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Stanford CS224W: Node Embeddings

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

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Stanford CS224W: Announcements

CS224W: Machine Learning with Graphs
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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

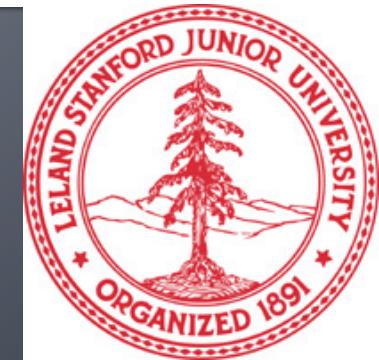
- **Colab 1 will be released today by 9PM on our course website**
- **Colab 1:**
 - Will cover material from Lectures 1-2, so you can get started right away!
 - Due on Thursday 10/12 (2 weeks from today)
 - Submit written answers and code on Gradescope

Stanford CS224W: Node Embeddings

CS224W: Machine Learning with Graphs

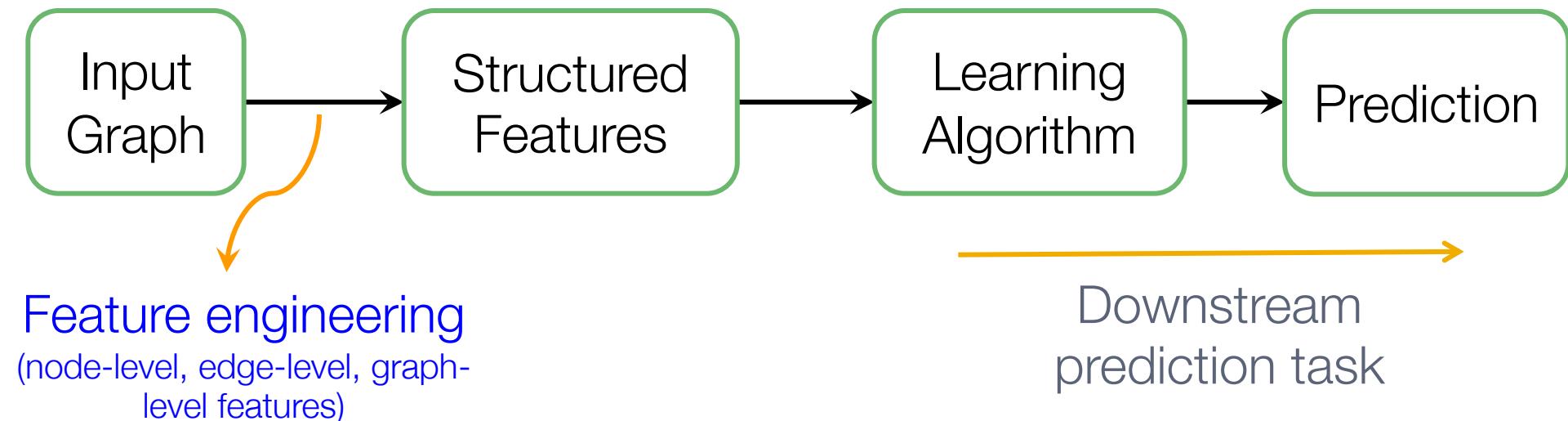
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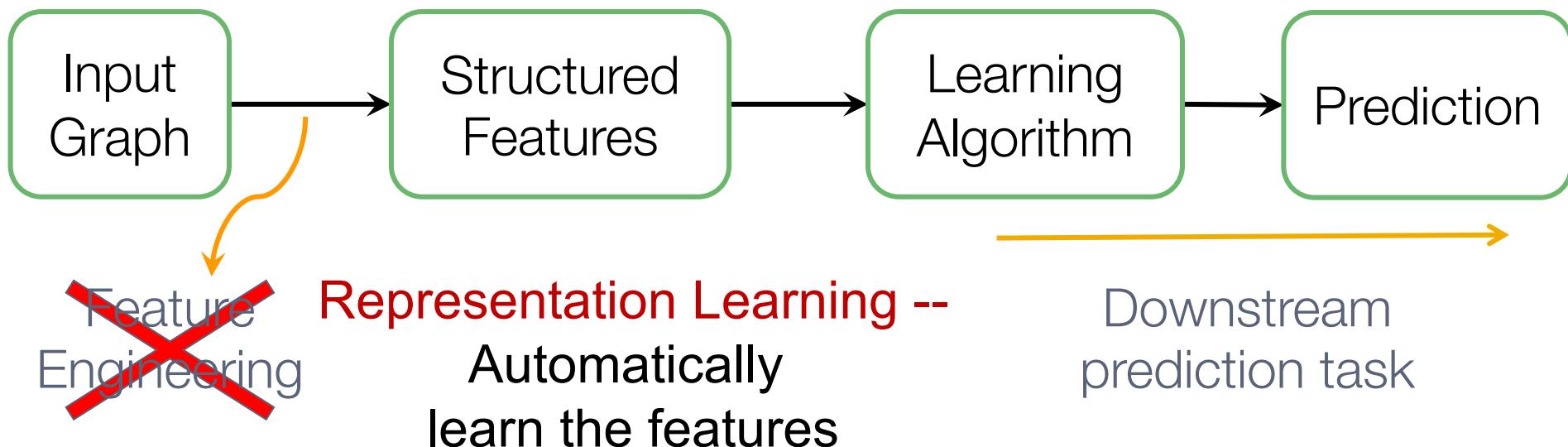
Recap: Traditional ML for Graphs

