Stanford CS224W: Graph as Matrix: PageRank, Random Walks and Embeddings

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

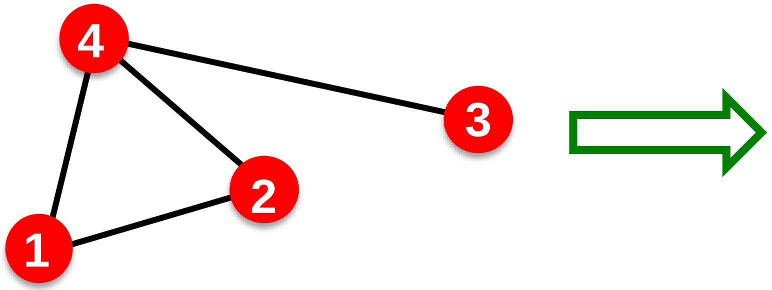
ANNOUNCEMENTS

- **Homework 1 will be released after class**
- **Next Thursday (10/07):** Colab 1 due, Colab 2 out
  - **Do Colab 0**! It has almost everything you need to complete Colab 1.
- **Office hours:** we've added Zoom links to our OH calendar.
  - See http://web.stanford.edu/class/cs224w/oh.html for OH calendar, Zoom links, and QueueStatus link.

Graph as Matrix

In this lecture, we investigate graph analysis and learning from a matrix perspective.

- Treating a graph as a matrix allows us to:
  - Determine node importance via **random walk** (PageRank)
  - Obtain node embeddings via **matrix factorization (MF)**
  - View other **node embeddings** (e.g. Node2Vec) as MF
- **Random walk, matrix factorization and node embeddings are closely related!**



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

Stanford CS224W: PageRank (aka the Google Algorithm)

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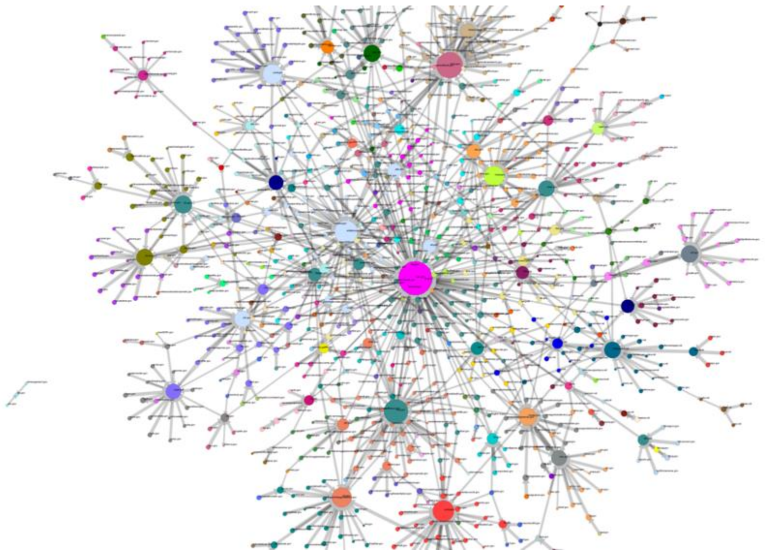
Example: The Web as a Graph

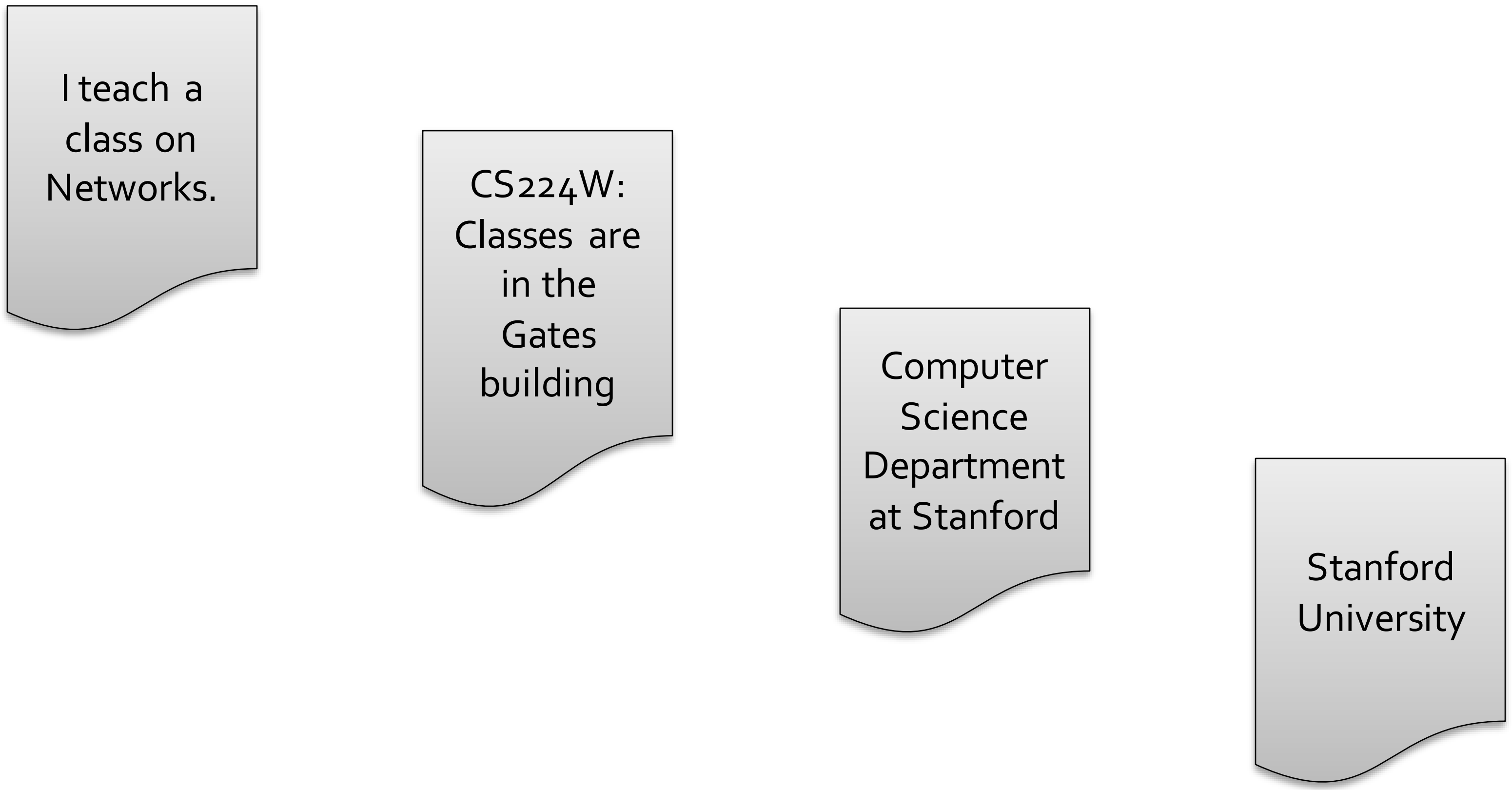
Q: What does the Web "look like" at a global level?

- **Web as a graph:**
  - Nodes = web pages
  - Edges = hyperlinks

  - **Side issue:** What is a node?
    - Dynamic pages created on the fly
    - "dark matter" – inaccessible database generated pages



The Web as a Graph



I teach a class on Networks.

