# Stanford CS224W: Node Embeddings

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

# Stanford CS224W: Announcements

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# Announcements

- No class on November 7th (Election Day)
  - Lectures 13 (Advanced Topics in GNNs) to 17 (Link Prediction and Causality) will be pushed back by one class
  - Lecture 18 (Frontiers of GNN Research) will be skipped
- First assignments released on course website: Colab 0 and Colab 1
  - Links can be found under the **Schedule** section of the website

# Course Logistics: Colab 0

- **Colab 0 will be released today by 9PM on our course website**
- **Colab 0:**
  - Overview of NetworkX and PyTorch Geometric
  - Does not need to be handed in
  - TAs will hold a recitation session to walk you through Colab 0:
    - Time: Friday (09/29), 3-4pm PT
    - Location: Zoom, link will be posted on Ed
    - Session will be recorded

# Course Logistics: Colab 1

- **Colab 1 will be released today by 9PM on our course website**
- **Colab 1:**
  - Will cover material from Lectures 1-2, so you can get started right away!
  - Due on Thursday 10/12 (2 weeks from today)
  - Submit written answers and code on Gradescope

# Stanford CS224W: Node Embeddings

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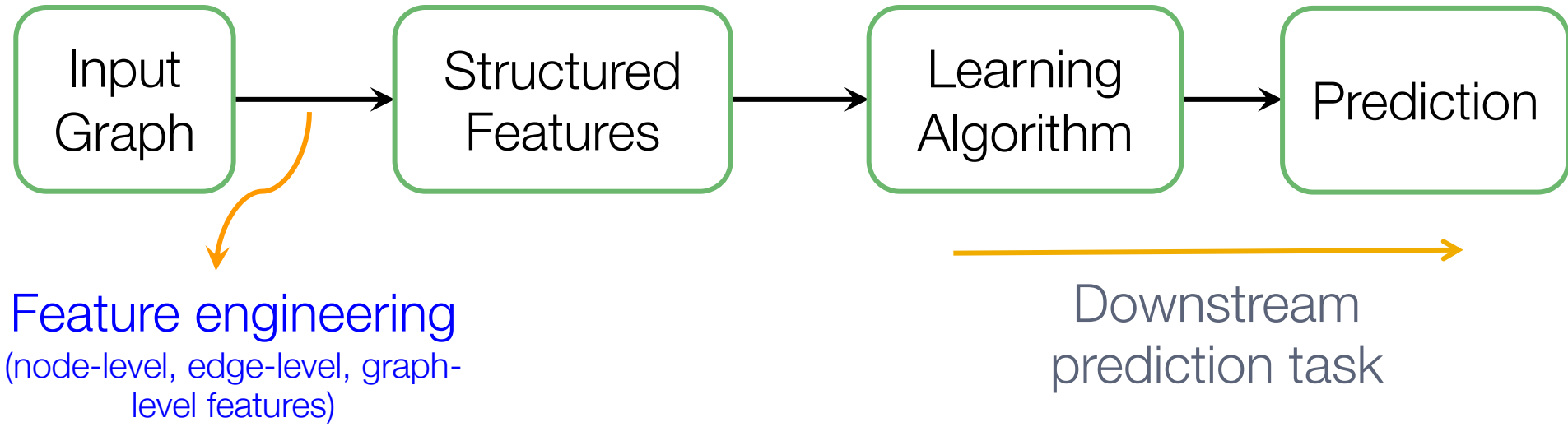
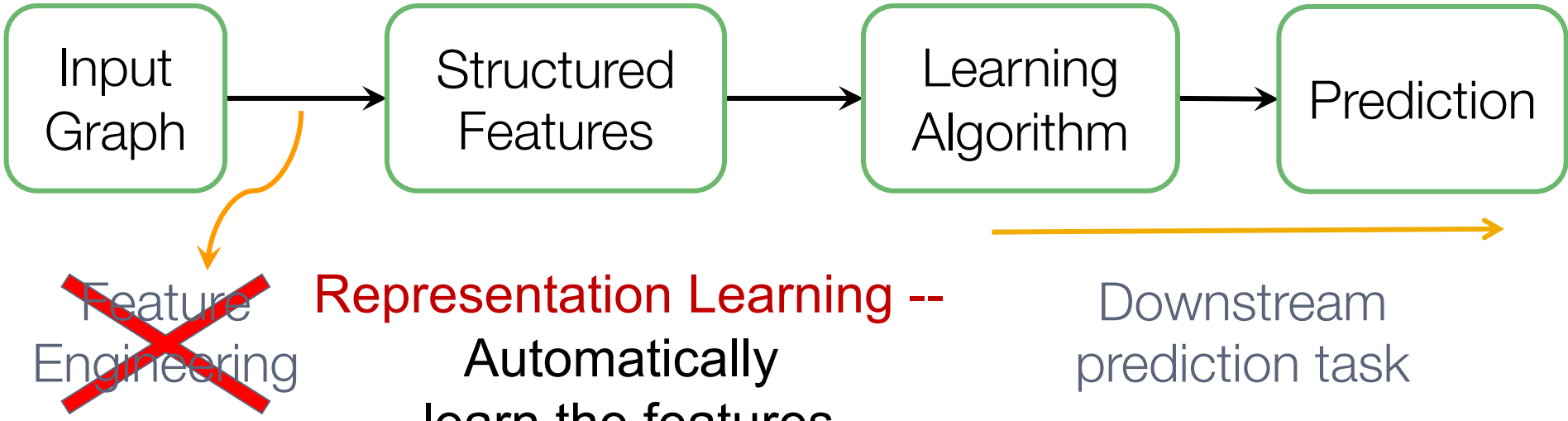
# Recap: Traditional ML for Graphs