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



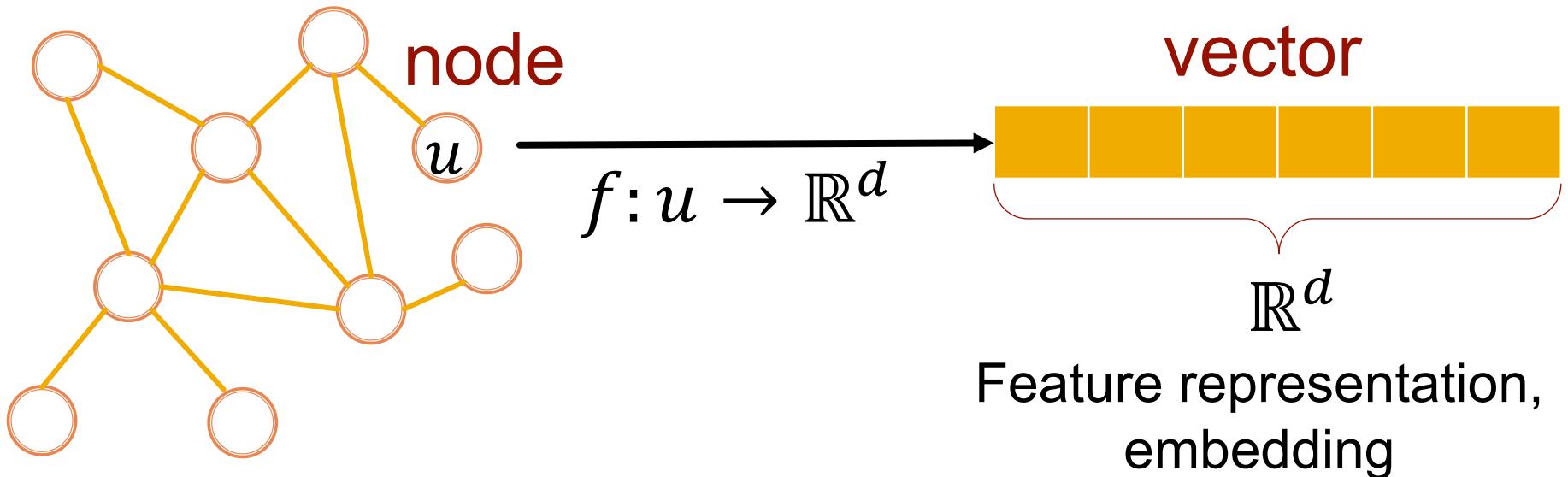
Graph Representation Learning

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



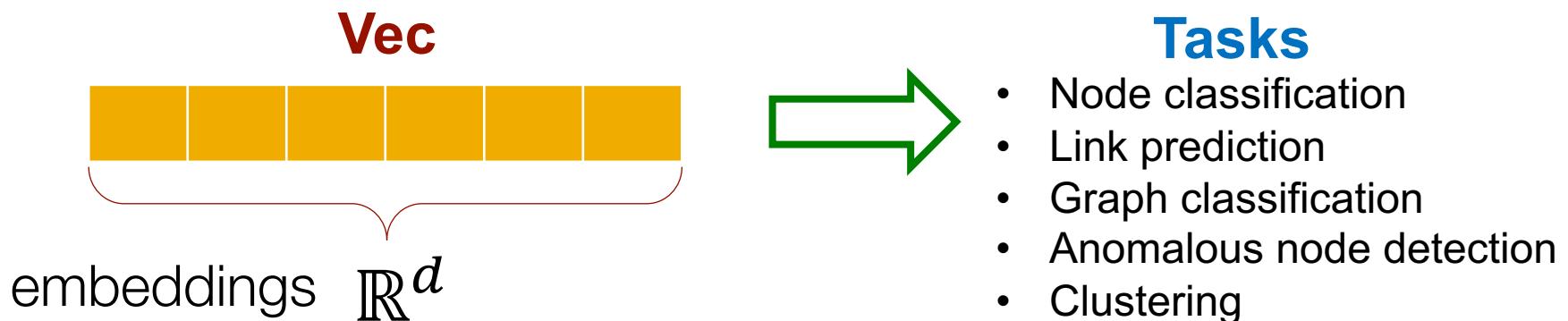
Graph Representation Learning

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

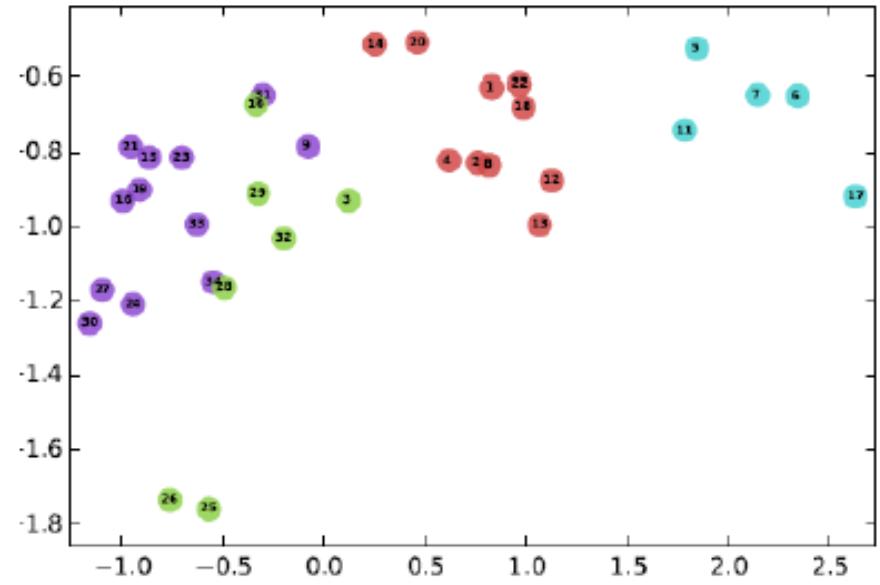


Example Node Embedding

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



Input



Output

Image from: [Perozzi et al.](#). DeepWalk: Online Learning of Social Representations. *KDD 2014*.

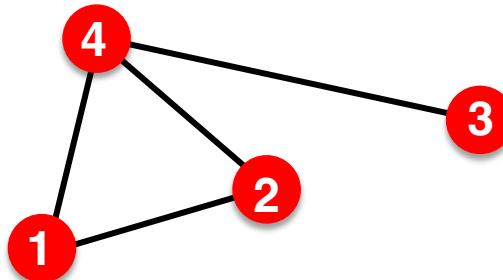
Stanford CS224W: **Node Embeddings:** **Encoder and Decoder**

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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**