CS224W: Classes are in the Gates building

Computer Science Department at Stanford

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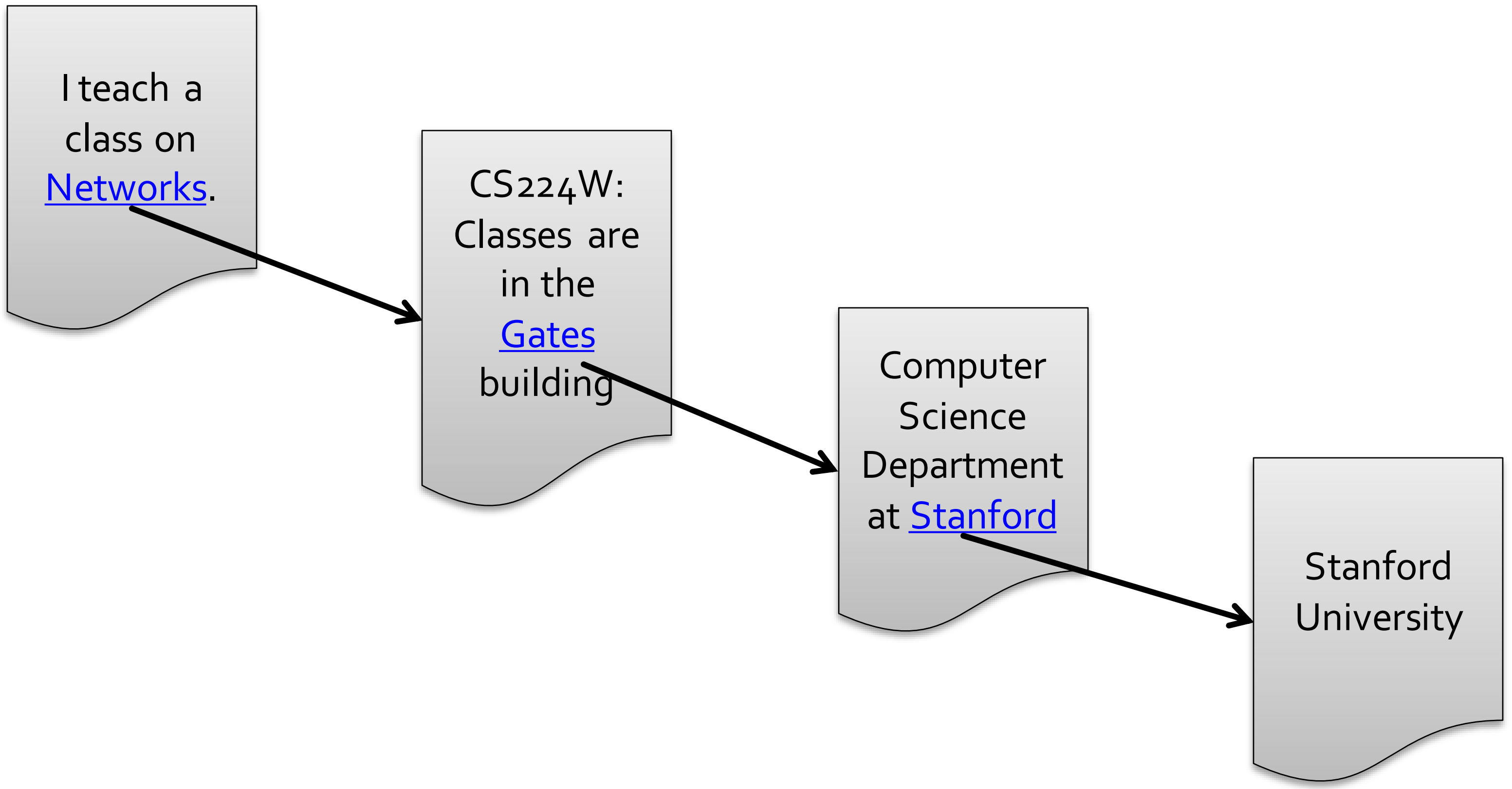
The Web as a Graph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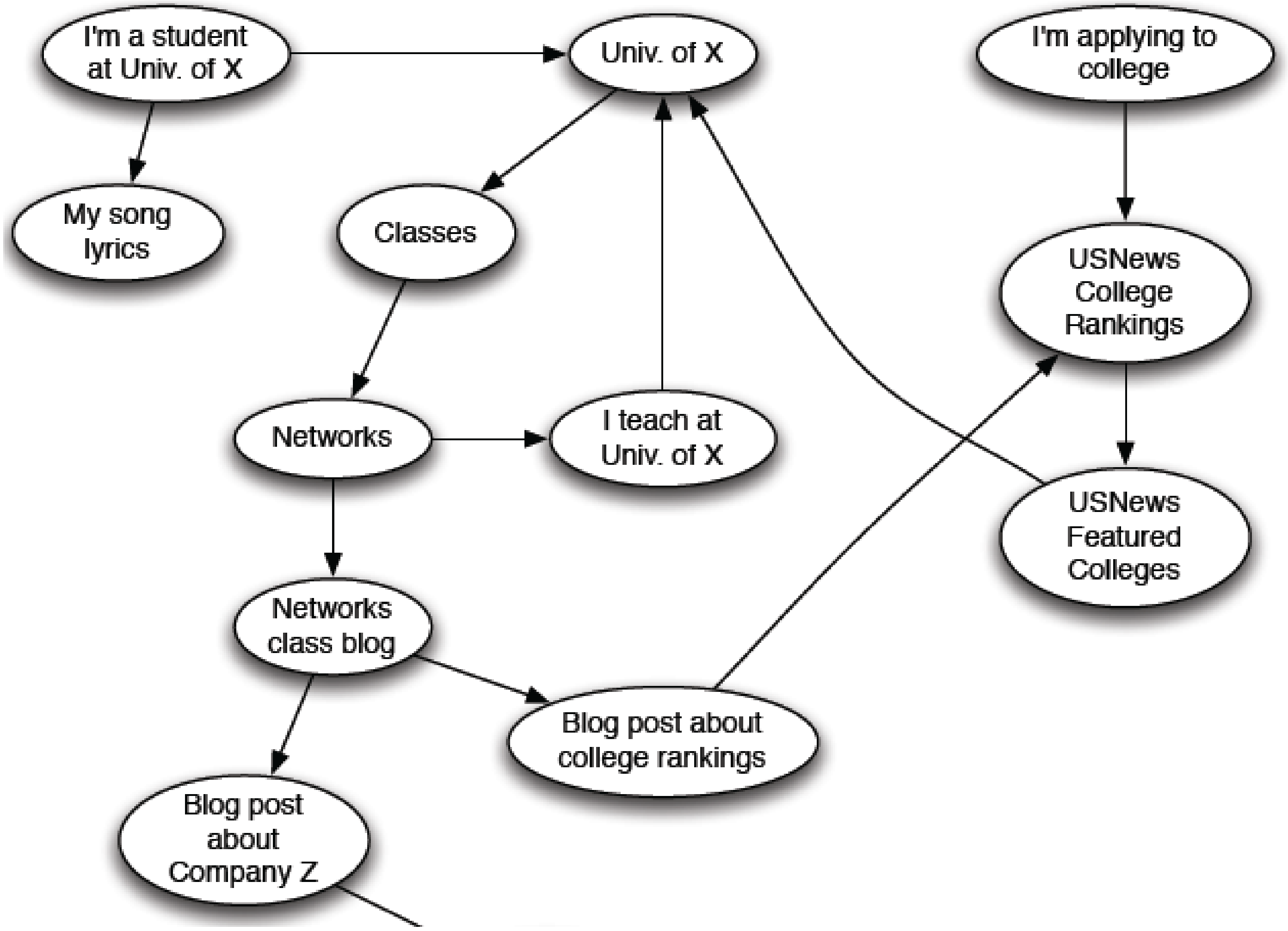
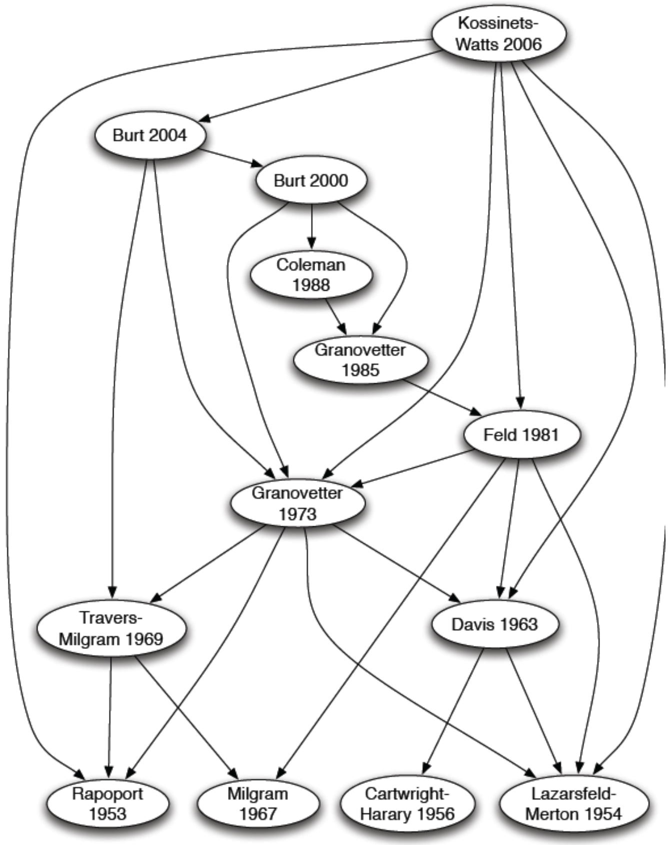
- In early days of the Web links were **navigational**
- Today many links are **transactional** (used not to navigate from page to page, but to post, comment, like, buy, …)

