Stanford CS224W: Node Embeddings

CS224W: Machine Learning with Graphs
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http://cs224w.stanford.edu

如何把节点映射成D维向量？

- 人工特征工程：节点重要度，集群系数，graphlet
- 图表示学习：通过随机游走构造自监督学习任务
  deepwalk，node2vec
- 矩阵分解
- 深度学习：GNN

Graph Embedding

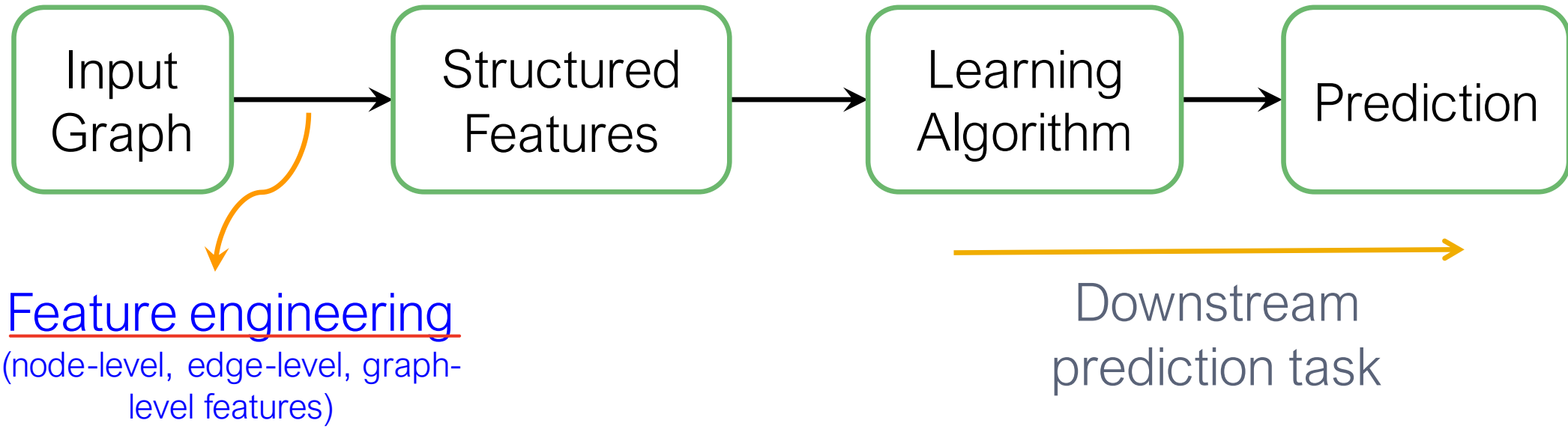
- 节点
- 边
- 子图
- 全图

基于

- 手工构造特征
- 矩阵分解
- 随机游走
- GNN

Recap: Traditional ML for Graphs

Given an input graph, extract node, link and graph-level features, learn a model (SVM, neural network, etc.) that maps features to labels.

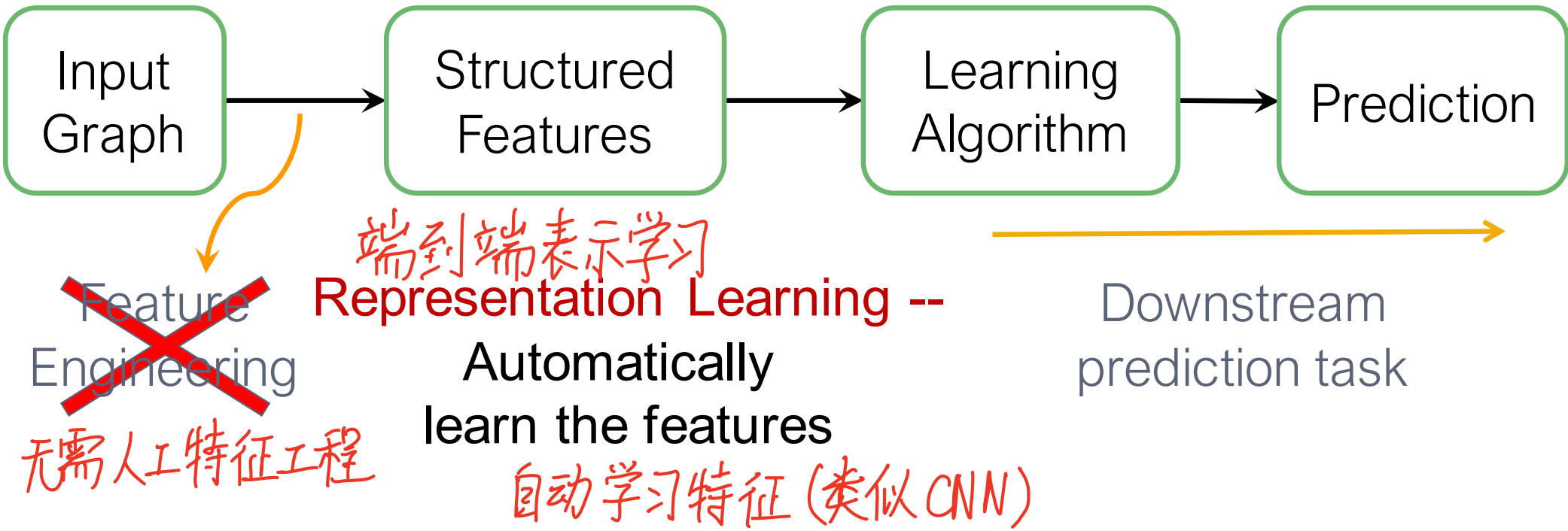


Graph Representation Learning

图表示学习：自动学习特征

减轻

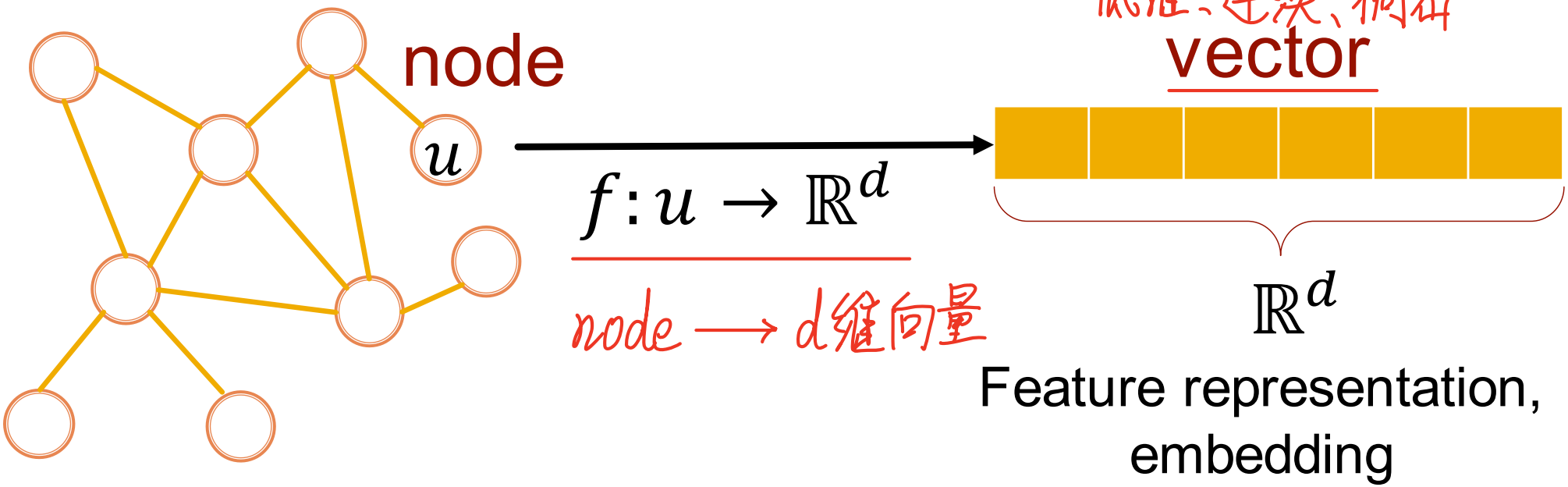
Graph Representation Learning alleviates the need to do feature engineering every single time.



Graph Representation Learning

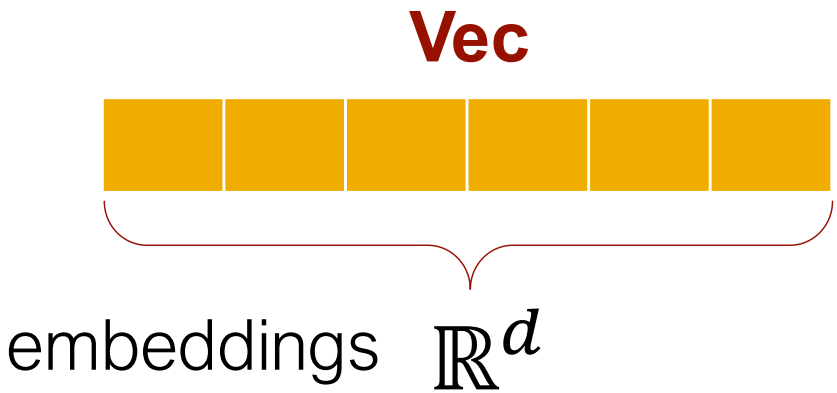
与下游任务无关

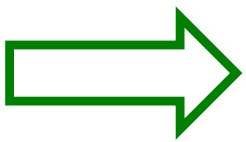
Goal: Efficient task-independent feature learning for machine learning with graphs!



Why Embedding?

- **Task: Map nodes into an embedding space**
  - Similarity of embeddings between nodes indicates their similarity in the network. For example: 向量相似度反映节点相似度
    - Both nodes are close to each other (connected by an edge)
  - Encode network information embedding还包含network的连接信息
  - Potentially used for many downstream predictions





Tasks

- Node classification
- Link prediction
- Graph classification
- Anomalous node detection
- Clustering 社群检测(聚类)
- ….

