Graph Representation Learning

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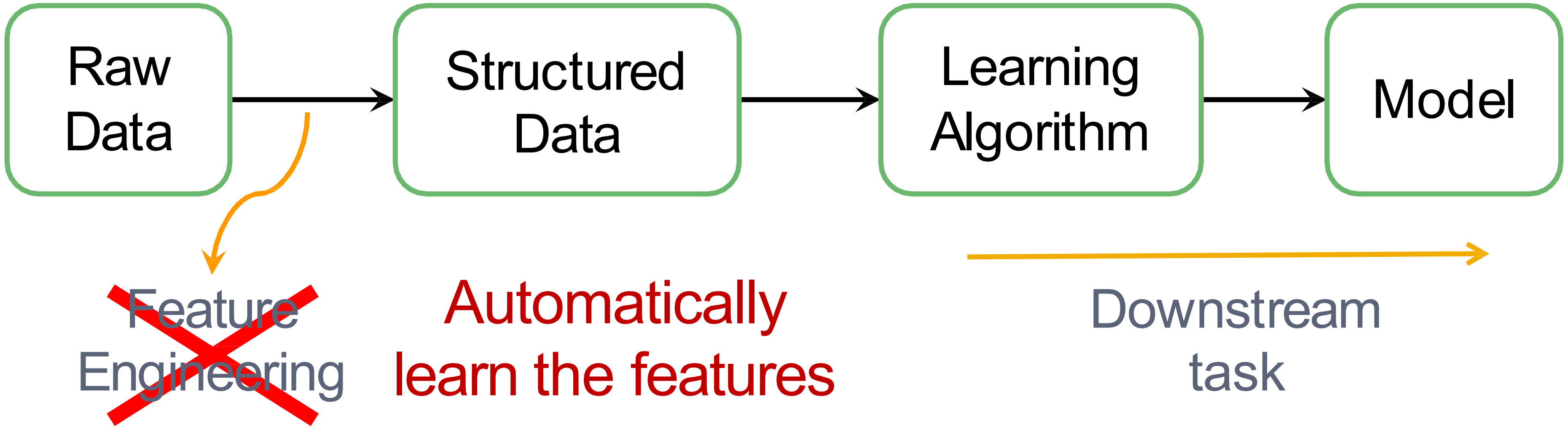
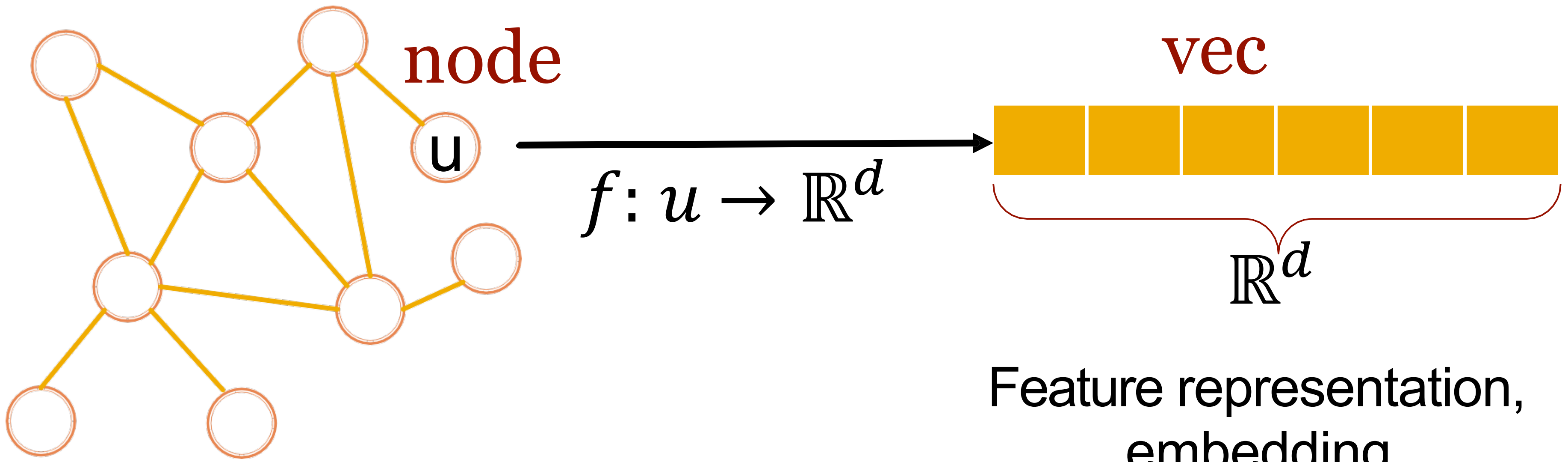
Machine Learning Lifecycle

Machine Learning Lifecycle requires feature engineering. Feature engineering is painful! How can we make it easy?



Feature Learning in Graphs

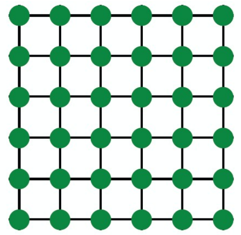
- **Goal:** Efficient task-independent feature learning for machine learning in graphs!

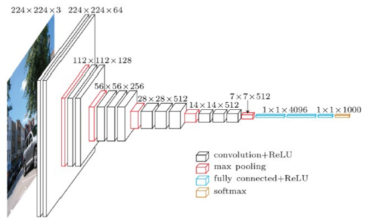


Feature representation, embedding

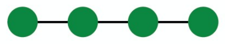
Why is it hard?

