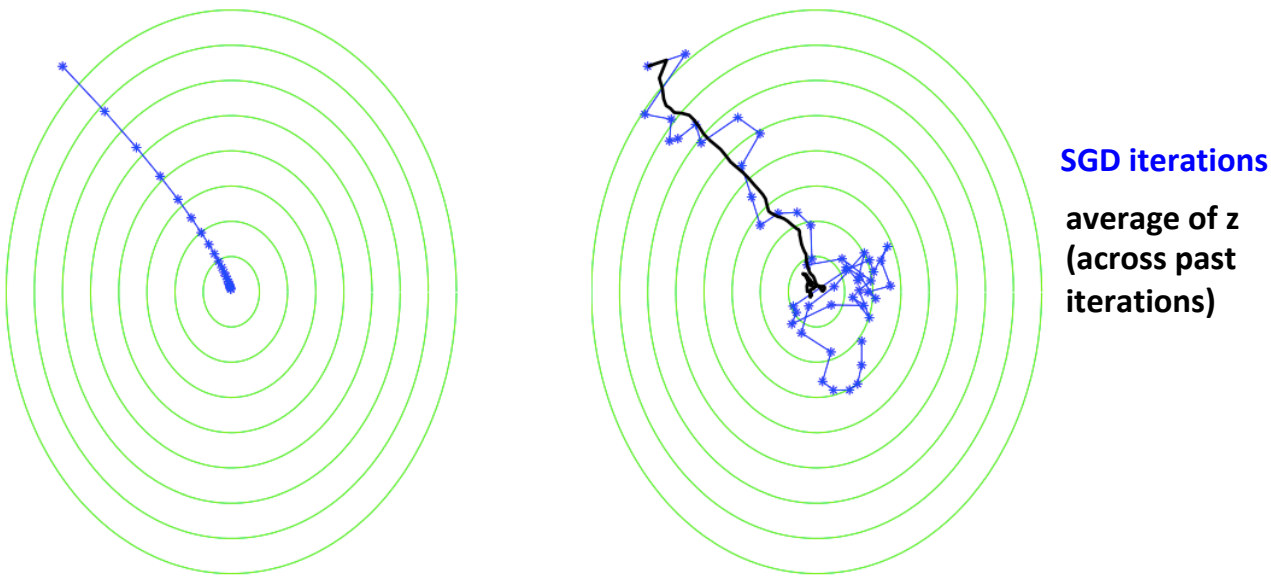
η is called *learning rate*; sometimes a *time dependent* η is used (e.g., "move" more at the beginning than at the end)

Stochastic Gradient Descent (SGD)

Idea: instead of using exactly the gradient, we take a (random) vector with *expected value* equal to the gradient direction.

SGD algorithm:

$\mathbf{z} \leftarrow$ random vector in $\mathbb{R}^d$;
while *not converged* **do**
    choose $\mathbf{v}$ at random from a distribution such that $\mathbb{E}[\mathbf{v}|\mathbf{z}] \in \nabla f(\mathbf{z})$;
    `/* v has expected value equal to the gradient of` $f(\mathbf{z})$ `*/`
    $\mathbf{z} \leftarrow \mathbf{z} - \eta\mathbf{v}$;
return $\mathbf{z}$;



Adjacency-based Similarity Embeddings: GD

Adjacency-based Similarity Embeddings: SGD

Adjacency-based Similarity Embeddings: Limitation

While useful, adjacency-based similarity only considers direct connections among nodes

Extended-Neighborhood Similarity Embeddings: Cons

Idea: define similarity between u and v as a measure of similarity between their neighborhoods $\mathcal{N}(u)$ and $\mathcal{N}(v)$

Jaccard-Similarity

Definition

Given two vertices u and v, the *Jaccard similarity* between their neighborhoods is:

$$J(\mathcal{N}(u), \mathcal{N}(v)) = \frac{|\mathcal{N}(u) \cap \mathcal{N}(v)|}{|\mathcal{N}(u) \cup \mathcal{N}(v)|}$$