Example Node Embedding

- **2D embedding of nodes of the Zachary's Karate Club network:**

空手道俱乐部

颜色通过聚类(无监督)得到

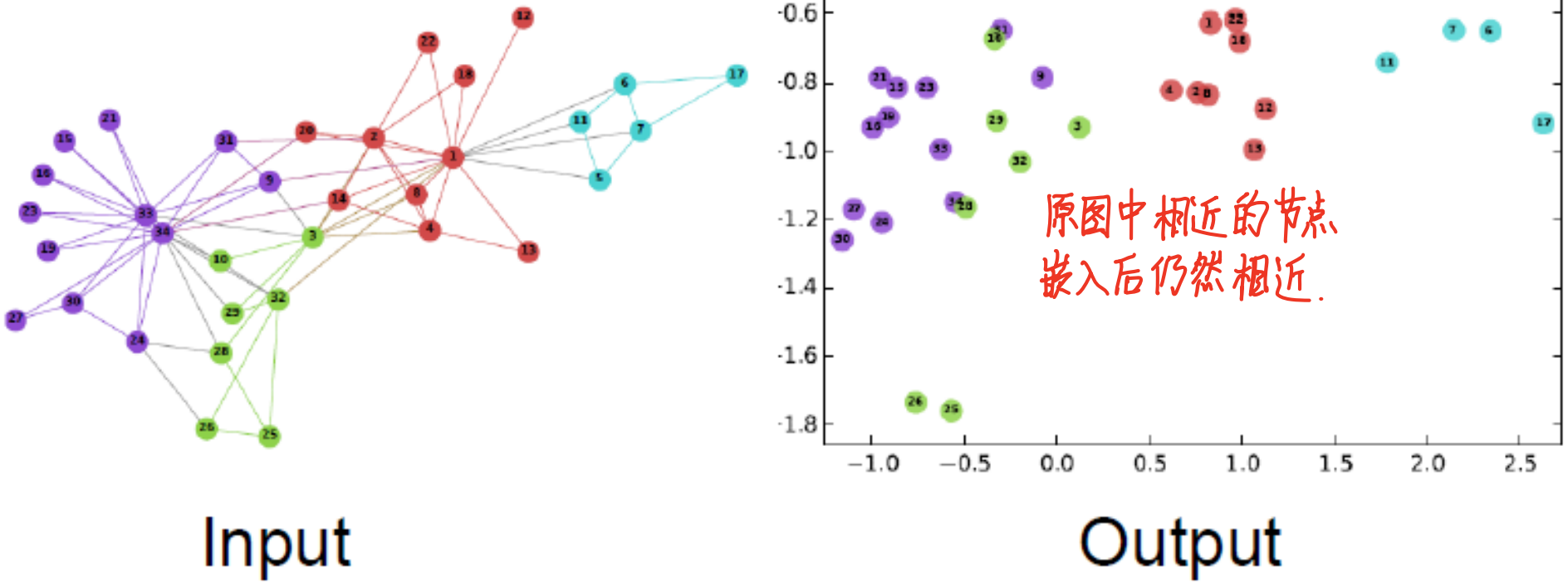


Image from: Perozzi et al. DeepWalk: Online Learning of Social Representations. *KDD 2014.*

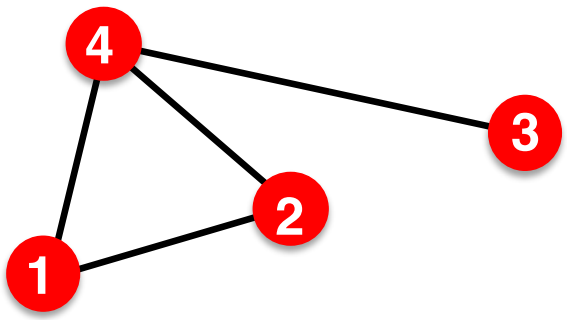
Stanford CS224W: Node Embeddings: Encoder and Decoder

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Setup

- **Assume we have a graph G:**
  - V is the vertex set.
  - A is the adjacency matrix (assume binary). 无权图
  - **For simplicity: No node features or extra information is used**

仅利用节点连接信息、
没有利用节点属性信息、



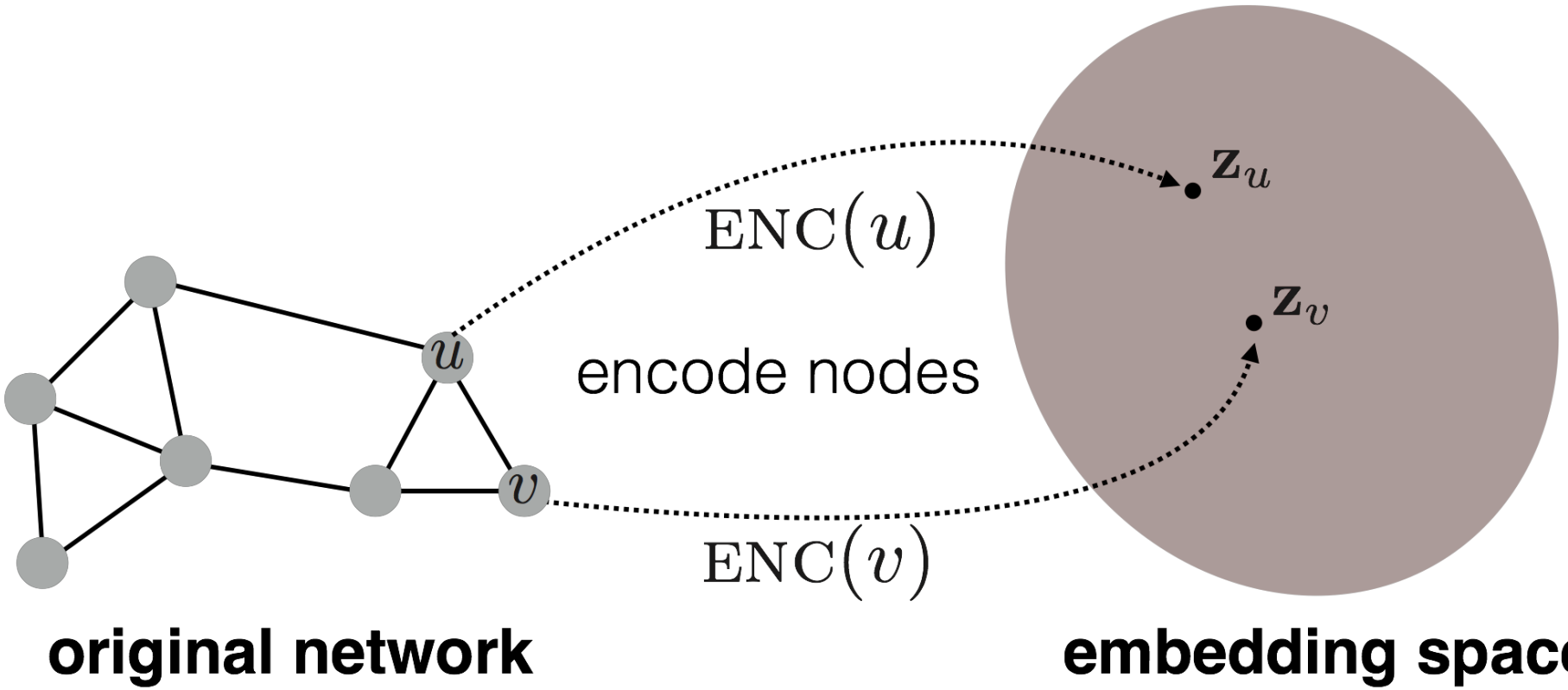
V: {1, 2, 3, 4}

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Embedding Nodes

向量的点乘数值(余弦相似度)反映节点的相似度

- Goal is to encode nodes so that similarity in the embedding space (e.g., dot product) approximates similarity in the graph



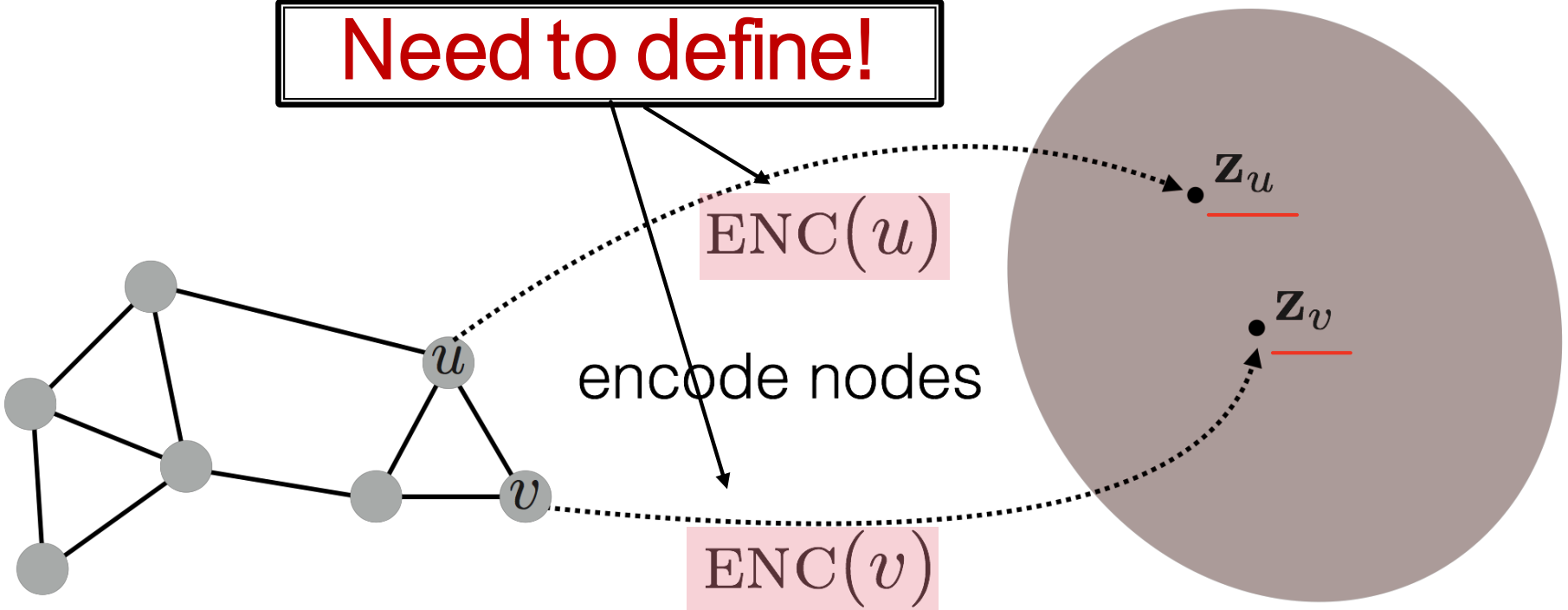
Embedding Nodes

Goal: $\text{similarity}(u, v) \approx \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$

in the original network

Similarity of the embedding

Need to define!



