Graph Representation Learning

CS547 Machine Learning for Big Data

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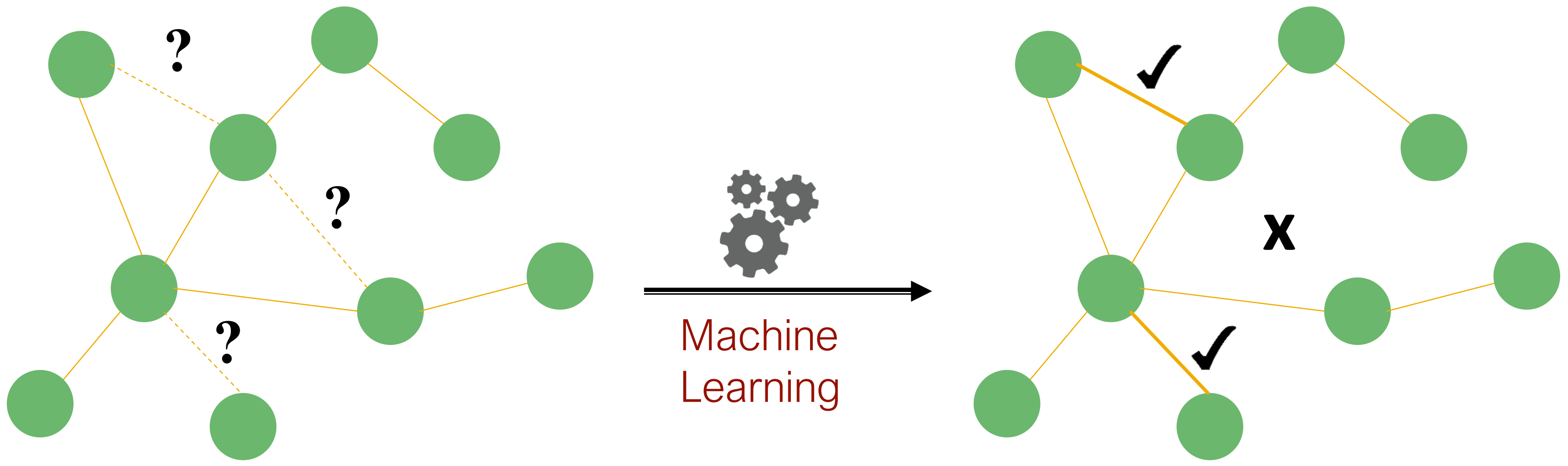
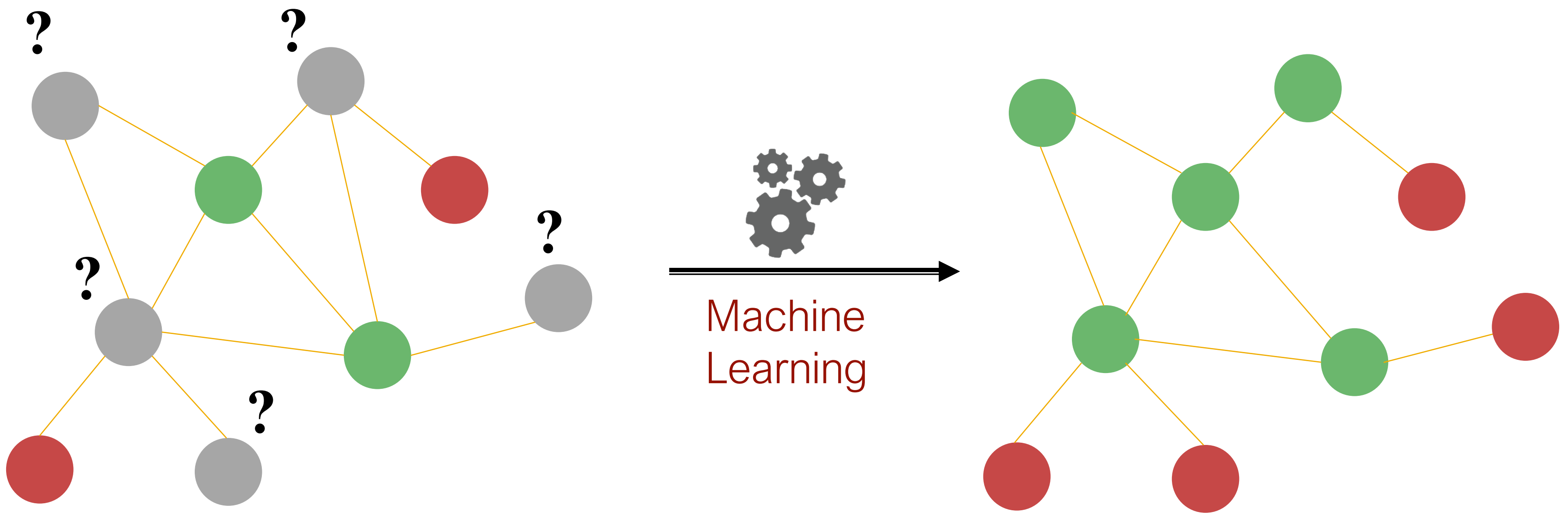
Example: Link Prediction