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



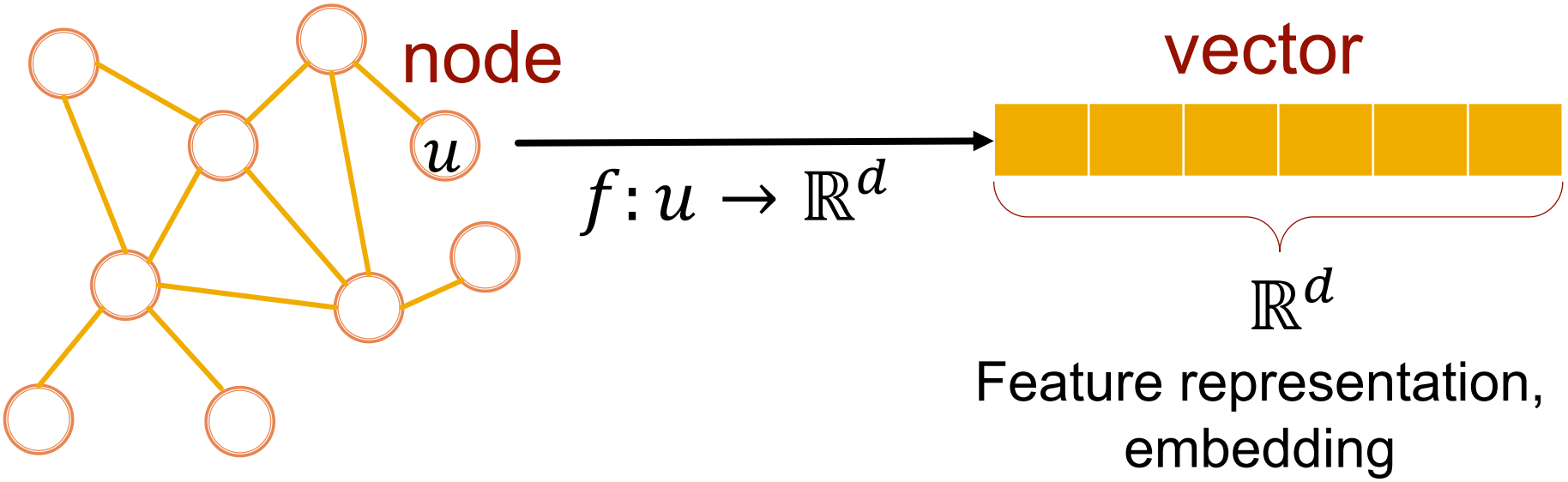
# Graph Representation Learning

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



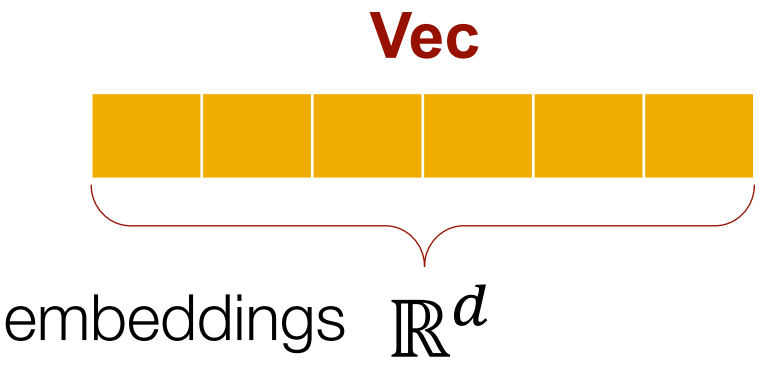
# Graph Representation Learning

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:
    - Both nodes are close to each other (connected by an edge)
  - Encode network information
  - Potentially used for many downstream predictions




**Tasks**

- Node classification
- Link prediction
- Graph classification
- Anomalous node detection
- Clustering
- ….

# Example Node Embedding

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

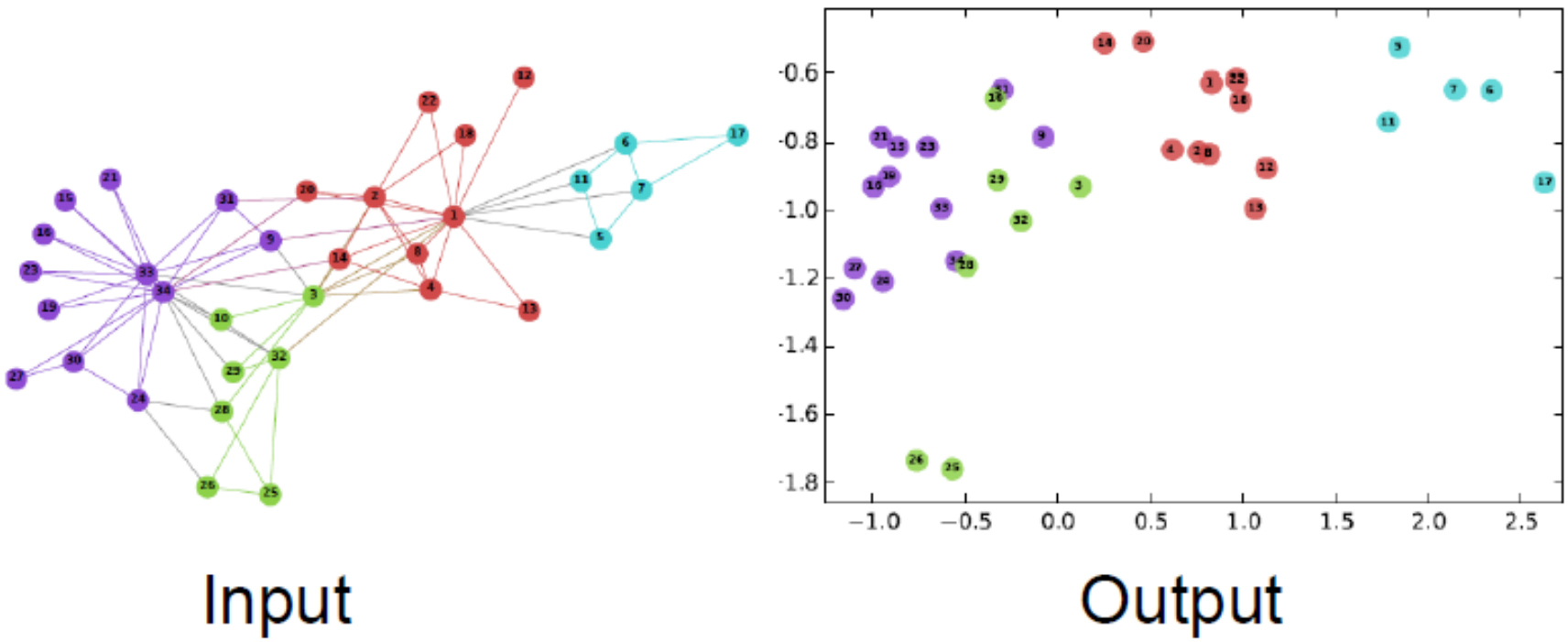



Image from: Perozzi et al. DeepWalk: Online Learning of Social Representations. *KDD 2014.*

# Stanford CS224W: Node Embeddings: Encoder and Decoder

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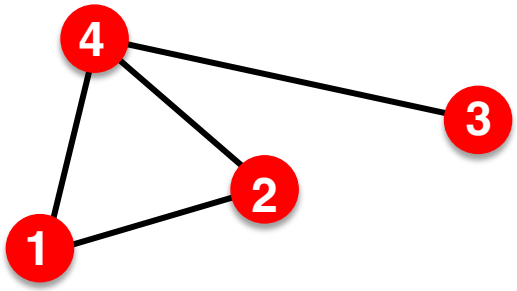
# Setup

