# Graph Representation Learning

CS246: Mining Massive Datasets
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# Announcements

- Regrade requests for homework 1 are due tonight
- Colab 6 out today
- Colab 5 due today

# ML as Optimization

- Machine learning is about *Optimization*
- Three key components:
  1. Training Data $\mathrm{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  2. Model $\boldsymbol{f_\theta(x)}$
  3. Loss function $\boldsymbol{\mathcal{L}}$
- Optimize $\boldsymbol{f_\theta(x)}$ on $D$ w.r.t loss function $\boldsymbol{\mathcal{L}}$:
  - find the parameter $\theta$ that minimizes the expected loss on the training data

$$\min_f J(f) = \min_f \frac{1}{\mathrm{n}} \sum_{i=1}^{\mathrm{n}} \mathcal{L}(f_\theta(x_i), y_i)$$

# Two Dominant ML Paradigms

- **Supervised learning**:
  - Given "labeled data" $\{x, y\}$, learn $f(x) = y$
  - Ex: classification, regression
    - In linear regression, the model $f_\theta(x) = Wx + b$
    - Parameters are $\theta = \{W, b\}$
    - The loss function is mean square error (MSE)

- **Unsupervised learning**:
  - Given only "unlabeled data" $\{x\}$, learn $f(x)$
  - Ex: Dimensionality reduction, clustering
    - In SVD, the model is $f(x) = \hat{x} = V^T x$ where $V$ are the right singular vectors of input matrix.
    - The loss function is L2 loss: $L(x, \hat{x}) = \sum \|x - \hat{x}\|^2$

# Input Feature Vectors

- All ML methods work with the input feature vectors $\{x_1, x_2, \ldots, x_n\}$ and almost all of them require input features to be numerical

- From ML perspective, there are four types of features:
  - **Numerical** (continues or discrete)
    - Continues: height
    - Discrete: age
  - **Categorical** (ordinal or nominal)
    - Ordinal: level={beginner, intermediate, advanced}
    - Nominal: gender={male, female}, color={red, blue, green}
  - **Time series:**
    - Average of home sale price over years
  - **Text:**
    - Bag of words

# Categorical Features

- There are two ways to encode categorical var:
  - Integer encoding
  - One-hot encoding (and multi-hot encoding)
- Consider the following movie dataset:

| Title | provider | IMDB genres | Release year | IMDB rating |
|---|---|---|---|---|
| Stranger Things | Netflix | drama, fantasy, horror | 2016 | 8.7 |
| Cocomelon | Prime Video | animation, comedy, family | 2019 | 4.7 |
| 100 Foot Waves | HBO Max | documentary, sport | 2021 | 8.1 |
| I, Tonya | Hulu | biography, drama, comedy | 2017 | 7.5 |

# Integer Encoding

- Assigns each category value with an integer
  - *provider :=[Netflix, Prime Video, HBO Max, Hulu],* we assign them integers 1, 2, 3 and 4 respectively.

- Pros: dense representation
- Cons: It implies ordering between different categories:
  *Netflix < Prime Video < HBO Max < Hulu*

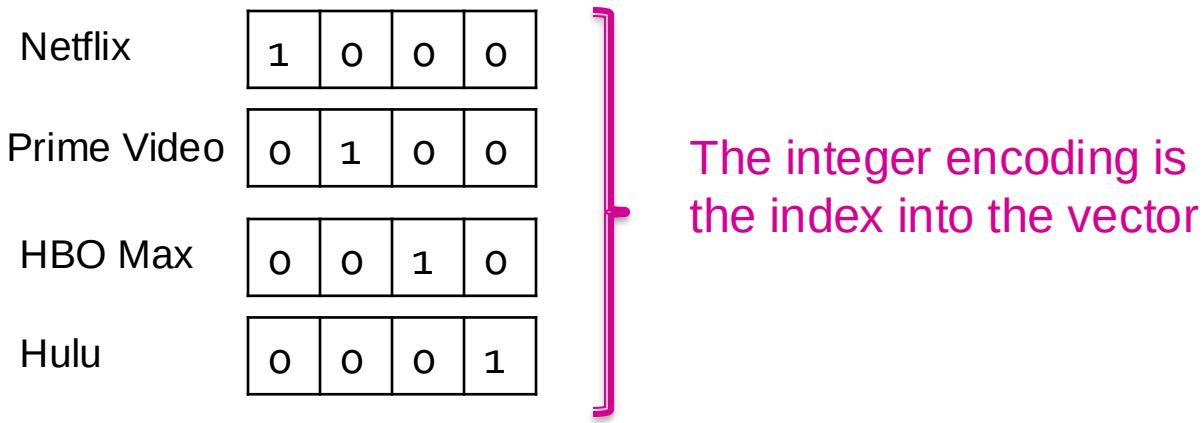
| Title | provider | IMDB genres | Release year | IMDB rating |
|---|---|---|---|---|
| Stranger Things | 1 | drama, fantasy, horror | 2016 | 8.7 |
| Cocomelon | 2 | animation, comedy, family | 2019 | 4.7 |
| 100 Foot Waves | 3 | documentary, sport | 2021 | 8.1 |
| I, Tonya | 4 | biography, drama, comedy | 2017 | 7.5 |

- Makes more sense to use it for ordinal variables:
  - Such as "Education"= {Diploma, Undergrad, Masters, Phd }
  - But still it implies values are equally spaced out

# One-hot Encoding

- First do integer encoding, then create a binary vector that represents the numerical values
  - Ex: following integer encoding on provider:

    Netflix -> 1, Prime Video -> 2, HBO Max ->3 , Hulu -> 4
  - Create a binary vector of length 4 for each value:



# Multi-hot Encoding

- An extension of one-hot encoding when categorical variable can take multiple values at the same time
  - Ex: There are 28 distinct IMDB genres

a movie can take multiple genres, e.g. *stranger things is drama, fantasy, horror.*

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Stranger things | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Cocomelon | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 100 foot wave | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| I, Tonya | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**IMDB genres**

```
[(1, 'Action'),
 (2, 'Comedy'),
 (3, 'Short'),
 (4, 'Western'),
 (5, 'Drama'),
 (6, 'Horror'),
 (7, 'Music'),
 (8, 'Thriller'),
 (9, 'Animation'),
 (10, 'Adventure'),
 (11, 'Family'),
 (12, 'Fantasy'),
 (13, 'Sport'),
 (14, 'Romance'),
 (15, 'Crime'),
 (16, 'Sci-Fi'),
 (17, 'Biography'),
 (18, 'Musical'),
 (19, 'Mystery'),
 (20, 'History'),
 (21, 'Documentary'),
 (22, 'Film-Noir'),
 (23, 'News'),
 (24, 'Game-Show'),
 (25, 'Reality-TV'),
 (26, 'War'),
 (27, 'Talk-Show'),
 (28, 'Adult')]
```

# Applying encodings on Movies dataset

| | provider | | | | IMDB genres | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Stranger things | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2016 | 8.7 |
| cocomelon | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2019 | 4.7 |
| 100 foot waves | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2021 | 8.1 |
| I, Tonya | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2017 | 7.5 |

- Data dimensions increased from 4 to 34. It will blow up to thousands or a million if we multi-hot encode title!

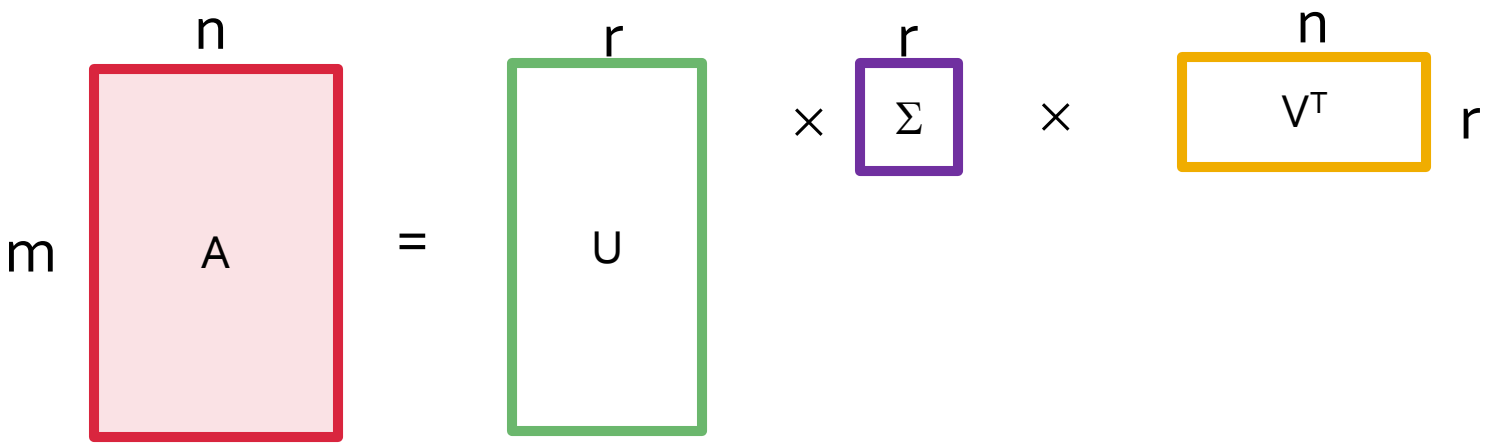
- One-hot and multi-hot encodings are not practical for features with large value sets.