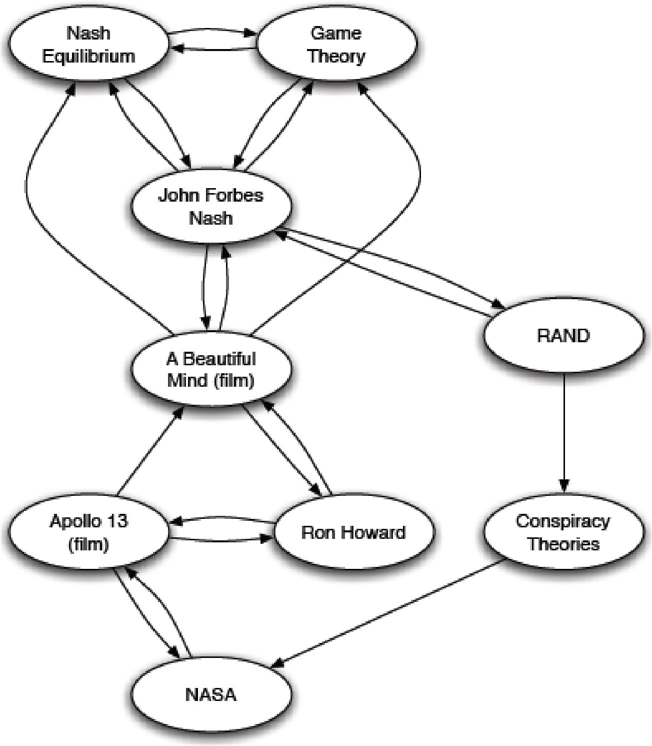
The Web as a Directed Graph



Other Information Networks



Citations



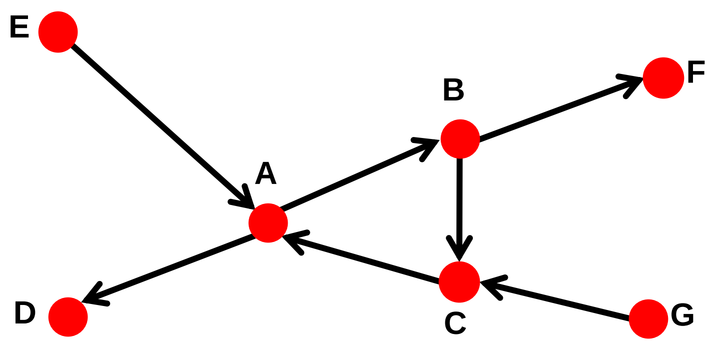
References in an Encyclopedia

What Does the Web Look Like?

- **How is the Web linked?**
- **What is the "map" of the Web?**

Web as a directed graph [Broder et al. 2000]:

- Given node v, what nodes can v reach?
- What other nodes can reach v?

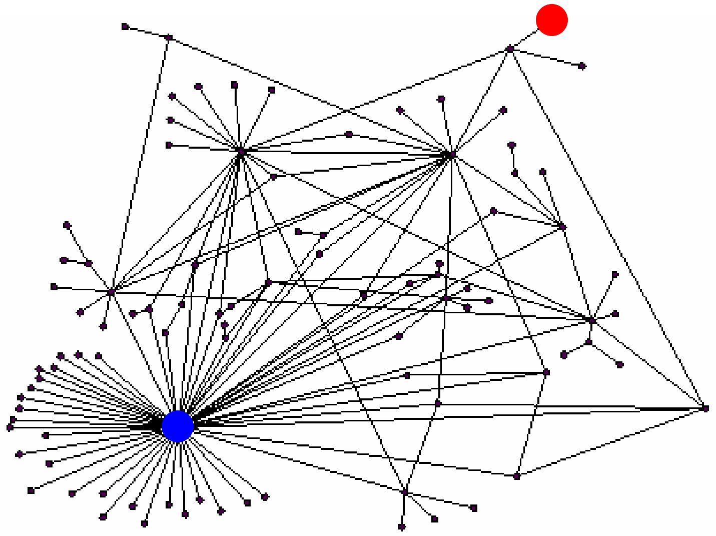


Ranking Nodes on the Graph

- **All web pages are not equally "important"**

  thispersondoesnotexist.com vs. www.stanford.edu

- There is large diversity in the web-graph node connectivity.
- **So, let's rank the pages using the web graph link structure!**



Link Analysis Algorithms

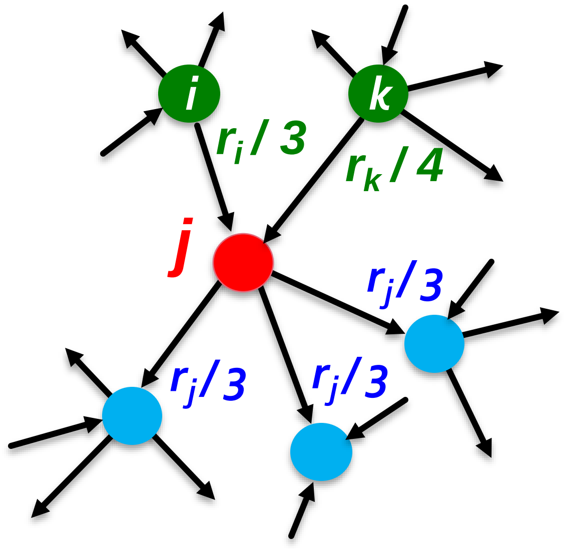
- We will cover the following **Link Analysis approaches** to compute the **importance** of nodes in a graph:
  - PageRank
  - Personalized PageRank (PPR)
  - Random Walk with Restarts

Links as Votes

- **Idea: Links as votes**
  - **Page is more important if it has more links**
    - In-coming links? Out-going links?
- **Think of in-links as votes:**
  - www.stanford.edu has 23,400 in-links
  - thispersondoesnotexist.com has 1 in-link
- **Are all in-links equal?**
  - Links from important pages count more
  - Recursive question!