Learning Node Embeddings

※encoder-decoder思想贯穿整门课.

1. **Encoder** maps from nodes to embeddings
2. **Define a node similarity function** (i.e., a measure of similarity in the original network)
3. **Decoder** **DEC** maps from embeddings to the similarity score
4. **Optimize the parameters of the encoder so that:**

$\mathrm{DEC}(\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u)$

$$\underbrace{\text{similarity}(u, v)}_{\text{in the original network}} \approx \underbrace{\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u}_{\text{Similarity of the embedding}}$$

迭代优化每个节点的D维向量,使得图中相似节点内积大
不相似节点内积小

Two Key Components

- **Encoder:** maps each node to a low-dimensional vector

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

d-dimensional embedding

node in the input graph

- **Similarity function:** specifies how the relationships in vector space map to the relationships in the original network

$$\text{similarity}(u, v) \approx \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$$

Decoder

Similarity of u and v in the original network

dot product between node embeddings

"Shallow" Encoding

Simplest encoding approach: **Encoder is just an embedding-lookup** 最简单的编码器：查表

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

$\mathbf{Z} \in \mathbb{R}^{d \times |\mathcal{V}|}$ matrix, each column is a node embedding [what we learn / optimize] 优化的对象是embedding

$v \in \mathbb{I}^{|\mathcal{V}|}$ indicator vector, all zeroes except a one in column indicating node *v*

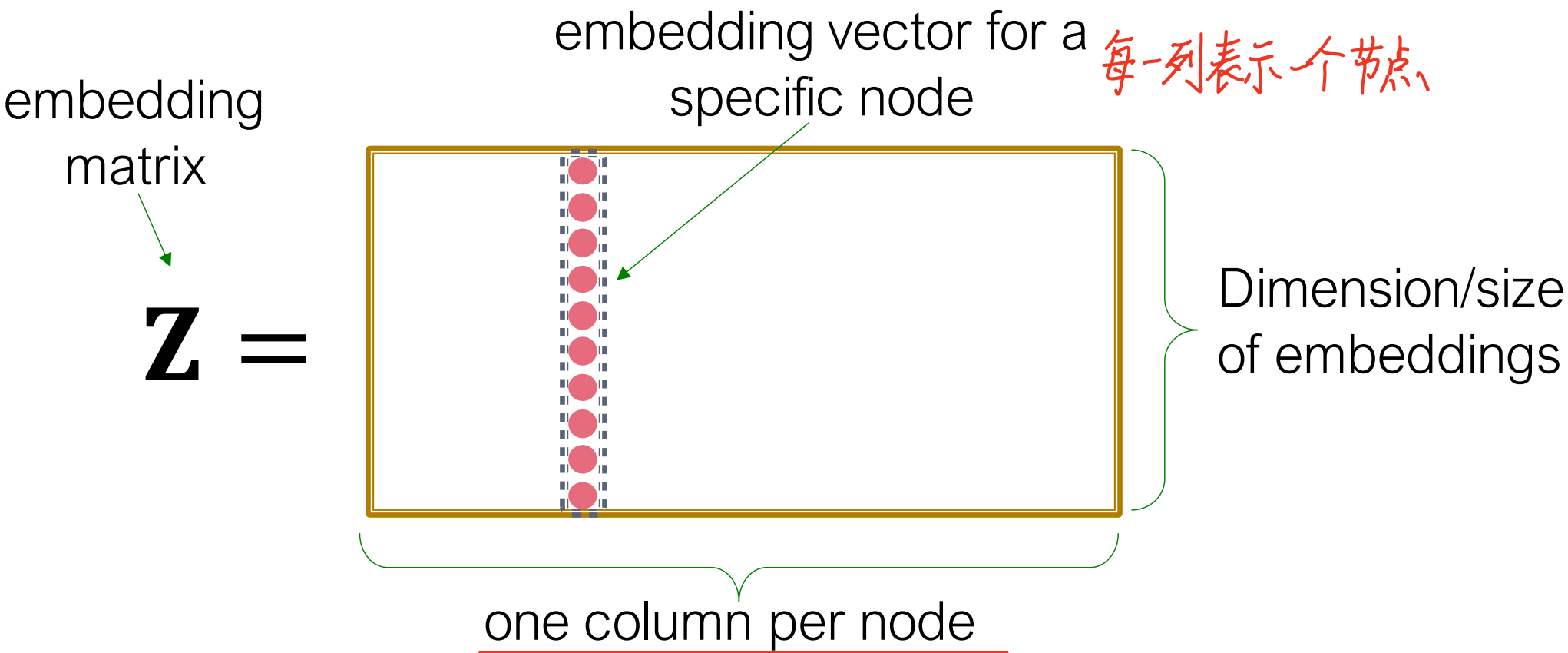
$$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

1. 直推式学习：Transductive Learning
   - 用于预测的节点在训练时就见过
   - 随机游走方法：DeepWalk，Node2Vec

2. 归纳式学习：Inductive Learning
   - 用于预测的节点在训练时没见过（泛化到新节点）
   - 图神经网络方法：GCN，GraphSAGE，GAT，GIN

"Shallow" Encoding

Simplest encoding approach: **encoder is just an embedding-lookup**



"Shallow" Encoding

Simplest encoding approach: **Encoder is just an embedding-lookup**

Each node is assigned a unique embedding vector
(i.e., we directly optimize the embedding of each node)

Many methods: DeepWalk, node2vec

Framework Summary

- **Encoder + Decoder Framework**
  - Shallow encoder: embedding lookup 查表
  - Parameters to optimize: $\mathbf{Z}$ which contains node embeddings $\mathbf{z}_u$ for all nodes $u \in V$
  - We will cover deep encoders in the GNNs (Lecture 6)

  - **Decoder:** based on node similarity.
  - **Objective:** maximize $\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$ for node pairs (u, v) that are **similar**

How to Define Node Similarity?

- Key choice of methods is **how they define node similarity.**

- Should two nodes have a similar embedding if they…
  - are linked? 直接相连
  - share neighbors? 间接相连
  - have similar "structural roles"? 相同功能角色
- We will now learn node similarity definition that uses **random walks**, and how to optimize embeddings for such a similarity measure.

Note on Node Embeddings

- This is **unsupervised/self-supervised** way of learning node embeddings.
  - We are **not** utilizing node labels
  - We are **not** utilizing node features
  - The goal is to directly estimate a set of coordinates (i.e., the embedding) of a node so that some aspect of the network structure (captured by DEC) is preserved.

直接优化嵌入向量

- These embeddings are **task independent**

与下游任务无关

  - They are not trained for a specific task but can be used for any task.