Machine Learning in Networks



Node classification

Example: Node Classification

Classifying the function of proteins in the interactome

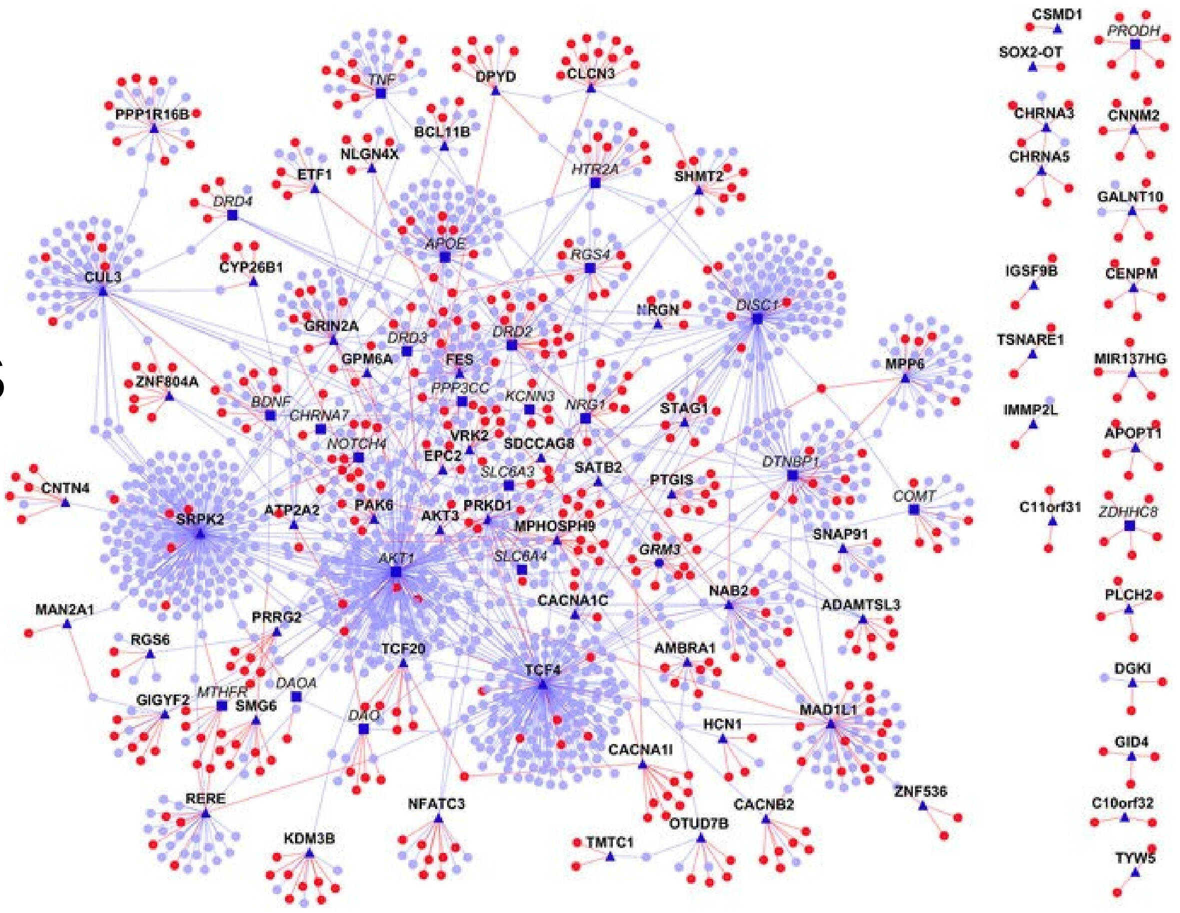
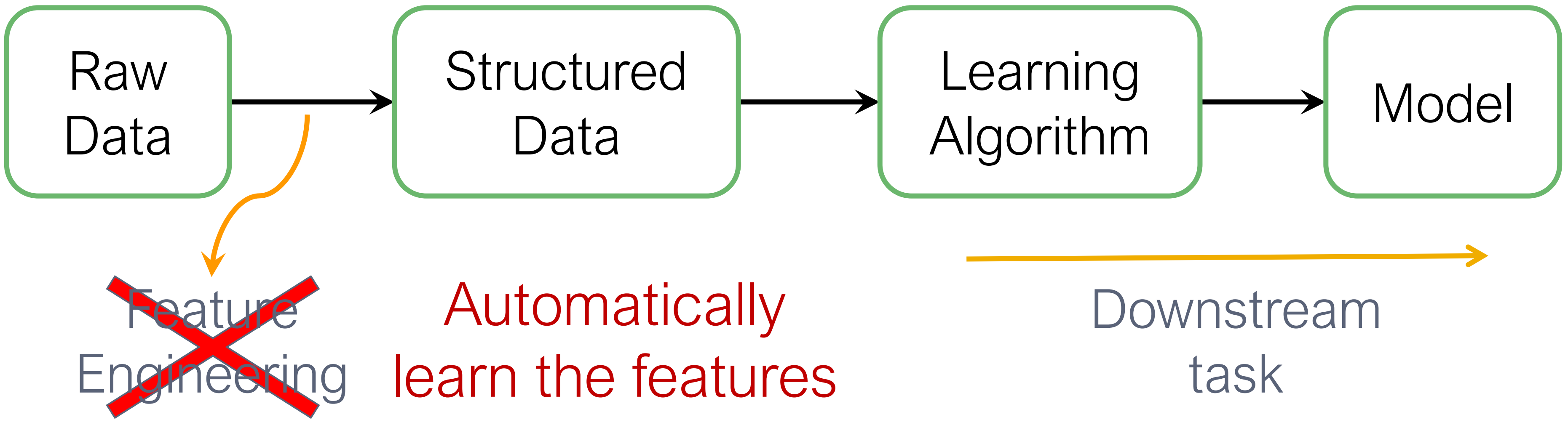


Image from: Ganapathiraju et al. 2016. Schizophrenia interactome with 504 novel protein–protein interactions. *Nature*.

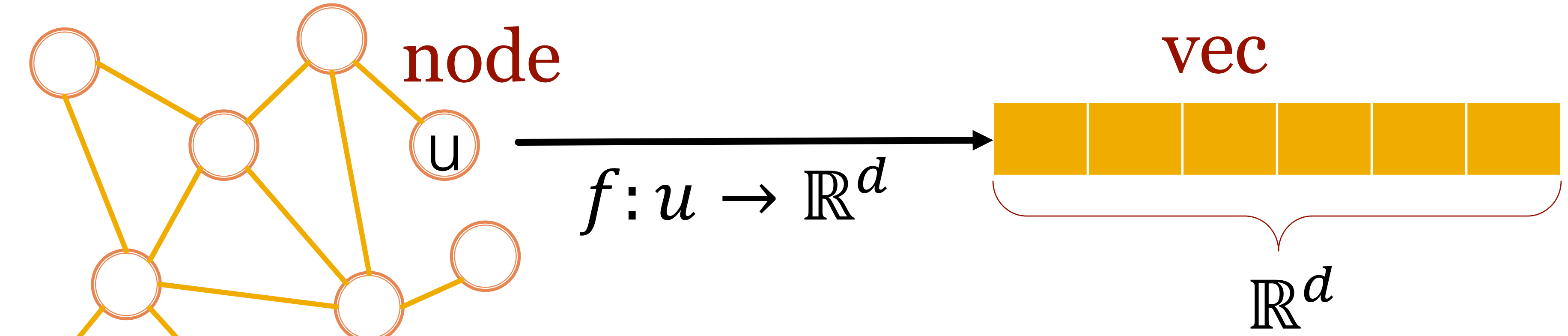
Machine Learning Lifecycle

- **(Supervised) Machine Learning Lifecycle requires feature engineering every single time!**



Feature Learning in Graphs

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

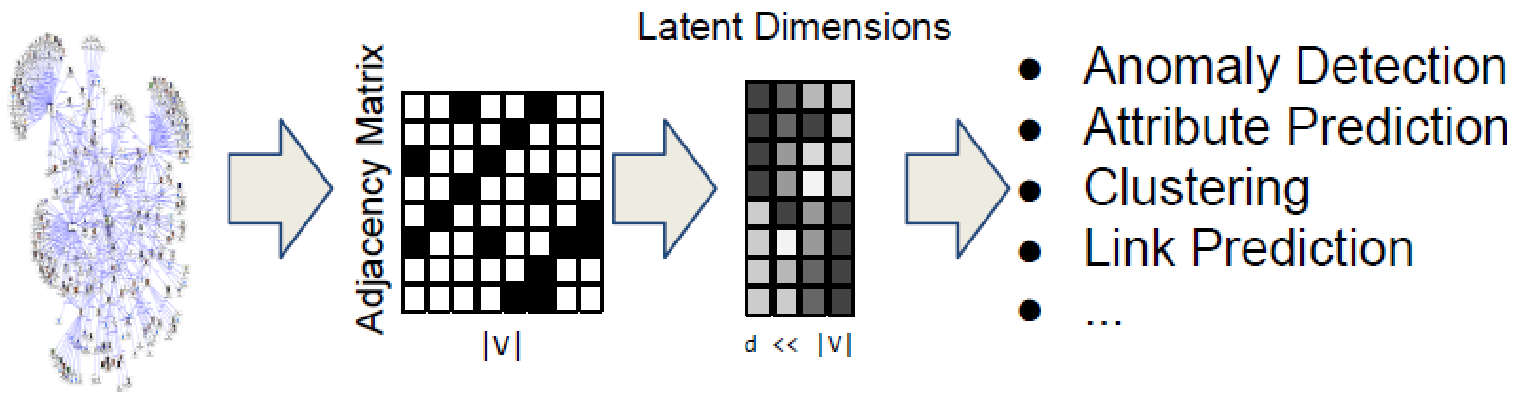


Feature representation, embedding

Why network embedding?