PageRank: The "Flow" Model

- **A "vote" from an important page is worth more:**
  - Each link's vote is proportional to the **importance** of its source page
  - If page ***i*** with importance r_i has d_i out-links, each link gets r_i / d_i votes
  - Page ***j***'s own importance r_j is the sum of the votes on its in-links



$$r_j = r_i/3 + r_k/4$$

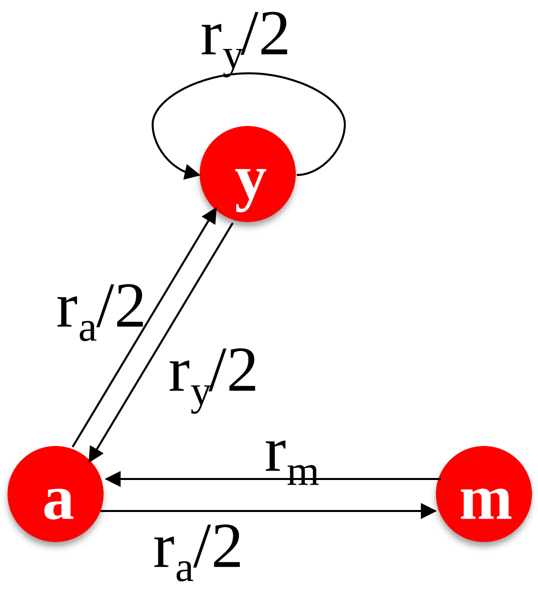
PageRank: The "Flow" Model

- **A page is important if it is pointed to by other important pages**
- **Define "rank" r_j for node j**

$$r_j = \sum_{i \to j} \frac{r_i}{d_i}$$

d_i … out-degree of node i

The web in 1839



"Flow" equations:

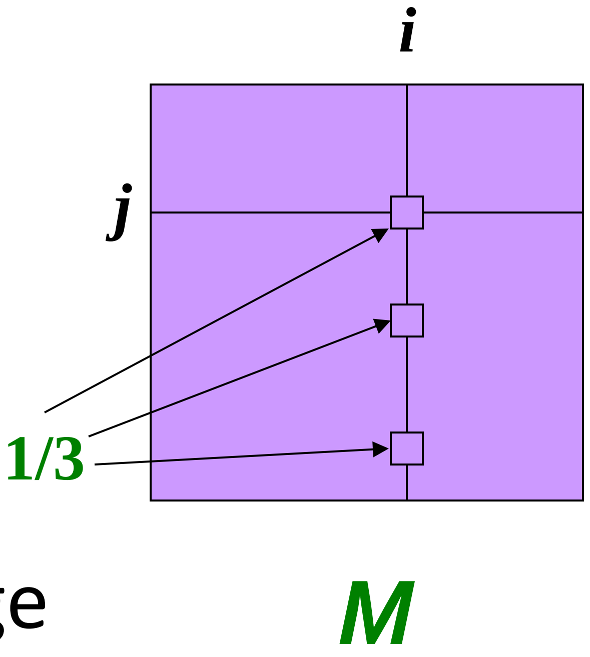
$$r_y = r_y/2 + r_a/2$$
$$r_a = r_y/2 + r_m$$
$$r_m = r_a/2$$

You might wonder: Let's just use Gaussian elimination to solve this system of linear equations. Bad idea!

PageRank: Matrix Formulation

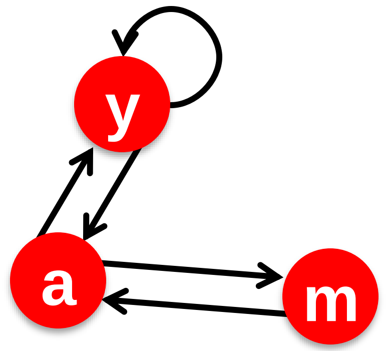
- **Stochastic adjacency matrix M**
  - d_i is the outdegree of node i
  - If $i \to j$, then $M_{ji} = \frac{1}{d_i}$
    - M is a **column stochastic matrix**
      - $\boxed{\textbf{Columns sum to 1}}$
- **Rank vector r:** An entry per page
  - r_i is the importance score of page i
  - $\boxed{\sum_i r_i = 1}$
- **The flow equations can be written**

$$r = M \cdot r$$



$$r_j = \sum_{i \to j} \frac{r_i}{d_i}$$

Example: Flow Equations & M



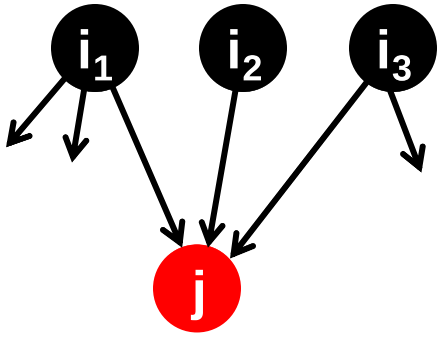
$$\begin{array}{c|c|c|c|}
 & r_y & r_a & r_m \\ \hline
r_y & \frac{1}{2} & \frac{1}{2} & 0 \\ \hline
r_a & \frac{1}{2} & 0 & 1 \\ \hline
r_m & 0 & \frac{1}{2} & 0 \\ \hline
\end{array}$$

$$r_y = r_y/2 + r_a/2$$
$$r_a = r_y/2 + r_m$$
$$r_m = r_a/2$$

$$\underset{\boldsymbol{r}}{\boxed{\begin{matrix} r_y \\ r_a \\ r_m \end{matrix}}} = \underset{\boldsymbol{M}}{\boxed{\begin{matrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 1 \\ 0 & \frac{1}{2} & 0 \end{matrix}}} \underset{\boldsymbol{r}}{\boxed{\begin{matrix} r_y \\ r_a \\ r_m \end{matrix}}}$$

Connection to Random Walk

- **Imagine a random web surfer:**
  - At any time $\boldsymbol{t}$, surfer is on some page i
  - At time $\boldsymbol{t+1}$, the surfer follows an out-link from $\boldsymbol{i}$ uniformly at random
  - Ends up on some page $\boldsymbol{j}$ linked from $\boldsymbol{i}$
  - Process repeats indefinitely
- **Let:**
  - $\boldsymbol{p(t)}$ … vector whose i^{th} coordinate is the prob. that the surfer is at page i at time t
  - So, $\boldsymbol{p(t)}$ is a probability distribution over pages

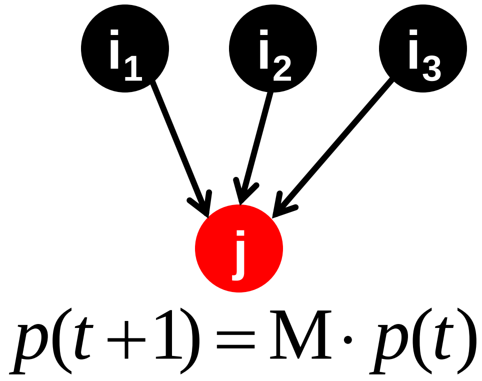


$$r_j = \sum_{i \to j} \frac{r_i}{d_i}$$

The Stationary Distribution

- **Where is the surfer at time *t+1*?**
  - Follow a link uniformly at random

$$\boldsymbol{p}(\boldsymbol{t}+1) = \boldsymbol{M}\cdot\boldsymbol{p}(\boldsymbol{t})$$