Stanford CS224W: Random Walk Approaches for Node Embeddings

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Notation

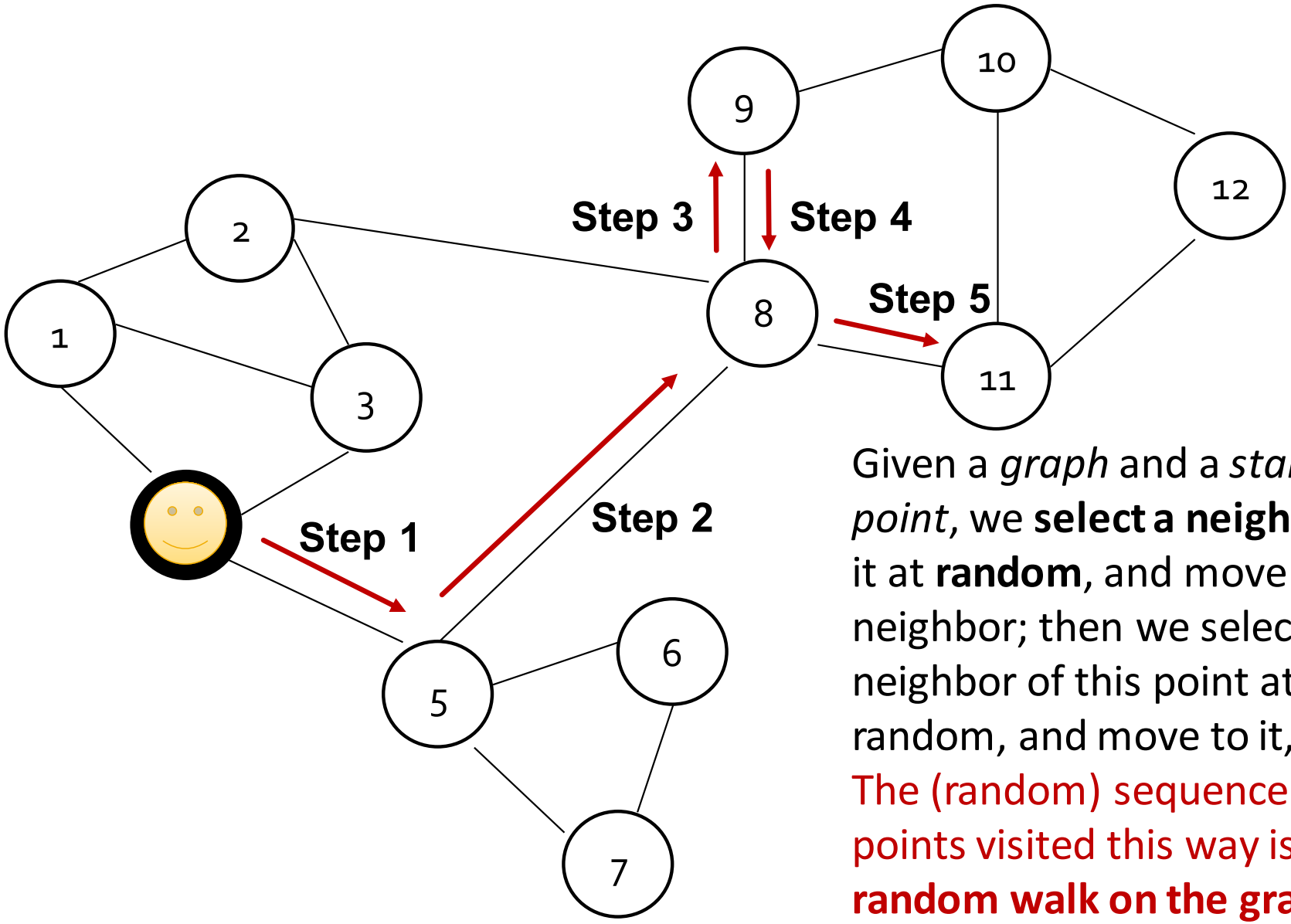
- **Vector** $\mathbf{z}_u$:
  - The embedding of node u (what we aim to find).
- **Probability** $P(v \mid \mathbf{z}_u)$: ⟸ Our model prediction based on $\mathbf{z}_u$
  - The **(predicted) probability** of visiting node v on random walks starting from node u.

从u节点出发的随机游走序列经过v节点的概率

Non-linear functions used to produce predicted **probabilities**

- **Softmax** function:
  - Turns vector of K real values (model predictions) into K probabilities that sum to 1: $\sigma(\boldsymbol{z})[i] = \frac{e^{\boldsymbol{z}[i]}}{\sum_{j=1}^{K} e^{\boldsymbol{z}[j]}}$
- **Sigmoid** function:
  - S-shaped function that turns real values into the range of (0, 1). Written as $S(x) = \frac{1}{1+e^{-x}}$.

Random Walk



Given a *graph* and a *starting point*, we **select a neighbor** of it at **random**, and move to this neighbor; then we select a neighbor of this point at random, and move to it, etc. The (random) sequence of points visited this way is a **random walk on the graph**.

图机器学习	NLP
图	文章
随机游走序列	句子
节点	单词
deepwalk	skip-gram
node embedding	word embedding

Random-Walk Embeddings

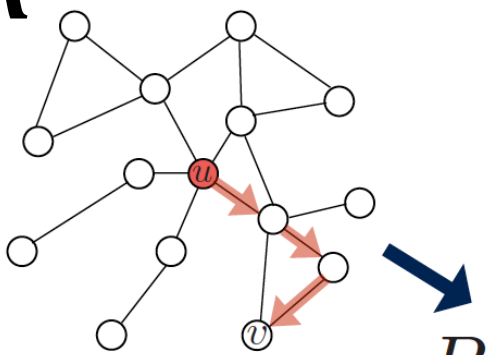
节点相似的定义：
共同出现在同一个随机游走序列

$$\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v \approx$$

probability that u and v co-occur on a random walk over the graph

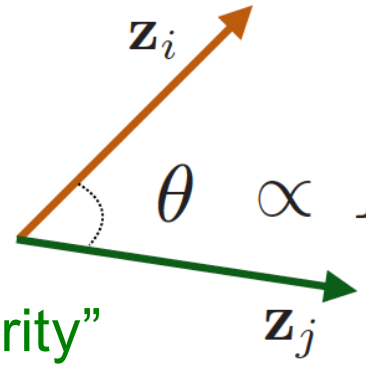
Random-Walk Embeddings

1. **Estimate probability of visiting node v on a random walk starting from node u using some random walk strategy R**



$$P_R(v|u)$$

2. **Optimize embeddings to encode these random walk statistics:**



$$\theta \propto P_R(v|u)$$

Similarity in embedding space (Here: dot product=$\cos(\theta)$) encodes random walk "similarity"

Why Random Walks?

表示能力

1. **Expressivity:** Flexible stochastic definition of node similarity that incorporates both local and higher-order neighborhood information
   Idea: if random walk starting from node u visits v with high probability, u and v are similar (high-order multi-hop information)

计算便捷　　多跳

2. **Efficiency:** Do not need to consider all node pairs when training; only need to consider pairs that co-occur on random walks

共现

Unsupervised Feature Learning

- Intuition: Find embedding of nodes in d-dimensional space that preserves similarity
- Idea: Learn node embedding such that nearby nodes are close together in the network
- Given a node u, how do we define nearby nodes?
  - $N_R(u)$ … neighbourhood of u obtained by some random walk strategy R

Feature Learning as Optimization

- Given $G = (V, E)$,
- Our goal is to learn a mapping $f: u \rightarrow \mathbb{R}^d$:
  $f(u) = \mathbf{z}_u$

- Log-likelihood objective:

$$\max_f \sum_{u \in V} \log \mathrm{P}(N_{\mathrm{R}}(u) | \mathbf{z}_u)$$

  - $N_R(u)$ is the neighborhood of node u by strategy R

- Given node u, we want to learn feature representations that are predictive of the nodes in its random walk neighborhood $N_R(u)$.

Random Walk Optimization

1. Run **short fixed-length random walks** starting from each node u in the graph using some random walk strategy R.
2. For each node u collect $N_R(u)$, the multiset* of nodes visited on random walks starting from u.
3. Optimize embeddings according to: Given node u, predict its neighbors $N_R(u)$.

$$\max_f \sum_{u \in V} \log \mathrm{P}(N_R(u) | \mathbf{z}_u) \Rightarrow$$ Maximum likelihood objective

*$N_R(u)$ can have repeat elements since nodes can be visited multiple times on random walks

Random Walk Optimization

Equivalently,

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

遍历所有节点

- **Intuition:** Optimize embeddings $\mathbf{z}_u$ to maximize the likelihood of random walk co-occurrences.

- **Parameterize $P(v|\mathbf{z}_u)$ using softmax:**

$$P(v|\mathbf{z}_u) = \frac{\exp(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_n)}$$

Why softmax?
We want node v to be most similar to node u (out of all nodes n).
Intuition: $\sum_i \exp(x_i) \approx \max_i \exp(x_i)$

Random Walk Optimization

Putting it all together:

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log\left(\frac{\exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_n)}\right)$$

sum over all nodes u

sum over nodes v seen on random walks starting from u

predicted probability of u and v co-occuring on random walk

Optimizing random walk embeddings =

Finding embeddings $\mathbf{z}_u$ that minimize $\mathcal{L}$

Random Walk Optimization

But doing this naively is too expensive!

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log\left(\frac{\exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_n)}\right)$$

Nested sum over nodes gives $O(|V|^2)$ complexity!

Random Walk Optimization

But doing this naively is too expensive!

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log\left(\frac{\exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^{\mathrm{T}} \mathbf{z}_n)}\right)$$

The normalization term from the softmax is the culprit… can we approximate it?

Negative Sampling

- **Solution:** Negative sampling

$$\log\left(\frac{\exp\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v\right)}{\sum_{n\in V}\exp\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_n\right)}\right)$$

Why is the approximation valid?
Technically, this is a different objective. But Negative Sampling is a form of Noise Contrastive Estimation (NCE) which approx. maximizes the log probability of softmax.

New formulation corresponds to using a logistic regression (sigmoid func.) to distinguish the target node v from nodes n_i sampled from background distribution P_v.

More at https://arxiv.org/pdf/1402.3722.pdf

$$\approx \log\left(\sigma\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v\right)\right) - \sum_{i=1}^{k}\log\left(\sigma\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_{n_i}\right)\right),\ n_i \sim P_V$$

sigmoid function
(makes each term a "probability" between 0 and 1)

random distribution over nodes

Instead of normalizing w.r.t. all nodes, just normalize against k random "**negative samples**" n_i

- Negative sampling allows for quick likelihood calculation.

Negative Sampling

$$\log\left(\frac{\exp\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v\right)}{\sum_{n\in V}\exp\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_n\right)}\right)$$

random distribution over nodes

$$\approx \log\left(\sigma\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v\right)\right) - \sum_{i=1}^{k}\log\left(\sigma\left(\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_{n_i}\right)\right), n_i \sim P_V$$

- Sample k negative nodes n_i each with prob. proportional to its degree.
- Two considerations for k (# negative samples):
  1. Higher k gives more robust estimates
  2. Higher k corresponds to higher bias on negative events

  In practice k =5-20.

Can negative sample be any node or only the nodes not on the walk? People often use any nodes (for efficiency). However, the most "correct" way is to use nodes not on the walk.

Stochastic Gradient Descent

- After we obtained the objective function, how do we optimize (minimize) it?