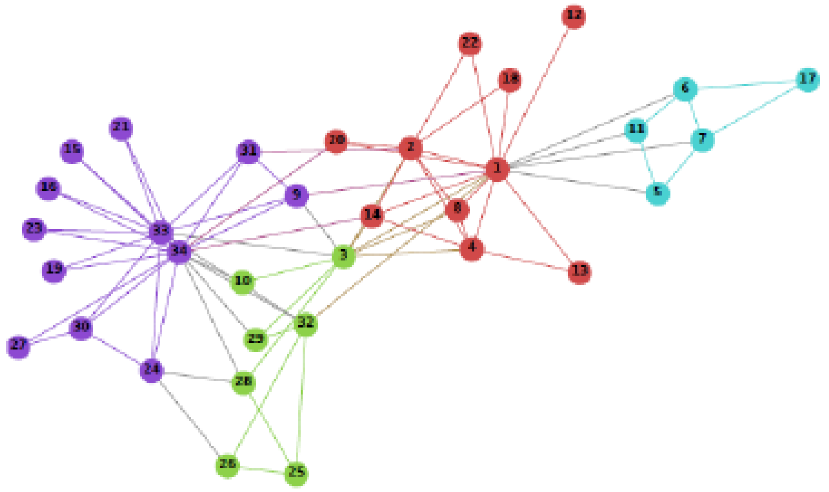
Task: We map each node in a network to a point in a low-dimensional space

- Distributed representation for nodes
- Similarity of embedding between nodes indicates their network similarity
- Encode network information and generate node representation

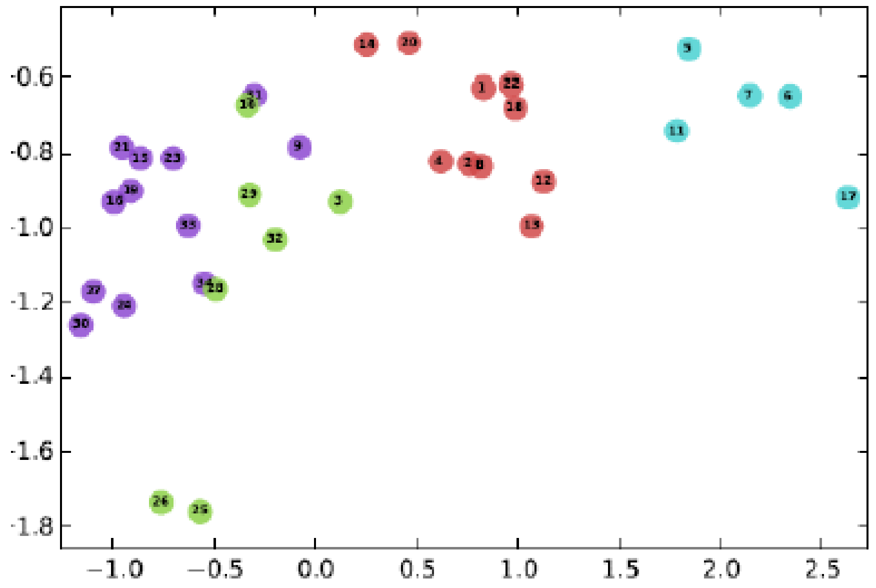


Example Node Embedding

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



Input

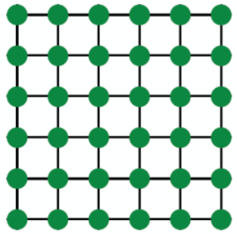


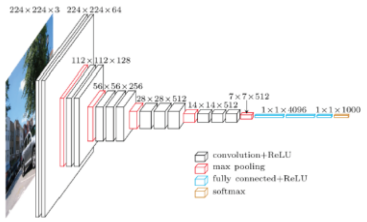
Output

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

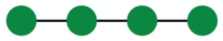
Why Is It Hard?

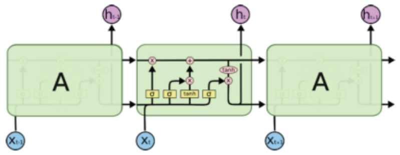
- **Modern deep learning toolbox is designed for simple sequences or grids**
  - CNNs for fixed-size images/grids….





  - RNNs or word2vec for text/sequences…

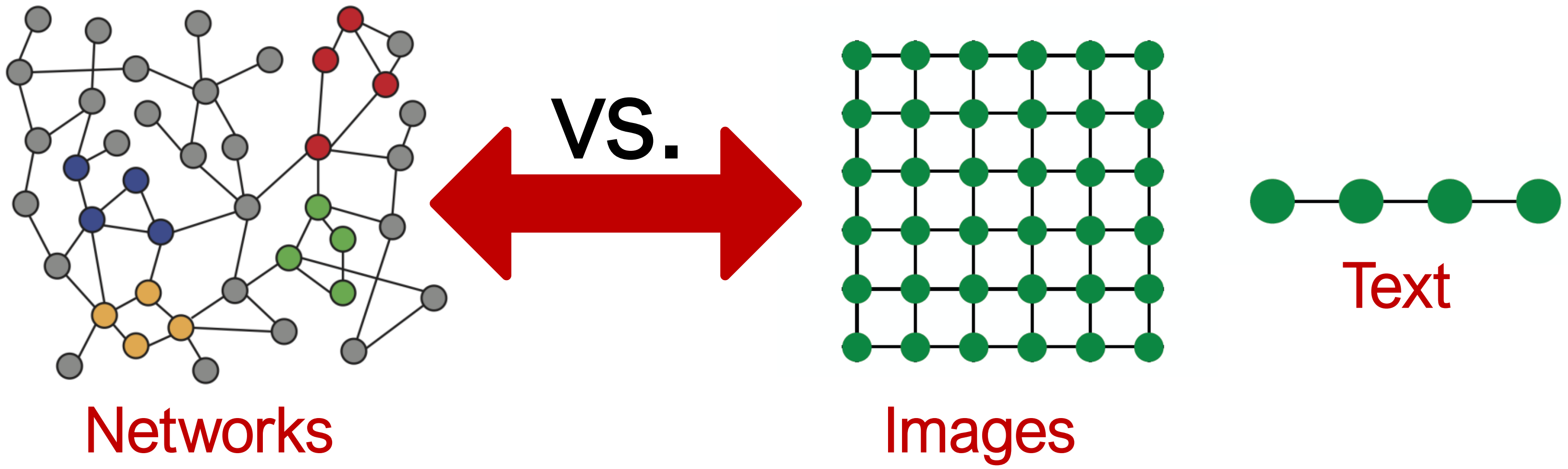




Why Is It Hard?

But networks are far more complex!

- Complex topographical structure (no spatial locality like grids)



- No fixed node ordering or reference point
- Often dynamic and have multimodal features.