Example

Embedding with Jaccard Similarity

Similarity: $S(u, v) = J(\mathcal{N}(u), \mathcal{N}(v))$

Encoder: shallow encoder $ENC(v) = \mathbf{Z} \times \mathbf{v} = \mathbf{z}_v$

Decoder: $DEC(\mathbf{z}_u, \mathbf{z}_v) = \mathbf{z}_u^T \mathbf{z}_v$

Loss function: squared-loss

$$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v)) = \left(\mathbf{z}_u^T \mathbf{z}_v - J(\mathcal{N}(u), \mathcal{N}(v))\right)^2$$

Embeddings with Jaccard Similarity (continue)

Empirical loss:

$$\begin{aligned}\mathcal{L} &= \sum_{u,v \in V \times V} \ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u,v)) \\ &= \sum_{u,v \in V \times V} \left(\mathbf{z}_u^T \mathbf{z}_v - J(\mathcal{N}(u), \mathcal{N}(v))\right)^2\end{aligned}$$

Therefore the embeddings $\mathbf{z}_v$ for each $v \in V$ are given by the solution $\mathbf{Z}^*$ to

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \sum_{u,v \in V \times V} \left(\mathbf{z}_u^T \mathbf{z}_v - J(\mathcal{N}(u), \mathcal{N}(v))\right)^2$$

Embeddings with Jaccard Similarity: Notes

How do we compute $\mathbf{Z}^*$?

This approach can be generalized to consider an *extended neighborhood* of nodes, e.g. all nodes within distance k from u

Node Embeddings: Random-Walk Approaches

Idea: the similarity between u and v is given by the probability of visiting v on a random walk of length k starting at node u

Definition

Given a graph $G = (V, E)$, we define $\Pr_k[v|u]$ as the probability of visiting node v on a random walk of length k starting at u.

Random Walks

What is a random walk of length k starting at u?

Algorithm `RandomWalk`(u, k)
Input: node $u \in V$ of graph $G = (V, E)$; $k \in \mathbb{N}$
Output: random walk of length k starting from u
$v^{(0)} \leftarrow u$;
for $i \leftarrow 1$ *to* k **do**
    $v^{(i)} \leftarrow$ random vertex chosen uniformly at random from $\mathcal{N}\left(v^{(i-1)}\right)$;
return;

Example

Example

Node Embeddings: Random-Walk Approaches (continue)

Observation: in general, $\Pr_k[v|u] \neq \Pr_k[u|v]$

Random-Walk Approaches: Motivation

Why Random Walks?

Expressivity: flexible stochastic definition of node similarity that incorporates both *local* and *higher-order* neighborhood information

Efficiency: no need to consider all node pairs to learn the embedding, only need to consider pairs that co-occur on random walks.

Random-Walk Approaches: Components

Similarity: $S(u, v) = \Pr_k[v|u]$

Encoder: shallow encoder $ENC(v) = \mathbf{Z} \times \mathbf{v} = \mathbf{z}_v$

Decoder: $DEC(\mathbf{z}_u, \mathbf{z}_v) = \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$ (softmax function)

Note: the values $DEC(\mathbf{z}_u, \mathbf{z}_v)$ for all $v \in V$ define a *probability distribution*

Random-Walk Approaches: Loss Function

Loss function: measure of distance between the true values $\Pr_k[v|u]$ and the predicted values $DEC(\mathbf{z}_u, \mathbf{z}_v) = \frac{e^{\mathbf{z}_u^T z_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T z_i}}$

The loss function is

$$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v)) = -\Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Random-Walk Approaches: Empirical Loss

Empirical loss:

$$\mathcal{L} = - \sum_{u,v \in V \times V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Therefore the embeddings $\mathbf{z}_v$ for each $v \in V$ are given by the solution $\mathbf{Z}^*$ to

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} - \sum_{u,v \in V \times V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T z_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T z_i}}$$

Loss Function: Motivation

Let's go back to the loss function:

$$\ell(DEC(\mathbf{z}_u, \mathbf{z}_v), S(u, v)) = -\Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Where does it come from?

Loss function: measure of distance between the true values $\Pr_k[v|u]$ for all $v \in V$ and the corresponding predicted values $DEC(\mathbf{z}_u, \mathbf{z}_v) = \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$ for all $v \in V$

$\Rightarrow$ measure of the difference between two sets of probabilities

Loss Function: Motivation (continue)

Cross-entropy $H(p, q)$ between two probability distributions p, q is a *measure of the difference* beween p and q.

