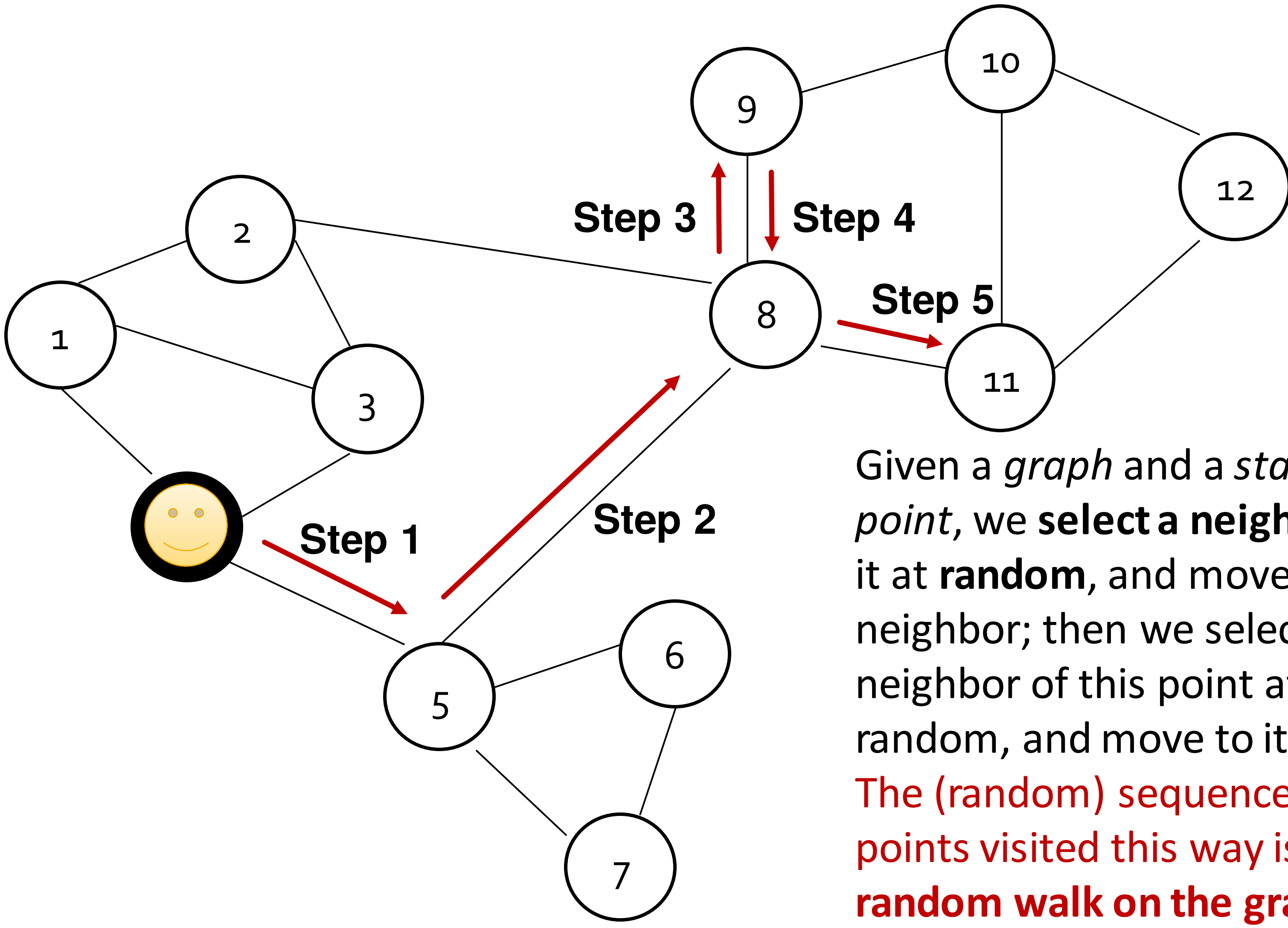
Notation

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



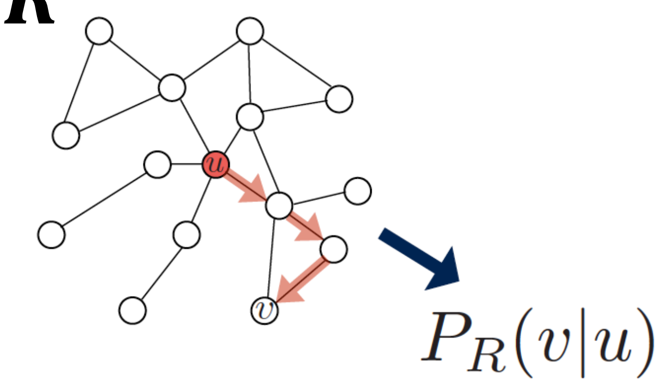
Given a *graph* and a *starting point*, we **select a neighbor** of it at **random**, and move to this neighbor; then we select a neighbor of this point at random, and move to it, etc. The (random) sequence of points visited this way is a **random walk on the graph**.

Random-Walk Embeddings

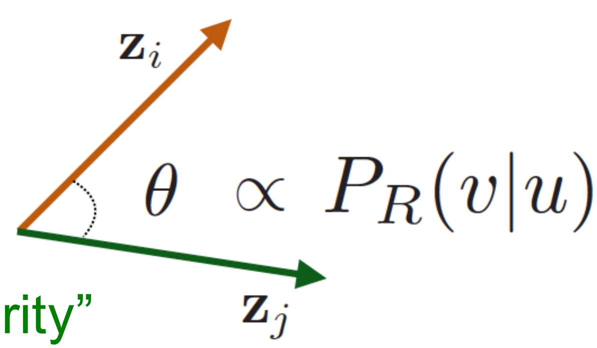
$$\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v \approx$$ probability that u and v co-occur on a random walk over the graph

Random-Walk Embeddings

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



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 $f: u \to \mathbb{R}^d$: $f(u) = \mathbf{z}_u$
- 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 $N_{\mathrm{R}}(u)$.

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

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