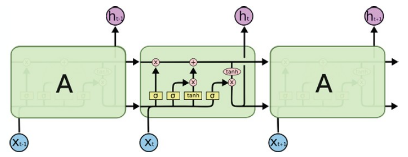
- **Modern deep learning toolbox is designed for simple sequences or grids**
  - CNNs for fixed-size images/grids….





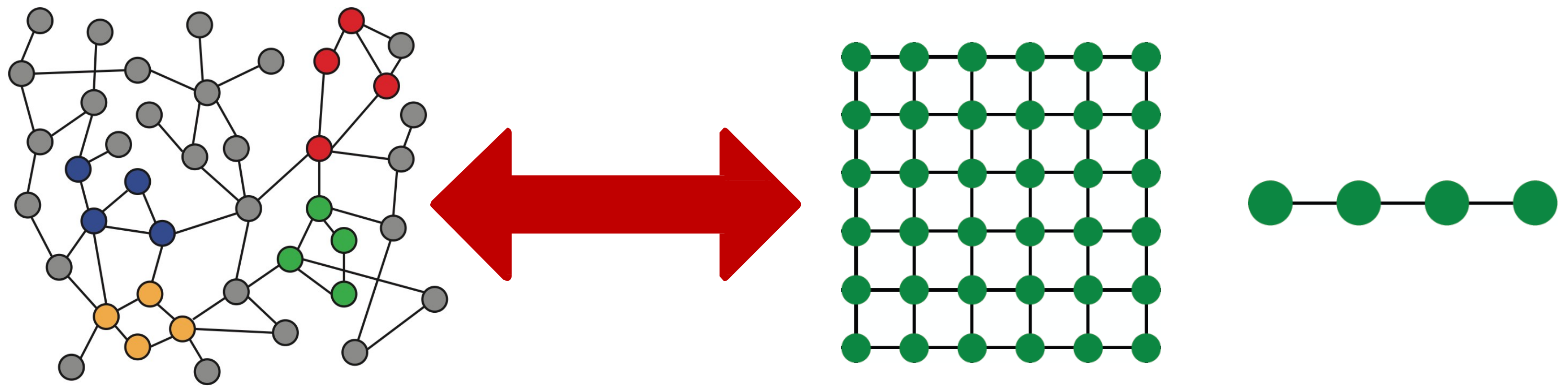
  - RNNs or word2vec for text/sequences…





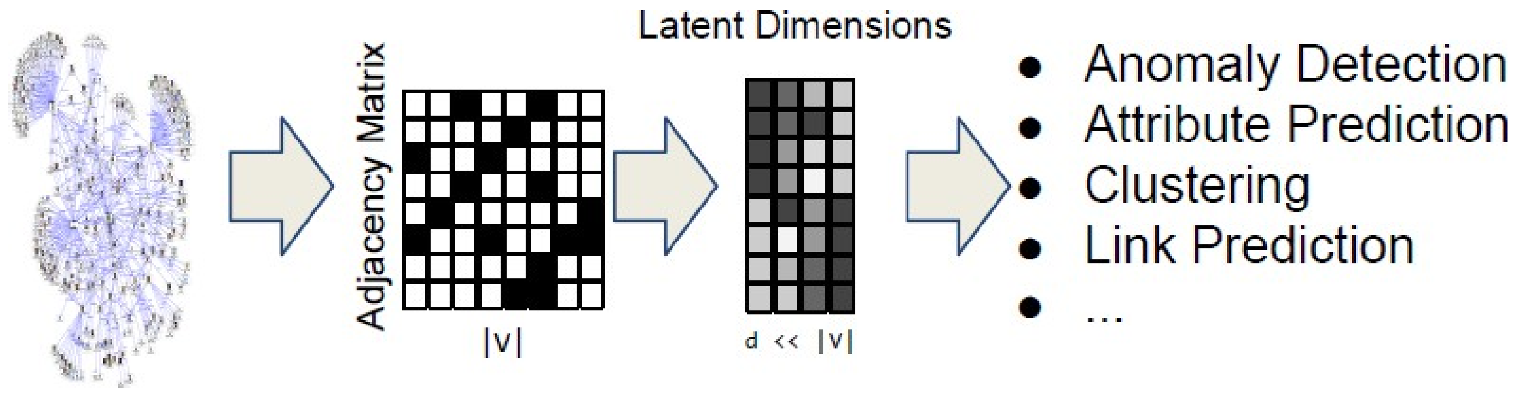
Why is it hard?

- **Networks are far more complex.**
  - Complex topographical structure
  - No fixed node ordering or reference point.