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

- **Gradient Descent**: a simple way to minimize $\mathcal{L}$:
  - Initialize z_u at some randomized value for all nodes u.
  - Iterate until convergence:
    - For all u, compute the derivative $\frac{\partial \mathcal{L}}{\partial z_u}$.
    - For all u, make a step in reverse direction of derivative: $z_u \leftarrow z_u - \eta \frac{\partial \mathcal{L}}{\partial z_u}$.

η: learning rate

Stochastic Gradient Descent

- **Stochastic Gradient Descent**: Instead of evaluating gradients over all examples, evaluate it for each **individual** training example.
  - Initialize z_u at some randomized value for all nodes u.
  - Iterate until convergence: $\mathcal{L}^{(u)} = \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$
    - Sample a node u, for all v calculate the derivative $\frac{\partial \mathcal{L}^{(u)}}{\partial z_v}$.
    - For all v, update: $z_v \leftarrow z_v - \eta \frac{\partial \mathcal{L}^{(u)}}{\partial z_v}$.

Random Walks: Summary

1. Run **short fixed-length** random walks starting from each node on the graph

2. For each node u collect $N_R(u)$, the multiset of nodes visited on random walks starting from u.

3. Optimize embeddings using Stochastic Gradient Descent:

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

We can efficiently approximate this using negative sampling!

How should we randomly walk?

- So far we have described how to optimize embeddings given a random walk strategy R
- **What strategies should we use to run these random walks?**
  - Simplest idea: **Just run fixed-length, unbiased random walks starting from each node** (i.e., DeepWalk from Perozzi et al., 2013)
    - The issue is that such notion of similarity is too constrained
- **How can we generalize this?**

Reference: Perozzi et al. 2014. DeepWalk: Online Learning of Social Representations. *KDD.*

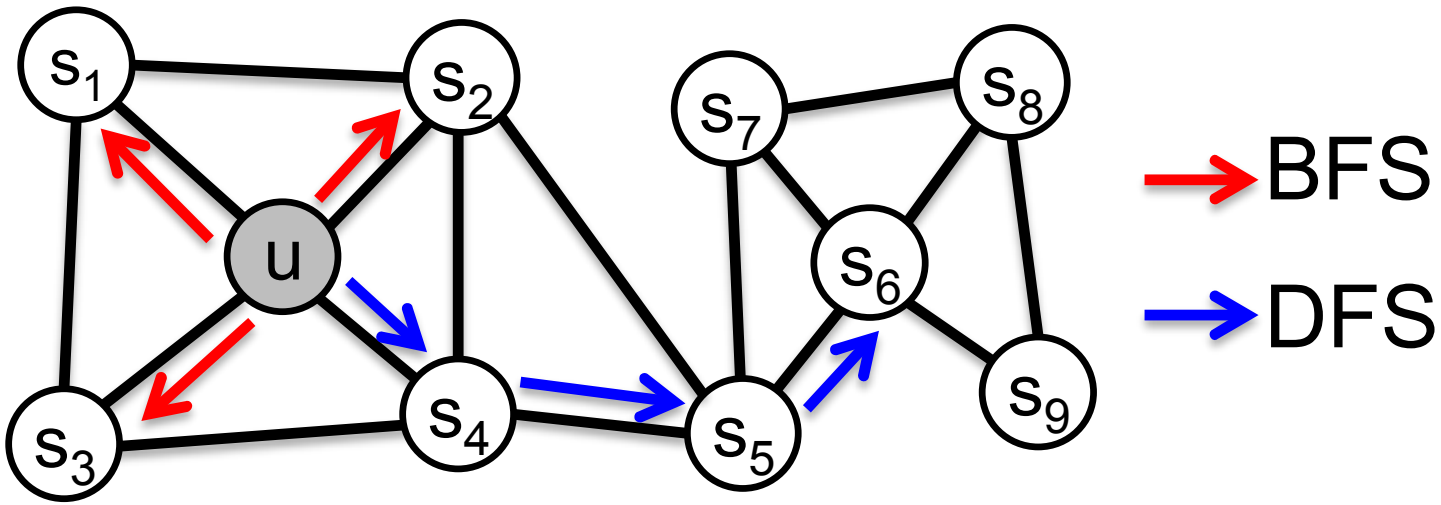
Overview of node2vec

- **Goal:** Embed nodes with similar network neighborhoods close in the feature space.
- We frame this goal as a maximum likelihood optimization problem, independent to the downstream prediction task.
- **Key observation:** Flexible notion of network neighborhood $N_R(u)$ of node u leads to rich node embeddings
- Develop biased 2nd order random walk R to generate network neighborhood $N_R(u)$ of node u

Reference: Grover et al. 2016. node2vec: Scalable Feature Learning for Networks. *KDD.*

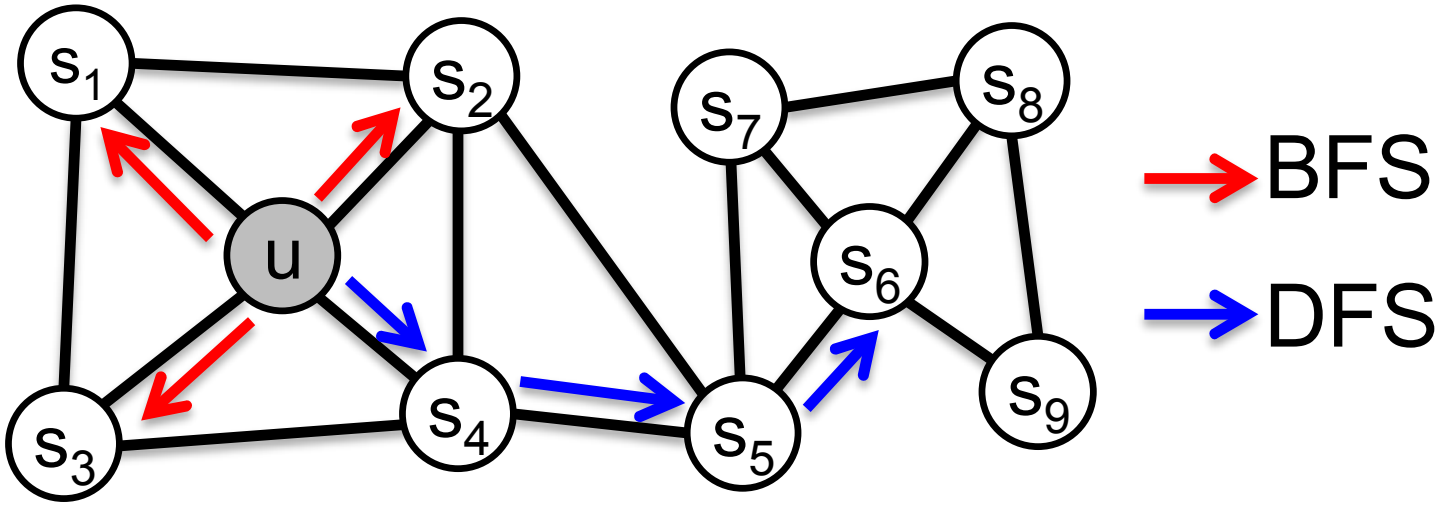
node2vec: Biased Walks

Idea: use flexible, biased random walks that can trade off between **local** and **global** views of the network (Grover and Leskovec, 2016).



node2vec: Biased Walks

Two classic strategies to define a neighborhood $N_R(u)$ of a given node u:

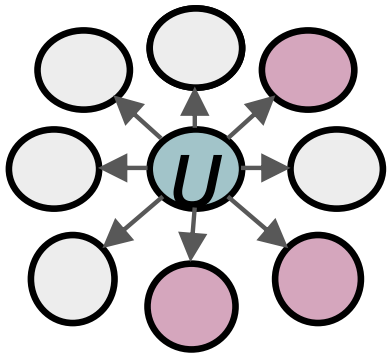


Walk of length 3 ($N_R(u)$ of size 3):

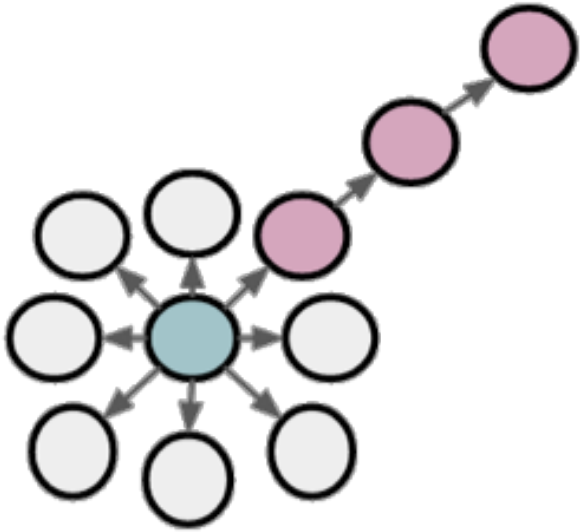
$N_{BFS}(u) = \{s_1, s_2, s_3\}$ Local microscopic view