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

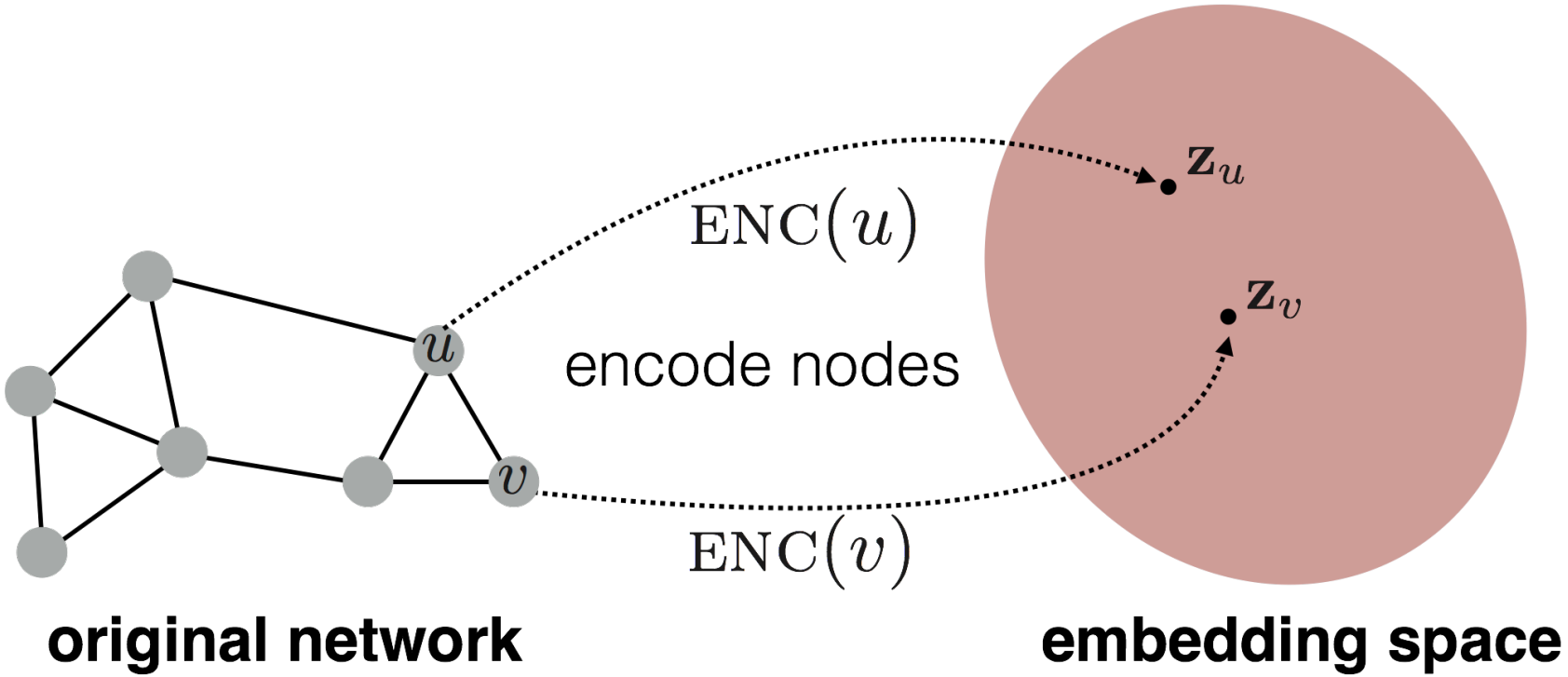



V: {1, 2, 3, 4}

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

# Embedding Nodes

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



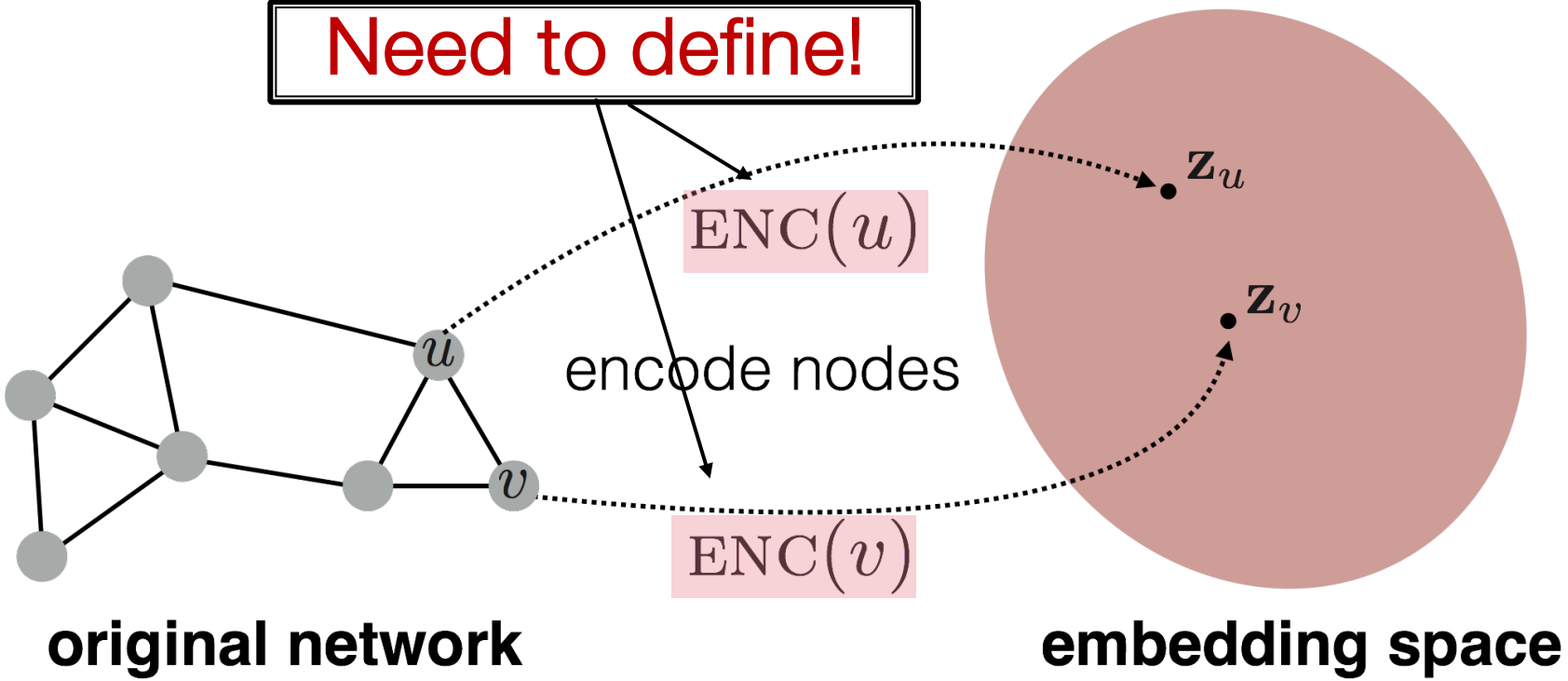
# Embedding Nodes

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

similarity($u, v$) in the original network

$\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$ Similarity of the embedding

Need to define!



# Learning Node Embeddings

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** $\mathbf{DEC}$ maps from embeddings to the similarity score
4. **Optimize the parameters of the encoder so that:**

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

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

in the original network — Similarity of the embedding

# 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**

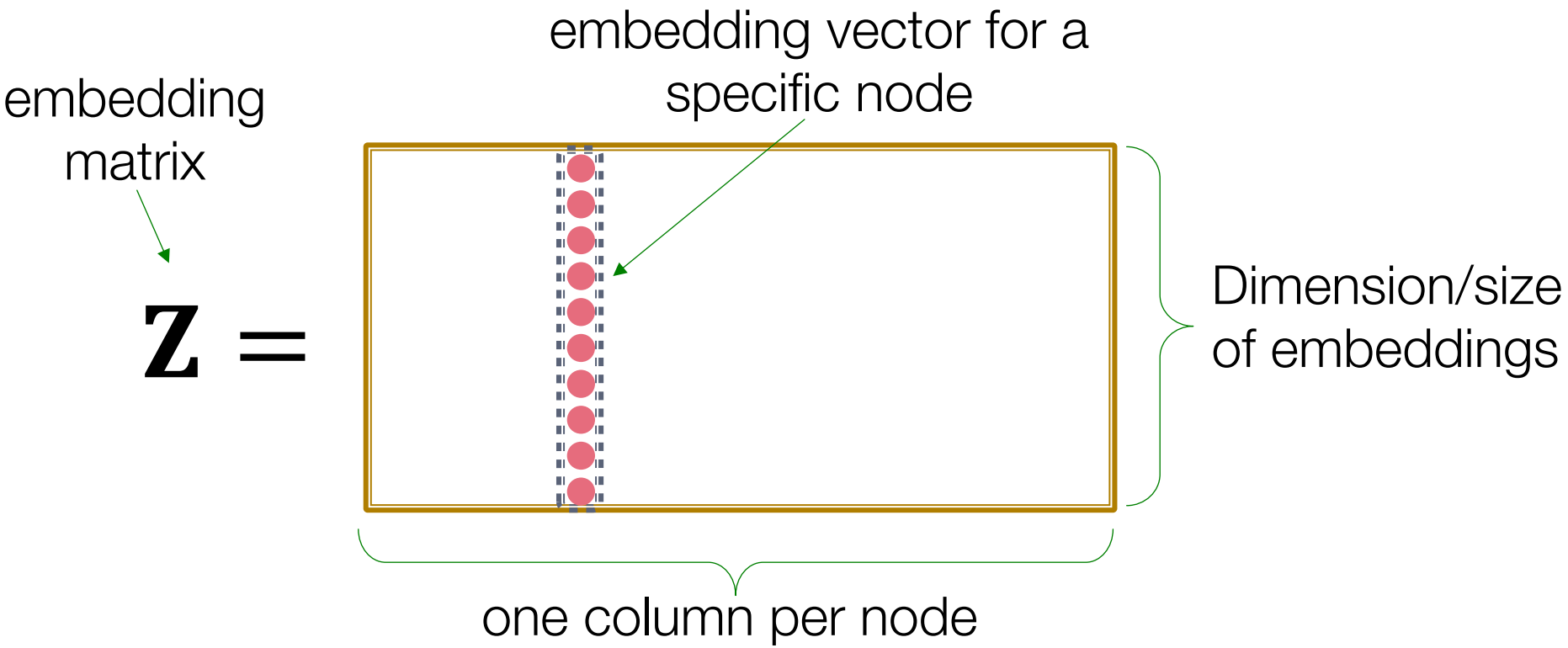
$$\text{ENC}(v) = \mathbf{z}_v = \mathbf{Z} \cdot v$$