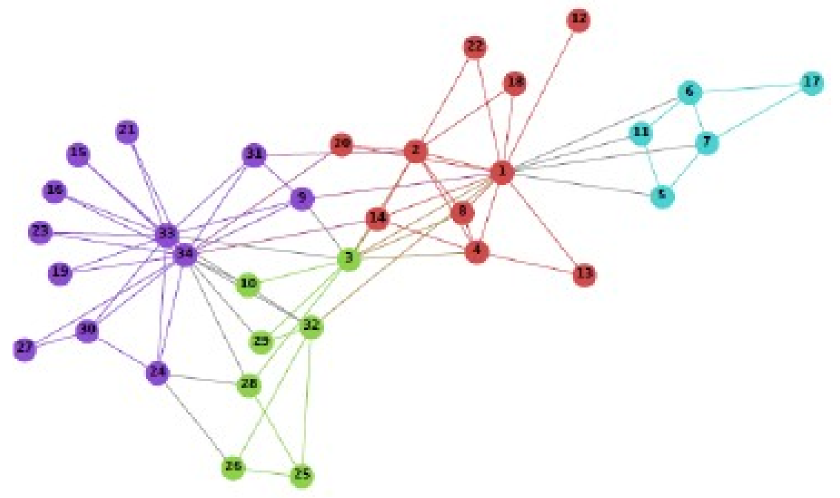
Node embedding

- **Task: Give a graph G, we map each node in a network to a point in a low-dimensional space**
  - Encode network information and generate node representation
  - Similarity of embedding between nodes approximates their original network similarity

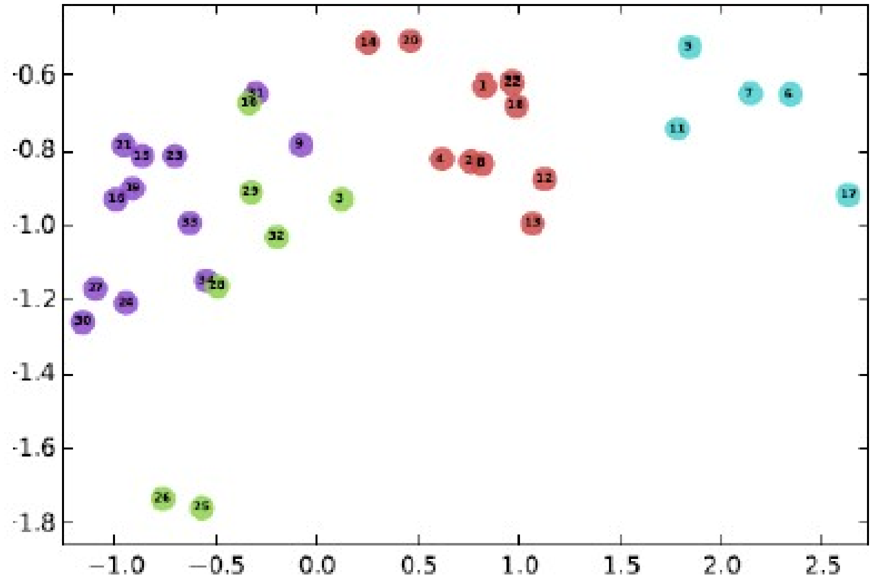


Example: Node Embedding

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



Input



Output

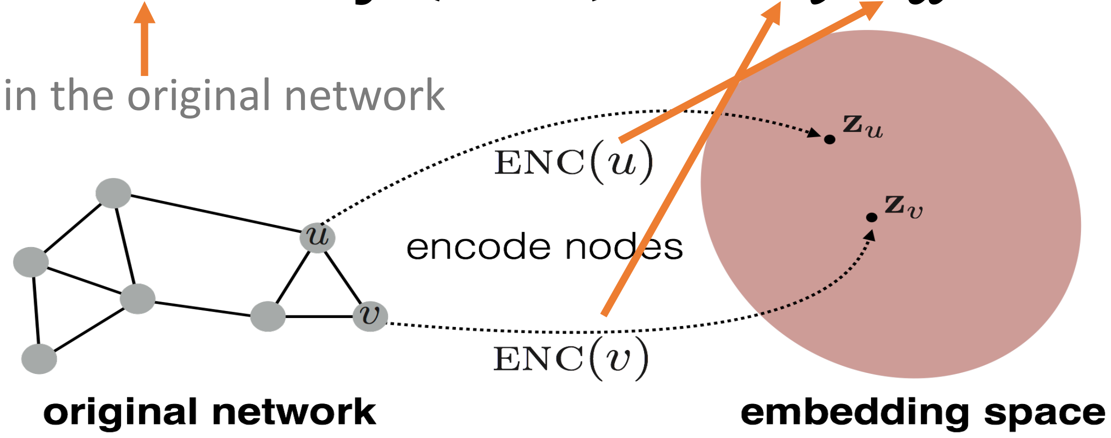
Image from: Perozzi et al. DeepWalk: Online Learning of Social Representations. *KDD 2014.*

Learning Node Embeddings

- Define a **node similarity function** $\text{similarity}(u, v)$
  - a measure of similarity in the original network
- **Encoder ENC** maps from nodes to embeddings $\text{ENC}(v) = z_v$
- **Decoder DEC** maps from embedding to the similarity score(e.g. dot product $\boldsymbol{z}_v^T \boldsymbol{z}_u$)
- **Optimize the parameters of the encoder so that:**