$N_{DFS}(u) = \{s_4, s_5, s_6\}$ Global macroscopic view

BFS vs. DFS



BFS:
Micro-view of neighbourhood



DFS:
Macro-view of neighbourhood

Interpolating BFS and DFS

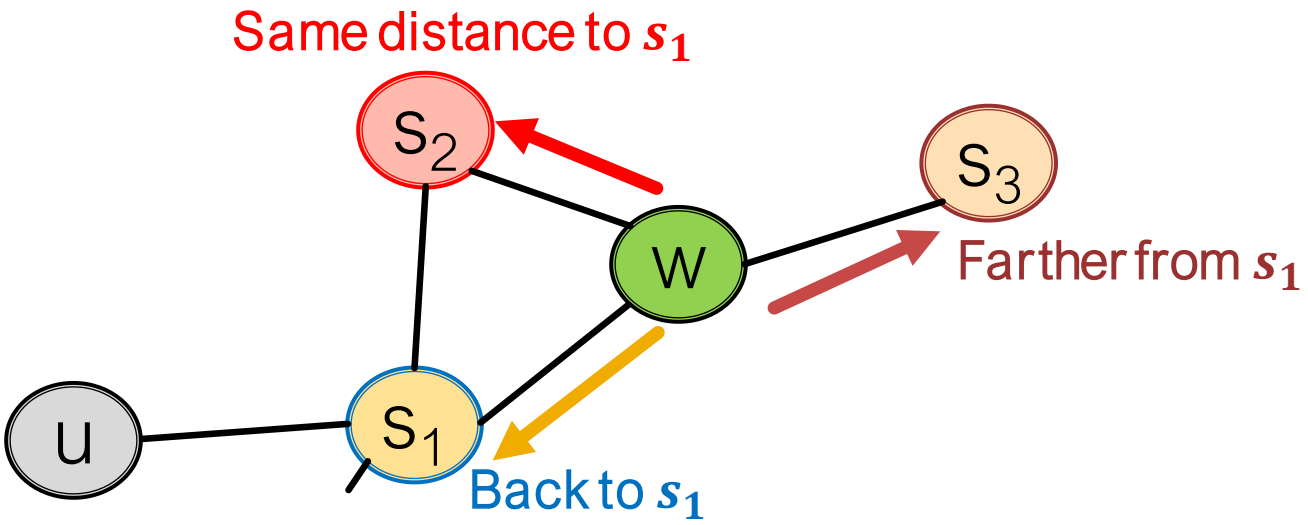
Biased fixed-length random walk R that given a node u generates neighborhood $N_R(u)$

- Two parameters:
  - **Return parameter p:**
    - Return back to the previous node
  - **In-out parameter q:**
    - Moving outwards (DFS) vs. inwards (BFS)
    - Intuitively, q is the "ratio" of BFS vs. DFS

Biased Random Walks

Biased 2nd-order random walks explore network neighborhoods:

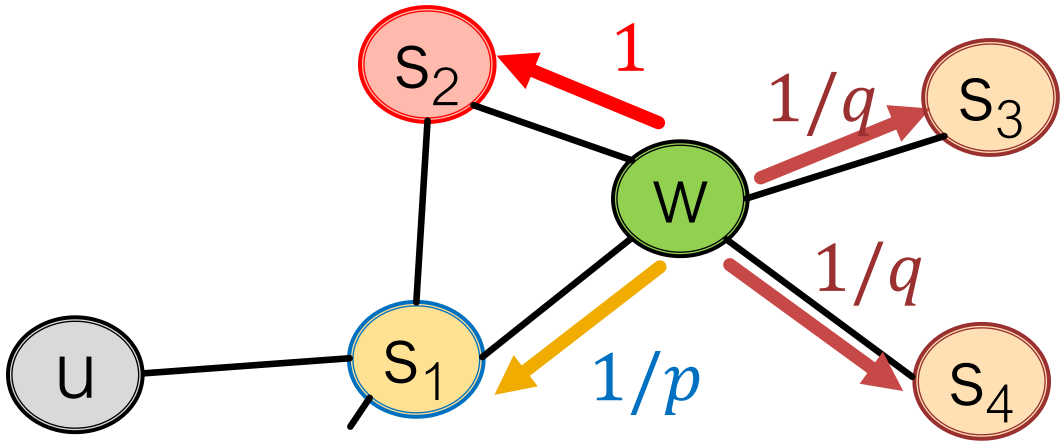
- Rnd. walk just traversed edge (s_1, w) and is now at w
- **Insight:** Neighbors of w can only be:



Idea: Remember where the walk came from

Biased Random Walks

- **Walker came over edge (s_1, w) and is at w. Where to go next?**

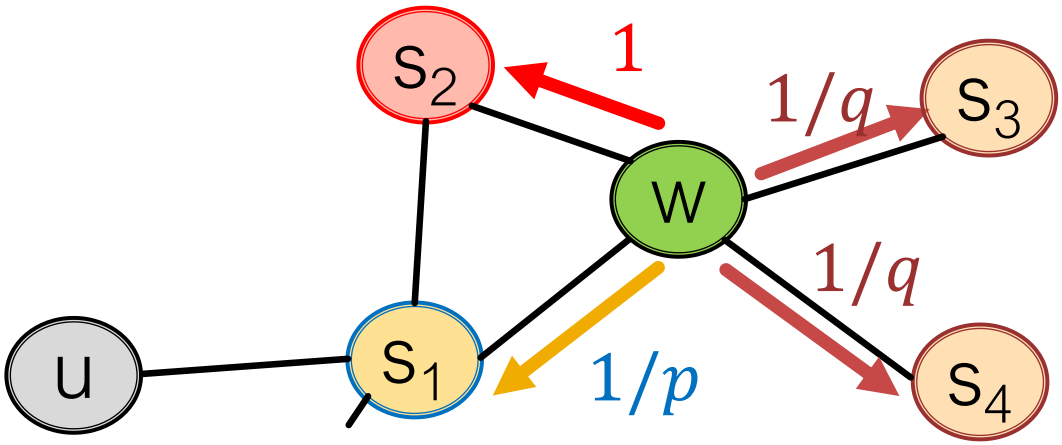


$1/p, 1/q, 1$ are unnormalized probabilities

- p, q model transition probabilities
  - p … return parameter
  - q … "walk away" parameter

Biased Random Walks

- **Walker came over edge (s_1, w) and is at w. Where to go next?**



$w \rightarrow$

Target t	Prob.	Dist. (s_1, t)
s_1	$1/p$	0
s_2	1	1
s_3	$1/q$	2
s_4	$1/q$	2

Unnormalized transition prob. segmented based on distance from s_1

- **BFS-like** walk: Low value of p
- **DFS-like** walk: Low value of q

$N_R(u)$ are the nodes visited by the biased walk

node2vec algorithm

- 1) Compute random walk probabilities
- 2) Simulate r random walks of length l starting from each node u
- 3) Optimize the node2vec objective using Stochastic Gradient Descent

- **Linear-time** complexity
- All 3 steps are individually parallelizable

Other Random Walk Ideas

- **Different kinds of biased random walks:**
  - Based on node attributes (Dong et al., 2017).
  - Based on learned weights (Abu-El-Haija et al., 2017)
- **Alternative optimization schemes:**
  - Directly optimize based on 1-hop and 2-hop random walk probabilities (as in LINE from Tang et al. 2015).
- **Network preprocessing techniques:**
  - Run random walks on modified versions of the original network (e.g., Ribeiro et al. 2017's struct2vec, Chen et al. 2016's HARP).

Summary so far

- **Core idea:** Embed nodes so that distances in embedding space reflect node similarities in the original network.
- **Different notions of node similarity:**
  - Naïve: Similar if two nodes are connected (next)
  - Neighborhood overlap (covered in Lecture 2)
  - Random walk approaches (covered today)

Summary so far

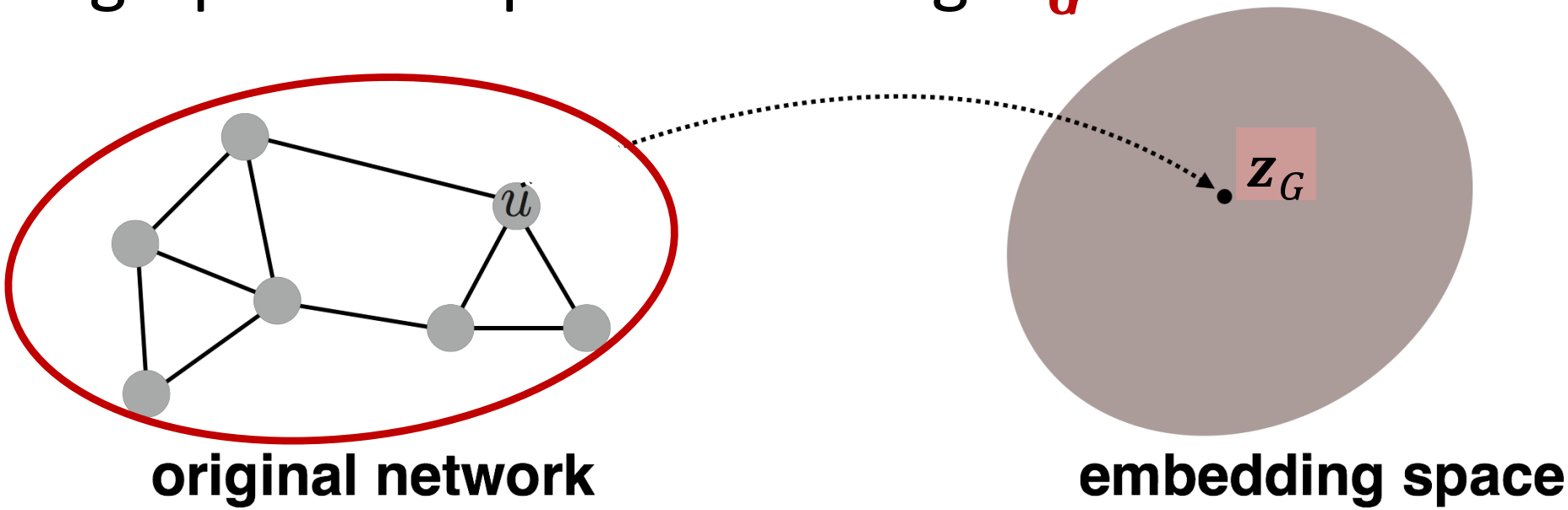
- **So what method should I use..?**
- No one method wins in all cases….
  - E.g., node2vec performs better on node classification while alternative methods perform better on link prediction (Goyal and Ferrara, 2017 survey).
- Random walk approaches are generally more efficient.
- **In general:** Must choose definition of node similarity that matches your application.