Random Walk Optimization

Equivalently,

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

- **Intuition:** Optimize embeddings $\boldsymbol{z}_u$ 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:

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

Optimizing random walk embeddings =

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

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

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

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

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.

Negative Sampling

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

random distribution over nodes

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

- Sample k negative nodes 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.*

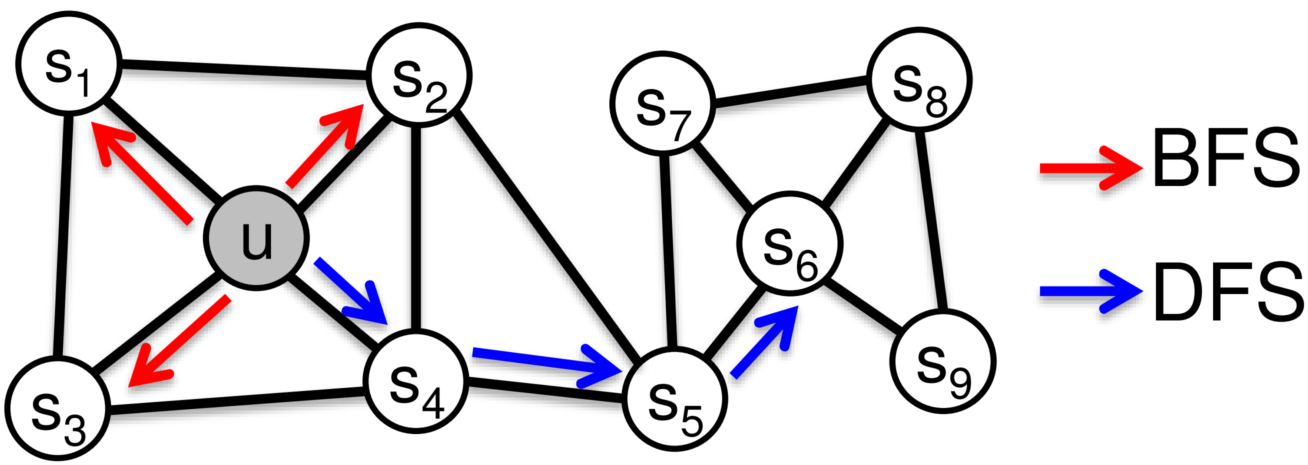
Overview of node2vec

- **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 2^{nd} 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.*