Definition

Given two discrete probability distributions p and q with the same support $\mathcal{X}$, the cross-entropy between p and q is:

$$-\sum_{x \in \mathcal{X}} p(x) \log q(x)$$

Therefore, for a given u, the difference between the true values $\Pr_k[v|u]$ and their predicted values $\frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T z_i}}$ is

$$-\sum_{v \in V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Loss Function: Motivation (continue)

Summing such difference for all nodes u gives:

$$-\sum_{u\in V}\sum_{v\in V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i\in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

that is exactly the empirical loss

$$-\sum_{u,v\in V\times V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i\in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Random-Walk Approaches: Computation

How do we find the best embedding $\mathbf{Z}^*$?

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} - \sum_{u,v \in V \times V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

From the previous slides:

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \mathcal{L}$$

$$= - \sum_{u \in V} \sum_{v \in V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Complexity to *evaluate* $\mathcal{L}$? $\Theta\left(|V|^2\right)$
$\Rightarrow$ too expensive for large networks!

Random-Walk Approaches: Optimizations

$$-\sum_{u \in V} \sum_{v \in V} \Pr_k[v|u] \log \frac{e^{\mathbf{z}_u^T z_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T z_i}}$$

Instead of considering all terms $\Pr_k[v|u]$, consider only vertices v with *high* $\Pr_k[v|u]$.

Given u, how do we find vertices v with high $\Pr_k[v|u]$?

$\Pr_k[v|u]$ as the probability of visiting node v on a random walk of length k starting at u

$\Rightarrow$ run random walks of length k from u: if $\Pr_k[v|u]$ is high, v will appear in the random walks!

Random-Walk Approaches: Optimizations (continue)

Definition

Let $\mathcal{N}_{RW,k}(u)$ be the *set* of nodes visited on a random walks of length k starting from node u.

Definition

Consider s random walks of length k starting from u. Let $n_{RW,k,s}(v|u)$ be the number of such walks containing v.

Example

Random-Walk Approaches: Optimizations (continue)

Note that $n_{RW,k,s}(v|u)$ is a random variable.

Proposition

$$\mathbb{E}\left[\frac{n_{RW,k,s}(v|u)}{s}\right] = \Pr_k[v|u]$$

Random-Walk Approaches: Optimizations (continue)

Let $\mathcal{M}_{RW,k,s}(u)$ be the *multiset* of nodes visited during s random walks of length k starting from u, where vertex v appears in $\mathcal{M}_{RW,k,s}(u)$ exactly $n_{RW,k,s}(v|u)$ times

Example

Random-Walk Approaches: Optimizations (continue)

We can use $\frac{n_{RW,k,s}(v|u)}{s}$ instead of $\Pr_k[v|u]$ in the empirical loss.

Random-Walk Approaches: Optimizations (continue)

Overall, the approach is:

1. run s random walks of length k from each node $u \in V$ to obtain $\mathcal{M}_{RW,k,s}(u)$
2. solve the following problem:

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \mathcal{L}$$

$$= -\sum_{u \in V} \sum_{v \in \mathcal{M}_{RW,k,s}(u)} \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Complexity? $\Theta\left(|V|^2\right)$...

DeepWalk

What we have described up to know corresponds to the method DeepWalk, described in Perozzi et al. (2014), *DeepWalk: online learning of social representations*, ACM KDD.

The paper presents also an optimization to reduce the complexity to $\Theta(|V| \log |V|)$

DeepWalk: Experimental Evaluation

From Perozzi et al. (2014), *DeepWalk: online learning of social representations*, ACM KDD.