Embedding Nodes

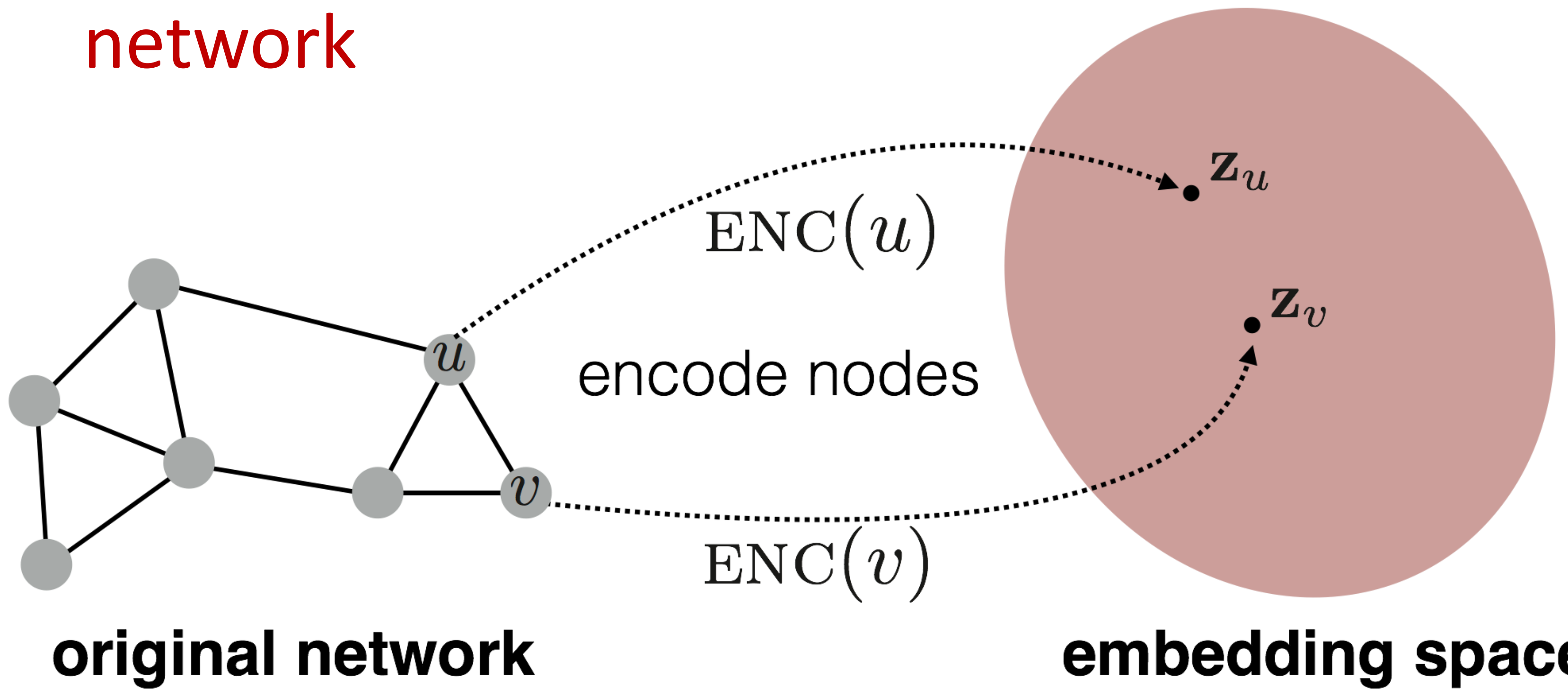
Setup

Assume we have a graph G:

- V is the vertex set
- $\mathbf{A}$ is the adjacency matrix (assume binary)
- **No node features or extra information is used!**

Embedding Nodes

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



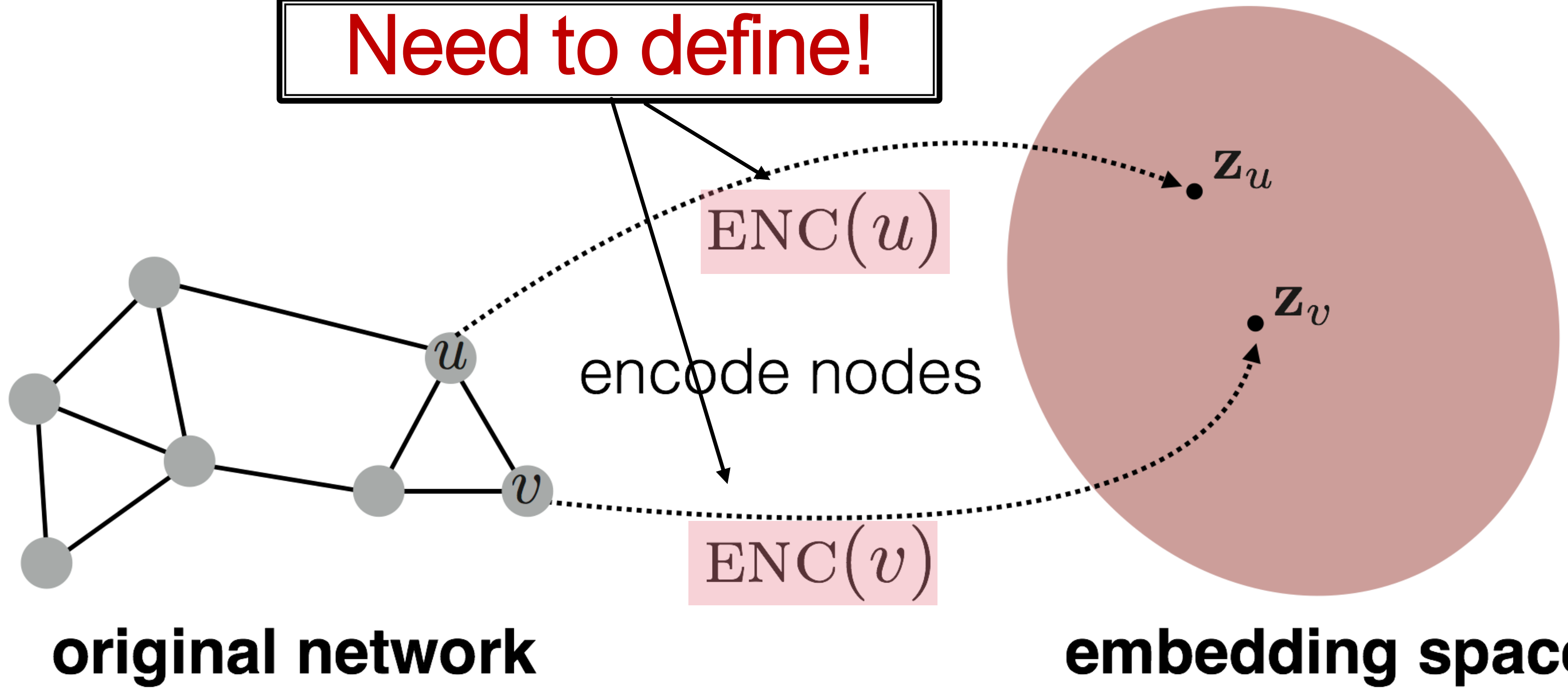
Embedding Nodes

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

in the original network

Similarity of the embedding

Need to define!