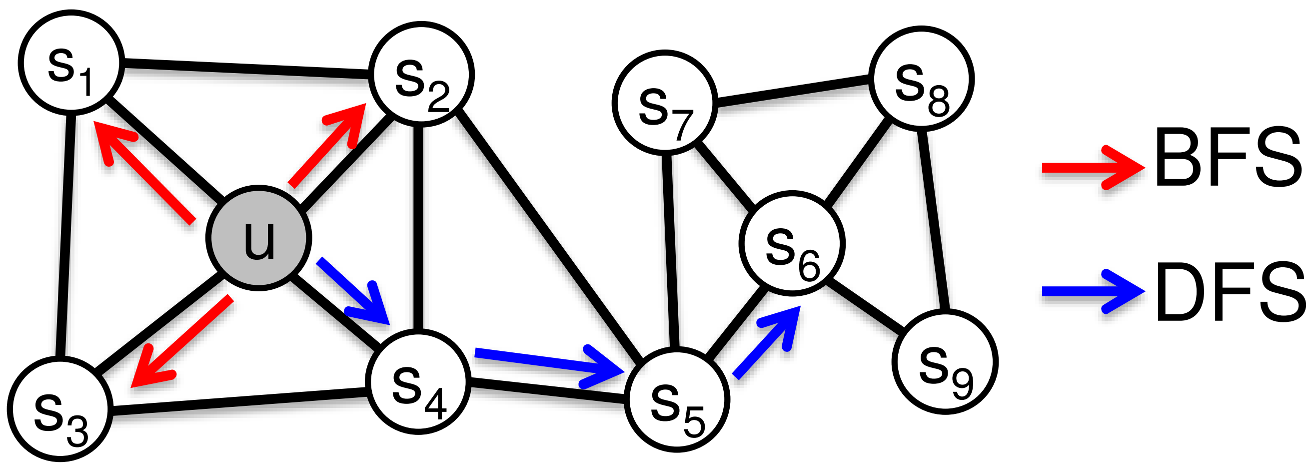
node2vec: Biased Walks

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 $\boldsymbol{N_R(u)}$ of a given node $\boldsymbol{u}$:

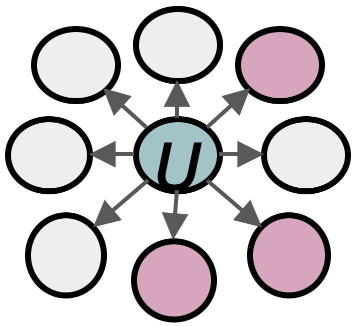


Walk of length 3 ($N_R(u)$ of size 3):

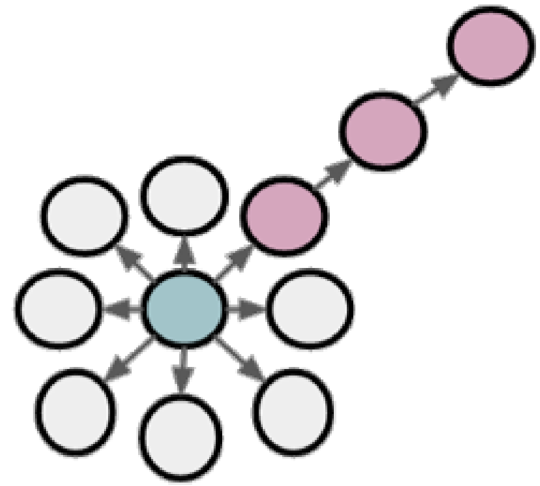
$$N_{BFS}(u) = \{\, s_1, s_2, s_3\}$$ Local microscopic view