Datasets:

Name	BlogCatalog	Flickr	YouTube
$\|V\|$	10,312	80,513	1,138,499
$\|E\|$	333,983	5,899,882	2,990,443
$\|\mathcal{Y}\|$	39	195	47
Labels	Interests	Groups	Groups

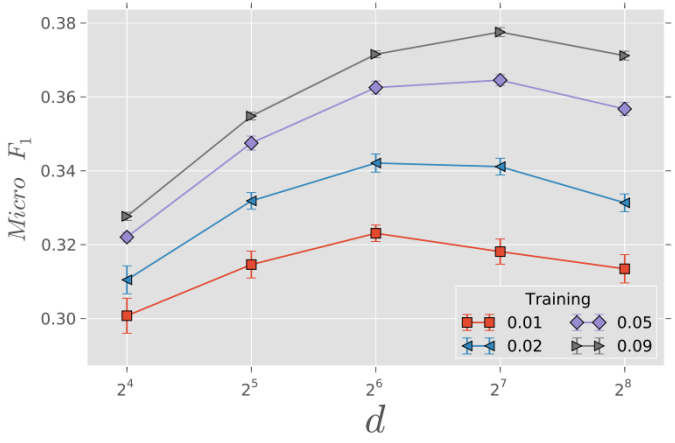
- randomly sample a portion of the labeled nodes, use them as training data
- rest of the nodes are used as test
- repeat the process 10 times, and report the average
- dimension $d = 128$ for DeepWalk
- use a one-vs-rest logistic regression for classification

DeepWalk: Experimental Evaluation (continue)

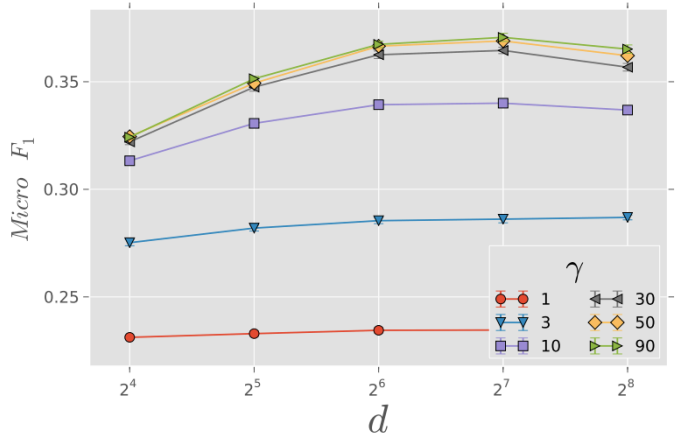
	% Labeled Nodes	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
Micro-F1(%)	DeepWalk	**32.4**	**34.6**	**35.9**	**36.7**	**37.2**	**37.7**	**38.1**	**38.3**	**38.5**	**38.7**
	SpectralClustering	27.43	30.11	31.63	32.69	33.31	33.95	34.46	34.81	35.14	35.41
	EdgeCluster	25.75	28.53	29.14	30.31	30.85	31.53	31.75	31.76	32.19	32.84
	Modularity	22.75	25.29	27.3	27.6	28.05	29.33	29.43	28.89	29.17	29.2
	wvRN	17.7	14.43	15.72	20.97	19.83	19.42	19.22	21.25	22.51	22.73
	Majority	16.34	16.31	16.34	16.46	16.65	16.44	16.38	16.62	16.67	16.71
Macro-F1(%)	DeepWalk	**14.0**	17.3	**19.6**	**21.1**	**22.1**	**22.9**	**23.6**	**24.1**	**24.6**	**25.0**
	SpectralClustering	13.84	**17.49**	19.44	20.75	21.60	22.36	23.01	23.36	23.82	24.05
	EdgeCluster	10.52	14.10	15.91	16.72	18.01	18.54	19.54	20.18	20.78	20.85
	Modularity	10.21	13.37	15.24	15.11	16.14	16.64	17.02	17.1	17.14	17.12
	wvRN	1.53	2.46	2.91	3.47	4.95	5.56	5.82	6.59	8.00	7.26
	Majority	0.45	0.44	0.45	0.46	0.47	0.44	0.45	0.47	0.47	0.47