Learning Node Embeddings

1. **Define an encoder** (i.e., a mapping from nodes to embeddings)
2. **Define a node similarity function** (i.e., a measure of similarity in the original network)
3. **Optimize the parameters of the encoder so that:**

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

Two Key Components

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

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

d-dimensional embedding

node in the input graph

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

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

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**

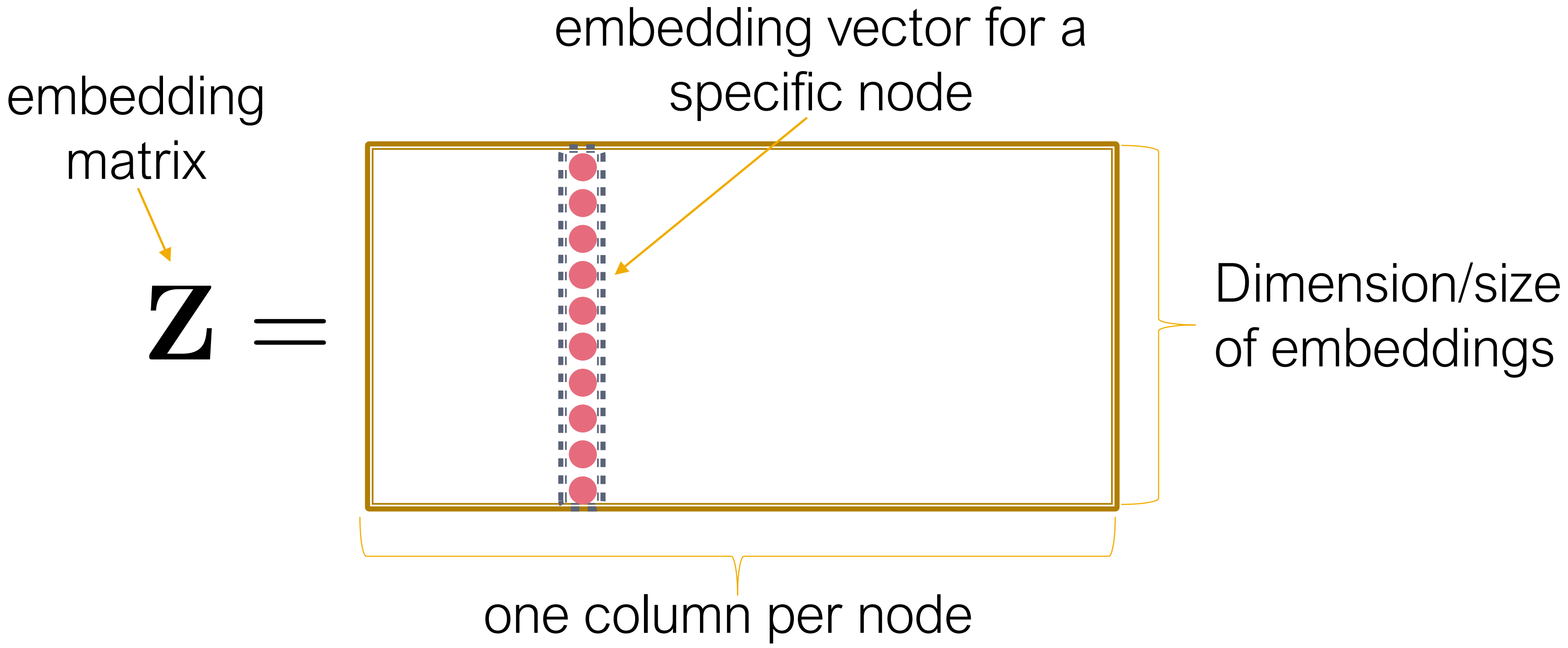
$$\mathrm{ENC}(v) = \mathbf{Z}\mathbf{v}$$

$\mathbf{Z} \in \mathbb{R}^{d \times |\mathcal{V}|}$ Matrix, each column is d-dim node embedding [what we learn!]

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

"Shallow" Encoding

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


embedding matrix
$\mathbf{Z} =$
embedding vector for a specific node
Dimension/size of embeddings
one column per node

“Shallow” Encoding

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

Each node is assigned a unique embedding vector

Many methods: node2vec, DeepWalk, LINE

How to Define Node Similarity?

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

E.g., should two nodes have similar embeddings if they….

- are connected?
- share neighbors?
- have similar "structural roles"?
- …?

Random Walk Approaches to Node Embeddings

Material based on:

- Perozzi et al. 2014. DeepWalk: Online Learning of Social Representations. *KDD.*
- Grover et al. 2016. node2vec: Scalable Feature Learning for Networks. *KDD.*

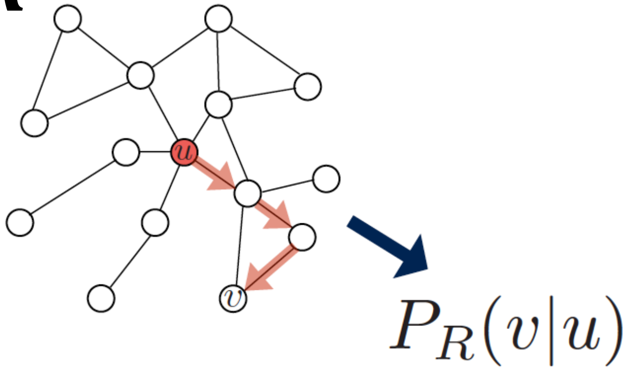
Random-walk Embeddings

$$\mathbf{z}_u^\top \mathbf{z}_v \approx$$ Probability that u and v co-occur on a random walk over the network

z_u … embedding of node u

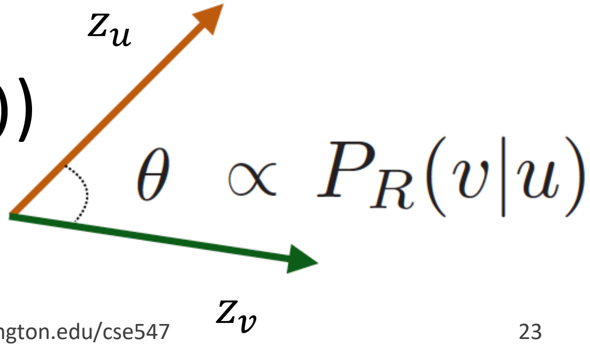
Random-walk Embeddings

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 (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

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 to d-dimensional space so that node similarity is preserved
- **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 strategy R

Feature learning as optimization

- Given $G = (V, E)$
- Our goal is to learn a mapping $z: u \to \mathbb{R}^d$
- Maximize log-likelihood objective:

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

  - where $N_R(u)$ is neighborhood of node u

- Given node u, we want to learn feature representations predictive of nodes in its neighborhood $N_{\mathrm{R}}(u)$

Random Walk Optimization

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

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

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

Random Walk Optimization

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

- **Assumption:** Conditional likelihood factorizes over the set of neighbors:

$$\log \mathrm{P}(N_{\mathrm{R}}(u)|z_u) = \sum_{v \in N_R(u)} \log \mathrm{P}(\mathrm{z}_v \mid z_u)$$

- **Softmax parametrization:**

$$\Pr(\mathrm{z}_v|z_u) = \frac{\exp(z_v \cdot \mathrm{z_u})}{\sum_{\mathrm{n} \in V} \exp(z_n \cdot \mathrm{z_u})}$$

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:

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

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 node embeddings z that minimize L

Random Walk Optimization

But doing this naively is too expensive!!

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

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

Random Walk Optimization

But doing this naively is too expensive!!