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

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

# "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
  - 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

  - **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?
  - share neighbors?
  - have similar "structural roles"?
- 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.
- These embeddings are **task independent:**
  - They are not trained for a specific task but can be used for any task.

# Stanford CS224W: Random Walk Approaches for Node Embeddings

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# Notation

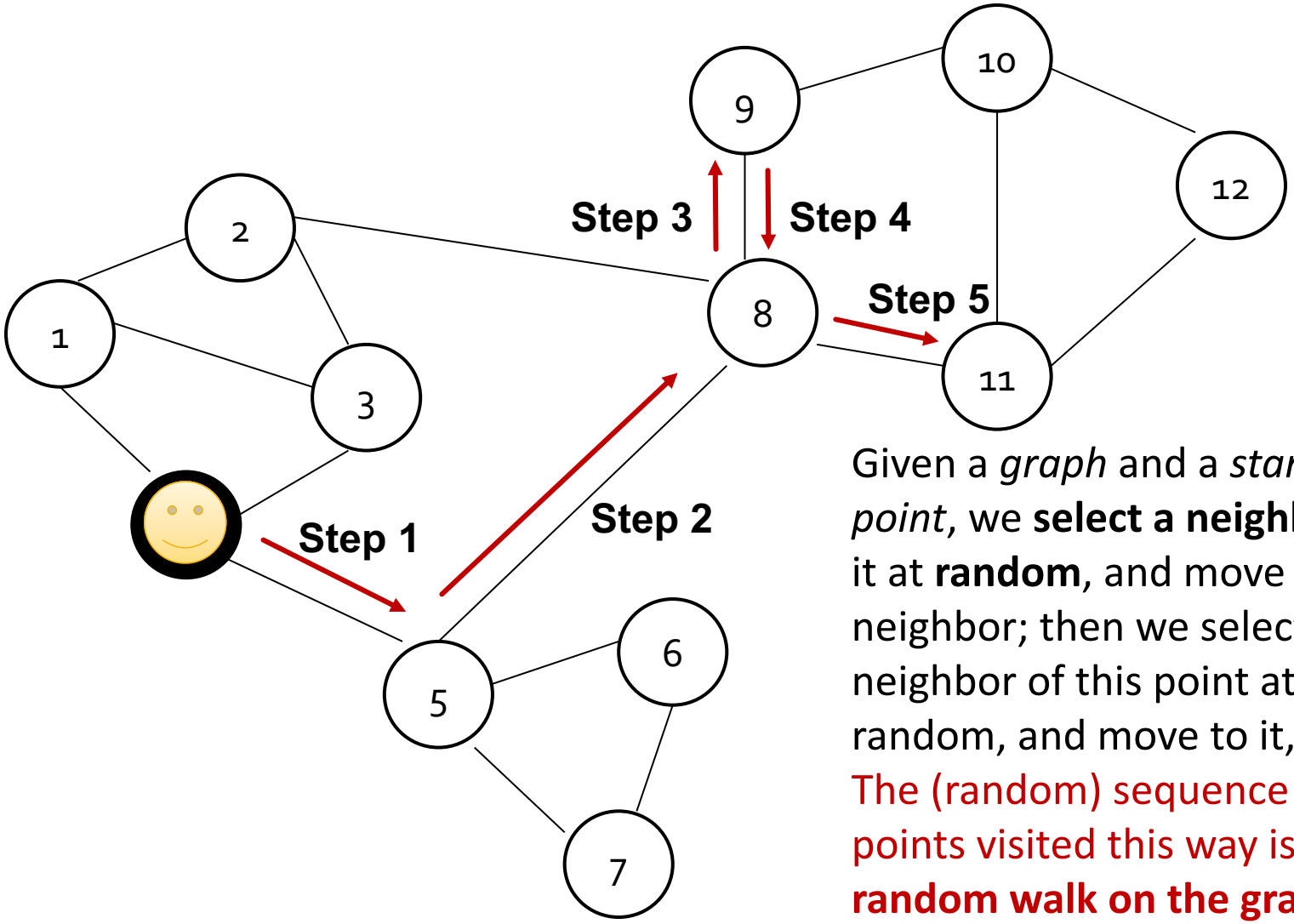
- **Vector** $\mathbf{z}_u$:
  - The embedding of node $u$ (what we aim to find).
- **Probability** $P(v \,|\mathbf{z}_u)$ : ⟸ Our model prediction based on $\mathbf{z}_u$
  - The **(predicted) probability** of visiting node $v$ on random walks starting from node $u$.

---

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

# 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**.

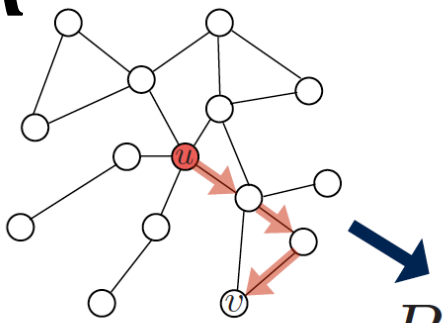
# Random-Walk Embeddings

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

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

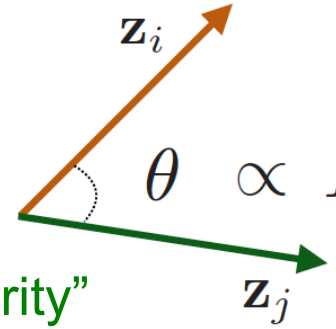
# Random-Walk Embeddings

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?

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)

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

# 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:

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

  - $N_R(u)$ 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 $N_{\mathrm{R}}(u)$.

$$\arg\max_{z} \sum_{u \in V} \log \mathrm{P}(N_{\mathrm{R}}(u) | \mathbf{z}_u) \Longrightarrow$$ Maximum likelihood objective

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

# Random Walk Optimization

Equivalently,

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

- **Intuition:** Optimize embeddings $\mathbf{z}_u$ to minimize the negative log-likelihood of random walk neighborhoods $N(u)$.
- **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 sample any node (for efficiency).