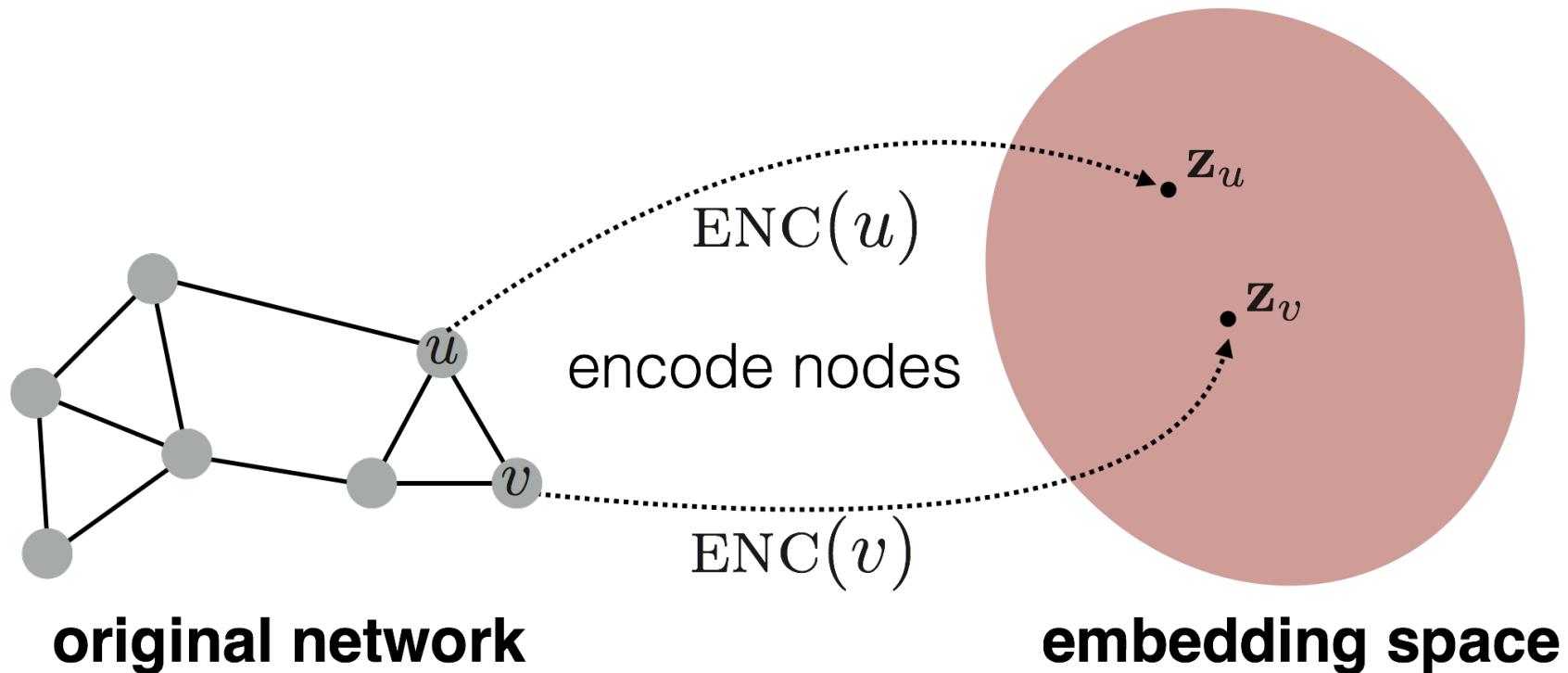


$V: \{1, 2, 3, 4\}$

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

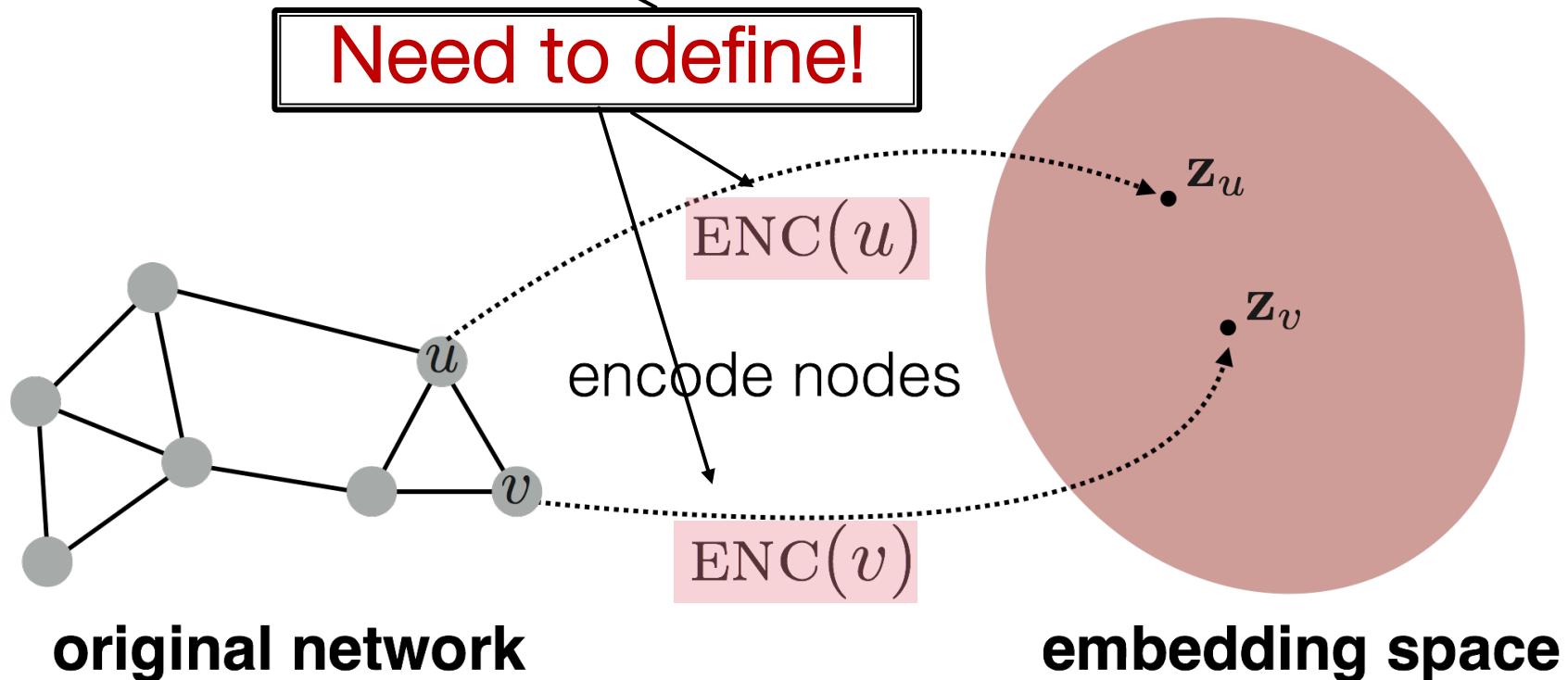
Embedding Nodes

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



Embedding Nodes

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



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 DEC** maps from embeddings to the similarity score
4. Optimize the parameters of the encoder so that:

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

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

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

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

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**

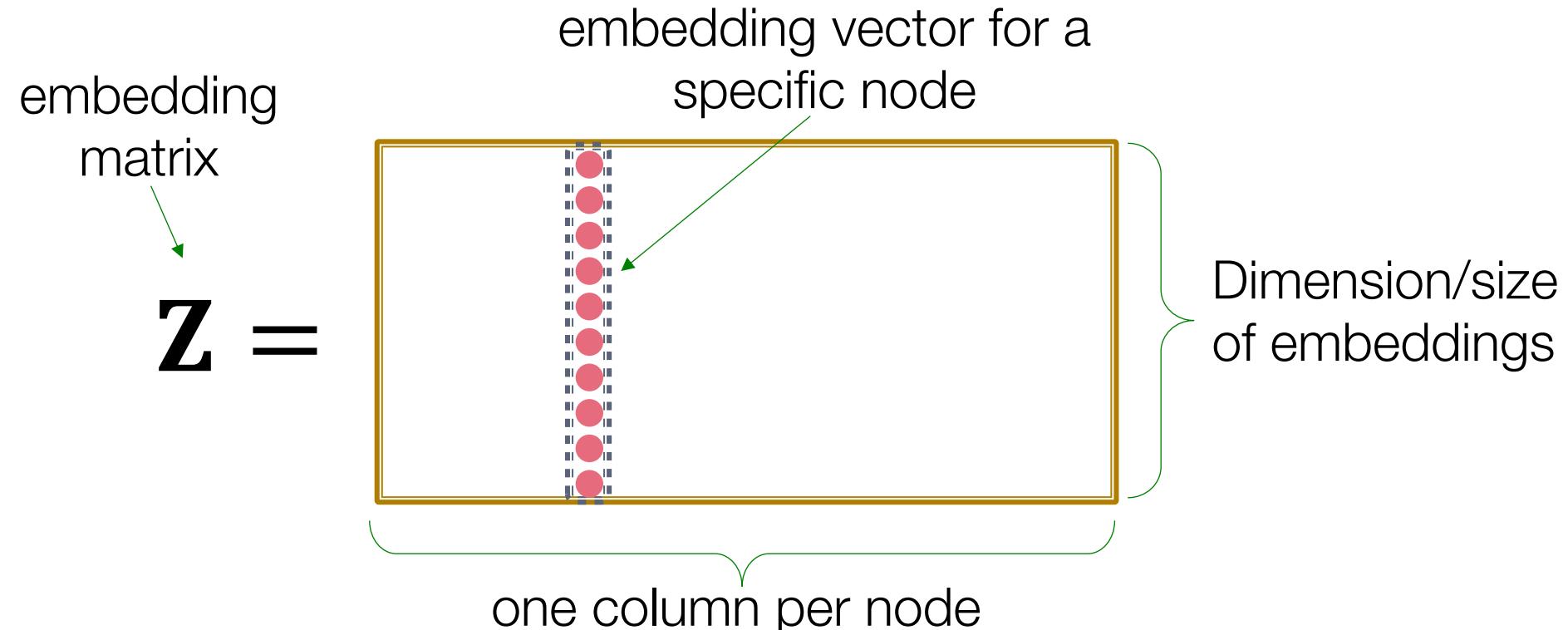
$$\text{ENC}(v) = z_v = Z \cdot v$$

$Z \in \mathbb{R}^{d \times |\mathcal{V}|}$ 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 $\mathbf{z}_v^T \mathbf{z}_u$ 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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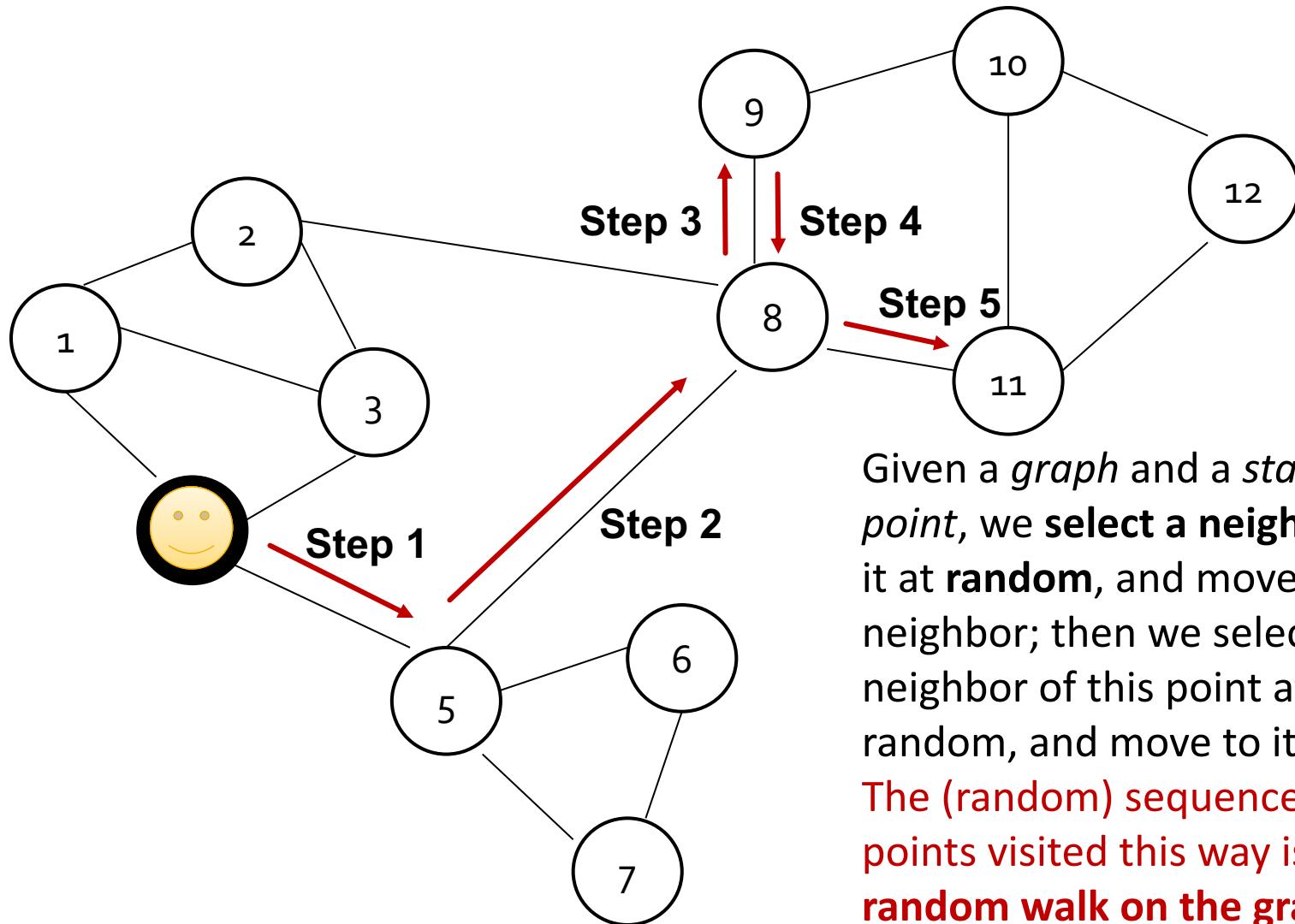
Notation

- **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: $S(\mathbf{z})[i] = \frac{e^{\mathbf{z}[i]}}{\sum_{j=1}^K e^{\mathbf{z}[j]}}$
- **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**.

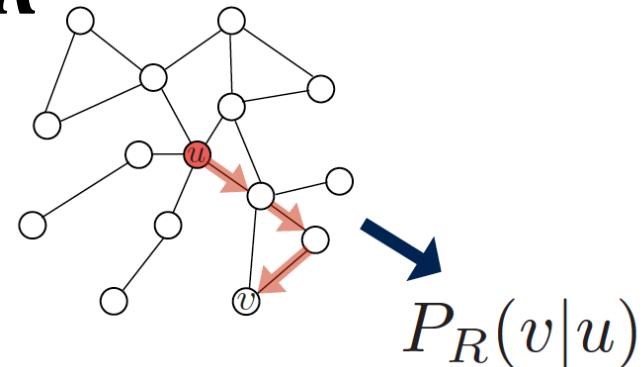
Random-Walk Embeddings

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

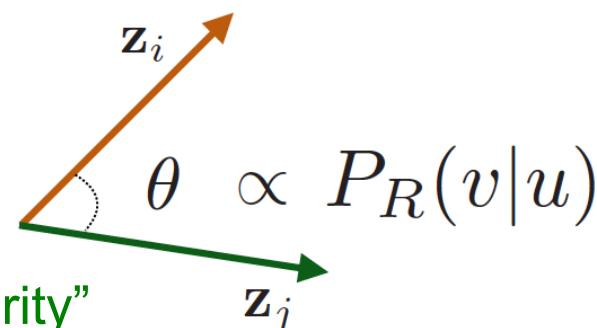
probability that u and v co-occur on a random walk over the graph