# From Encodings to Embeddings

- **One-hot/multi-hot encodings:**
  - **Pros**: Simple, robust, when trained on huge amounts of data they outperform complex systems trained on fewer data
  - **Cons**: Sparse and high dimensional, don't capture semantic similarity
- **In a corpus of documents with one million distinct words:**
  - High dimensional: Multi-hot encodings are 1-million dimensional
  - Sparse: An average document contains 500 words therefore the multi-hot encodings are > 99.95% sparse
  - Lack of semantics: Encoding of two words 'good' and 'great' are as different as encoding of 'good' and 'bad'!
- **An embedding is a translation of a high-dim vector into a low-dim space.** An embedding is a:
  - Dense representation (floating-point value)
  - Low-dimensional vector
  - Captures semantic similarity

# SVD as an Embedder

- Standard dimensionality Reduction methods
  - Singular value decompositions (SVD)




- **A**: **Input data matrix:** *m* x *n* matrix (e.g., *m* documents, *n* terms)
  (*r* : rank of the matrix **A** – often r < min(m,n) )
- **U**: **Left singular vectors:** *m* x *r* matrix (*m* documents, *r* concepts)
- **Σ**: **Singular values:** *r* x *r* diagonal matrix (strength of each 'concept')
- **V**: **Right singular vectors:** *n* x *r* matrix (*n* terms, *r* concepts)

# SVD as an Embedder

- ***U, V***: Column orthonormal
  - $U^T U = I$; $V^T V = I$ (***I***: identity matrix)
  - Columns are orthogonal unit vectors hence they define an r-dimensional subspace
    - ***U*** defines an r-dim subspace in $R^m$
    - ***V*** defines an r-dim subspace in $R^n$

- Projecting ***A*** onto ***V*** and ***U*** produces embeddings:
  - **Since $A = U \Sigma V^T$ then $AV = U \Sigma$ are row embeddings**
  - **Since $A = U \Sigma V^T$ then $U^T A = \Sigma V^T$ are col embeddings**

# SVD as an Embedder

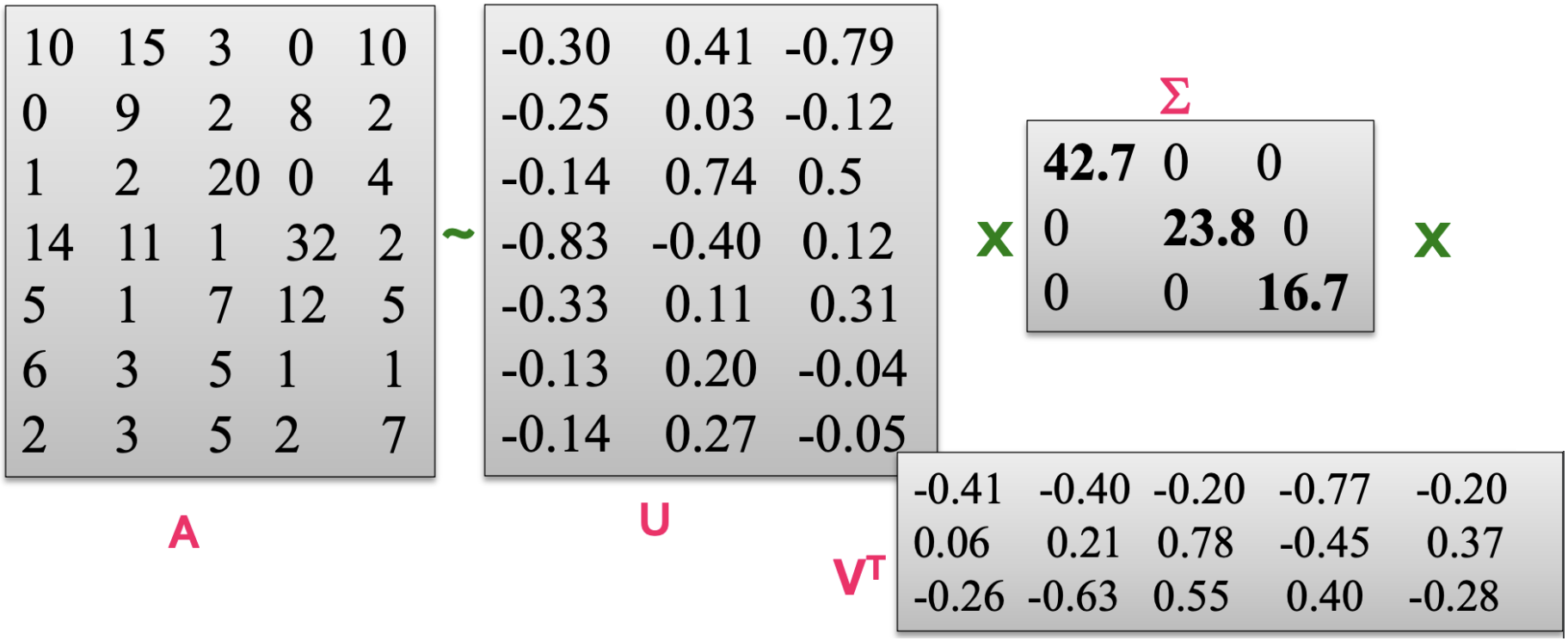
Ex: Compute document & word embeddings

Step 1: Given a corpus of documents convert it to BOW vectors ⇨ get a term-document matrix

| | data | science | spark | Stanford | learning |
|---|---|---|---|---|---|
| document 1 | 10 | 15 | 3 | 0 | 10 |
| document 2 | 0 | 9 | 2 | 8 | 2 |
| document 3 | 1 | 2 | 20 | 0 | 4 |
| document 4 | 14 | 11 | 1 | 32 | 2 |
| document 5 | 5 | 1 | 7 | 12 | 5 |
| document 6 | 6 | 3 | 5 | 1 | 1 |
| document 7 | 2 | 3 | 5 | 2 | 7 |

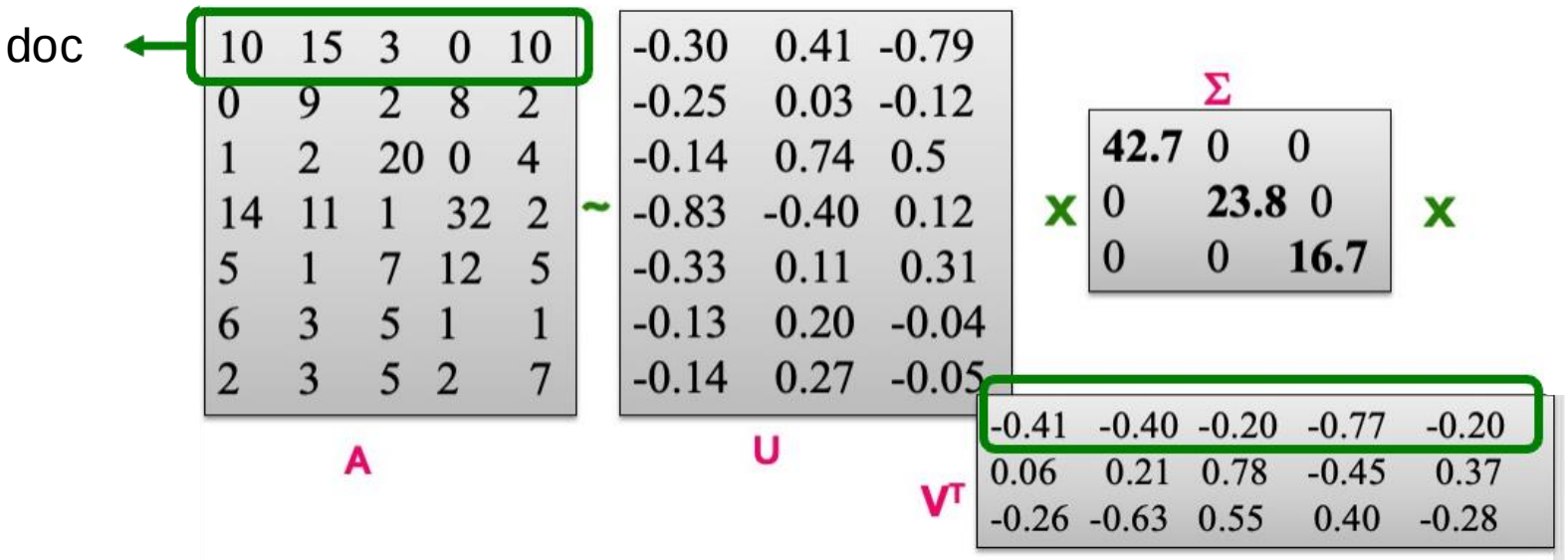
# SVD as an embedder

Step 2: apply SVD on the term-document matrix and pick a value $r \leq rank(A)$



# SVD as an embedder

Step 3: compute embedding of documents as
emb = [<doc, v1> , <doc, v2> , <doc, v3>]