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

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

Negative Sampling

- **Solution:** Negative sampling

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

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

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

random distribution over all nodes

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 and https://arxiv.org/pdf/1410.8251.pdf

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

Negative Sampling

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

$$\approx \log(\sigma(\mathbf{z}_u^\top \mathbf{z}_v)) - \sum_{i=1}^{k} \log(\sigma(\mathbf{z}_u^\top \mathbf{z}_{n_i})), n_i \sim \underset{\text{random distribution over all nodes}}{P_V}$$

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

  In practice k =5-20

Random Walks: Stepping Back

1. Run **short fixed-length** random walks starting from each node on the graph using some strategy R.
2. For each node u collect $\mathrm{N}_R(u)$, 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 random walk statistics
- **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?

Overview of node2vec

- **Goal:** Embed nodes with similar network neighborhoods close in the feature space

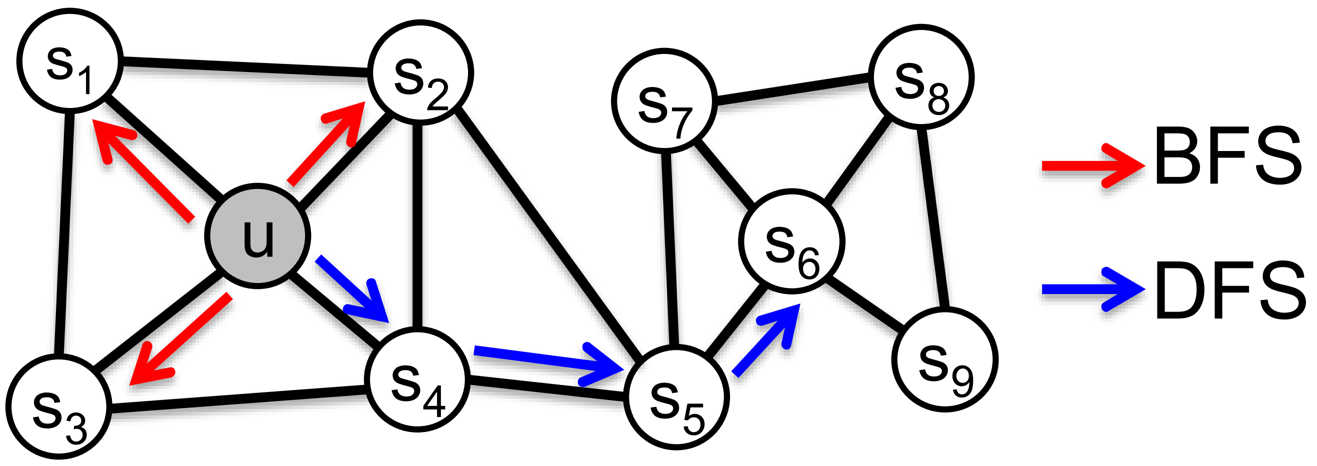
- We frame this goal as prediction-task independent maximum likelihood optimization problem

- **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

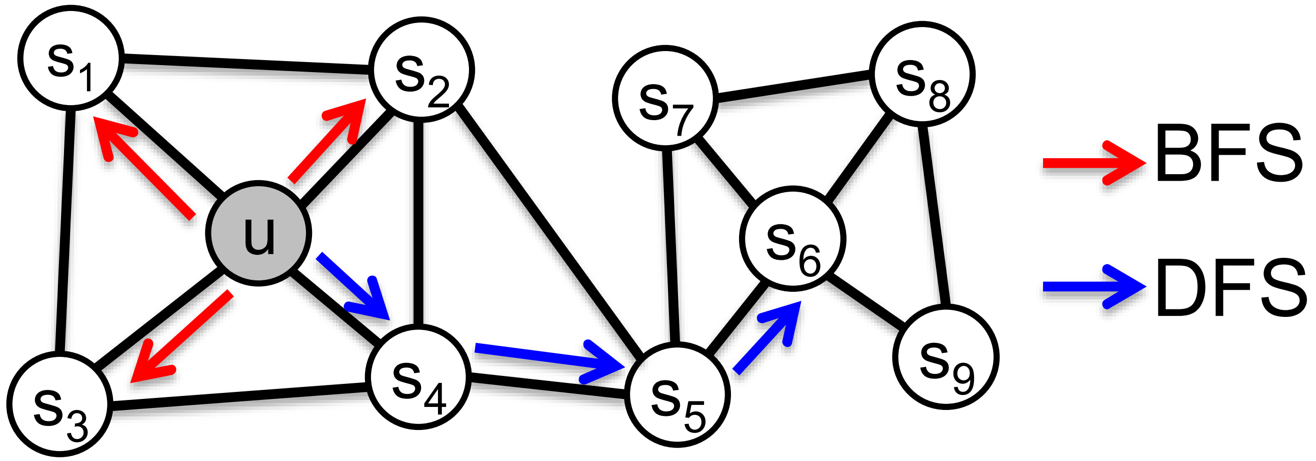
node2vec: Biased Walks

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

Interpolating BFS and DFS

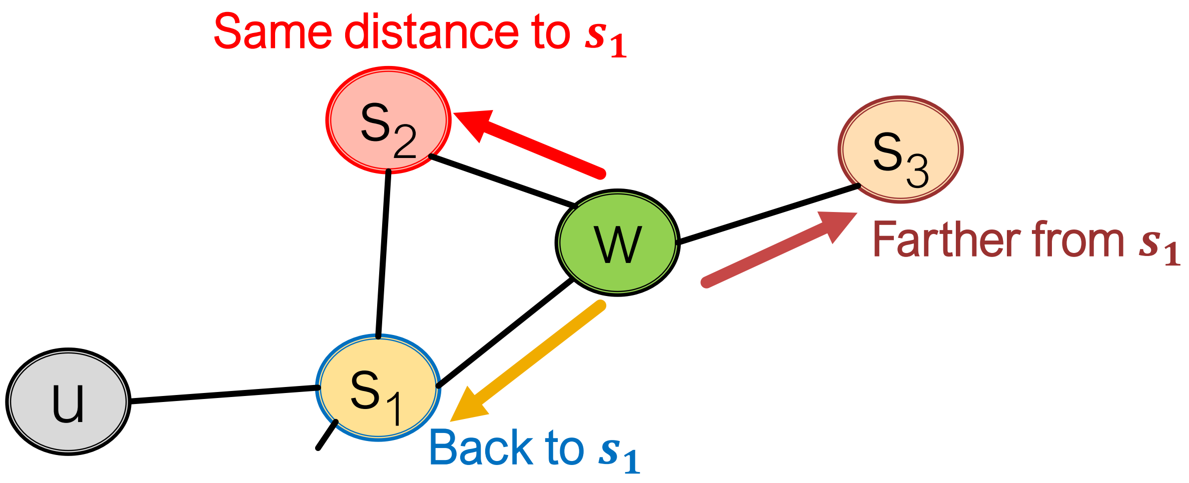
Biased fixed-length random walk R that given a node u generates neighborhood $N_R(u)$

- 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:

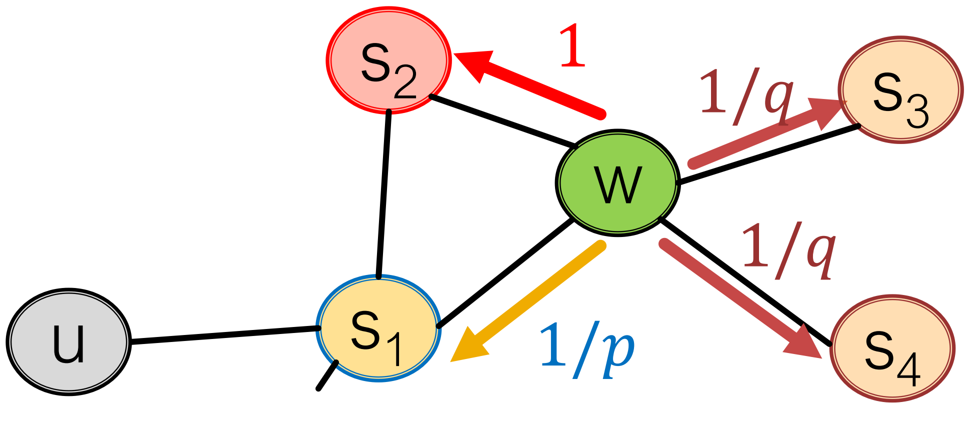
- Rnd. walk just traversed edge (s_1, w) and is now at w
- **Insight:** Neighbors of w can only be:



Idea: Remember where that walk came from

Biased Random Walks

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

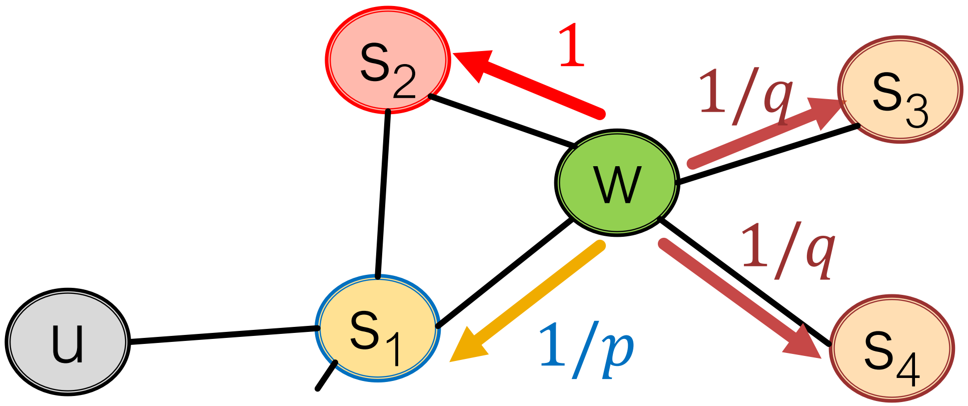


$1/p, 1/q, 1$ are "unnormalized" probabilities (weights we later convert to probability distribution)

- 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

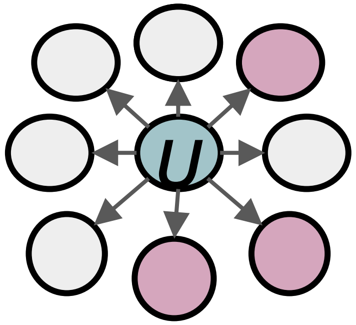
$N_R(u)$ are the nodes visited by the biased walk

node2vec algorithm

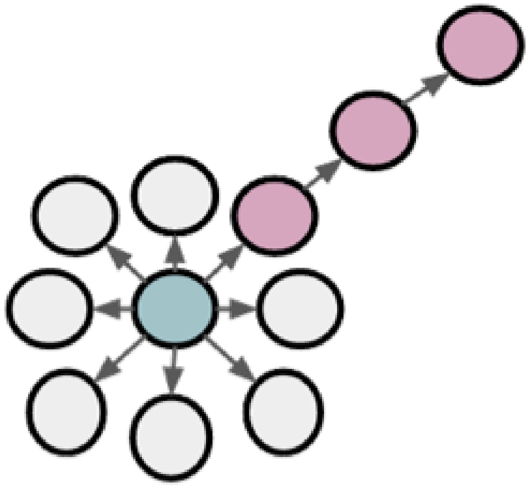
- 1) Compute random walk probabilities
- 2) Simulate r random walks of length l starting from each node u
- 3) Optimize the node2vec objective using Stochastic Gradient Descent

Linear-time complexity.
All 3 steps are individually parallelizable

BFS vs. DFS



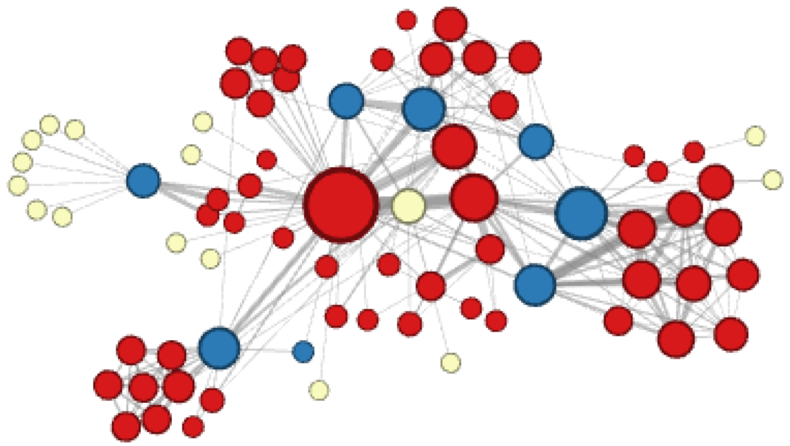
BFS:
Micro-view of neighbourhood



DFS:
Macro-view of neighbourhood

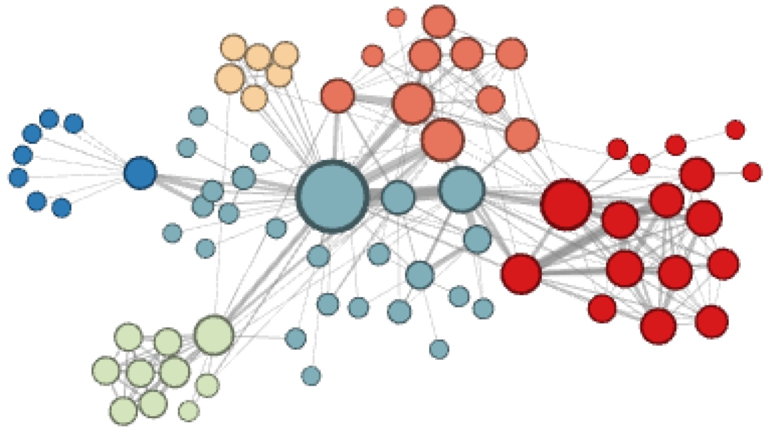
Experiments: Micro vs. Macro

Small network of interactions of characters in a novel:



p=1, q=2

Microscopic view of the network neighbourhood



p=1, q=0.5

Macroscopic view of the network neighbourhood

Other random walk ideas

(not covered in detailed here but for your reference)

- **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).