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

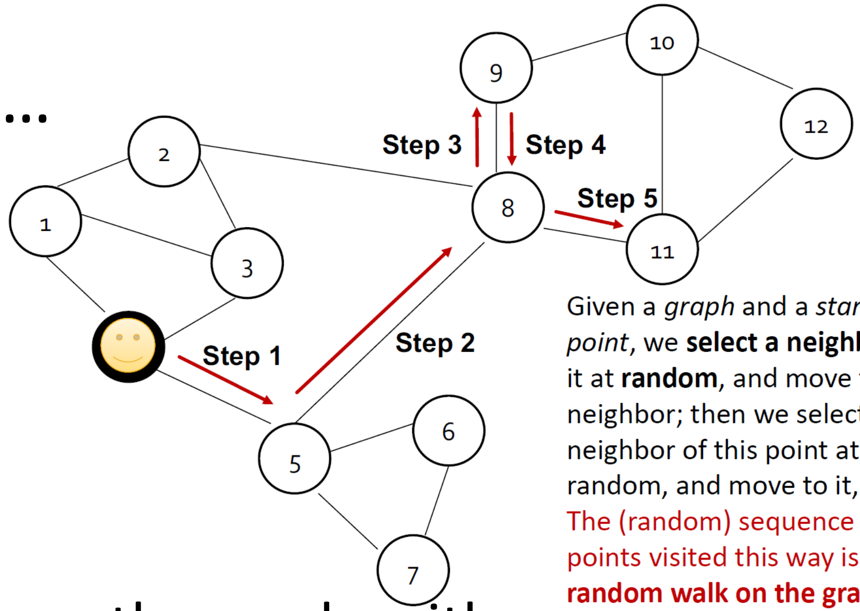
Similarity in the original network



How to define node similarity?

- Should two nodes have similar embeddings if they…
  - are connected?
  - share neighbors?
  - have similar "structural roles"?

- **Random walk approaches for node embedding!**
  - **Expressivity:** if random walk starting from a node visits another node with high probability, they are similar
  - **Efficiency:** only need to consider pairs that co-occur on random walks
- **We will introduce DeepWalk, node2vec.**

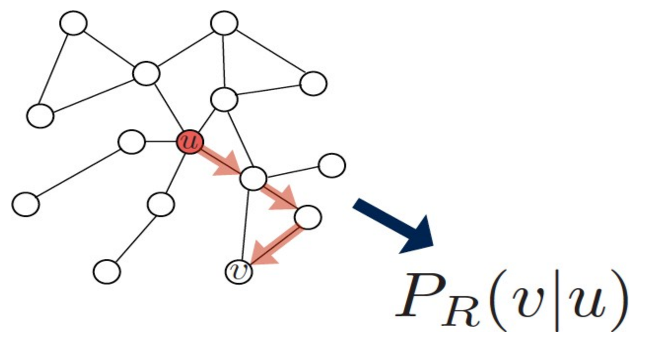


Given a *graph* and a *starting point*, we **select a neighbor** of it at **random**, and move to this neighbor; then we select a neighbor of this point at random, and move to it, etc. The (random) sequence of points visited this way is a **random walk on the graph**.

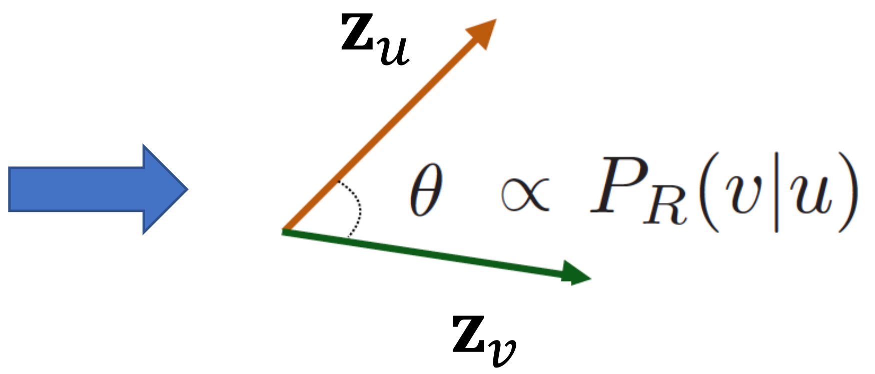
Perozzi, Bryan, Rami Al-Rfou, and Steven Skiena. "Deepwalk: Online learning of social representations." *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2014.
Grover, Aditya, and Jure Leskovec. "node2vec: Scalable feature learning for networks." *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*. 2016.

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



Estimate probability of visiting node $\boldsymbol{v}$ on a **random walk** starting from node $\boldsymbol{u}$ using some random walk **strategy** $\boldsymbol{R}$



Optimize embeddings to encode these random walk statistics

Notation

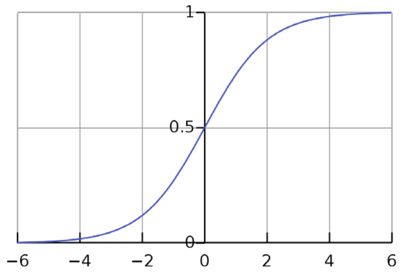
- **Vector** z_u: the embedding of node u
- **Probability** $P(v|z_u)$:
  - The predicted probability of visiting node v on random walks starting from node u (our model prediction based on z_u)

- **Softmax** function:

$$\sigma(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

Turns vector of K real values (model predictions) into K probabilities that sum to 1

- **Sigmoid** function:



$$S(x) = \frac{1}{1+e^{-x}}$$

S-shaped function that turns real values into the range of (0, 1).