- <doc, v1> = <[10,15,3,0,10] , v1>= -12.7
- <doc, v2> = <[10,15,3,0,10] , v2> = 9.79
- <doc, v3> = <[10,15,3,0,10] , v3>= -13.9

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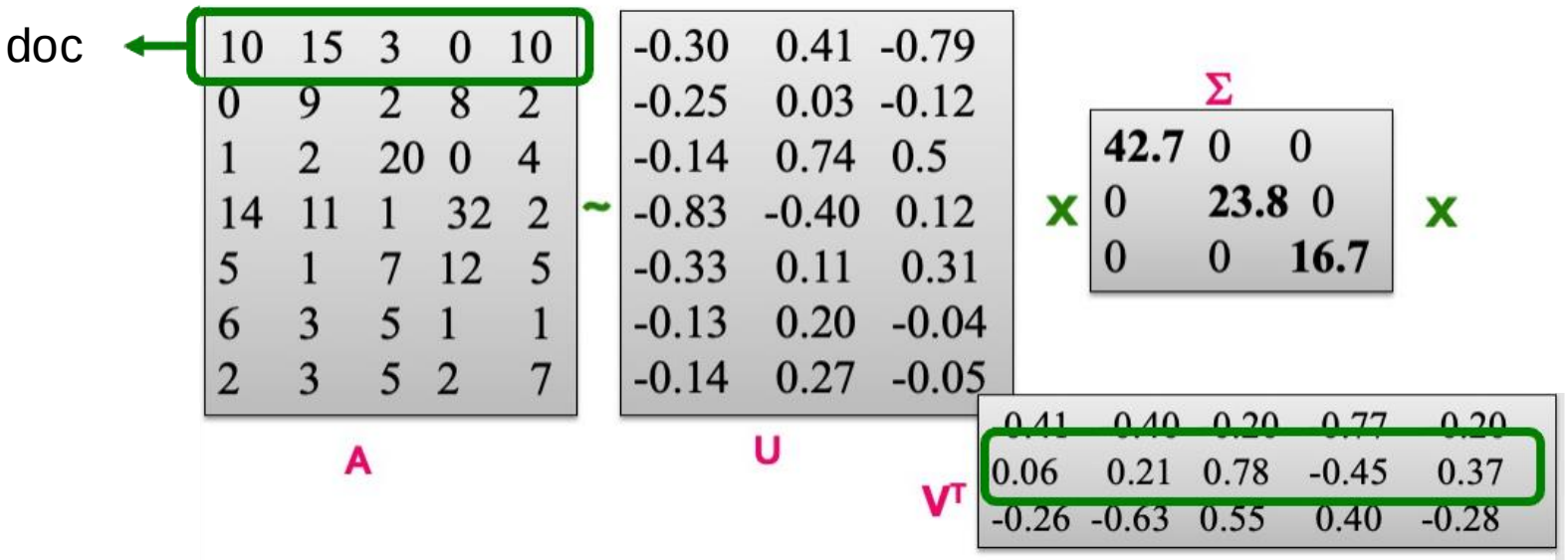


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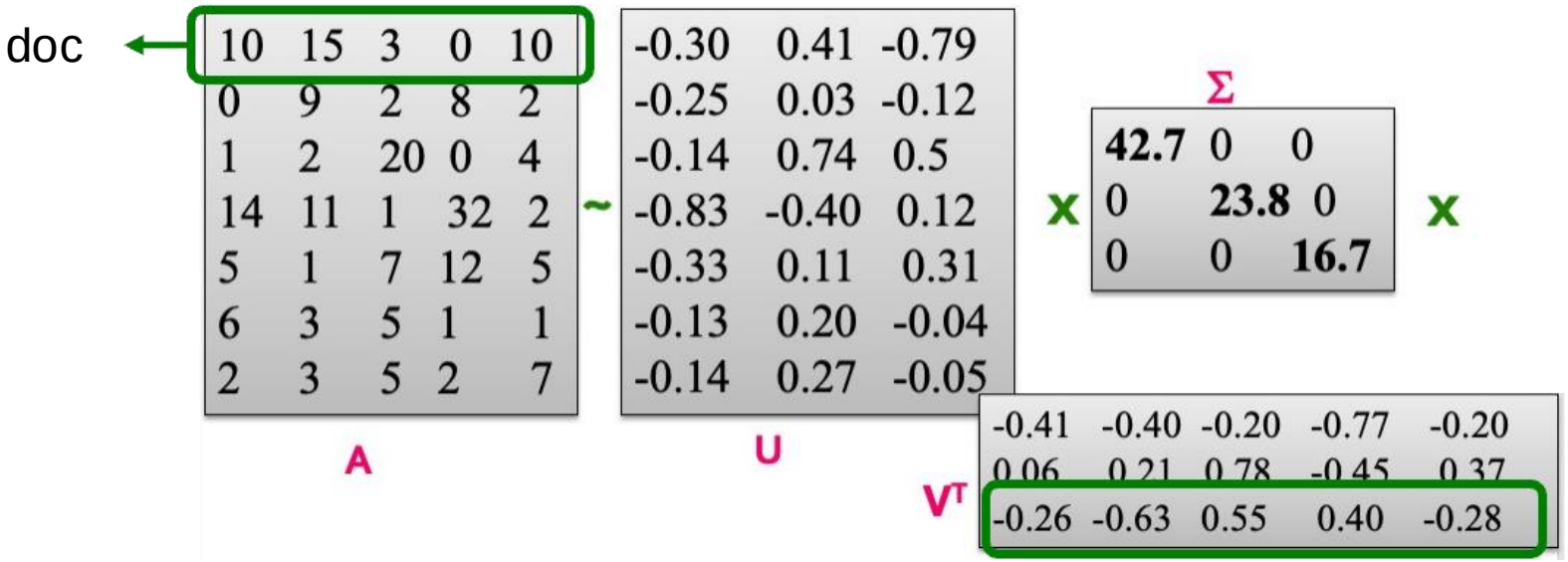


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# SVD as an embedder

SVD is impractical on many real-world datasets:

- For example, there are 0.5 billion wiki pages, and 4 billion words.
- SVD is computationally prohibitive, as it requires to load all data in memory
- SVD is a linear embedder
- SVD is not utilizing data sparsity
- Orthonormality constraint is an overkill