# 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: $z_u \leftarrow z_u - \eta \frac{\partial \mathcal{L}}{\partial z_u}$.

$\eta$: 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 gradient $\frac{\partial \mathcal{L}^{(u)}}{\partial z_v}$.
    - 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 $Z$ 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.*

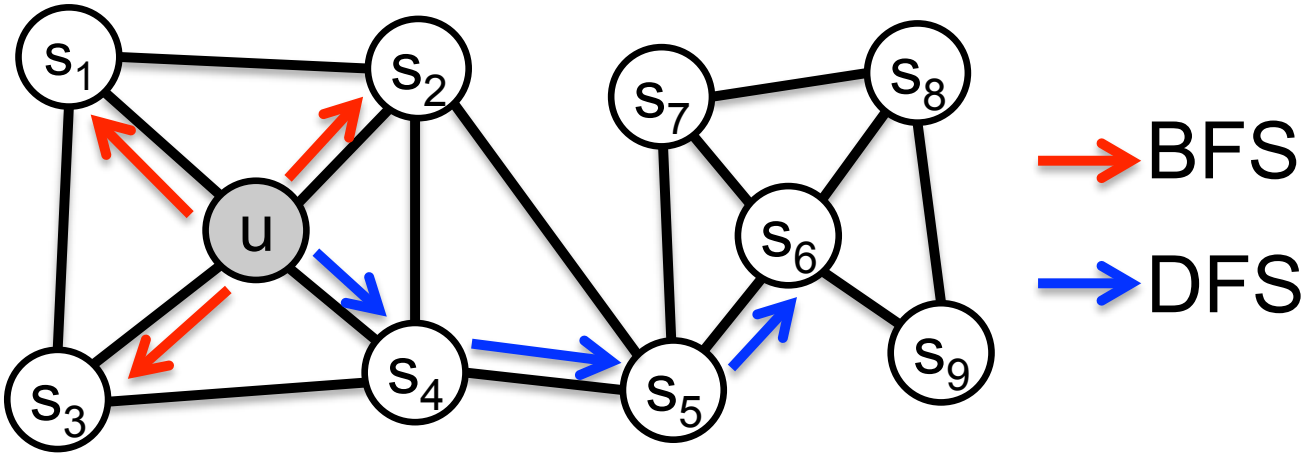
# Overview of node2vec

- **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.*

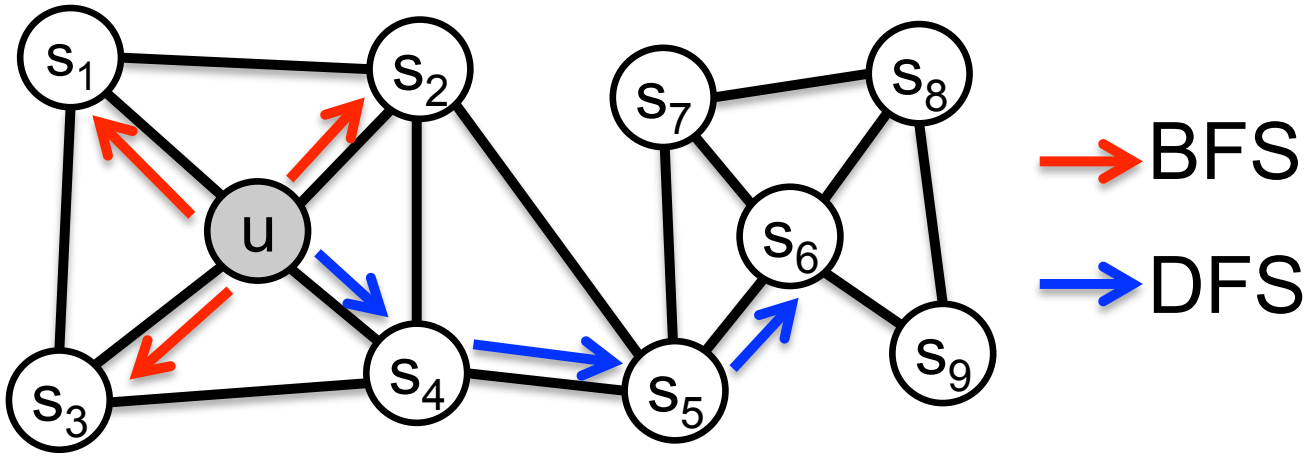
# node2vec: Biased Walks

**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 $u$:**

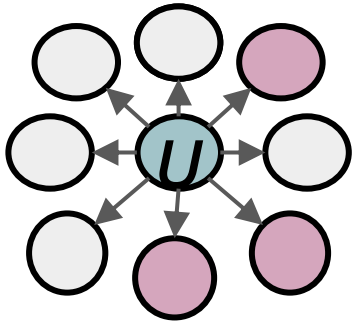



**Walk of length 3 ($N_R(u)$ of size 3):**

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

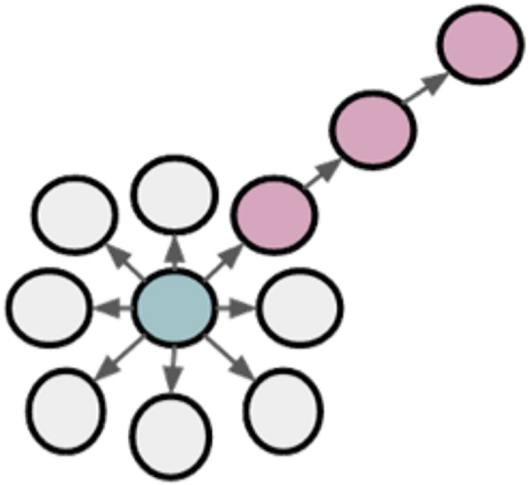
$N_{DFS}(u) = \{s_4, s_5, s_6\}$ Global macroscopic view

# BFS vs. DFS




BFS:

$N_R(\cdot)$ will provide a micro-view of neighbourhood



DFS:

$N_R(\cdot)$ will provide a macro-view of neighbourhood

# Interpolating BFS and DFS

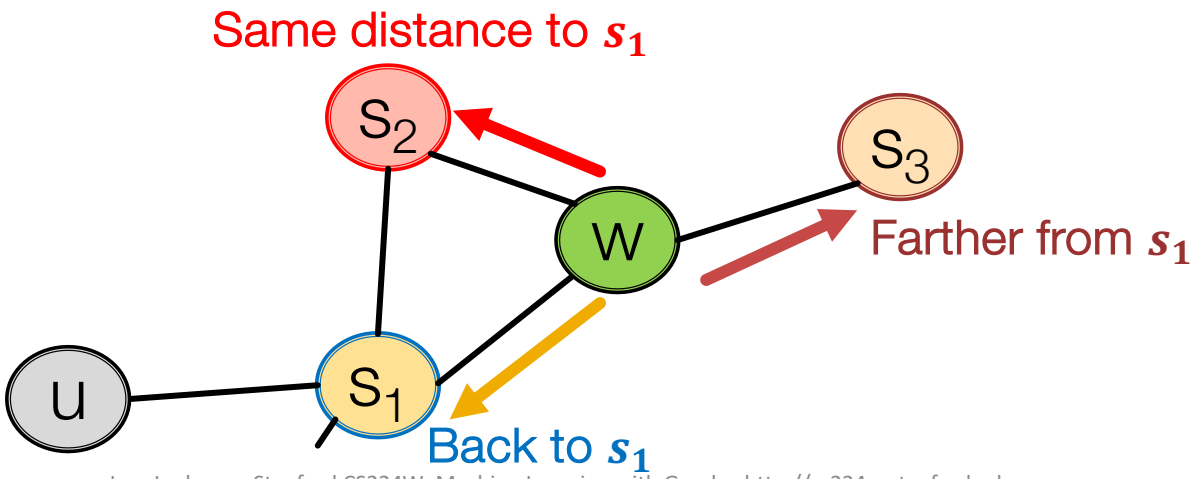
**Biased fixed-length random walk $R$ that given a node $u$ generates neighborhood $N_R(u)$**

- Random walk has two parameters:
  - **Return parameter $p$:**
    - Return back to the previous node
  - **In-out parameter $q$:**
    - Moving outwards (DFS) vs. inwards (BFS) from the previous node
    - Intuitively, $q$ is the "ratio" of BFS vs. DFS
- Next, we specify how a **single step** of biased random walk is performed.
- Random walk is then just a sequence of these steps.