Random-Walk Embeddings

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



2. Optimize embeddings to encode these random walk statistics:



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:

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

- $N_R(u)$ 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 $N_R(u)$.**

$$\arg \max_z \sum_{u \in V} \log P(N_R(u) | z_u) \Rightarrow \text{Maximum likelihood objective}$$

* $N_R(u)$ can have repeat elements since nodes can be visited multiple times on random walks
11/14/23 Jure Leskovec, Stanford CS224W: Machine Learning with Graphs, <http://cs224w.stanford.edu>

Random Walk Optimization

Equivalently,

$$\arg \min_z \mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|z_u))$$

- **Intuition:** Optimize embeddings z_u to **minimize** the negative log-likelihood of random walk neighborhoods $N(u)$.
- **Parameterize $P(v|z_u)$ using softmax:** Why softmax?

$$P(v|z_u) = \frac{\exp(z_u^T z_v)}{\sum_{n \in V} \exp(z_u^T z_n)}$$

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:

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

sum over all nodes u

sum over nodes v seen on random walks starting from u

predicted probability of u and v co-occurring 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!

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



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

Random Walk Optimization

But doing this naively is too expensive!

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

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

Negative Sampling

■ Solution: Negative sampling

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

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

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.

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>

Negative Sampling

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

random distribution
over nodes

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

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

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 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:

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

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*.

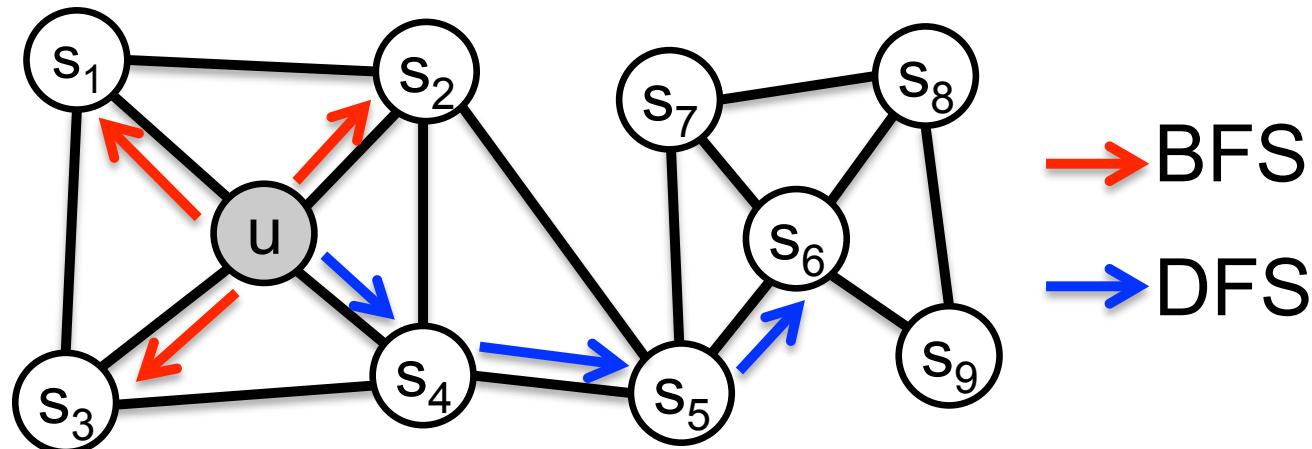
Overview of node2vec

- **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.

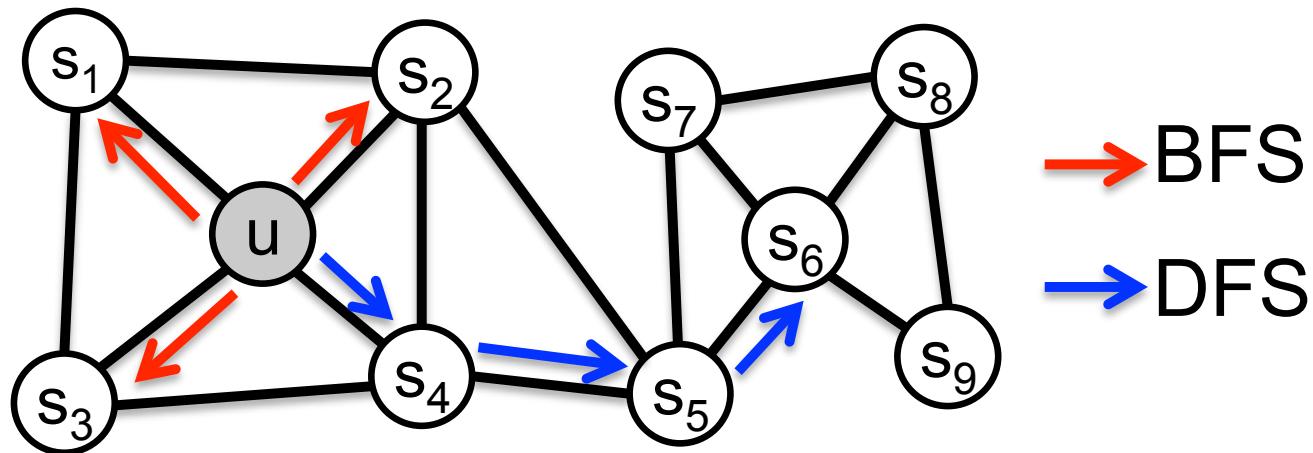
node2vec: Biased Walks

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 :

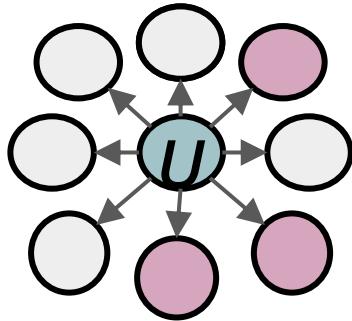


Walk of length 3 ($N_R(u)$ of size 3):

$$N_{BFS}(u) = \{ S_1, S_2, S_3 \} \quad \text{Local microscopic view}$$

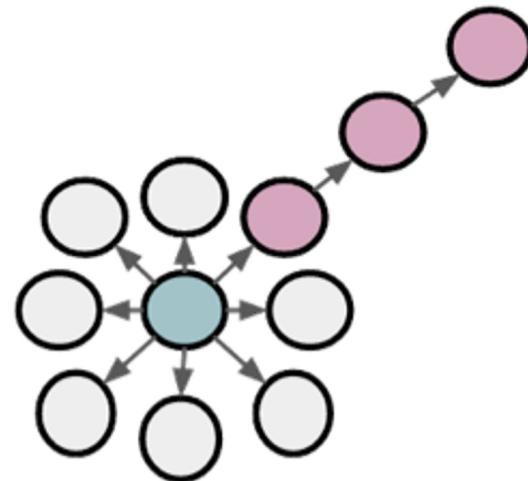
$$N_{DFS}(u) = \{ S_4, S_5, S_6 \} \quad \text{Global macroscopic view}$$