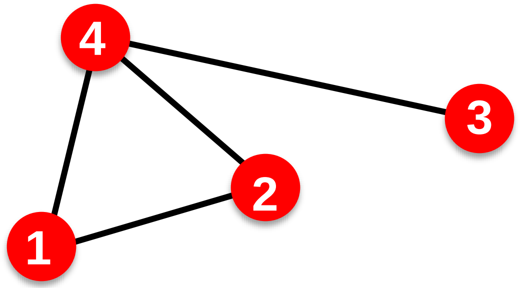
- Suppose the random walk reaches a state

$$\boldsymbol{p}(\boldsymbol{t}+1) = \boldsymbol{M}\cdot\boldsymbol{p}(\boldsymbol{t}) = \boldsymbol{p}(\boldsymbol{t})$$

  then $\boldsymbol{p}(t)$ is **stationary distribution** of a random walk
- **Our original rank vector** $\boldsymbol{r}$ satisfies $\boldsymbol{r} = \boldsymbol{M}\cdot\boldsymbol{r}$
  - **So, $\boldsymbol{r}$ is a stationary distribution for the random walk**

Recall Eigenvector of A Matrix

- Recall from lecture 2 (eigenvector centrality), let $\boldsymbol{A} \in \{\mathbf{0}, \mathbf{1}\}^{\boldsymbol{n \times n}}$ be an adj. matrix of undir. graph:



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

- Eigenvector of adjacency matrix: vectors satisfying $\boldsymbol{\lambda c} = \boldsymbol{Ac}$
- $\boldsymbol{c}$: eigenvector; $\boldsymbol{\lambda}$: eigenvalue

- Note:
  - This is the definition of eigenvector centrality (for undirected graphs).
  - PageRank is defined for directed graphs

Eigenvector Formulation

- **The flow equation:**
  $$1 \cdot \boldsymbol{r} = \boldsymbol{M} \cdot \boldsymbol{r}$$

$$\underbrace{\begin{bmatrix} r_y \\ r_a \\ r_m \end{bmatrix}}_{\boldsymbol{r}} = \underbrace{\begin{bmatrix} ½ & ½ & 0 \\ ½ & 0 & 1 \\ 0 & ½ & 0 \end{bmatrix}}_{\boldsymbol{M}} \underbrace{\begin{bmatrix} r_y \\ r_a \\ r_m \end{bmatrix}}_{\boldsymbol{r}}$$

- So the **rank vector** $\boldsymbol{r}$ is an **eigenvector** of the stochastic adj. matrix $\boldsymbol{M}$ (with eigenvalue 1)
  - Starting from any vector $\boldsymbol{u}$, the limit $\boldsymbol{M}(\boldsymbol{M}(\dots\boldsymbol{M}(\boldsymbol{M}\,\boldsymbol{u})))$ is the **long-term distribution** of the surfers.
    - PageRank = Limiting distribution = principal eigenvector of M
    - Note: If $\boldsymbol{r}$ is the limit of the product $\boldsymbol{MM}\dots\boldsymbol{Mu}$, then $\boldsymbol{r}$ satisfies the flow equation $1 \cdot \boldsymbol{r} = \boldsymbol{Mr}$
    - So $\boldsymbol{r}$ is the principal eigenvector of $\boldsymbol{M}$ with eigenvalue 1
- **We can now efficiently solve for *r*!**
  - The method is called **Power iteration**

PageRank: Summary

- **PageRank:**
  - Measures importance of nodes in a graph using the link structure of the web
  - Models a random web surfer using the stochastic adjacency matrix $\boldsymbol{M}$
  - PageRank solves $\boldsymbol{r} = \boldsymbol{M}\boldsymbol{r}$ where $\boldsymbol{r}$ can be viewed as both the principle eigenvector of $\boldsymbol{M}$ and as the stationary distribution of a random walk over the graph

Stanford CS224W: PageRank: How to solve?

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PageRank: How to solve?

Given a graph with *n* nodes, we use an iterative procedure:

- Assign each node an initial page rank
- Repeat until convergence ($\sum_i |r_i^{t+1} - r_i^t| < \epsilon$)
  - Calculate the page rank of each node

$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{d_i}$$

d_i …. out-degree of node i

Power Iteration Method

- **Given a web graph with *N* nodes, where the nodes are pages and edges are hyperlinks**
- **Power iteration:** a simple iterative scheme
  - Initialize: $\boldsymbol{r}^{(0)} = [1/N, \ldots., 1/N]^T$
  - Iterate: $\boldsymbol{r}^{(t+1)} = \boldsymbol{M} \cdot \boldsymbol{r}^{(t)}$
  - Stop when $|\boldsymbol{r}^{(t+1)} - \boldsymbol{r}^{(t)}|_1 < \varepsilon$

$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{d_i}$$

d_i …. out-degree of node i

$|\boldsymbol{x}|_1 = \sum_1^N |\boldsymbol{x_i}|$ is the **L1** norm
Can use any other vector norm, e.g., Euclidean

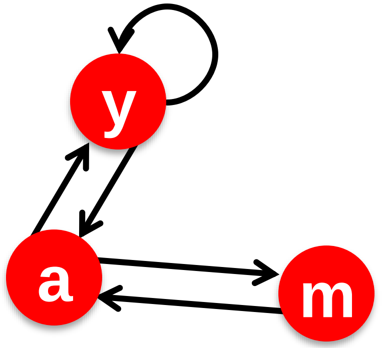
About 50 iterations is sufficient to estimate the limiting solution.

PageRank: How to solve?

- **Power Iteration:**
  - Set $r_j \leftarrow 1/N$
  - **1:** $r'_j \leftarrow \sum_{i \to j} \frac{r_i}{d_i}$
  - **2:** If $|r - r'| > \varepsilon$:
    - $r \leftarrow r'$
  - **3:** go to **1**
- **Example:**

$$\begin{bmatrix} r_y \\ r_a \\ r_m \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

Iteration 0, 1, 2, …



	y	a	m
y	½	½	0
a	½	0	1
m	0	½	0

$$\begin{aligned} r_y &= r_y/2 + r_a/2 \\ r_a &= r_y/2 + r_m \\ r_m &= r_a/2 \end{aligned}$$

PageRank: How to solve?

- **Power Iteration:**
  - Set $r_j \leftarrow 1/N$
  - **1:** $r'_j \leftarrow \sum_{i\to j} \frac{r_i}{d_i}$
  - **2:** If $|r - r'| > \varepsilon$:
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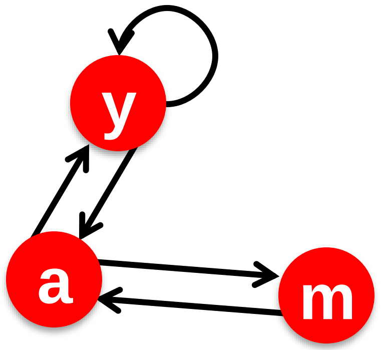
- **Example:**



$$\begin{array}{c|ccc} & y & a & m \\ \hline y & ½ & ½ & 0 \\ a & ½ & 0 & 1 \\ m & 0 & ½ & 0 \end{array}$$

$$\begin{aligned} r_y &= r_y/2 + r_a/2 \\ r_a &= r_y/2 + r_m \\ r_m &= r_a/2 \end{aligned}$$

$$\begin{pmatrix} r_y \\ r_a \\ r_m \end{pmatrix} = \quad \begin{pmatrix} 1/3 \\ 1/3 \\ 1/3 \end{pmatrix} \quad \begin{pmatrix} 1/3 \\ 3/6 \\ 1/6 \end{pmatrix} \quad \begin{pmatrix} 5/12 \\ 1/3 \\ 3/12 \end{pmatrix} \quad \begin{pmatrix} 9/24 \\ 11/24 \\ 1/6 \end{pmatrix} \quad \dots \quad \begin{pmatrix} 6/15 \\ 6/15 \\ 3/15 \end{pmatrix}$$

Iteration 0, 1, 2, …

PageRank: Three Questions

$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{d_i}$$ or equivalently $$r = Mr$$

- **Does this converge?**
- **Does it converge to what we want?**
- **Are results reasonable?**

PageRank: Problems

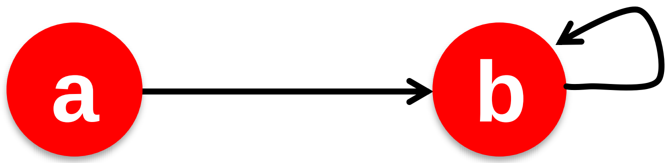
Two problems:

- **(1)** Some pages are **dead ends** (have no out-links)
  - Such pages cause importance to "leak out"

- **(2)** **Spider traps** (all out-links are within the group)
  - Eventually spider traps absorb all importance

Does this converge?