# One Step of the Biased Random Walk

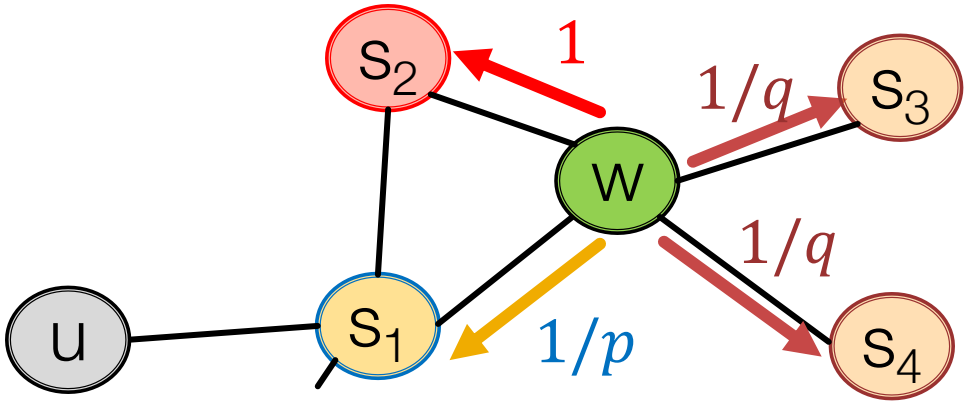
**Define the random walk by specifying the walk transition probabilities on edges adjacent to the current node $w$:**

- Rnd. walk just traversed edge $(s_1, w)$ and **is now at $w$**
- We specify edge transition probs. out of node $w$
- **Insight:** Neighbors of $w$ can only be:



# One Step of the Biased Random Walk

- **Walker came over edge $(s_1, w)$ and is now at $w$.**
  **How to set edge transition probabilities?**



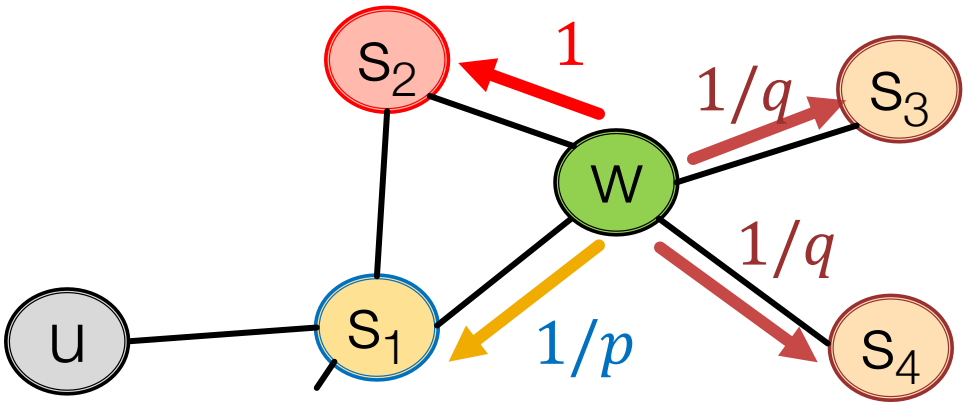

$1/p, 1/q, 1$ are unnormalized probabilities

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

# One Step of the Biased Random Walk

- **Walker came over edge $(s_1, w)$ and is at $w$.**

**How to set edge transition probabilities?**




$w \rightarrow$

| 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 edge transition probabilities:
  - For each edge $(s_1, w)$ we compute edge walk probabilities (based on $p, q$) of edges $(w, \cdot)$
- 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
  - 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