Table 3: Multi-label classification results in Flickr

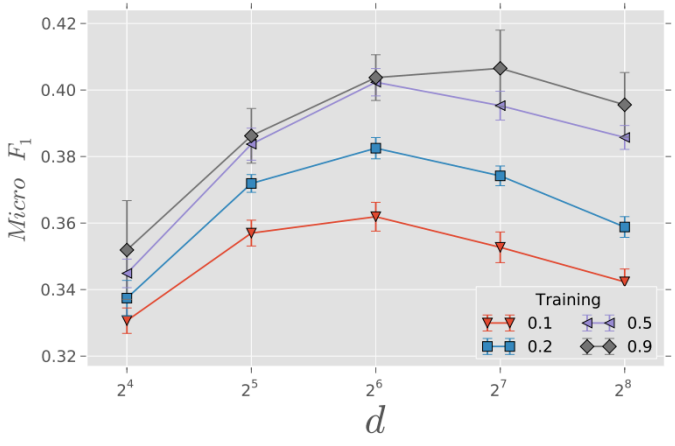
DeepWalk: Experimental Evaluation (continue)



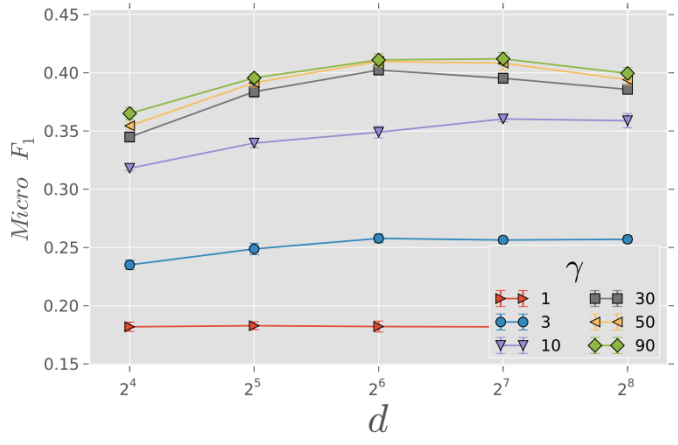
(a1) FLICKR, $\gamma = 30$



(a2) FLICKR, $T_R = 0.05$



(a3) BLOGCATALOG, $\gamma = 30$



(a4) BLOGCATALOG, $T_R = 0.5$

(a) Stability over dimensions, d

node2vec

A. Grover et al. (2016), *node2vec: Scalable Feature Learning for Networks*, ACM KDD.

Basic idea: as described for random walks approaches.

Presents a different approach to reduce the complexity.

Also based on a different type of random walks.

Recap

node2vec: Motivation

The random walk approach is:

1. run s random walks of length k from each node $u \in V$ to obtain $\mathcal{M}_{RW,k,s}(u)$
2. solve the following problem:

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \mathcal{L}$$

$$= -\sum_{u \in V} \sum_{v \in \mathcal{M}_{RW,k,s}(u)} \log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

Complexity is $\Theta\left(|V|^2\right)$, due to computation of $\log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$ for all $u \in V$

Can we approximate $\log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$?

Negative Sampling

Idea: the softmax

$$\log \frac{e^{\mathbf{z}_u^T \mathbf{z}_v}}{\sum_{i \in V} e^{\mathbf{z}_u^T \mathbf{z}_i}}$$

is a way to compare the (decoded) probability for node v (given node u) and the *background* probabilities of all nodes given u.

Therefore:

- use a different function to obtain a probability for a node v (given node u)
- sample random nodes to obtain the *background* probabilities

Negative Sampling (continue)

`node2vec` uses the following to compare the (decoded) probability for node v (given node u) and the *background* probability:

$$\log\left(\sigma(\mathbf{z}_u^T \mathbf{z}_v)\right) - \sum_{i=1}^{r} \log\left(\sigma(\mathbf{z}_u^T \mathbf{z}_i)\right)$$

where:

- i is a node chosen from $|V|$ *with probability proportional to its degree*
- $\sigma()$: sigmoid function

The r samples are called **negative events**.

Negative Sampling (continue)

What about the choice of r?