- **The "Spider trap" problem:**



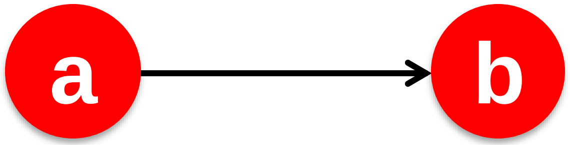
$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{d_i}$$

- **Example:**

	Iteration:	**0,**	**1,**	**2,**	**3…**
r_a	=	1	0	0	0
r_b		0	1	1	1

Does it converge to what we want?

- The "Dead end" problem:



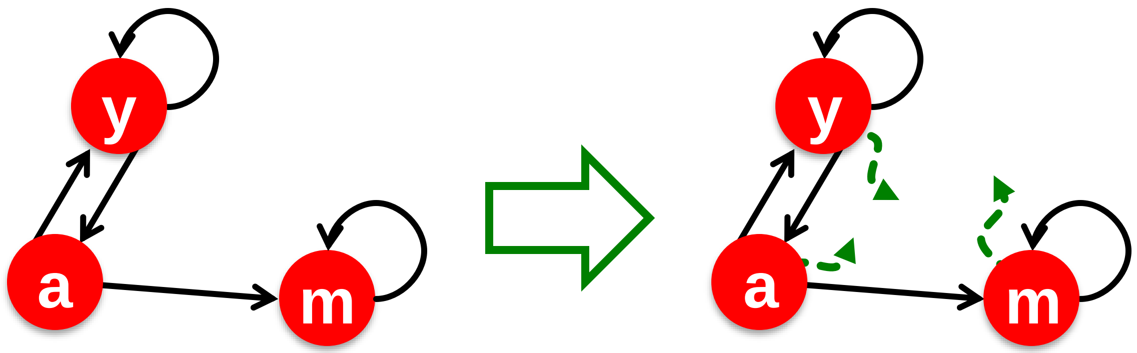
$$r_j^{(t+1)} = \sum_{i \to j} \frac{r_i^{(t)}}{d_i}$$

- Example:

Iteration:	0,	1,	2,	3…
r_a =	1	0	0	0
r_b	0	1	0	0

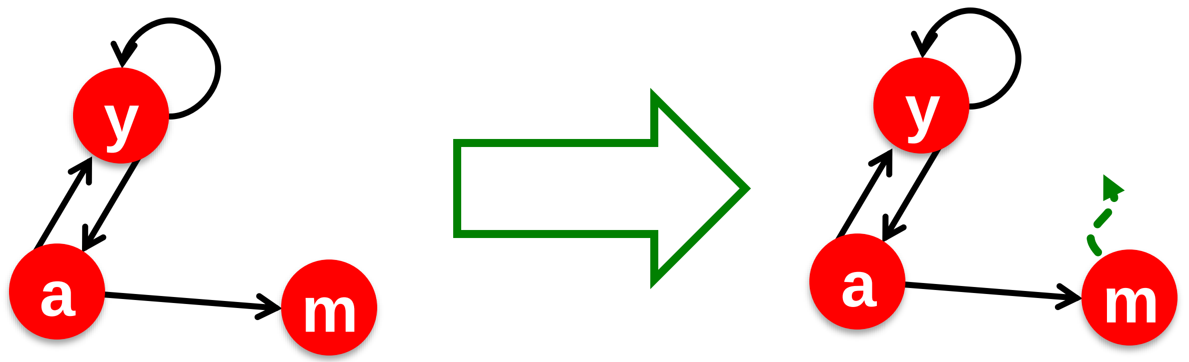
Solution to Spider Traps

- **Solution for spider traps: At each time step, the random surfer has two options**
  - With prob. β, follow a link at random
  - With prob. **1-β,** jump to a random page
  - Common values for β are in the range 0.8 to 0.9
- **Surfer will teleport out of spider trap within a few time steps**



Solution to Dead Ends

- **Teleports:** Follow random teleport links with total probability **1.0** from dead-ends
  - Adjust matrix accordingly



$$\begin{array}{c|ccc} & y & a & m \\ \hline y & \frac{1}{2} & \frac{1}{2} & 0 \\ a & \frac{1}{2} & 0 & 0 \\ m & 0 & \frac{1}{2} & 0 \end{array} \quad\Rightarrow\quad \begin{array}{c|ccc} & y & a & m \\ \hline y & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} \\ a & \frac{1}{2} & 0 & \frac{1}{3} \\ m & 0 & \frac{1}{2} & \frac{1}{3} \end{array}$$

Why Teleports Solve the Problem?

Why are dead-ends and spider traps a problem and why do teleports solve the problem?

- **Spider-traps** are not a problem, but with traps PageRank scores are **not** what we want
  - **Solution:** Never get stuck in a spider trap by teleporting out of it in a finite number of steps
- **Dead-ends** are a problem
  - The matrix is not column stochastic so our initial assumptions are not met
  - **Solution:** Make matrix column stochastic by always teleporting when there is nowhere else to go

Solution: Random Teleports

- **Google's solution that does it all:**
  At each step, random surfer has two options:
  - With probability β, follow a link at random
  - With probability $1\text{-}\beta$, jump to some random page

- **PageRank equation** [Brin-Page, 98]

$$r_j = \sum_{i \to j} \beta \frac{r_i}{d_i} + (1-\beta)\frac{1}{N}$$

d_i … out-degree of node i

This formulation assumes that M has no dead ends. We can either preprocess matrix M to remove all dead ends or explicitly follow random teleport links with probability 1.0 from dead-ends.