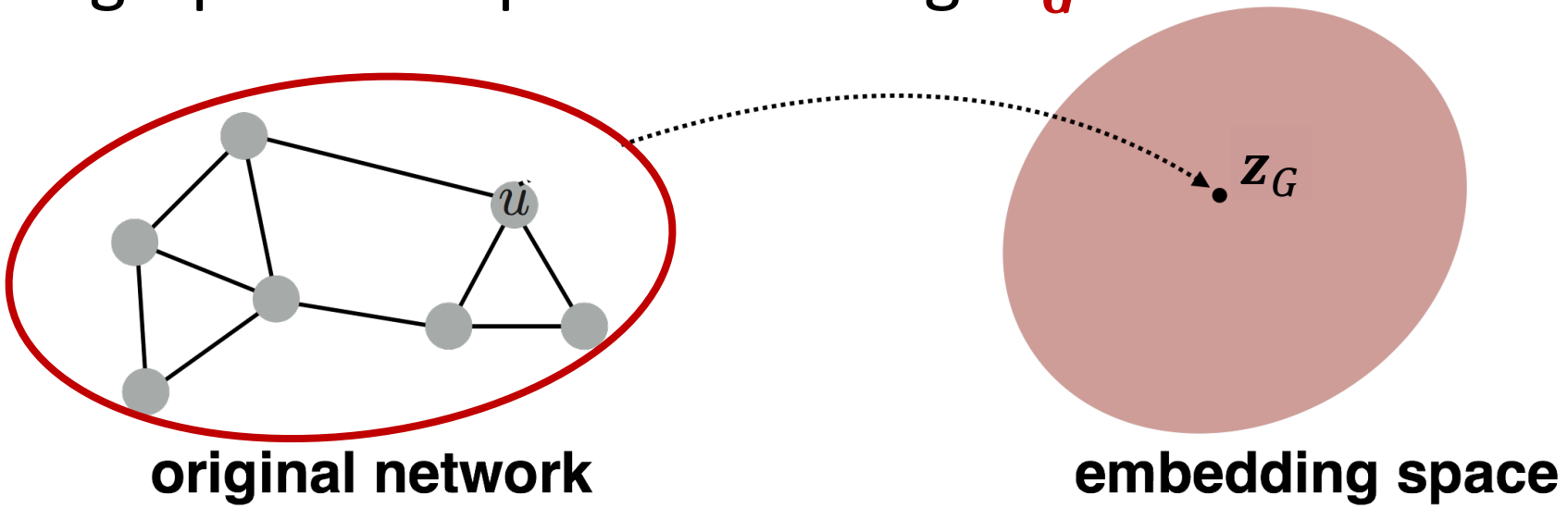
CS224W: Machine Learning with Graphs

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:**

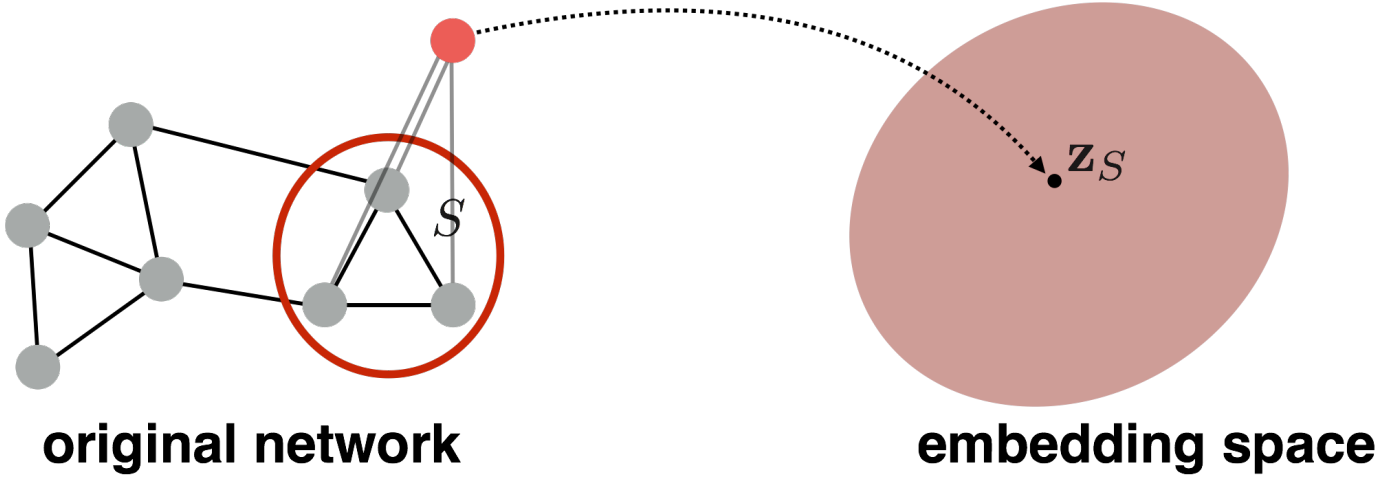
- Run a standard graph embedding technique *on* the (sub)graph $G$.
- Then just sum (or average) the node embeddings in the (sub)graph $G$.