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

BFS vs. DFS



BFS:
Micro-view of neighbourhood



DFS:
Macro-view of neighbourhood

Interpolating BFS and DFS

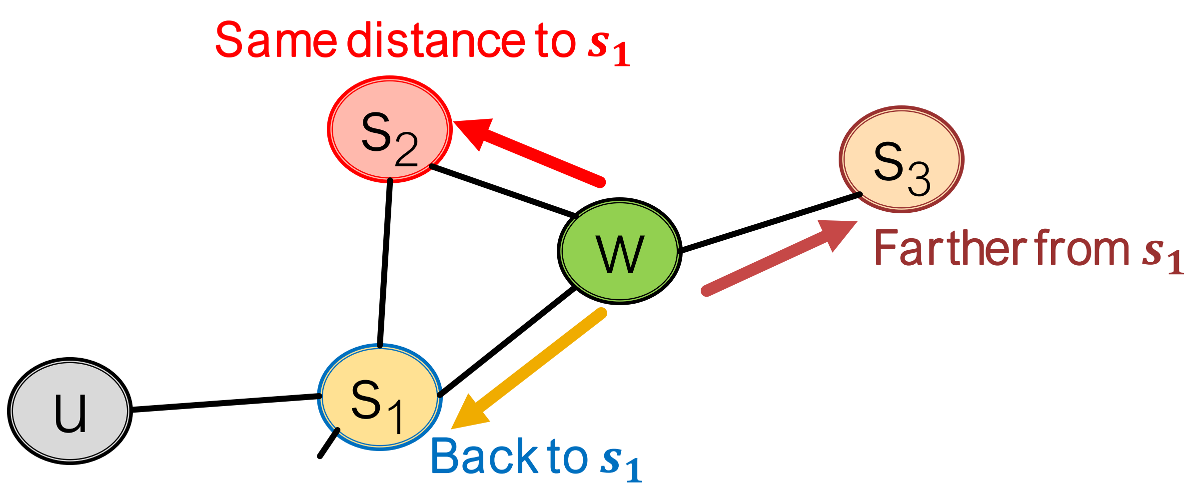
Biased fixed-length random walk R that given a node u generates neighborhood $N_R(u)$

- 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:

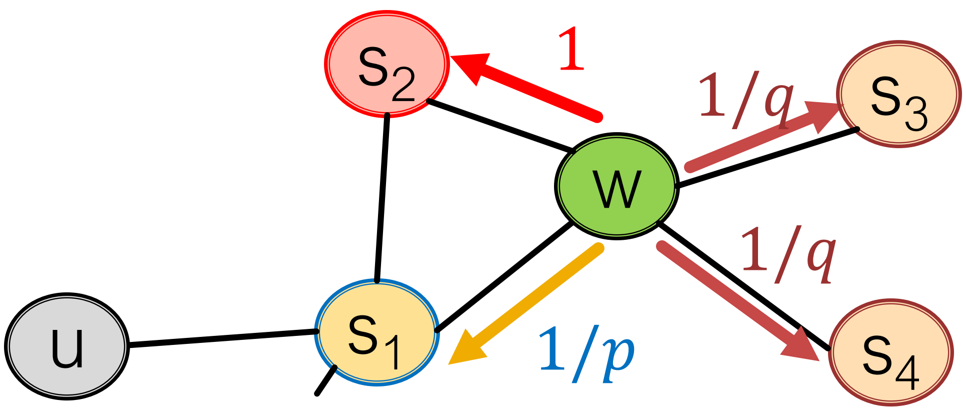
- Rnd. walk just traversed edge (s_1, w) and is now at w
- **Insight:** Neighbors of w can only be:



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?**

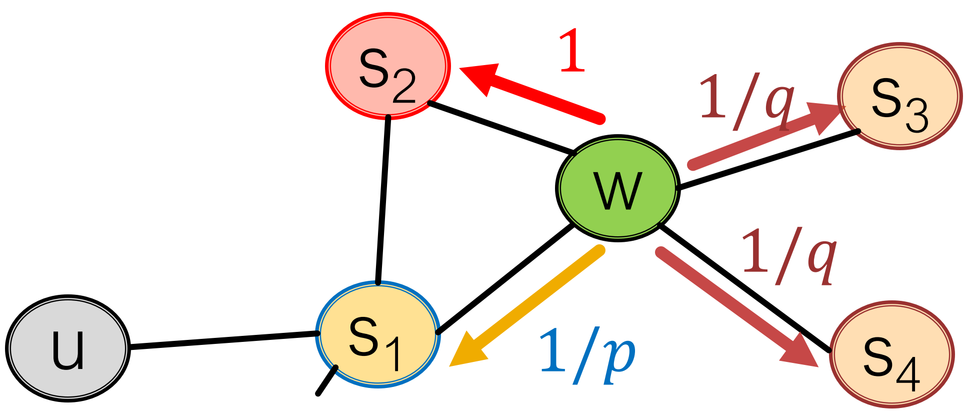


$1/p, 1/q, 1$ are unnormalized probabilities

- 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?**



$\mathrm{w} \rightarrow$

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
  - 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.