The Google Matrix

- **PageRank equation** [Brin-Page, '98]

$$r_j = \sum_{i \to j} \beta \frac{r_i}{d_i} + (1-\beta)\frac{1}{N}$$

- **The Google Matrix *G*:**

$[1/N]_{NxN}$…N by N matrix where all entries are 1/N

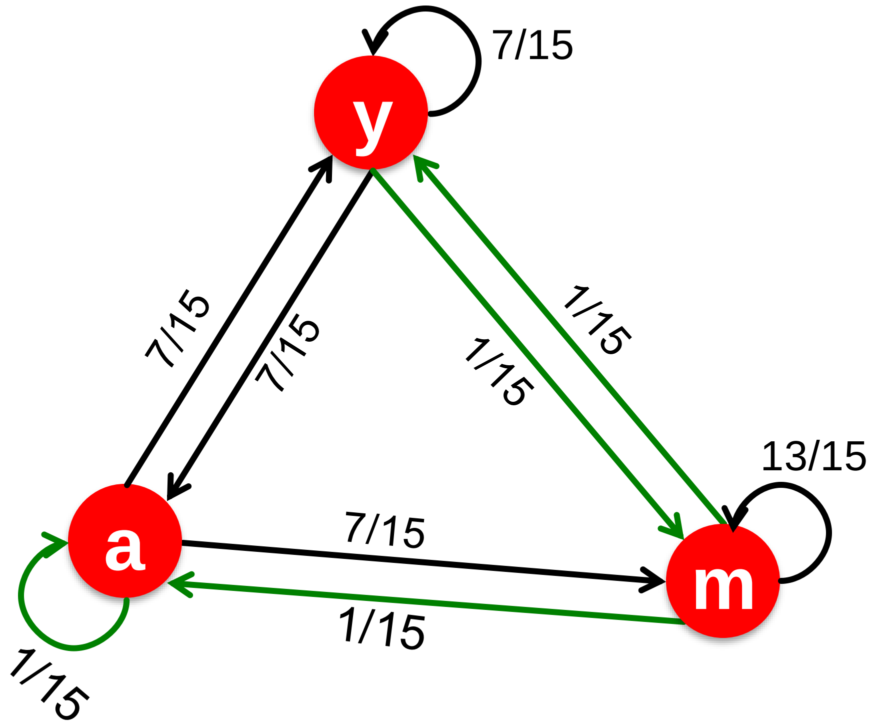
$$G = \beta\, M + (1-\beta)\left[\frac{1}{N}\right]_{N\times N}$$

- **We have a recursive problem: $\boldsymbol{r} = \boldsymbol{G} \cdot \boldsymbol{r}$**

  And the Power method still works!

- **What is β ?**
  - In practice β =0.8,0.9 (make 5 steps on avg., jump)

Random Teleports ($\beta = 0.8$)



$$0.8 \begin{array}{c} \mathbf{M} \\ \boxed{\begin{matrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 0 \\ 0 & 1/2 & 1 \end{matrix}} \end{array} + 0.2 \begin{array}{c} \mathbf{[1/N]_{NxN}} \\ \boxed{\begin{matrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{matrix}} \end{array}$$

$$\begin{array}{c|ccc|} y & 7/15 & 7/15 & 1/15 \\ a & 7/15 & 1/15 & 1/15 \\ m & 1/15 & 7/15 & 13/15 \end{array}$$

G

$$\begin{matrix} y \\ a \\ m \end{matrix} = \begin{matrix} 1/3 \\ 1/3 \\ 1/3 \end{matrix} \quad \begin{matrix} 0.33 \\ 0.20 \\ 0.46 \end{matrix} \quad \begin{matrix} 0.24 \\ 0.20 \\ 0.52 \end{matrix} \quad \begin{matrix} 0.26 \\ 0.18 \\ 0.56 \end{matrix} \quad \ldots \quad \begin{matrix} 7/33 \\ 5/33 \\ 21/33 \end{matrix}$$

PageRank Example

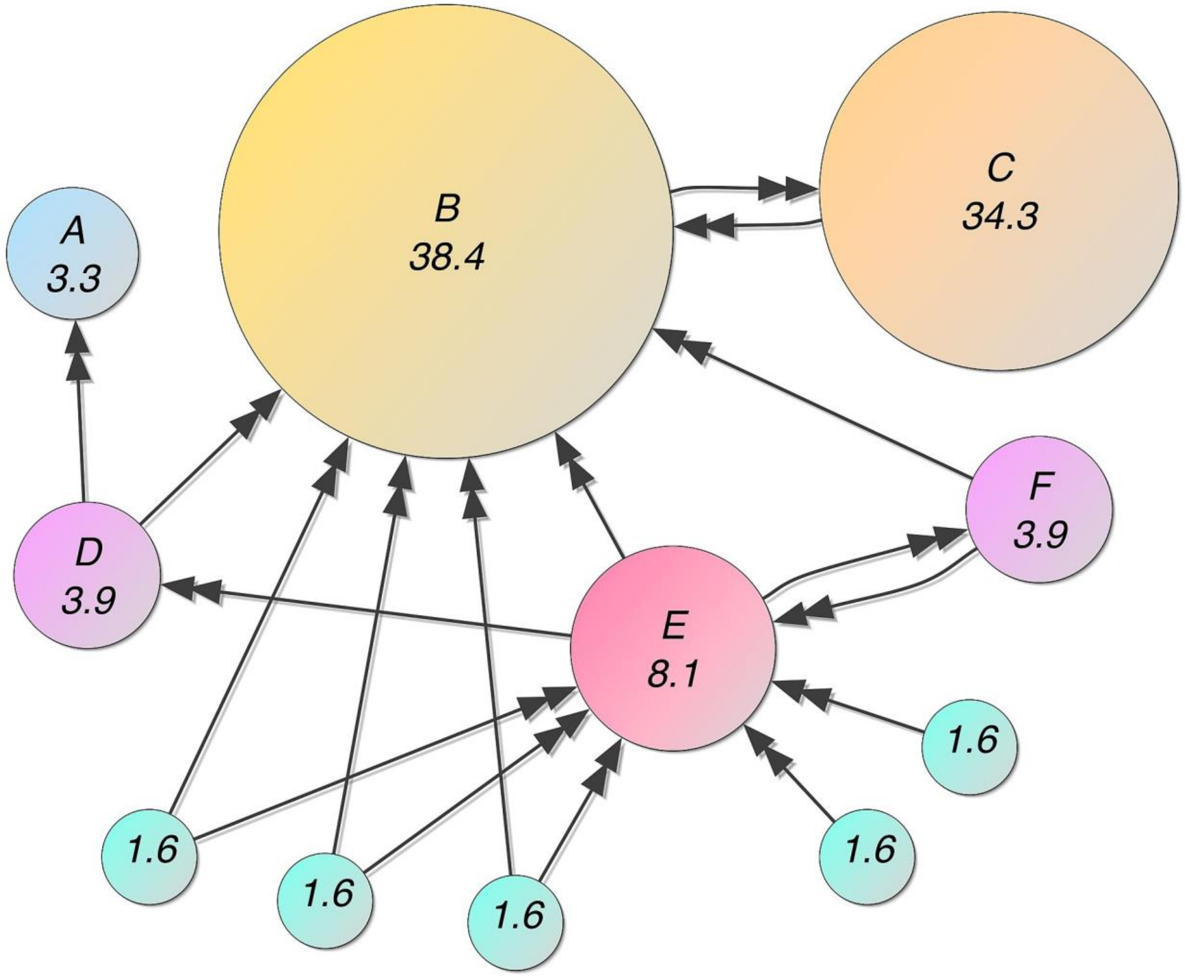


Image credit: [Wikipedia]()

Solving PageRank: Summary

- PageRank solves for $\boldsymbol{r} = \boldsymbol{Gr}$ and can be efficiently computed by power iteration of the stochastic adjacency matrix ($\boldsymbol{G}$)
- Adding random uniform teleportation solves issues of dead-ends and spider-traps