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

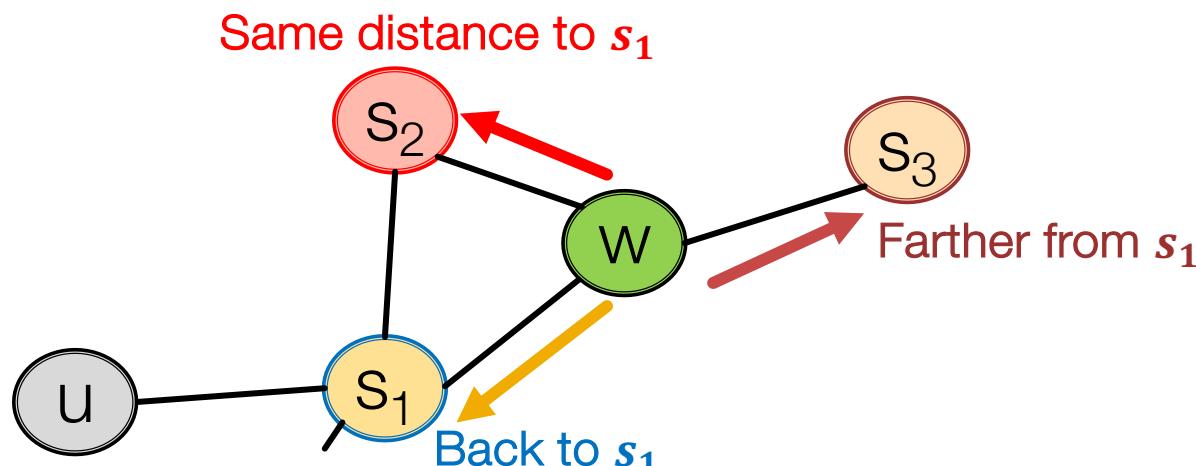
Biased fixed-length random walk R that given a node u generates neighborhood $N_R(u)$

- 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

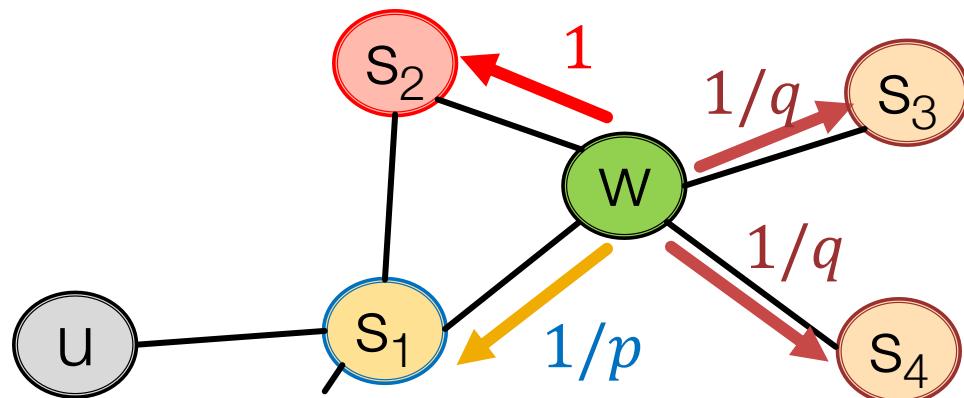
Define the random walk by specifying the walk transition probabilities on edges adjacent to the current node w :

- 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?



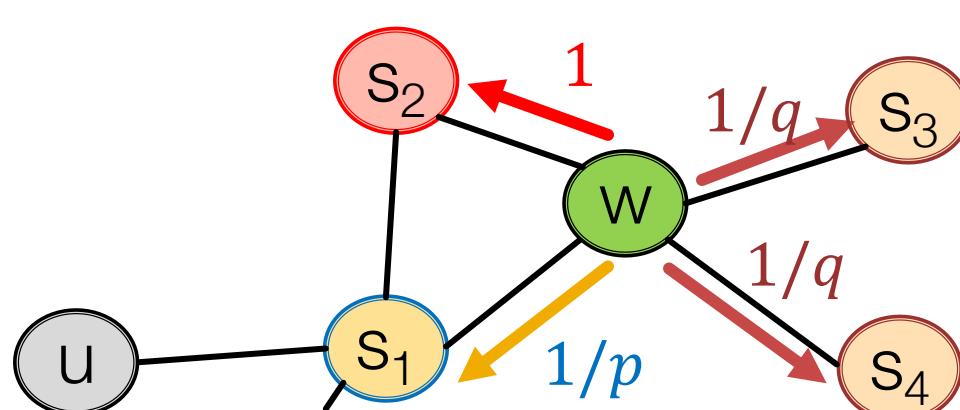
$1/p, 1/q, 1$ are
unnormalized
probabilities

- 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?



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

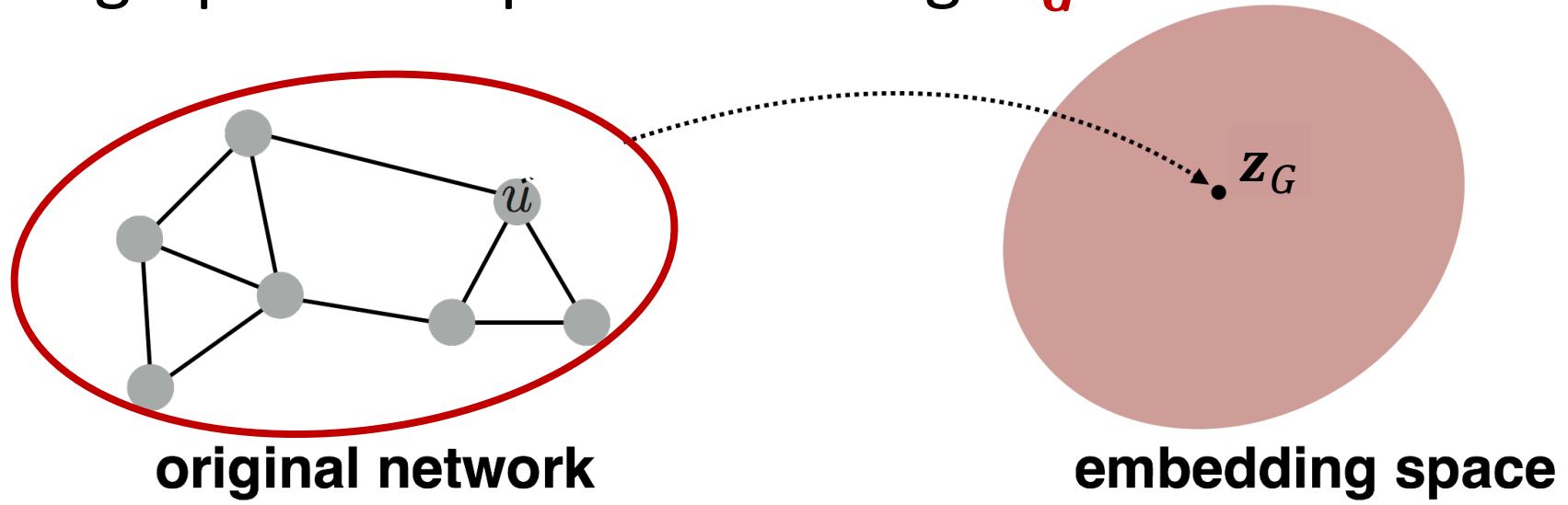
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Embedding Entire Graphs