- large $r \Rightarrow$ robust estimates
- large $r \Rightarrow$ stronger focus on negative events

In practice: $r \in \{5, \ldots, 20\}$

Putting everything together, the problem to be solved is

$$\mathbf{Z}^* = \arg\min_{\mathbf{Z}} \mathcal{L}$$

$$= \arg\min_{\mathbf{Z}} - \sum_{u \in V} \sum_{v \in \mathcal{M}_{RW,k,s}(u)} \left(\log \left(\sigma(\mathbf{z}_u^T \mathbf{z}_v) \right) - \sum_{i=1}^{r} \log \left(\sigma(\mathbf{z}_u^T \mathbf{z}_i) \right) \right)$$

How to find $\mathbf{Z}^*$?

node2vec: Random Walks

Other difference between DeepWalk and node2vec: type of random walks used:

- DeepWalk: random walks as presented before
- node2vec: uses *biased random walks*

node2vec: Biased Random Walks

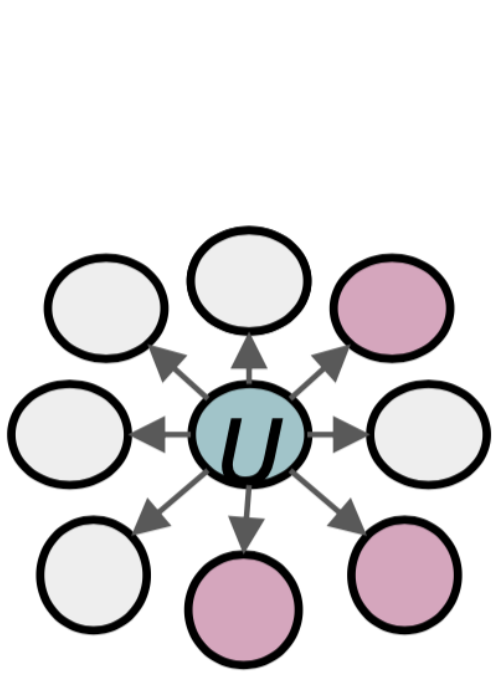
Idea: in iteration i and the current node $v^{(i)}$, compute weights to choose the next node $v^{(i+1)}$ in the node; the weights depend on the distance of a candidate next node from the previous vertex $v^{(i-1)}$.

Algorithm `RandomWalk`(u, k, p)
Input: node $u \in V$ of graph $G = (V, E)$; $k \in \mathbb{N}$; function $p : V \times V \to [0, 1]$
Output: random walk of length k starting from u
$v^0 \leftarrow u$;
for $i \leftarrow 1$ *to* k **do**
    $v^{(i)} \leftarrow$ vertex chosen from $\mathcal{N}\left(v^{(i-1)}\right)$ according to the probabilities $p(v^{(i-1)}, v^{(i)})$;
return;

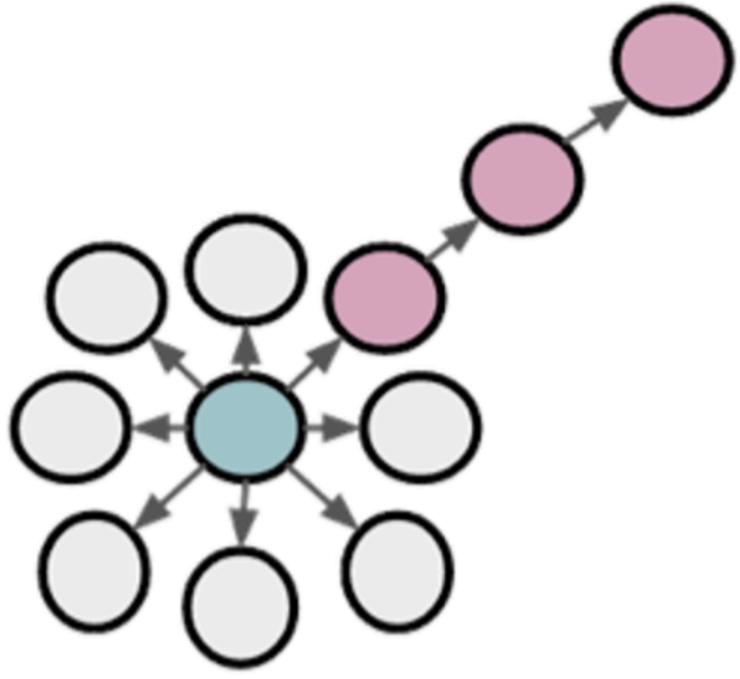
node2vec: Biased Random Walks (continue)