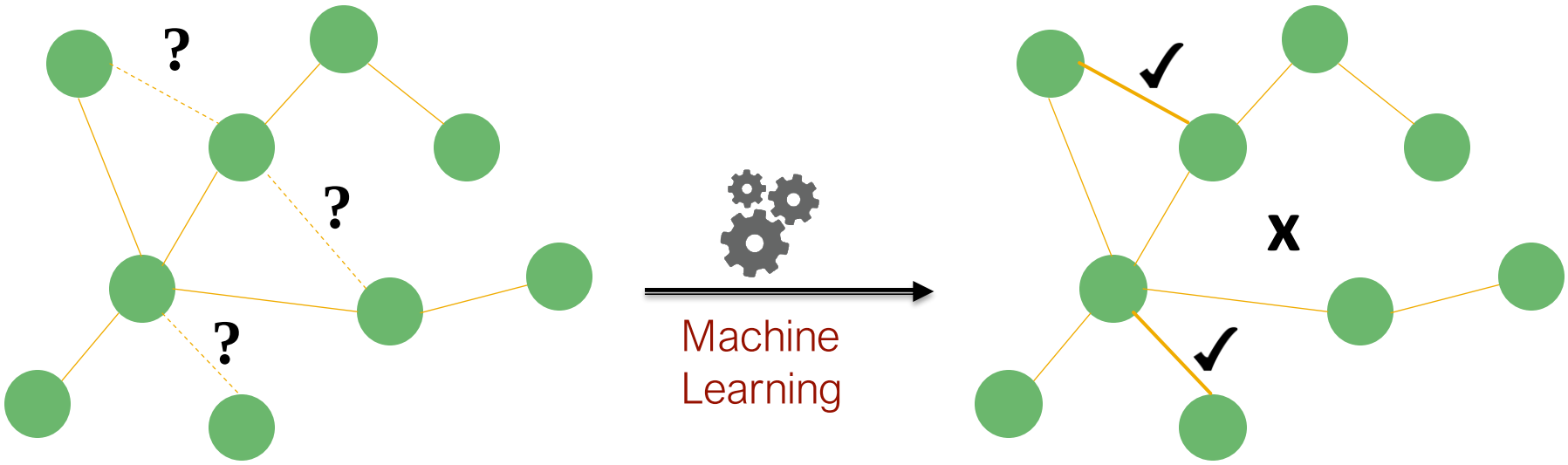
# SVD to Neural Networks

- State of the art embedders are among neural networks

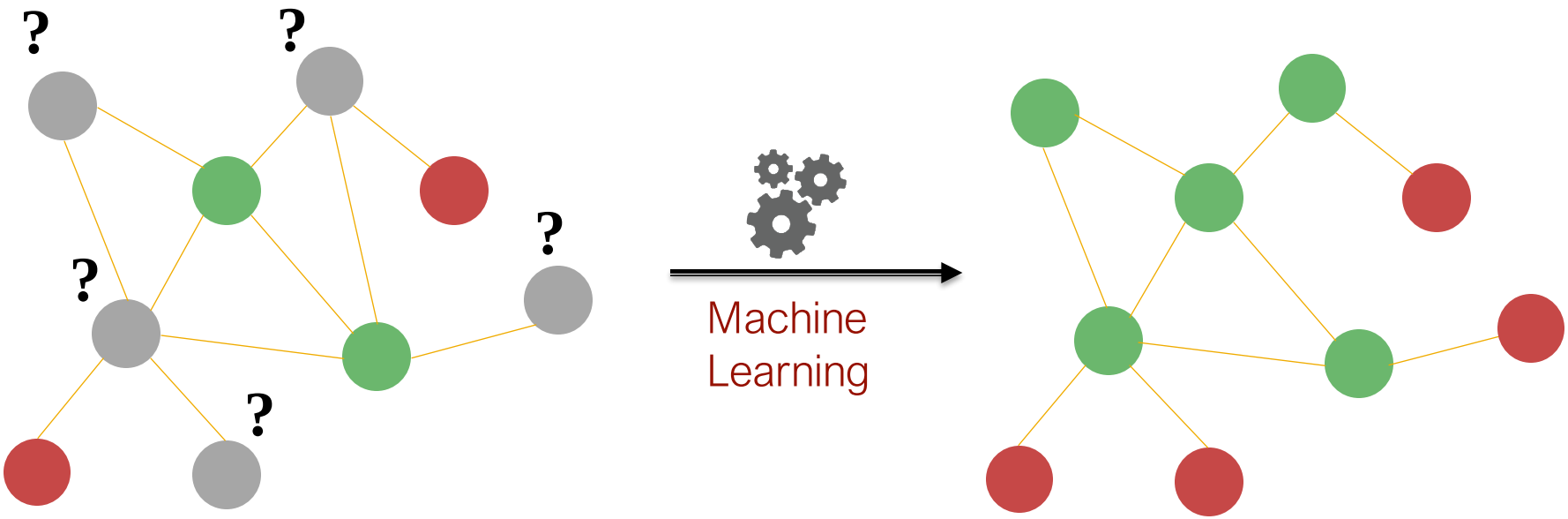
- Can we use neural networks to create non-linear embedding?

# Embedding for Graphs

# Example: Link Prediction



# Machine Learning in Networks




Node classification

# Example: Node Classification

Classifying the function of proteins in the interactome

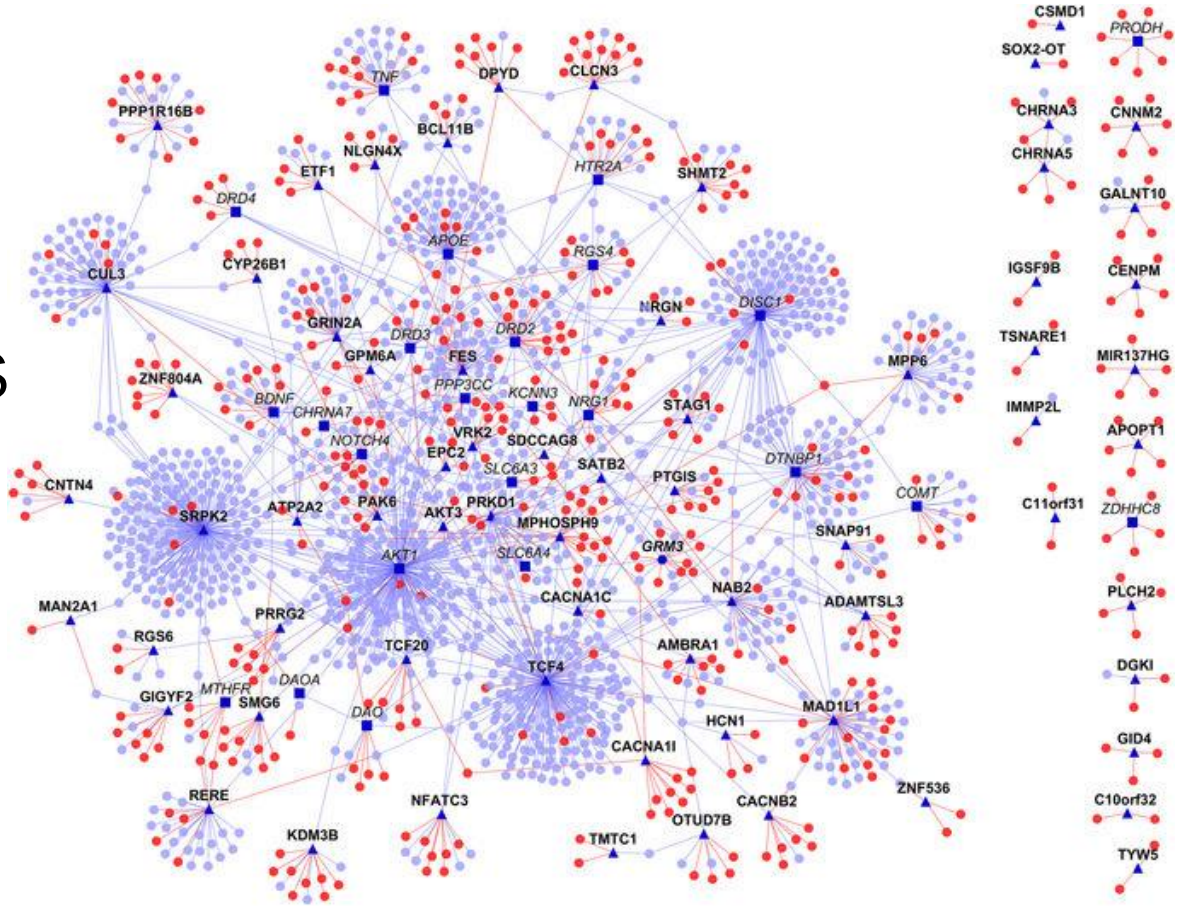
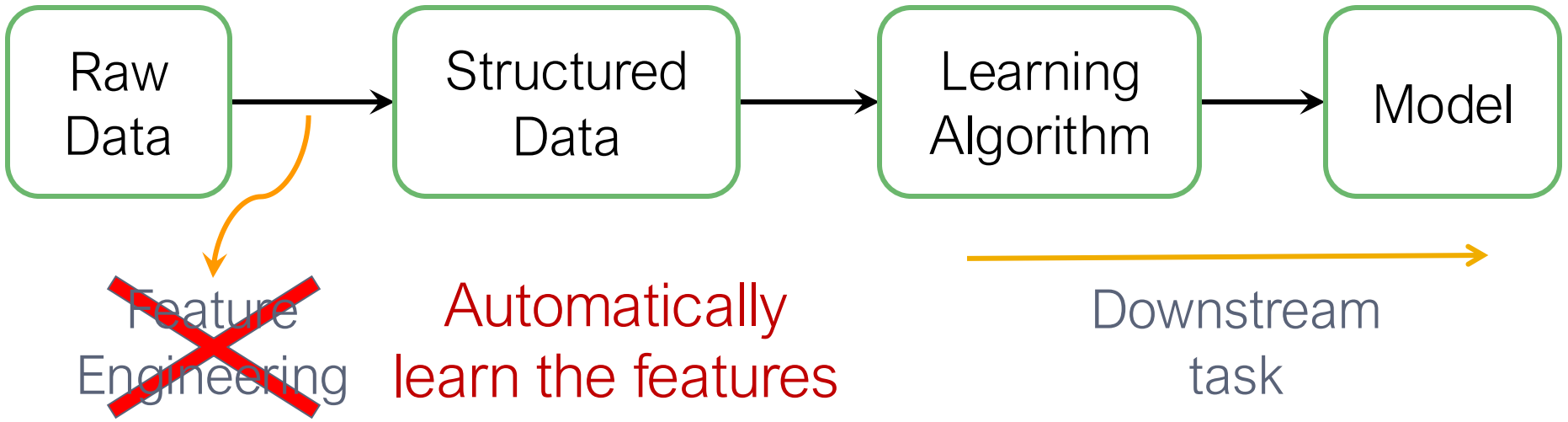



Image from: Ganapathiraju et al. 2016. Schizophrenia interactome with 504 novel protein–protein interactions. *Nature*.