- **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:

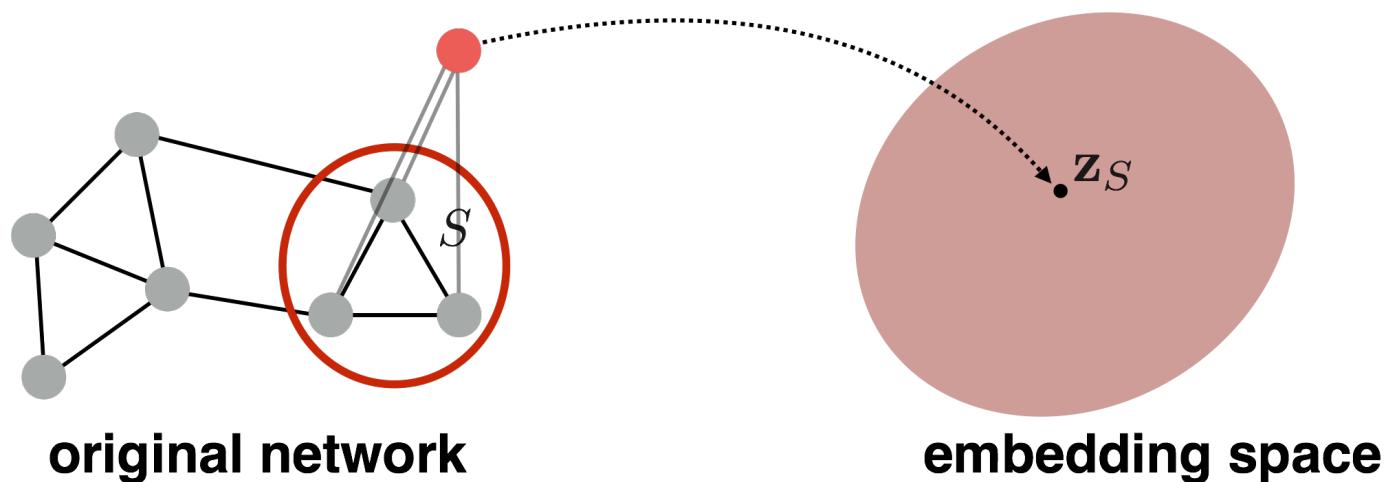
- Run a standard graph embedding technique *on* the (sub)graph G .
- Then just sum (or average) the node embeddings in the (sub)graph G .

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

- 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

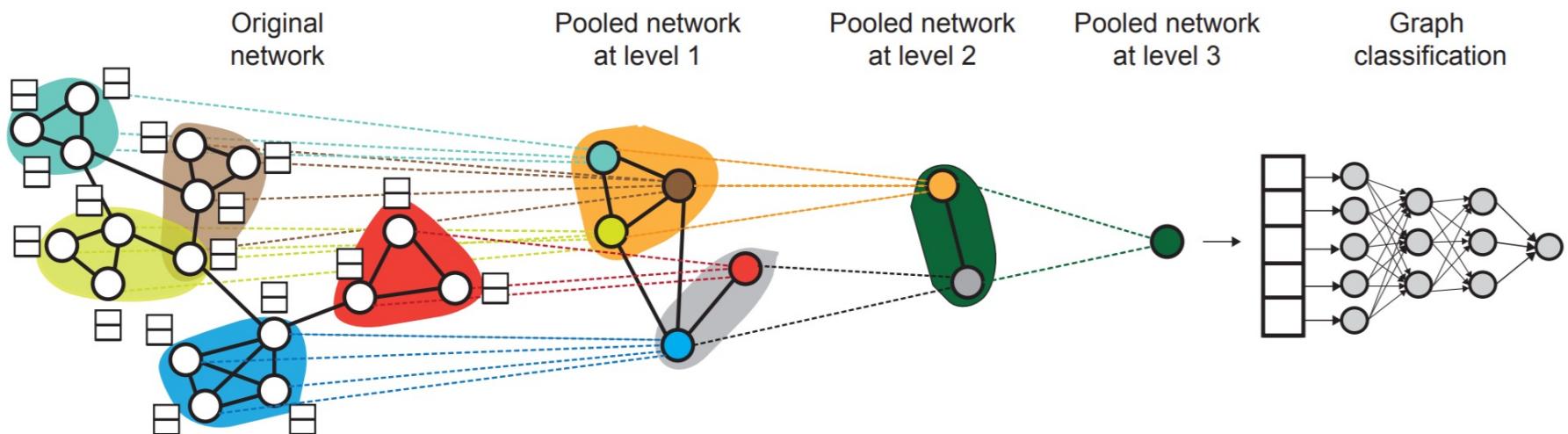
Summary

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

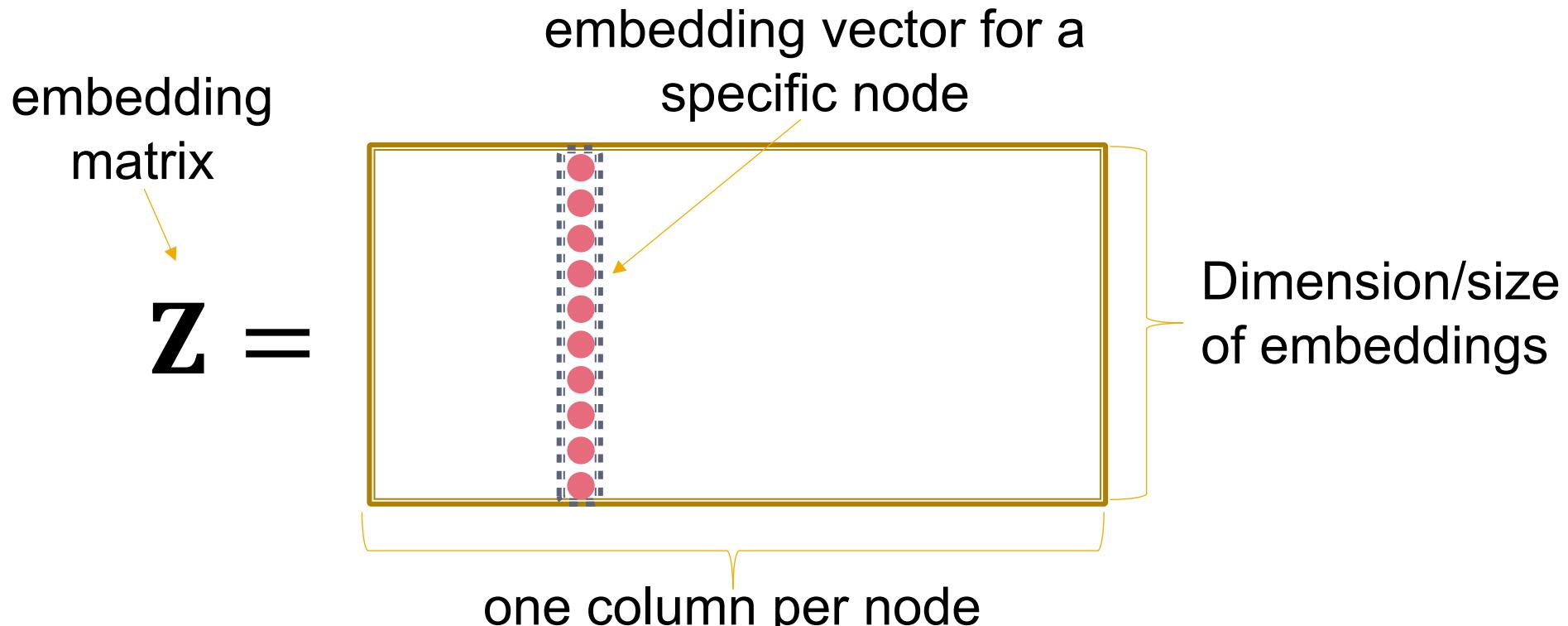
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<http://cs224w.stanford.edu>