How to Use Embeddings

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

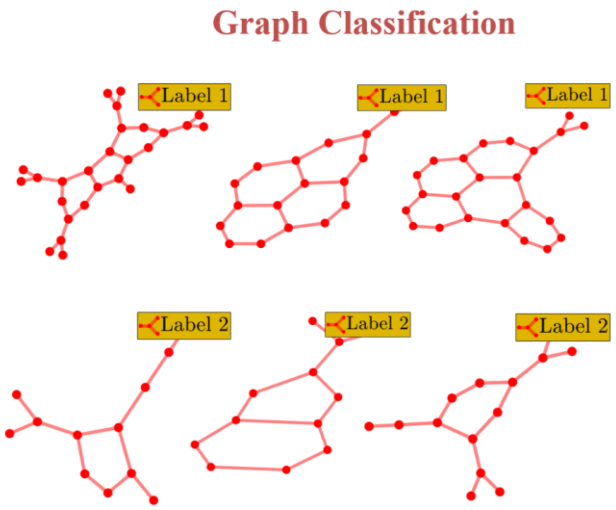
Summary so far

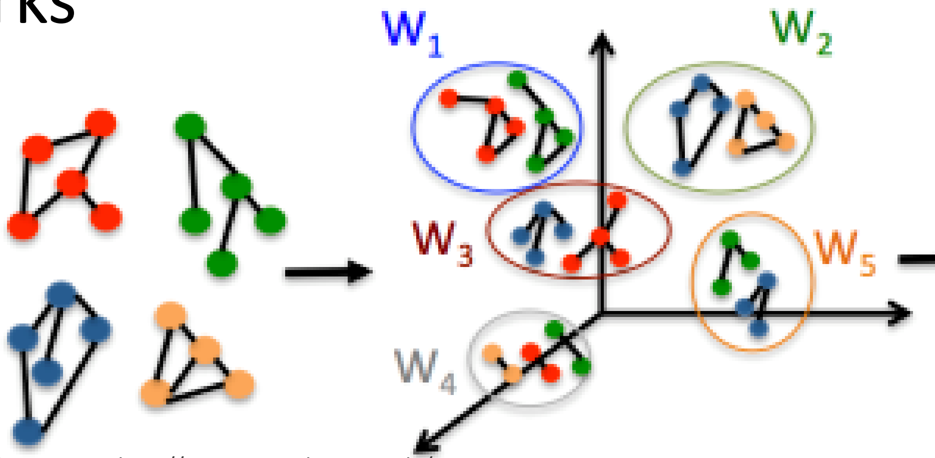
- **So what method should I use..?**
- No one method wins in all cases....
  - E.g., node2vec performs better on node classification while multi-hop methods performs better on link prediction (Goyal and Ferrara, 2017 survey)
- Random walk approaches are generally more efficient
- **In general:** Must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

Embedding Entire Graphs

Graph Classification

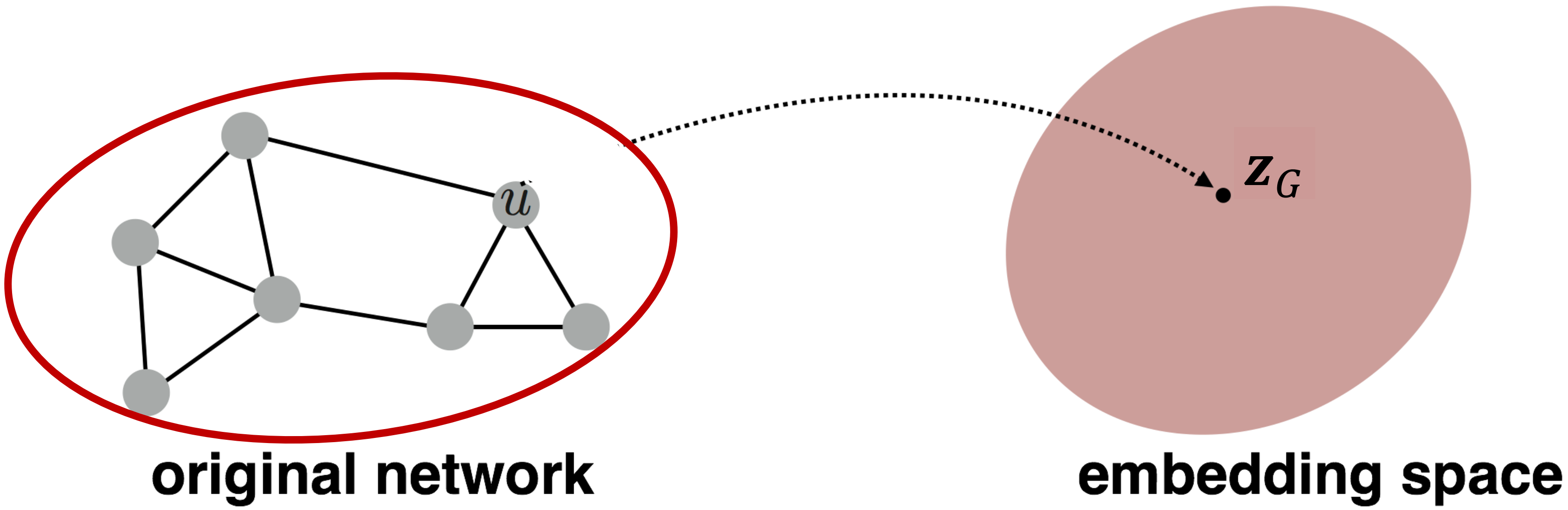
- **Tasks:**
  - Classifying toxic vs. non-toxic molecules
  - Identifying cancerogenic molecules
  - Graph anomaly detection
  - Classifying social networks





Embedding Entire Graphs

- **Goal:** Want to embed an entire graph G



Approach 1

Simple idea:

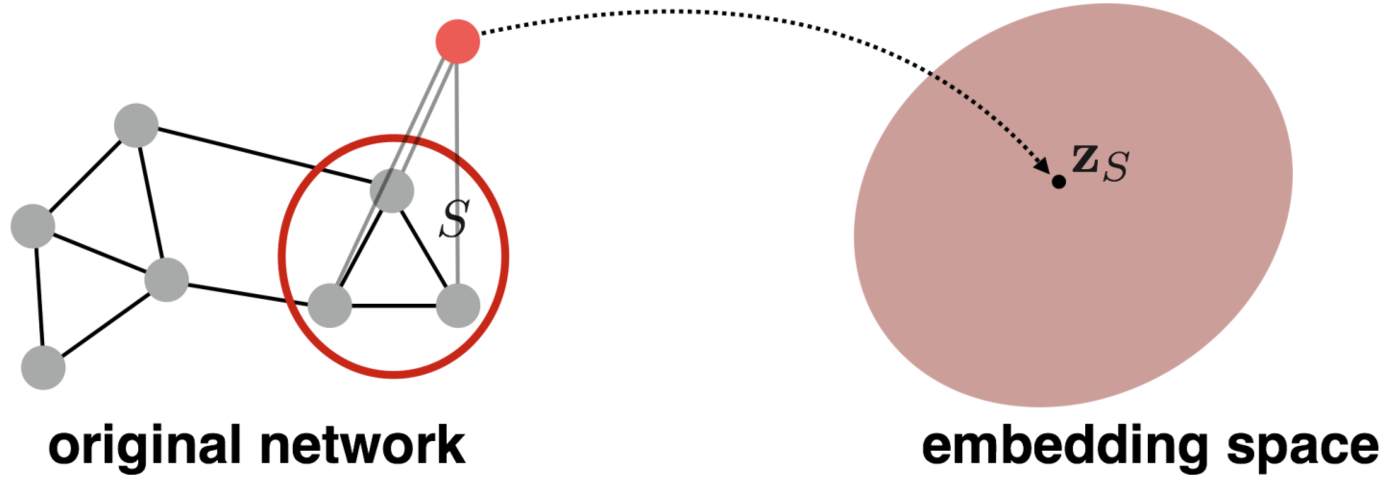
- Run a standard node embedding technique *on* the (sub)graph G
- Then just sum (or average) the node embeddings in the (sub)graph G

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

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

Approach 2

- **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