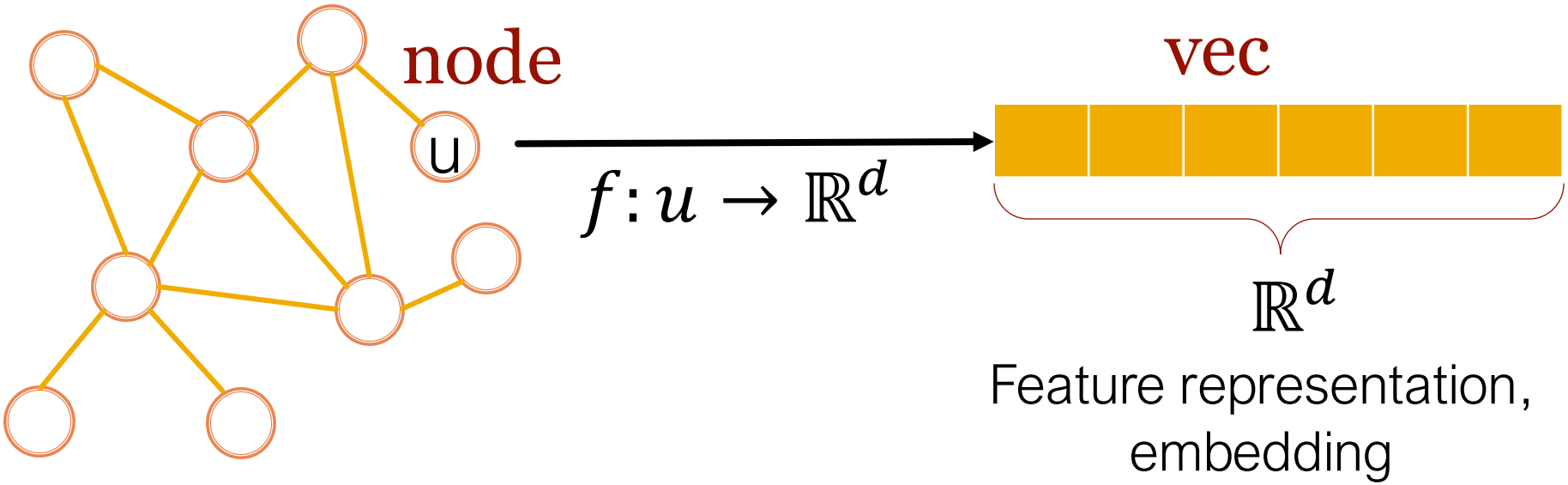
# Machine Learning Lifecycle

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



# Feature Learning in Graphs

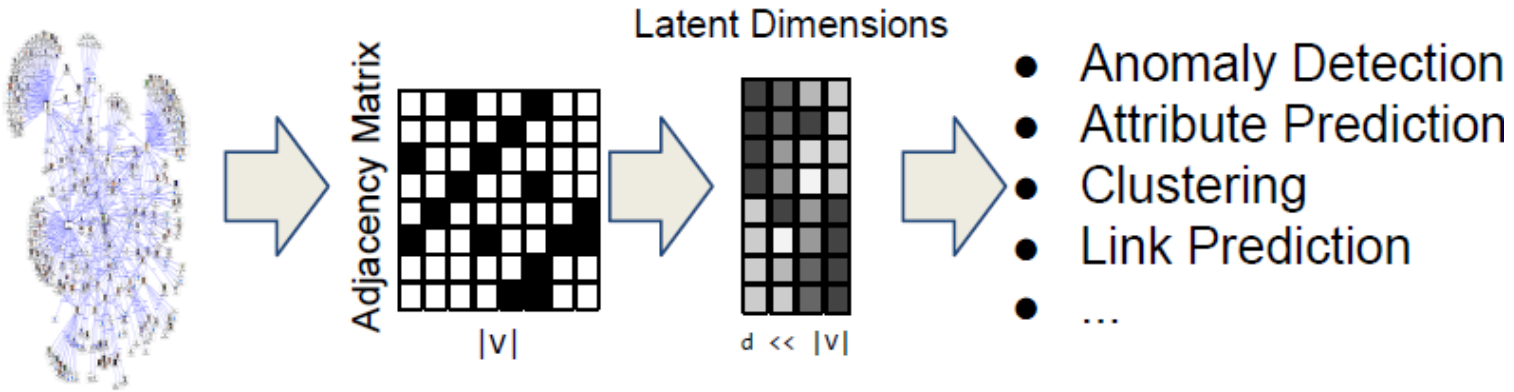
Goal: Efficient task-independent feature learning for machine learning in networks!



# 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:**

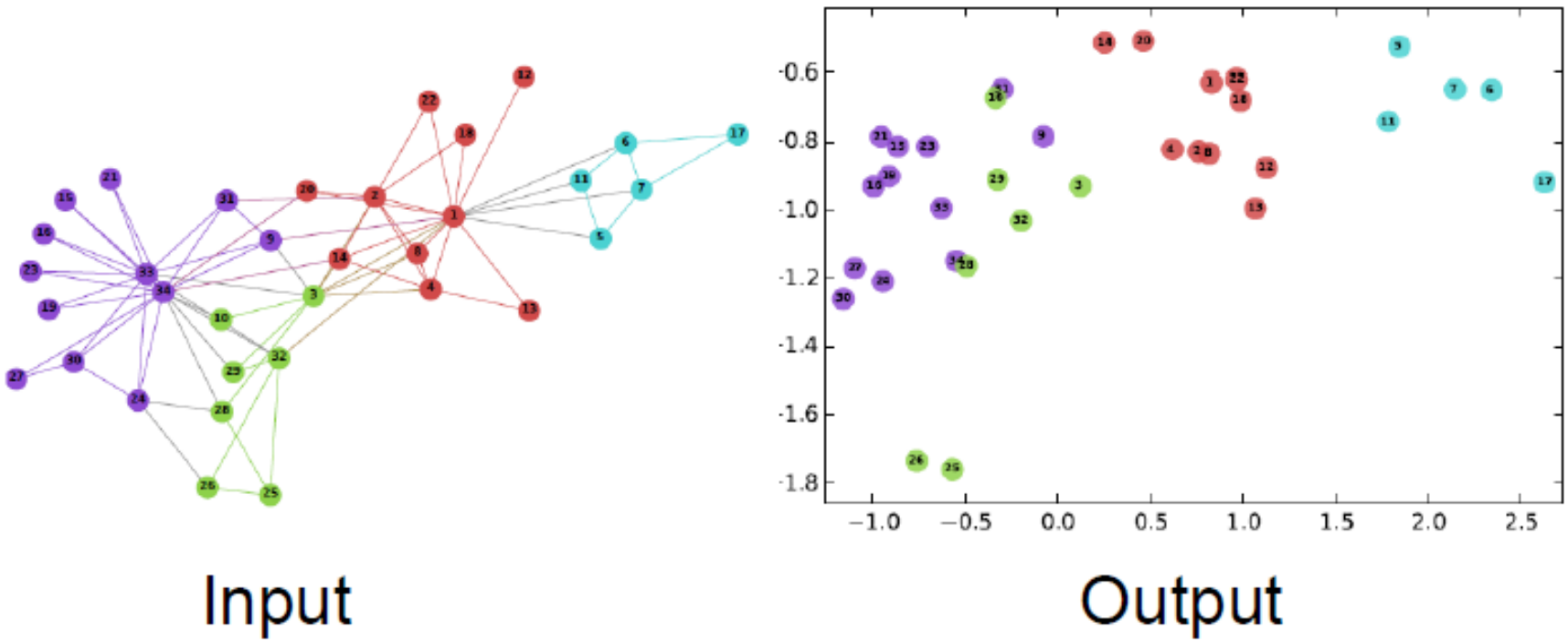



Image from: Perozzi et al. DeepWalk: Online Learning of Social Representations. *KDD 2014.*