Idea: the weights are chosen to combine and balance BFS-like visits and DFS-like visits

BFS vs DFS



BFS



DFS

BFS: micro-view of the neighborhood
DFS: macro-view of the neighborhood

node2vec: Biased Random Walks (continue)

node2vec uses random walks of length k where given a node u the weights of edges between u and the nodes in $\mathcal{N}(u)$ depend on two parameters:

- *return parameter* p: regulates the probability to go back to the previous node in the walk
- *in-out parameter* q: regulates the "ratio" of BSF moves vs DFS moves

node2vec: Biased Random Walks (continue)

Assume the random walk has just moved from node u to node v.

Observation: the neighbours of v can only be:

- the previous node u
- at the same distance of v from u
- further than v from u

Assign to each edge (v, z), with $z \in \mathcal{N}$, a weight $w(v, z)$ as follows:

- $w(v, u) = \frac{1}{p}$
- $w(v, z) = 1$ if $z \in \mathcal{N}(u)$
- $w(v, z) = \frac{1}{q}$ if $z \notin \mathcal{N}(u)$

Then the probability $p(v, z)$ is

$$p(v, z) = \frac{w(v, z)}{\sum_{z' \in \mathcal{N}(v)} w(v, z')}$$

Example

node2vec: Biased Random Walks (continue)

The parameters p and q control the *type* of random walk performed.

Assume the random walk has just moved from node u to node v.

Impact of p:

- p is "high" ($> \max\{q, 1\}$): reduced probability to go back to u, encourages moderate exploration
- p is low ($< \min\{q, 1\}$): lead the walk to *backtrack* a step, keep the walk "local"

Impact of q:

- q is "high" (> 1): random walk is biased towards nodes close to node $u \Rightarrow$ BFS-like walk
- q is low (< 1): random walk is biased towards nodes far frmo node $u \Rightarrow$ DFS-like walk