Stanford CS224W: Embedding Entire Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Embedding Entire Graphs

- **Goal:** Want to embed a subgraph or an entire graph G. Graph embedding: $\mathbf{z}_G$.



- **Tasks:**
  - Classifying toxic vs. non-toxic molecules
  - Identifying anomalous graphs

Approach 1

Simple (but effective) approach 1:

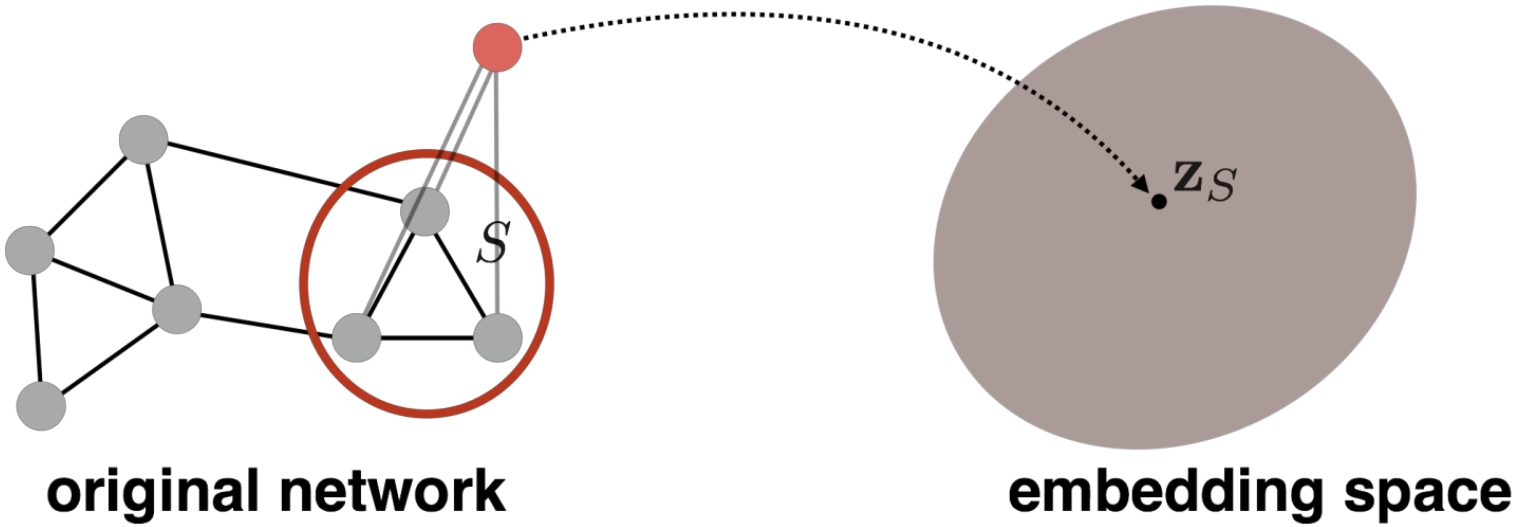
- Run a standard graph embedding technique *on* the (sub)graph G.
- Then just sum (or average) the node embeddings in the (sub)graph G.

$$\boldsymbol{z_G} = \sum_{v \in G} \boldsymbol{z_v}$$

- Used by Duvenaud et al., 2016 to classify molecules based on their graph structure

Approach 2

- **Approach 2:** Introduce a **"virtual node"** to represent the (sub)graph and run a standard graph embedding technique



- Proposed by Li et al., 2016 as a general technique for subgraph embedding

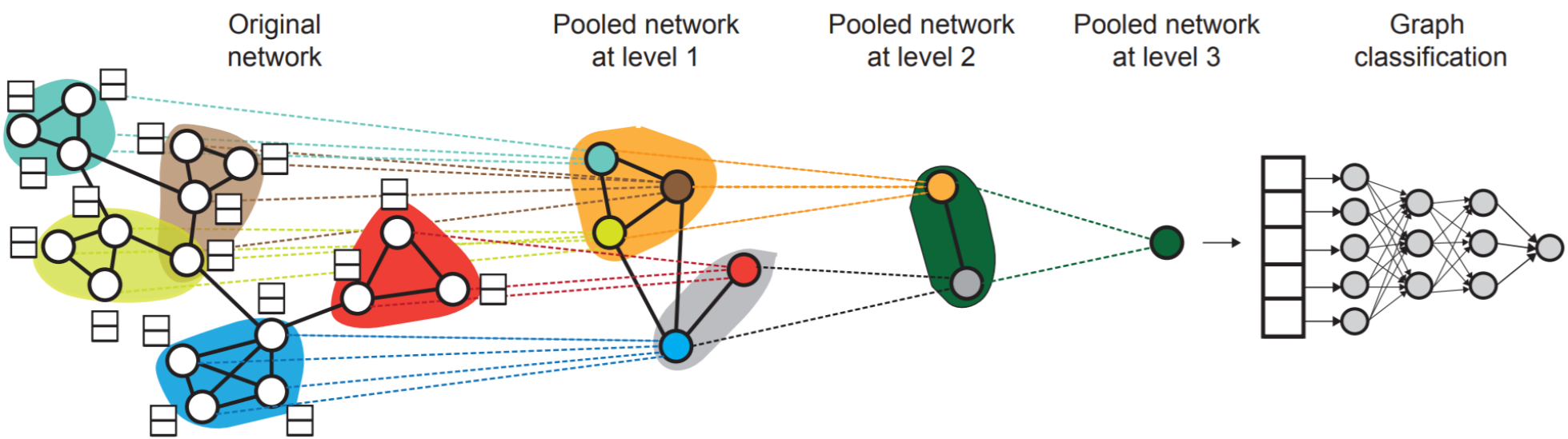
Summary

We discussed 3 ideas to graph embeddings:

- **Approach 1:** Embed nodes and sum/avg them
- **Approach 2:** Create super-node that spans the (sub) graph and then embed that node.

Preview: Hierarchical Embeddings

- We can **hierarchically** cluster nodes in graphs, and **sum/avg** the node embeddings according to these clusters.

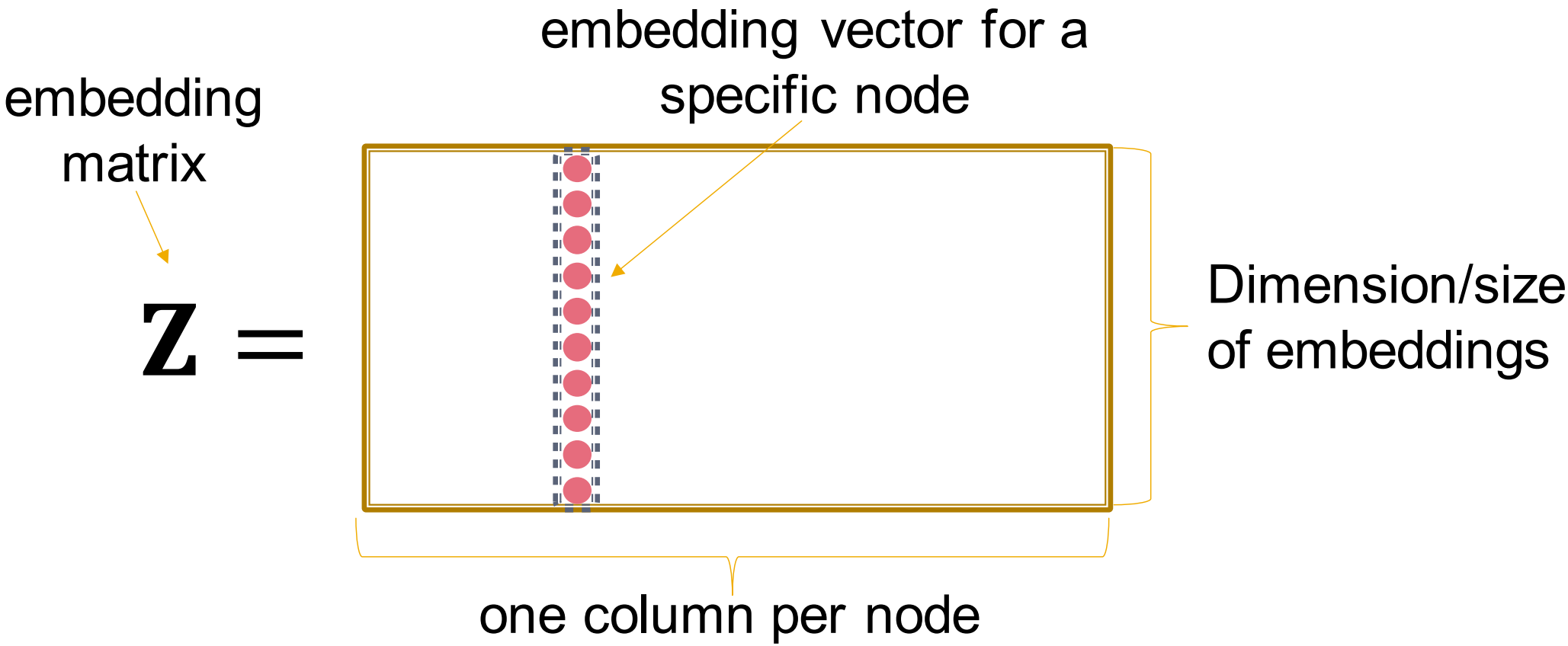


Stanford CS224W: Matrix Factorization and Node Embeddings

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Embeddings & Matrix Factorization