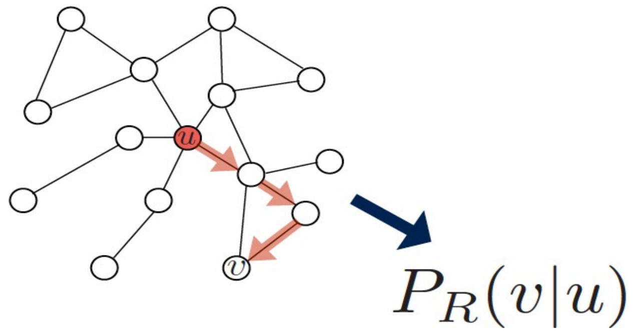
Feature Learning Objective

- Our **goal** is to learn a mapping $z: u \rightarrow \mathbb{R}^{d}$

Such that:

$$\max_{z} \sum_{u \in V} \log P(N_R(u) | z_u)$$

$N_R(u)$ neighborhood of u obtained by strategy R



Idea: Learn node embedding such that nearby nodes are close together in the network

Random Walk Optimization $N_R(u)$

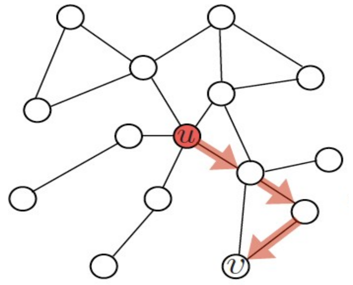
- Run short fixed-length random walks starting from each node on the graph using some strategy R
- For each node u collect $N_R(u)$, the multiset of nodes visited on random walks starting from u
- Optimize embeddings according to: Given node u, predict its neighbors $N_R(u)$

$$\max_z \sum_{u \in V} \log P(N_R(u) | z_u)$$

Random Walk Optimization $P(N_R(u)|z_u)$

- **Assumption:** Conditional likelihood factorizes over the set of neighbors $P(N_R(u)|z_u) = \Pi_{v \in N_R(u)} P(v|z_u)$
- The objective becomes:

$$\max_z \sum_{u \in V} \sum_{v \in N_R(u)} \log P(v|z_u)$$



- Softmax parametrization $P(v|z_u)$:

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

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 together

Computation cost is high! $O(V^2)$

$$\mathcal{L} = \underbrace{\sum_{u \in V}}_{\text{sum over all nodes } u} \underbrace{\sum_{v \in N_R(u)}}_{\text{sum over nodes } v \text{ seen on random walks starting from } u} - \log \left(\underbrace{\frac{\exp(\mathbf{z}_u^\top \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^\top \mathbf{z}_n)}}_{\text{predicted probability of } v \text{ appearing in random walk starting from } u} \right)$$

- Optimization random walk embedding is finding node embedding that minimize this loss function

Negative Sampling

- **Reduce Computation Cost: Negative sampling**

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

分母很复杂，就不全算，算一个很小的子集

Detailed proof is here

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

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

random distribution over all nodes

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

Negative Sampling

- $n_i \sim P_v$
- Sample k negative nodes proportional to **degree**
- Two considerations for k (# negative samples):
  - Higher k gives more **robust** estimates
  - Higher k corresponds to higher **prior** on **negative events**. In practice, $k = 5 \sim 20$

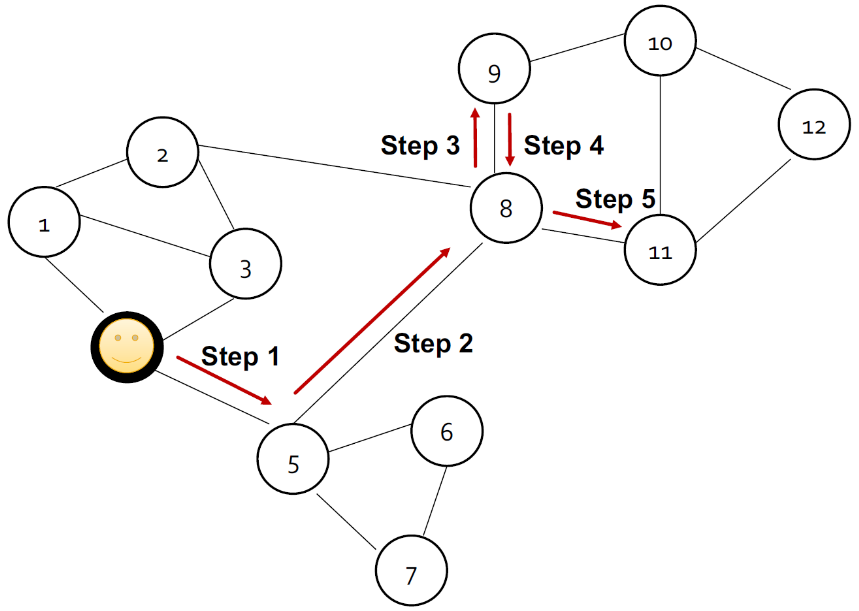
Random Walk Embedding Framework

- Run **short fixed-length** random walks starting from each node on the graph using some strategy R.
- For each node u collect $N_R(u)$, the multiset of nodes visited on random walks starting from u
- Optimize embeddings using **stochastic gradient descent** with loss function