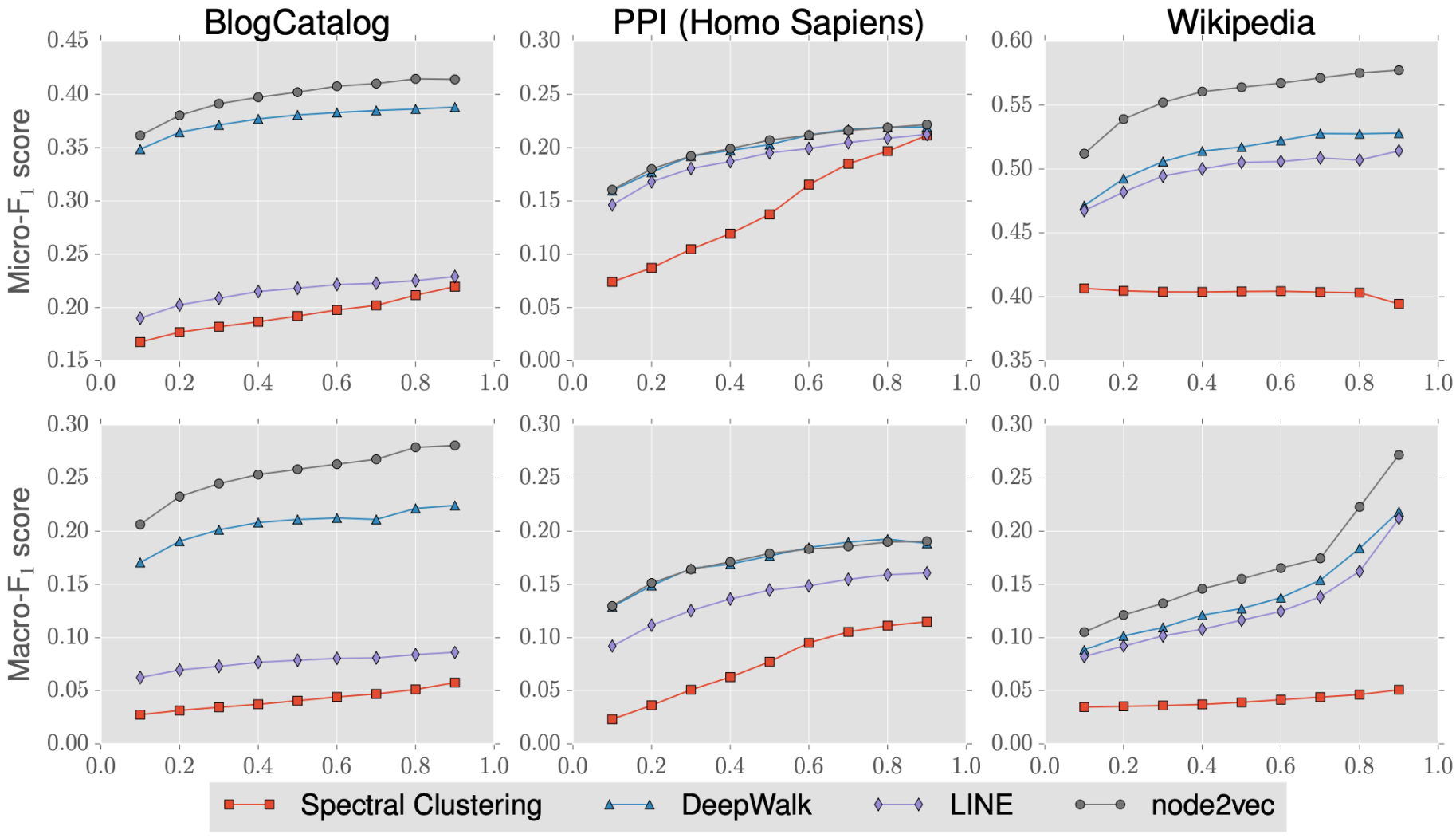
node2vec: Summary

The node2vec algorithm consists of the following steps:

1. compute random walk probabilities $p(u, v)$ for all $u \in V$ and all $v \in \mathcal{N}(u)$
2. perform s biased random walks of length k from each $u \in V$ to compute $\mathcal{M}_{RW,k,s}(u)$
3. use SGD to find $\mathbf{Z}$ that minimizes

$$-\arg\min_{\mathbf{Z}} \sum_{u \in V} \sum_{v \in \mathcal{M}_{RW,k,s}(u)} \left(\log\left(\sigma(\mathbf{z}_u^T \mathbf{z}_v)\right) - \sum_{i=1}^{r} \log\left(\sigma(\mathbf{z}_u^T \mathbf{z}_i)\right) \right)$$

node2vec: Experimental Evaluation



Random Walks: Other Approaches

Several other approaches based on random walks have been proposed.

- different kinds of biased random walks
  - using node attributes (Dong et al., 2017)
  - using weights learned from data (Abu-El-Haija et al., 2017)
- other optimization approaches
  - optimize 1-hop and 2-hop random walk probabilities (e.g., `LINE` from Tang et al., 2015)
- run random walks on modified versions of the initial graph (e.g., `HARP` from Chen et al., 2016; `struct2vec` from Ribeiro et al, 2017)

No method is the best in all situations!

In general: must choose the definition of node similarity that best suits the application

Graph Embeddings

Goal: embed an entire graph (or a subgraph) G into an embedding $\mathbf{z}_G \in \mathbb{R}^d$

Useful for several **tasks**:

- classifying toxic vs. non-toxic molecules
- identifying anomalous graphs
- ...

We are going to see approaches based on *node embeddings*

Graph Embeddings: Approach 1

1. run a node embedding technique on the (sub)graph G
2. the embedding of G is just the sum (or the average) of the embeddings of nodes in G

Example: used in *Convolutional Networks on Graphs for Learning Molecular Fingerprints.* Duvenaud et al., NeurIPS 2016.

Graph Embeddings: Approach 2

Idea: introduce a "virtual node: to represent the (sub)graph G and use its embedding as embedding of G

1. introduce a node g connected to all nodes in G
2. run a node embedding technique on the (sub)graph G (including g)
3. the embedding of G is the embedding $\mathbf{z}_g$ of g

Example: proposed in *Gated Graph Sequence Neural Networks.* Li et al., ICLR 2016.