Embeddings & Matrix Factorization

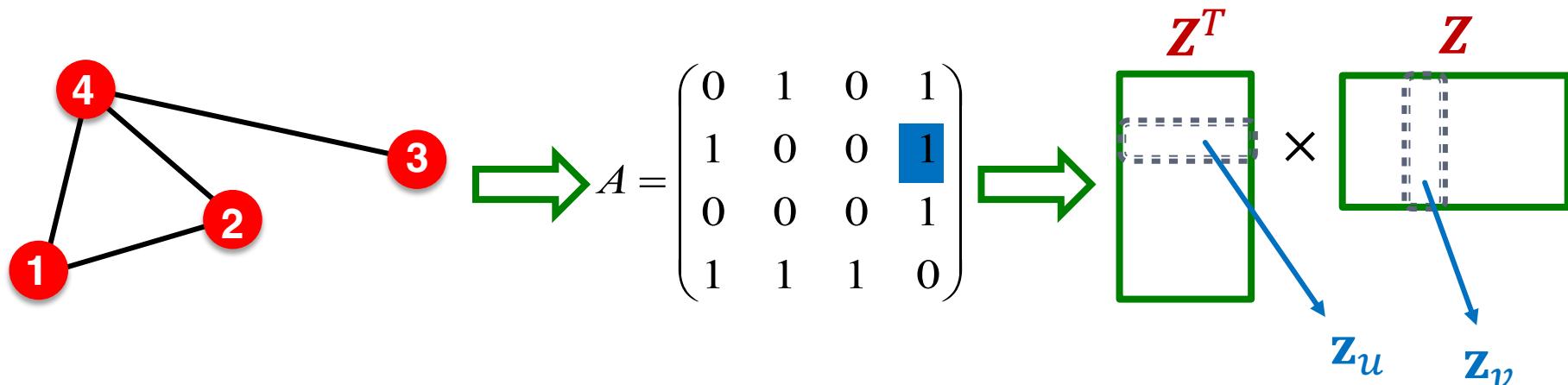
- Recall: encoder as an embedding lookup



Objective: maximize $\mathbf{z}_v^T \mathbf{z}_u$ 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: $\mathbf{z}_v^T \mathbf{z}_u = A_{u,v}$ which is the (u, v) entry of the graph adjacency matrix A
- Therefore, $\mathbf{Z}^T \mathbf{Z} = A$



Matrix Factorization

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

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

- 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

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

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

context window size

See Lec 3 slide 30:

$$T = |N_R(u)|$$

Diagonal matrix D
 $D_{u,u} = \deg(u)$

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

Today's Summary

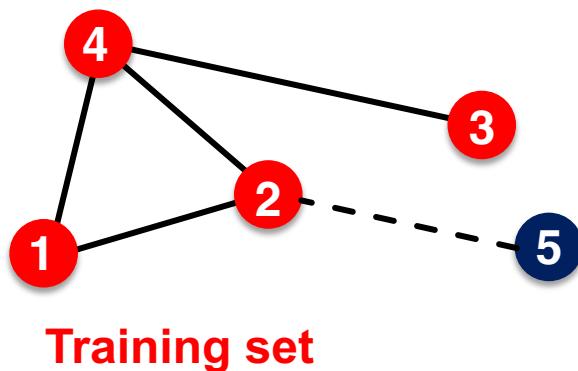
We discussed **graph representation learning**, a way to learn **node and graph embeddings** for downstream tasks, **without feature engineering**.

- **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.

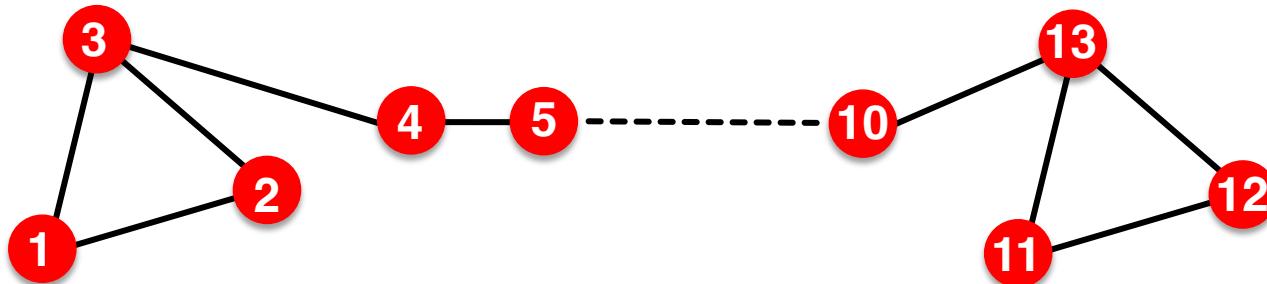


A newly added node 5 at test time
(e.g., new user in a social network)

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

Limitation (2)

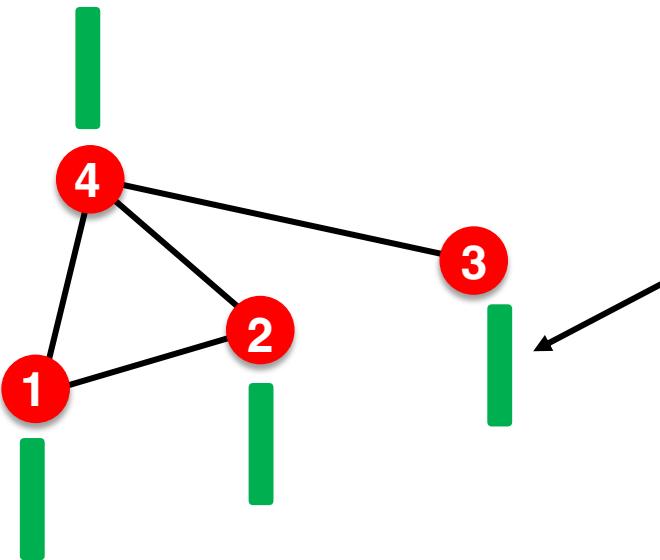
- Cannot capture **structural similarity**:



- 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)