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

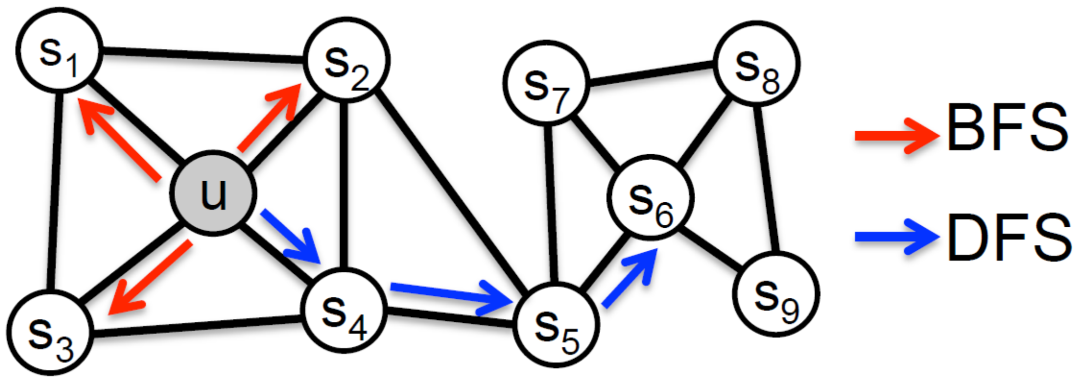
How should we randomly walk?

- **What strategies should we use to run these random walks?**
- Simplest idea: **Just run fixed-length, unbiased random walks starting from each node** （**DeepWalk** from Perozzi et al., 2013）
  - The issue is that such notion of similarity is too constrained
- How can we generalize this?



Biased Random Walk

- Second order random walk R: remember the previous step.
    - Richer node structures
- Use flexible, biased random walks that can trade off between local and global views of the network (**Node2Vec**, 2016).



Two strategies to define neighborhoods:
Breadth First Search(BFS)
Depth First Search(DFS).

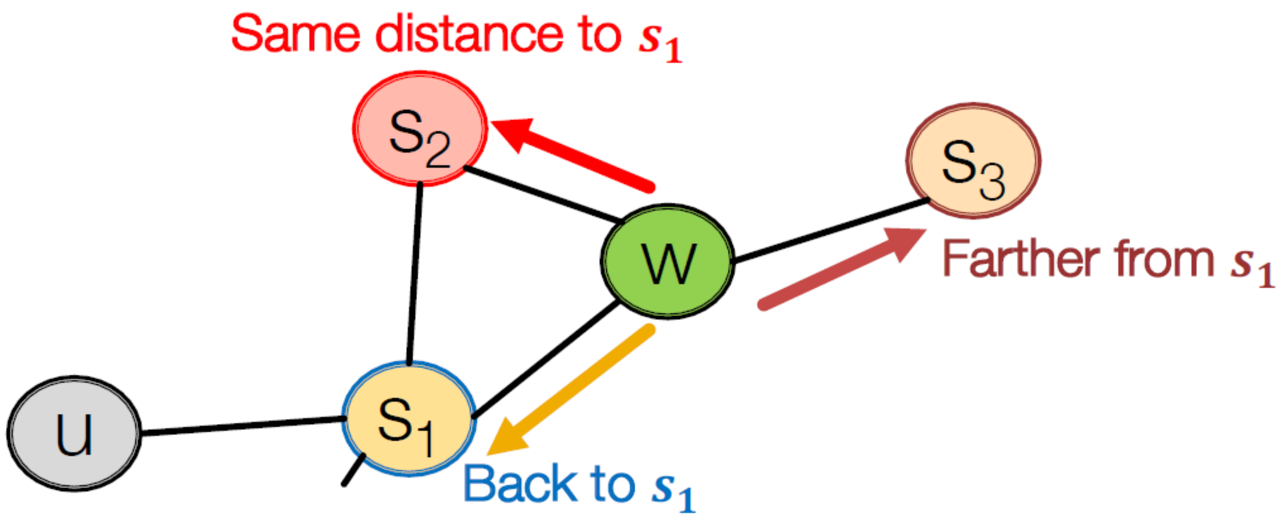
Walk of length 3 ($N_R(u)$ of size 3):

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

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

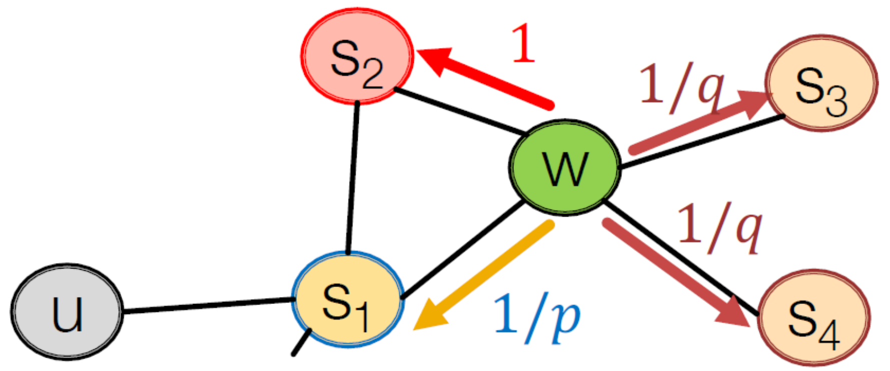
Biased Random Walks

- Biased second order random walks to explore neighborhoods:
  - Random walk just traversed edge (s_1, w) and is now at w
  - Neighbors of w can only be:



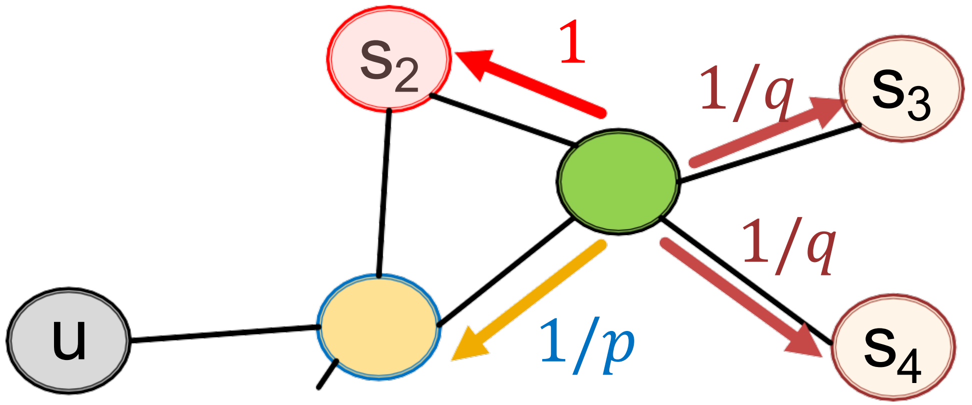
Tadeoff between BFS and DFS

- Two parameters to tune:
  - Return parameter p: the ratio between **BFS** and **return** to the previous node
  - In-out parameter q: the ratio between **BFS** and **DFS**



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

Biased Random Walk



$w \rightarrow$

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

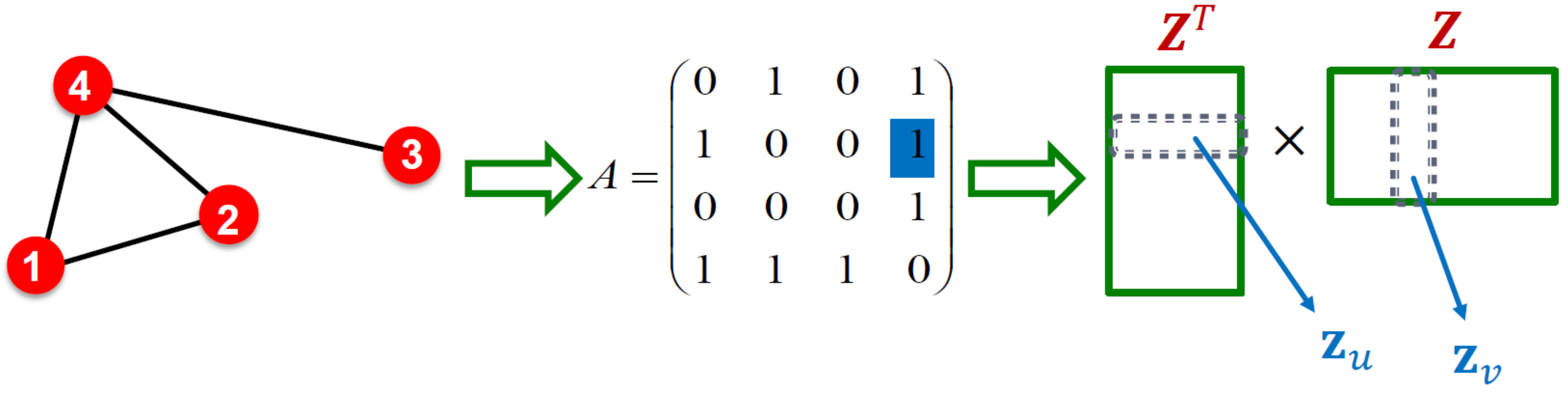
Node2vec Algorithm

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

Network Embedding as Matrix Factorization

- Inner product decoder with node similarity defined by edge connectivity is equivalent to matrix factorization of adjacency matrix A
  - Exact factorization $A = Z^T Z$ is generally not possible
  - We can approximate by

$$\min_{Z} \left\| A - Z^T Z \right\|_2$$



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

What does DeepWalk do?

- **DeepWalk** have a more complex **node similarity** definition based on random walks, equivalent to matrix factorization of:

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

Power of normalized adjacency matrix

Number of negative samples

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

Qiu, Jiezhong, et al. "Network embedding as matrix factorization: Unifying deepwalk, line, pte, and node2vec." *WSDM 2018*

How to use node embedding

- Node classification: predict label based on embedding
- Link prediction: predict edge (i, j) based on $f(z_i, z_j)$, where we can concatenate, avg, product, or take a difference between 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)