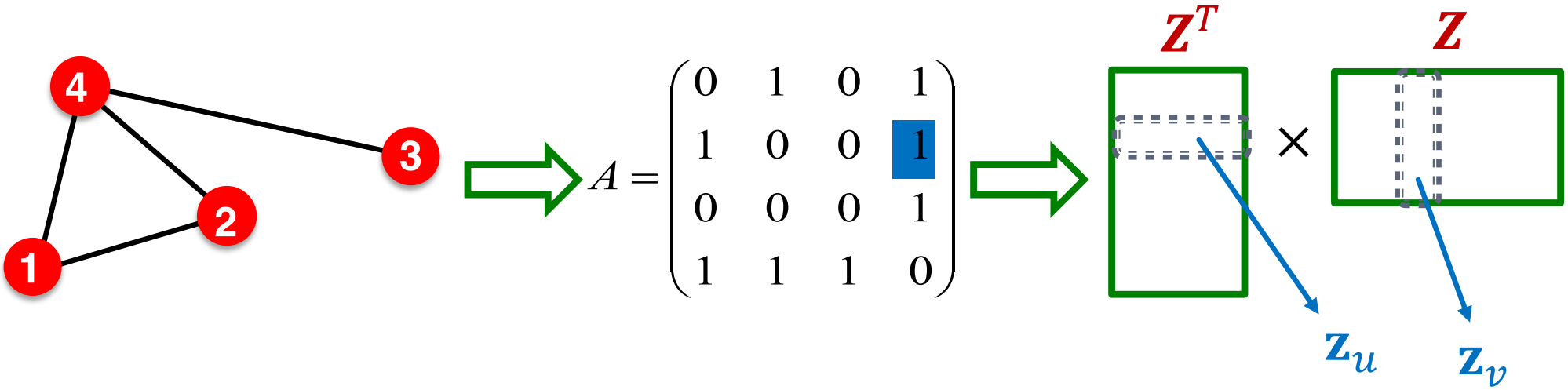
- **Recall:** encoder as an embedding lookup



Objective: maximize $\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u$ for node pairs (u, v) that are **similar**

Connection to Matrix Factorization

- Simplest **node similarity**: Nodes u, v are similar if they are connected by an edge
- This means: $\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u = A_{u,v}$ which is the (u, v) entry of the graph adjacency matrix A
- Therefore, $\boldsymbol{Z}^T \boldsymbol{Z} = A$



Matrix Factorization

- The embedding dimension d (number of rows in $\boldsymbol{Z}$) is much smaller than number of nodes n.
- Exact factorization $A = \boldsymbol{Z}^{\boldsymbol{T}}\boldsymbol{Z}$ is generally not possible
- However, we can learn $\boldsymbol{Z}$ approximately
- **Objective**: $\min_{\boldsymbol{Z}} \| \mathrm{A} - \boldsymbol{Z}^{T}\boldsymbol{Z} \|_2$
  - We optimize $\boldsymbol{Z}$ such that it minimizes the L2 norm (Frobenius norm) of $\mathrm{A} - \boldsymbol{Z}^{T}\boldsymbol{Z}$
  - Note today we used softmax instead of L2. But the goal to approximate A with $\boldsymbol{Z}^{T}\boldsymbol{Z}$ is the same.
- Conclusion: **Inner product decoder with node similarity defined by edge connectivity is equivalent to matrix factorization of A.**

Random Walk-based Similarity

- **DeepWalk** and **node2vec** have a more complex **node similarity** definition based on random walks
- **DeepWalk** is equivalent to matrix factorization of the following complex matrix expression:

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

  - Explanation of this equation is on the next slide.

Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec, WSDM 18

Random Walk-based Similarity

Volume of graph

$$vol(G) = \sum_i \sum_j A_{i,j}$$

Diagonal matrix D

$$D_{u,u} = \deg(u)$$

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

context window size

See Lec 3 slide 30:

$T = |N_R(u)|$

Power of normalized adjacency matrix

Number of negative samples

- **Node2vec** can also be formulated as a matrix factorization (albeit a more complex matrix)
- Refer to the paper for more details:

Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec, WSDM 18

How to Use Embeddings

- **How to use embeddings z_i of nodes:**
  - **Clustering/community detection:** Cluster points z_i
  - **Node classification:** Predict label of node i based on z_i
  - **Link prediction:** Predict edge (i, j) based on (z_i, z_j)
    - Where we can: concatenate, avg, product, or take a difference between the embeddings:
      - Concatenate: $f(z_i, z_j) = g([z_i, z_j])$
      - Hadamard: $f(z_i, z_j) = g(z_i * z_j)$ (per coordinate product)
      - Sum/Avg: $f(z_i, z_j) = g(z_i + z_j)$
      - Distance: $f(z_i, z_j) = g(||z_i - z_j||_2)$
  - **Graph classification**: Graph embedding z_G via aggregating node embeddings or virtual-node.
    Predict label based on graph embedding z_G.

Today's Summary

We discussed **graph representation learning**, a way to learn **node and graph embeddings** for downstream tasks, **without feature engineering**.

- **Encoder-decoder framework:**
  - **Encoder: embedding lookup**
  - **Decoder: predict score based on embedding to match node similarity**
- **Node similarity measure: (biased) random walk**
  - **Examples: DeepWalk, Node2Vec**
- **Extension to Graph embedding: Node embedding aggregation**

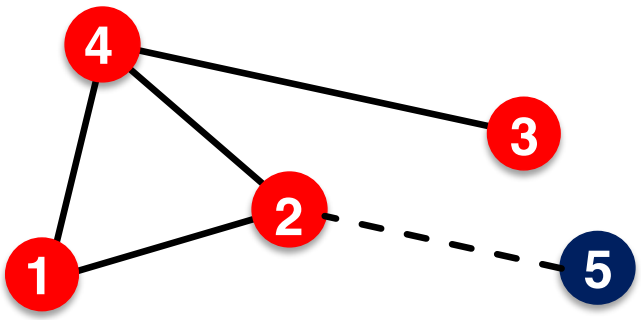
Limitations (1)

Limitations of node embeddings via matrix factorization and random walks

pagerank

- Cannot obtain embeddings for nodes not in the training set

无法立刻泛化到新加入的节点，某种程度的过拟合.



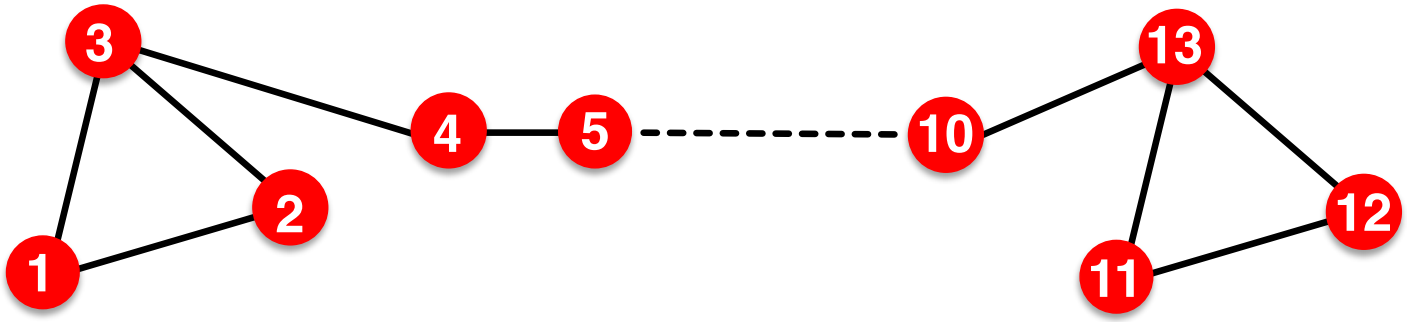
Training set

A newly added node 5 at test time (e.g., new user in a social network)

Cannot compute its embedding with DeepWalk / node2vec. Need to recompute all node embeddings.

Limitation (2)

- Cannot capture **structural similarity**: 功能、结构、角色

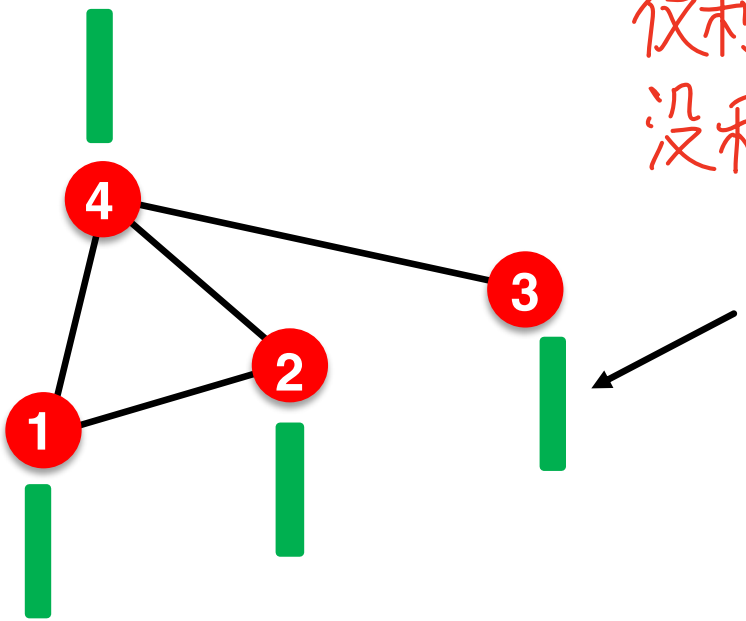


- Node 1 and 11 are **structurally similar** – part of one triangle, degree 2, …
- However, they have very **different** embeddings.
  - It's unlikely that a random walk will reach node 11 from node 1.
- **DeepWalk and node2vec do not capture structural similarity.**

Limitations (3)

- Cannot utilize node, edge and graph features

仅利用图本身的连接信息，
没利用属性信息。



Feature vector
(e.g. protein properties in a protein-protein interaction graph)

DeepWalk / node2vec embeddings do not incorporate such node features

Solution to these limitations: Deep Representation Learning and Graph Neural Networks
(To be covered in depth next)