# Embedding Nodes

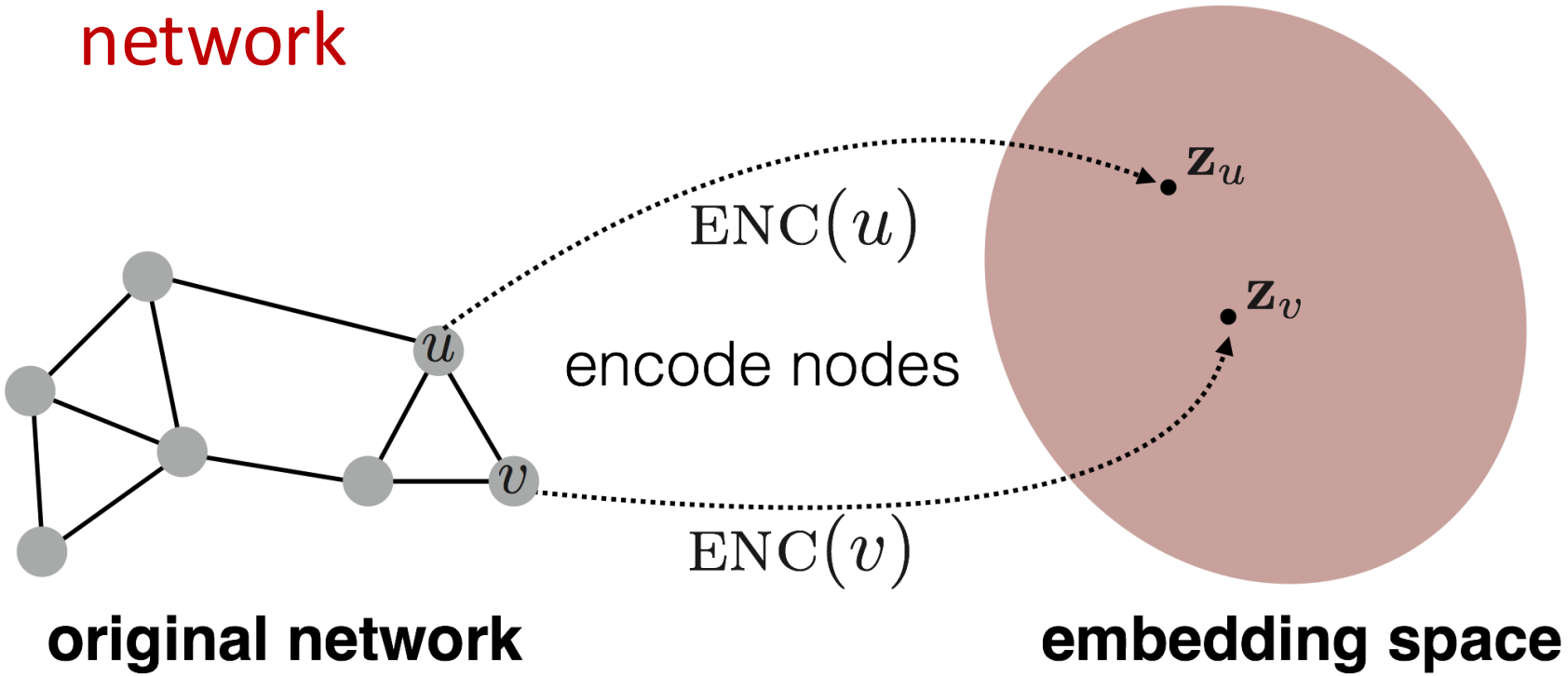
# Setup

**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



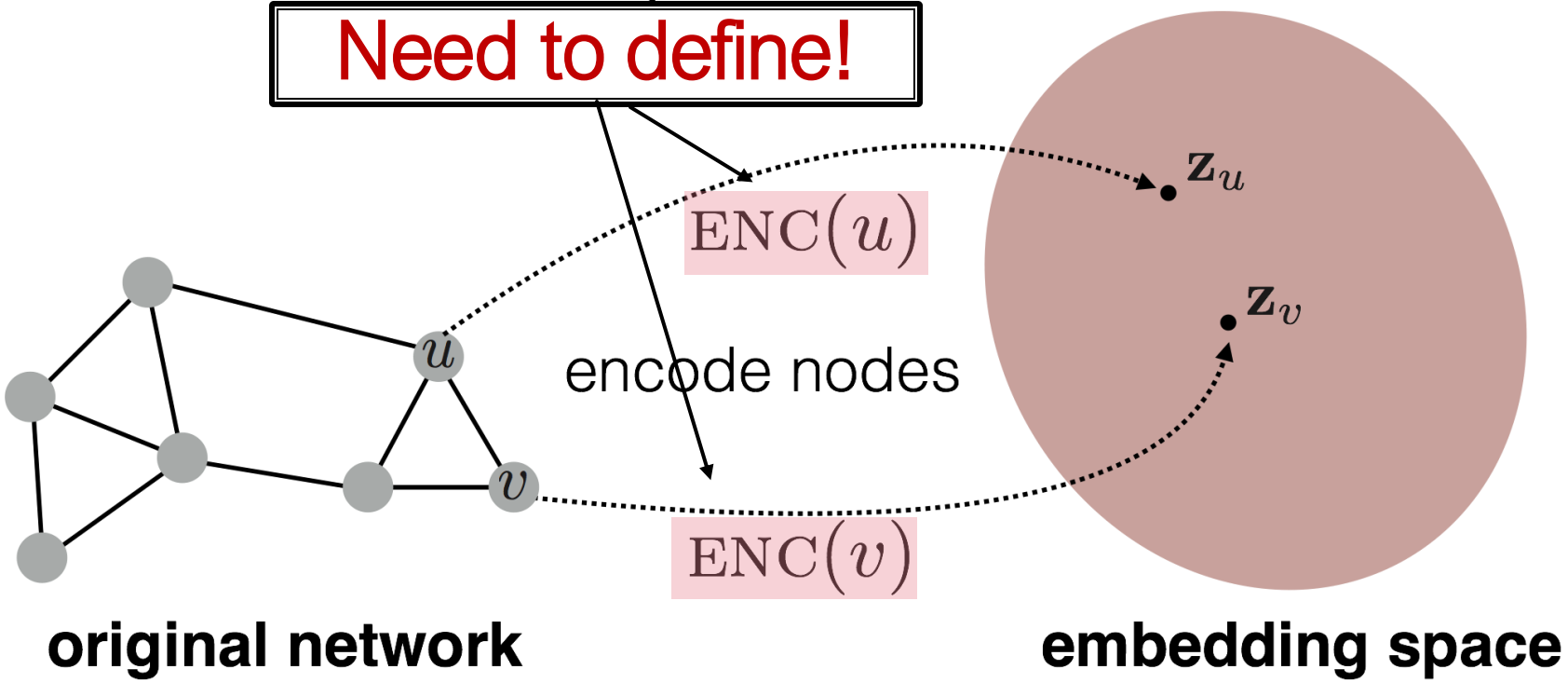
# Embedding Nodes

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

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

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**

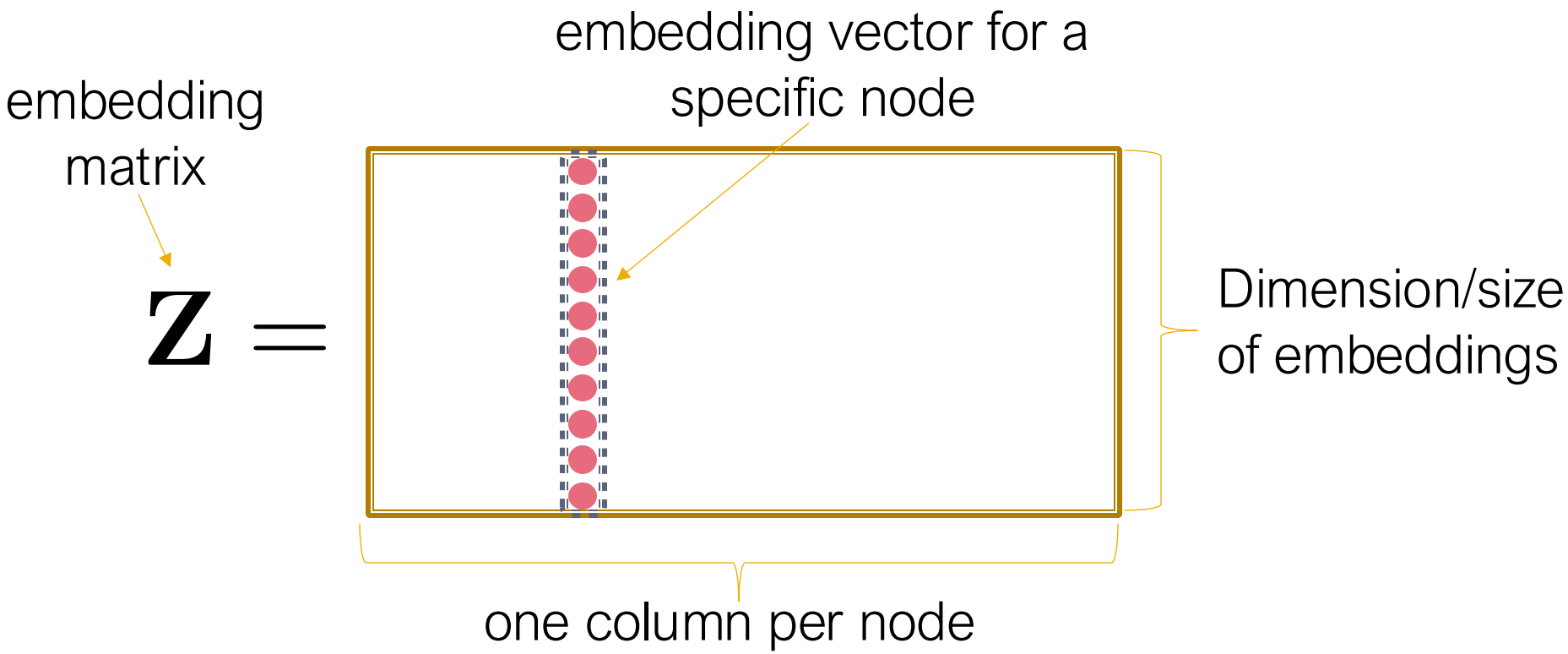
$$\text{ENC}(v) = \mathbf{Z}\mathbf{v}$$

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

$\mathbf{v} \in \mathbb{I}^{|\mathcal{V}|}$ Indicator vector, all zeroes except for a "1" at the position that corresponds to 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**

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

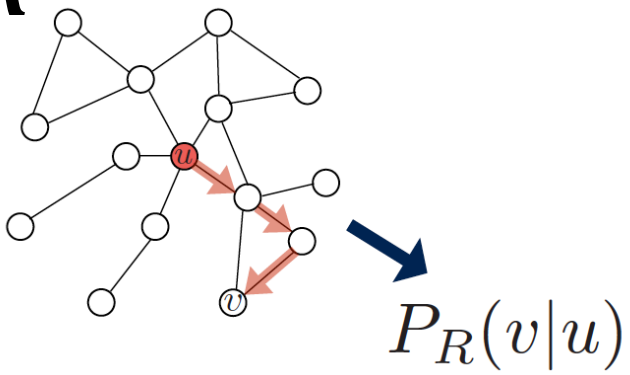
$$\mathbf{z}_u^\top \mathbf{z}_v \approx$$