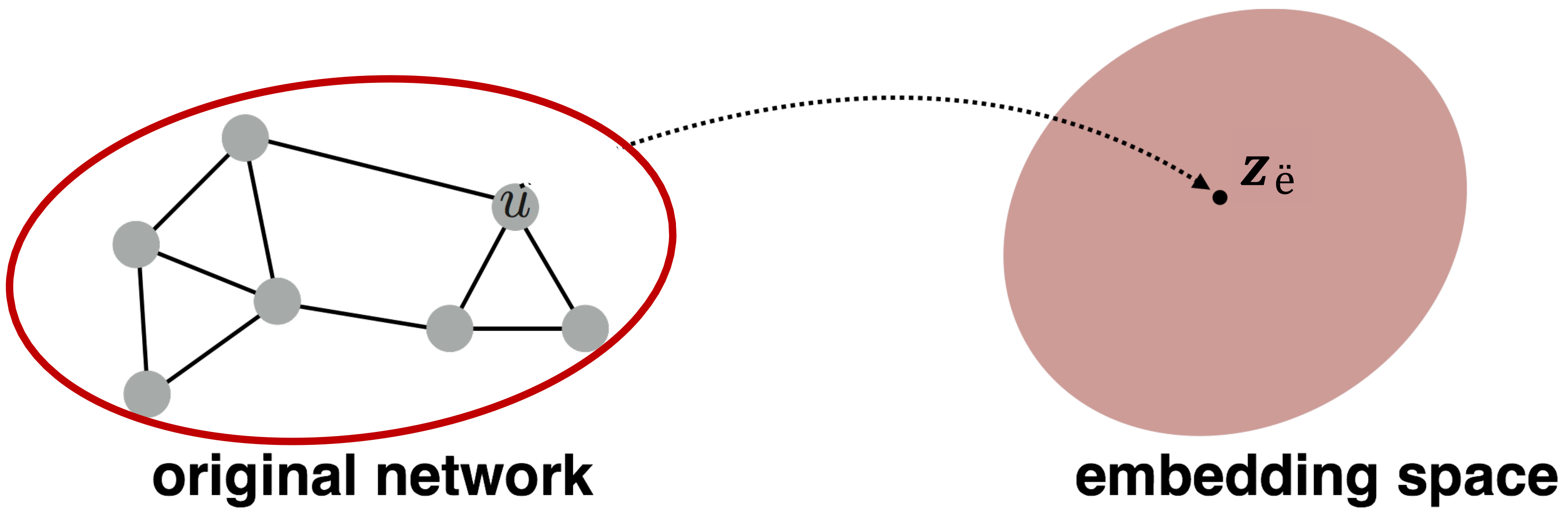
  Sum/Avg: $f(z_i, z_j) = g(z_i + z_j)$

  Distance: $f(z_i, z_j) = g(||z_i - z_j||_2)$

- No one method wins in all cases!
- Must choose node similarity that matches your application.

Embedding Entire Graphs

- **Goal:** Embed an entire graph G



Approach

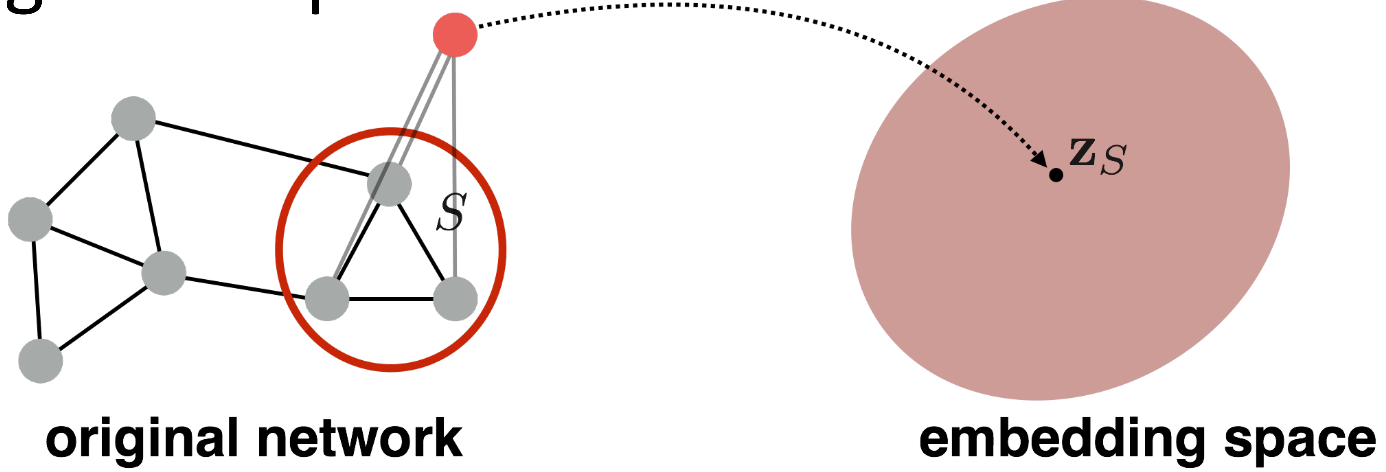
- Run a standard graph embedding
- Then just sum the node embeddings in the subgraph

$$Z_G = \sum_{v \in G} Z_v$$

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

Approach

- **Idea:** 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

Recommended Readings

- Different kinds of biased random walks:
  - Based on node attributes (Dong et al., 2017).
  - Based on a 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).

Note on Random Walk Embeddings

- This is **unsupervised** way of learning node embeddings
  - We are **not** utilizing node labels or features
  - The goal is to directly estimate a set of coordinates of a node so that some aspect of the network structure is preserved
- These embeddings are **task independent**
  - They are not trained for a specific task but can be used for **any task**

Limitations of Random Walk Embedding

- **Limitations** of random walk based embedding methods:
  - $\boldsymbol{O}(|\boldsymbol{V}|)$ parameters are needed:
    - No sharing of parameters between nodes
    - Every node has its own unique embedding
  - Inherently **"transductive"**:
    - Cannot generate embeddings for nodes that are not seen during training
  - Do **not** incorporate node **features:**
    - Many graphs have features that we can and should leverage