$$\mathbf{z}_G = \sum_{v \in G} \mathbf{z}_v$$

- 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

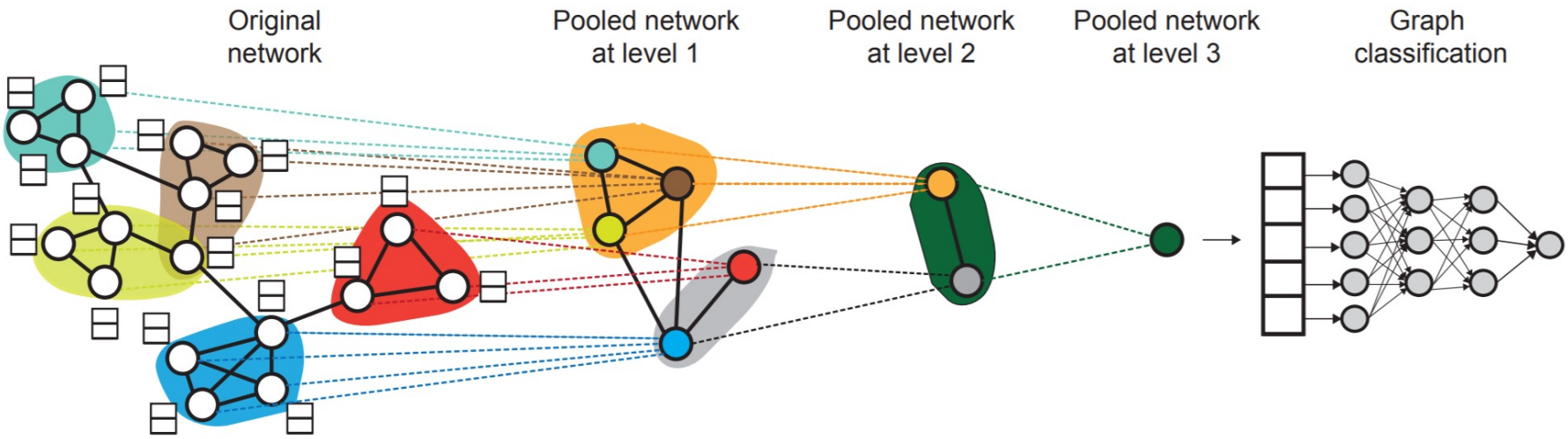
# Summary

## 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

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

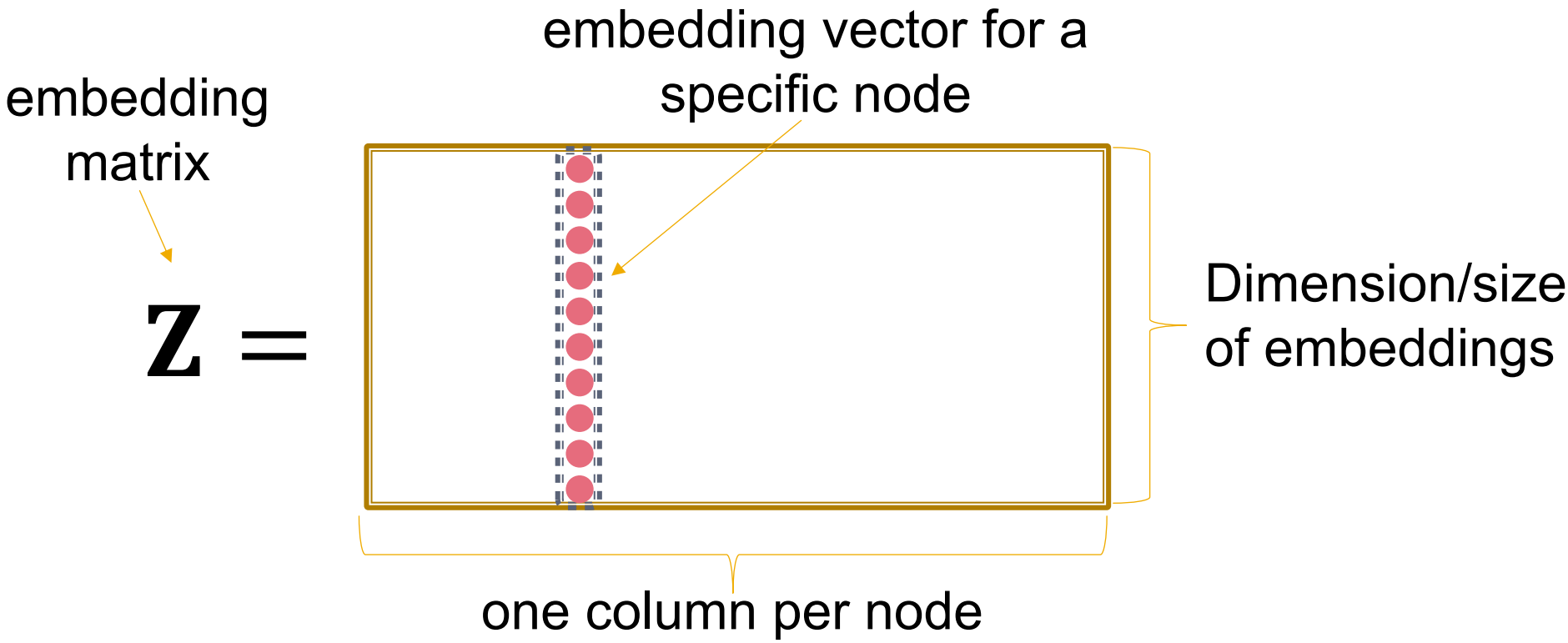


# Stanford CS224W: Matrix Factorization and Node Embeddings

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

# Embeddings & Matrix Factorization

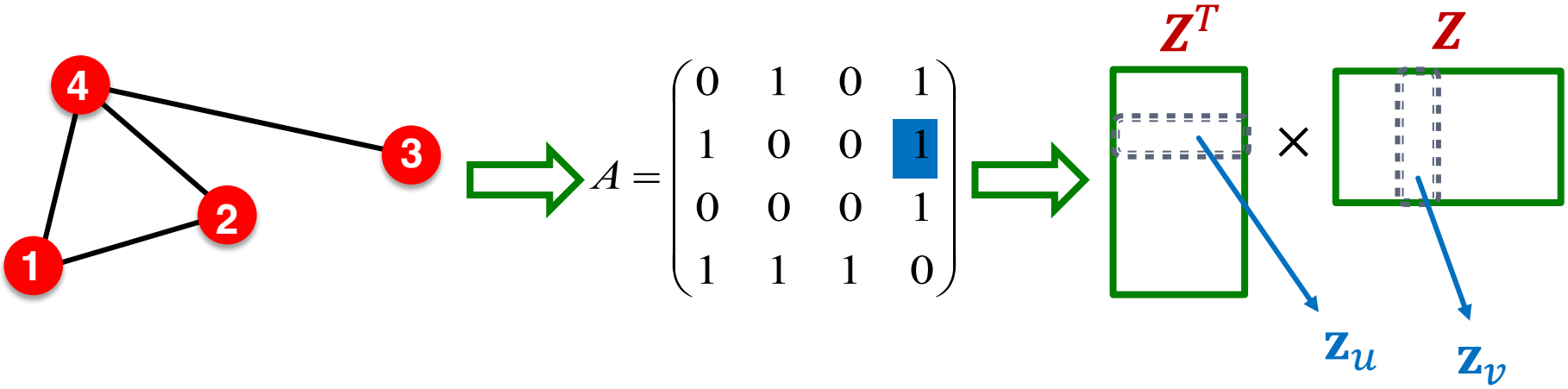
- **Recall:** encoder as an embedding lookup




**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**: $\min_{\mathbf{Z}} \| \mathrm{A} - \boldsymbol{Z}^{T}\boldsymbol{Z} \|_2$
  - 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 $\mathrm{A}$ 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 $\boldsymbol{z_i}$
  - **Node classification:** Predict label of node $i$ based on $\boldsymbol{z_i}$
  - **Link prediction:** Predict edge $(i, j)$ based on $(\boldsymbol{z_i}, \boldsymbol{z_j})$
    - Where we can: concatenate, avg, product, or take a difference between the embeddings:
      - Concatenate: $f(\boldsymbol{z}_i, \boldsymbol{z}_j) = g([\boldsymbol{z}_i, \boldsymbol{z}_j])$
      - Hadamard: $f(\boldsymbol{z}_i, \boldsymbol{z}_j) = g(\boldsymbol{z}_i * \boldsymbol{z}_j)$ (per coordinate product)
      - Sum/Avg: $f(\boldsymbol{z}_i, \boldsymbol{z}_j) = g(\boldsymbol{z}_i + \boldsymbol{z}_j)$
      - Distance: $f(\boldsymbol{z}_i, \boldsymbol{z}_j) = g(||\boldsymbol{z}_i - \boldsymbol{z}_j||_2)$
  - **Graph classification**: Graph embedding $\boldsymbol{z_G}$ via aggregating node embeddings or virtual-node.
    Predict label based on graph embedding $\boldsymbol{z}_G$.

# Today's Summary

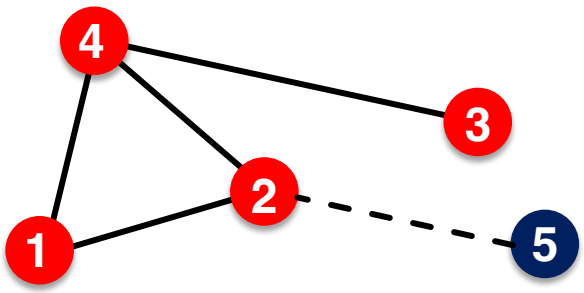
We discussed **graph representation learning**, a way to learn **node and graph embeddings** for downstream tasks, **without feature engineering**.

- **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

- **Transductive (not inductive) method:** Cannot obtain embeddings for nodes not in the training set. Cannot apply to new graphs, evolving graphs.



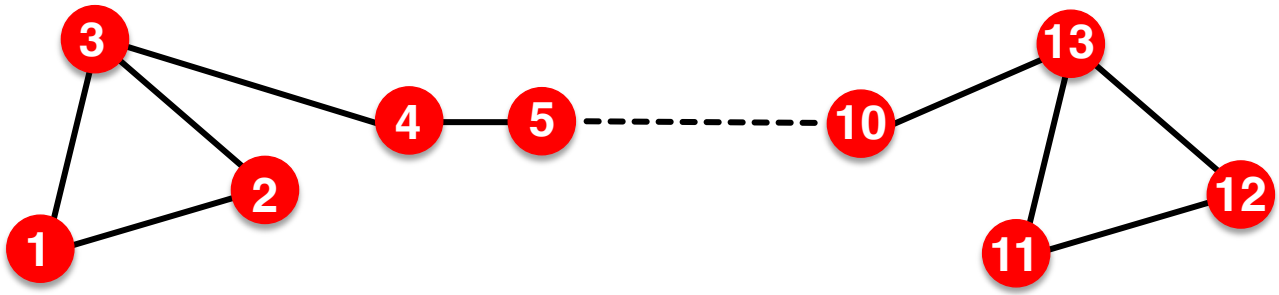

Training set

**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**:

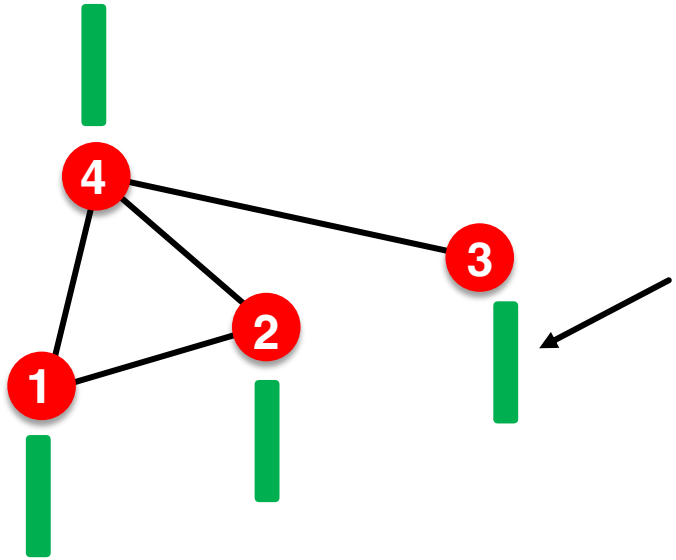



  - Node 1 and 11 are **structurally similar** – part of one triangle, degree 2, …
  - However, they have very **different** embeddings.
    - It's unlikely that a random walk will reach node 11 from node 1.

- **DeepWalk and node2vec do not capture structural similarity.**

# Limitations (3)

- Cannot utilize node, edge and graph features




**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)