Probability that $u$ and $v$ co-occur on a random walk over the network

$z_u$ … embedding of node $u$

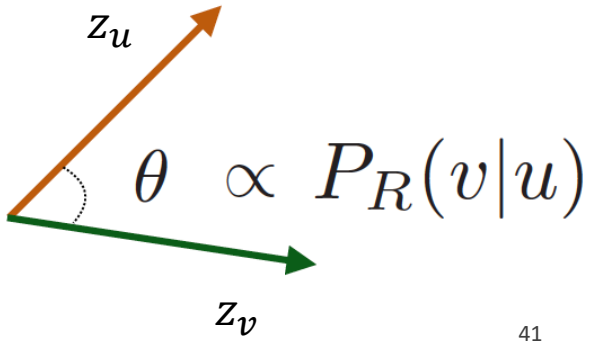
# Random-walk Embeddings

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 in $d$-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 $z: u \rightarrow \mathbb{R}^d$

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

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

*$N_R(u)$ 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:**

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

**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:**

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

sum over all nodes $u$

sum over nodes $v$ seen on random walks starting from $u$

predicted probability of $v$ appearing in random walk starting from $u$

**Optimizing random walk embeddings =**

**Finding node embeddings $z$ that minimize $\mathcal{L}$**

# Random Walk Optimization

**But doing this naively is too expensive!!**

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

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

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

# Negative Sampling

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

random distribution over all nodes

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

- 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?

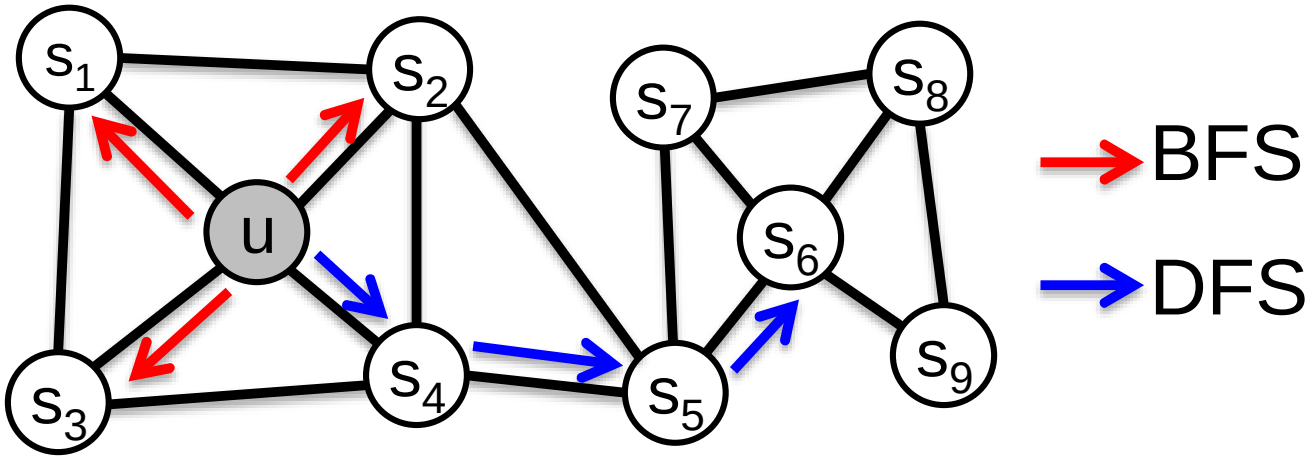
- So far we have described how to optimize embeddings given random walk statistics
- **What strategies should we use to run these random walks?**
  - Simplest idea: **Just run fixed-length, unbiased random walks starting from each node** (i.e., DeepWalk from Perozzi et al., 2013).
    - The issue is 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 $u$

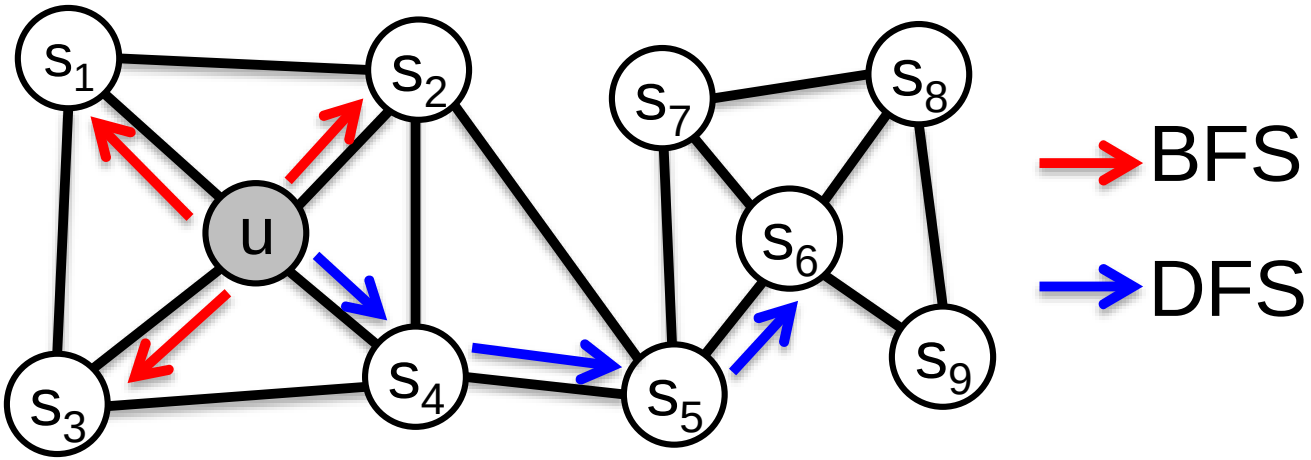
# node2vec: Biased Walks

**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

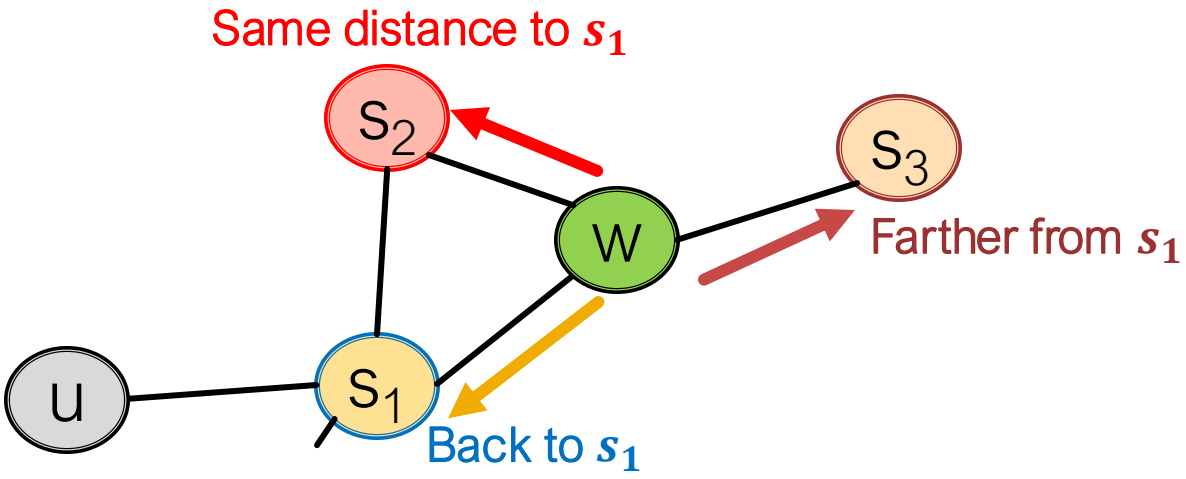
**Biased fixed-length random walk $R$ that given a node $u$ generates neighborhood $N_R(u)$**

- Two parameters:
  - **Return parameter $p$:**
    - Return back to the previous node
  - **In-out parameter $q$:**
    - Moving outwards (DFS) vs. spreading (BFS)
    - Intuitively, $q$ is the "ratio" of BFS vs. DFS

# Biased Random Walks

Biased 2nd-order random walks explore network neighborhoods:

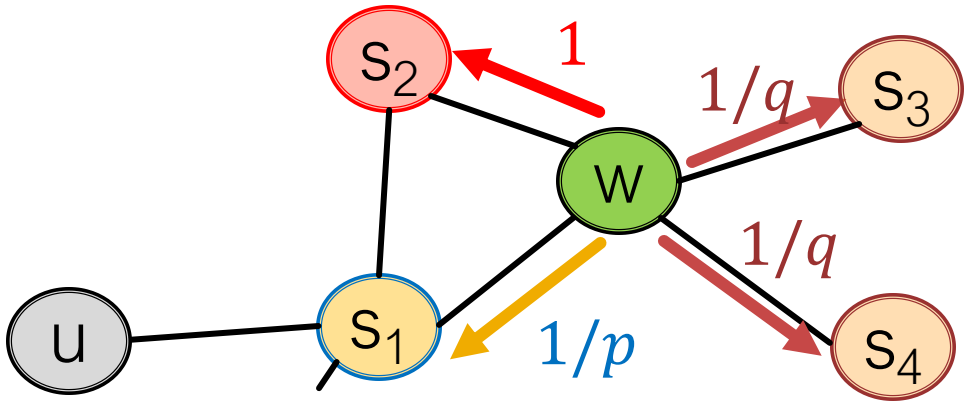
- Rnd. walk just traversed edge $(s_1, w)$ and is now at $w$
- **Insight:** Neighbors of $w$ can only be:




**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?

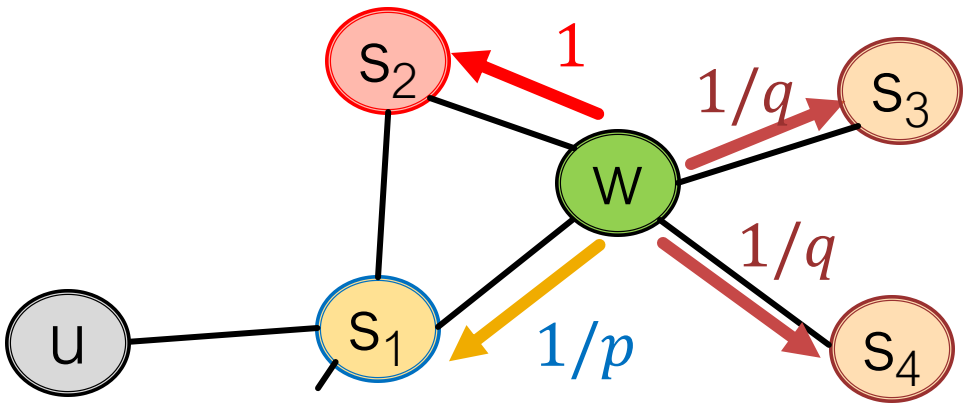



$1/p, 1/q, 1$ are unnormalized probabilities

- $p, q$ 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?




$w \rightarrow$

| 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 $q$

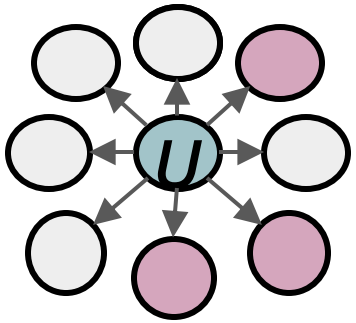
$N_R(u)$ are the nodes visited by the biased walk

# node2vec algorithm

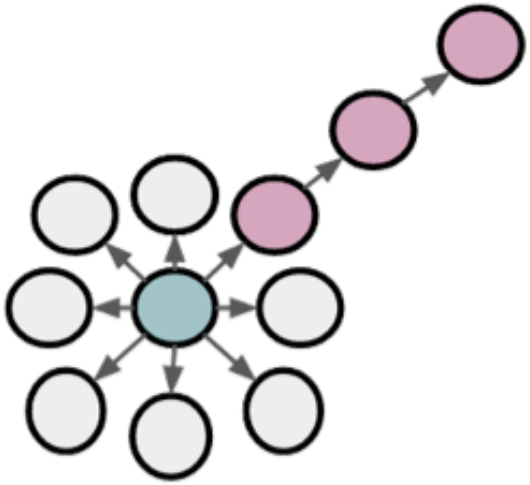
- 1) Compute random walk probabilities
- 2) Simulate $r$ random walks of length $l$ starting from each node $u$
- 3) Optimize the node2vec objective using Stochastic Gradient Descent

Linear-time complexity.
All 3 steps are individually parallelizable

# BFS vs. DFS



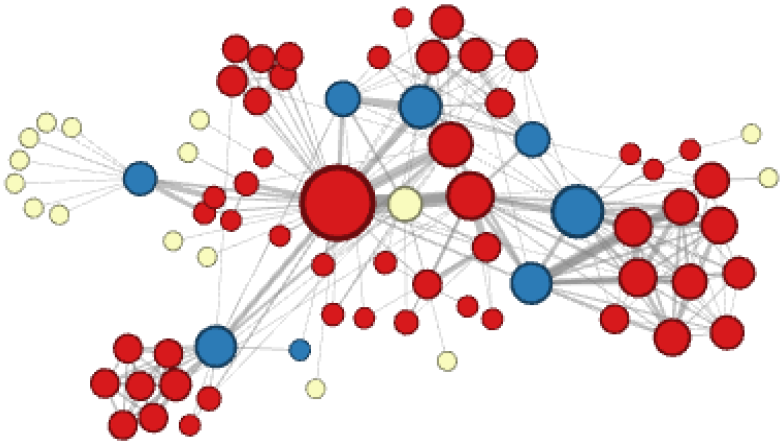

BFS:
Micro-view of neighbourhood



DFS:
Macro-view of neighbourhood

# Experiments: Micro vs. Macro

**Small network of interactions of characters in a novel:**



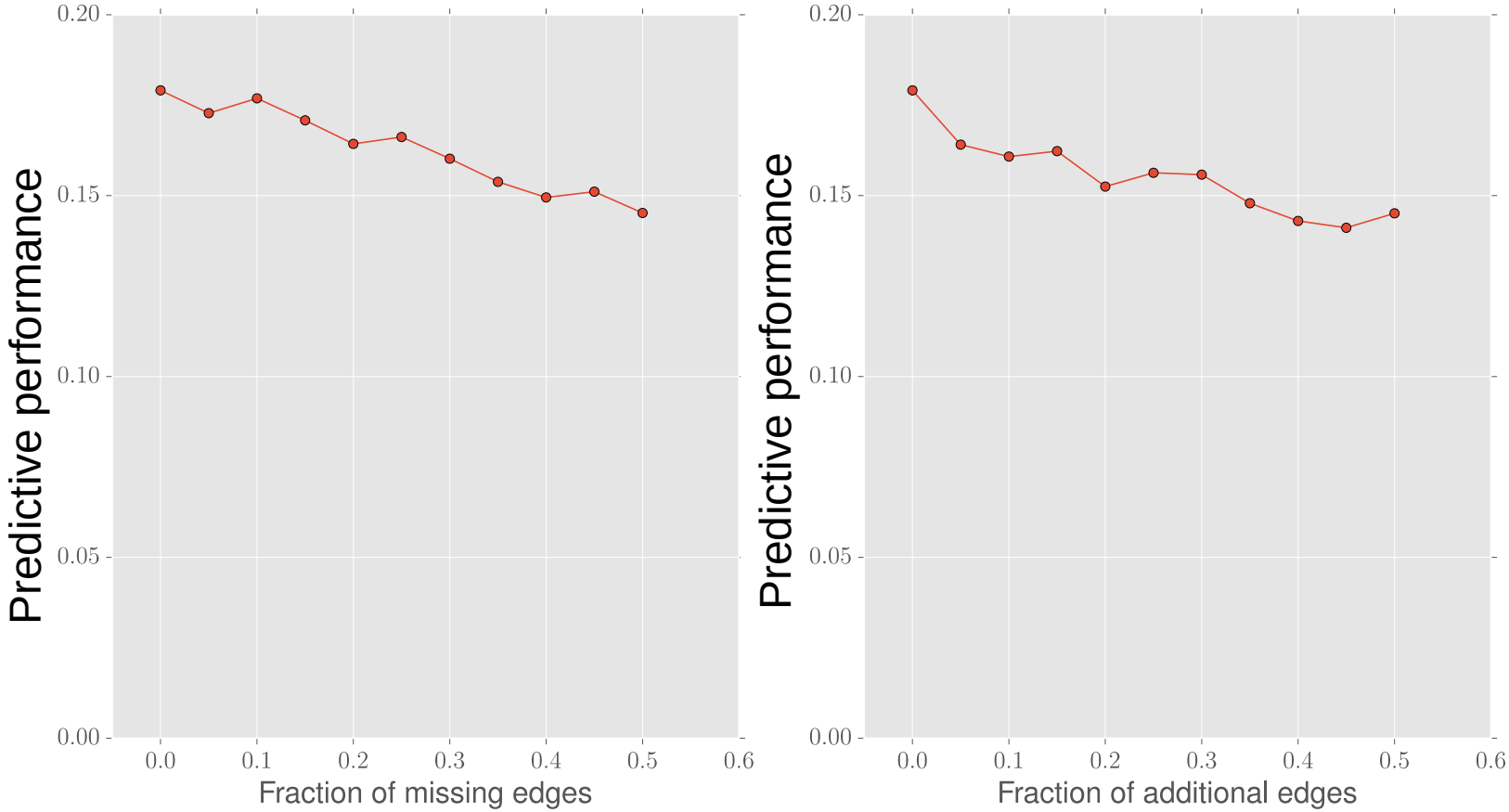
p=1, q=2

Microscopic view of the network neighbourhood

p=1, q=0.5

Macroscopic view of the network neighbourhood

# Node2vec: Incomplete Network




**How does predictive performance change as we**

- randomly remove a fraction of edges (left)
- randomly add a fraction of edges (right)

# 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

- **Basic idea:** Embed nodes so that similarities in embedding space reflect node similarities in the original network.

- **Different notions of node similarity:**
  - Adjacency-based (i.e., similar if connected)
  - Multi-hop similarity definitions.
  - Random walk approaches **(covered today)**

# Summary

- **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 perform 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!