Stanford CS224W: Random Walk with Restarts and Personalized PageRank

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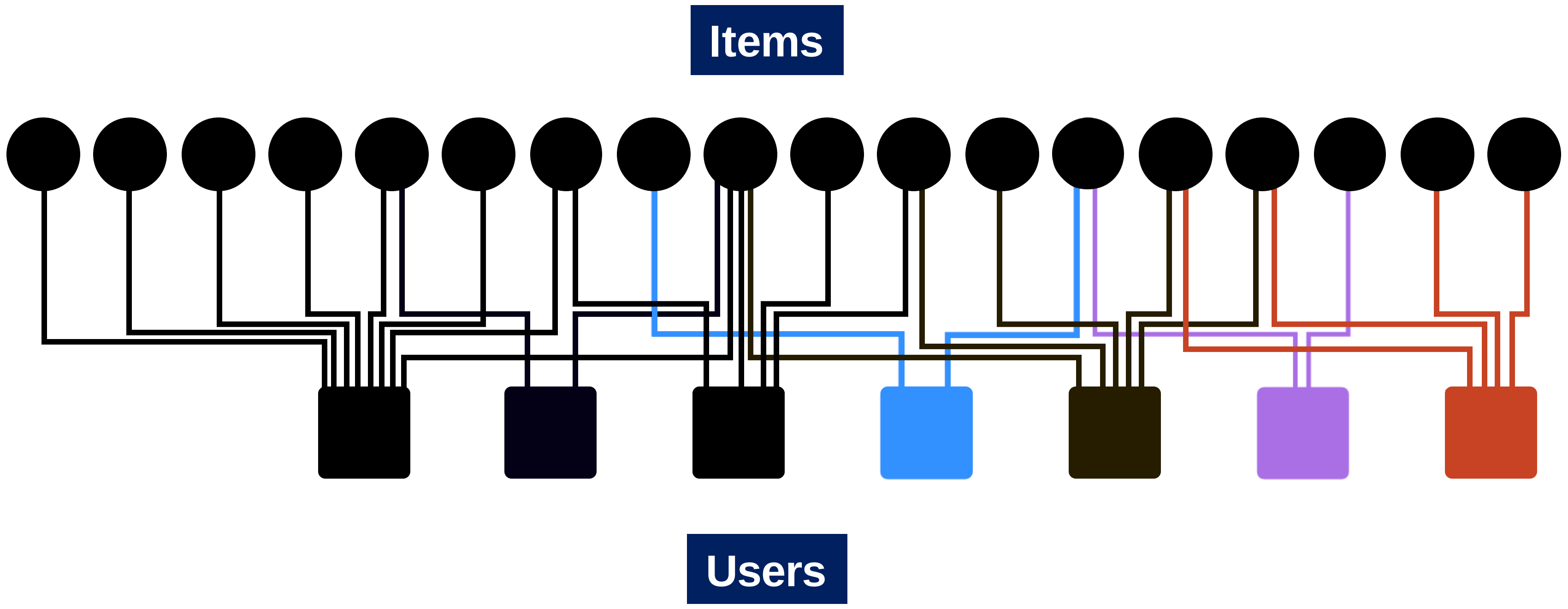
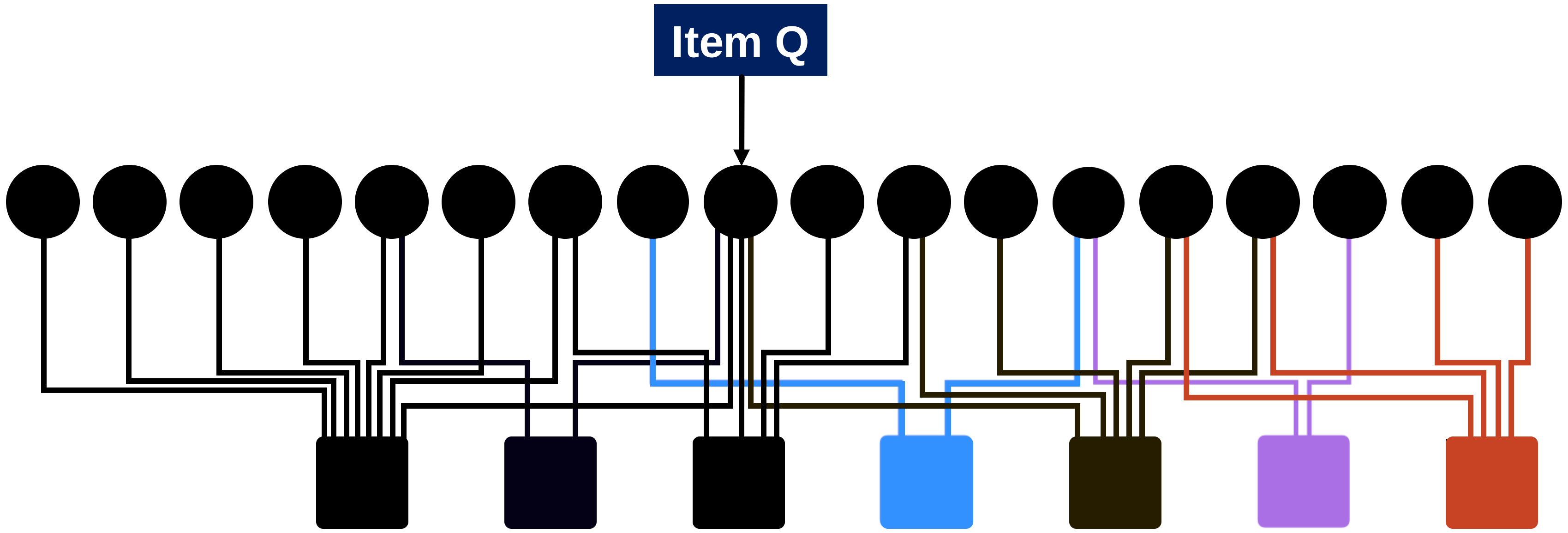
Example: Recommendation

- **Given:**
  A bipartite graph representing user and item interactions (e.g. purchase)



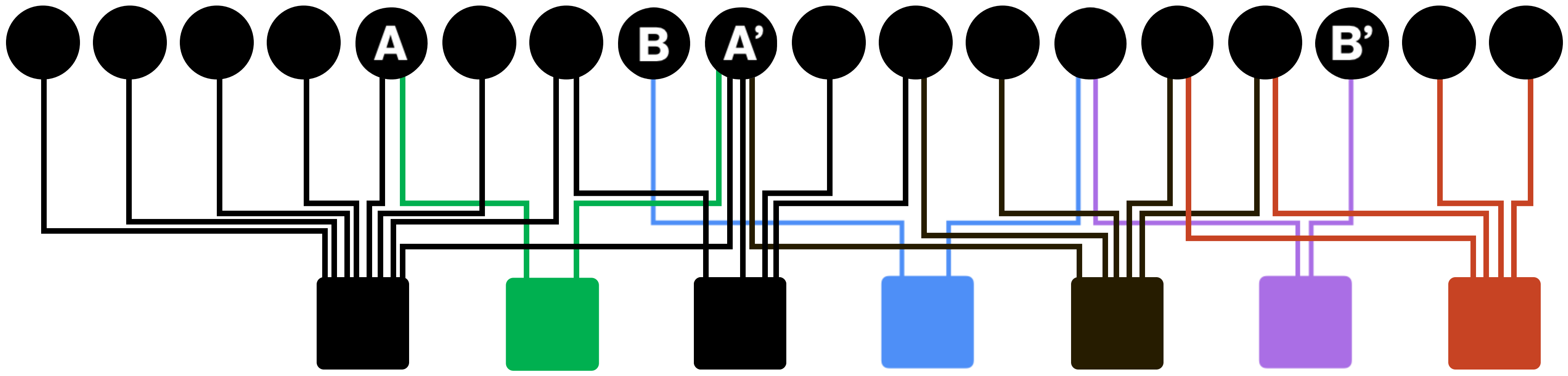
Bipartite User-Item Graph

- **Goal:** Proximity on graphs
  - **What items should we recommend to a user who interacts with item Q?**
  - **Intuition**: if items Q and P are interacted by similar users, recommend P when user interacts with Q



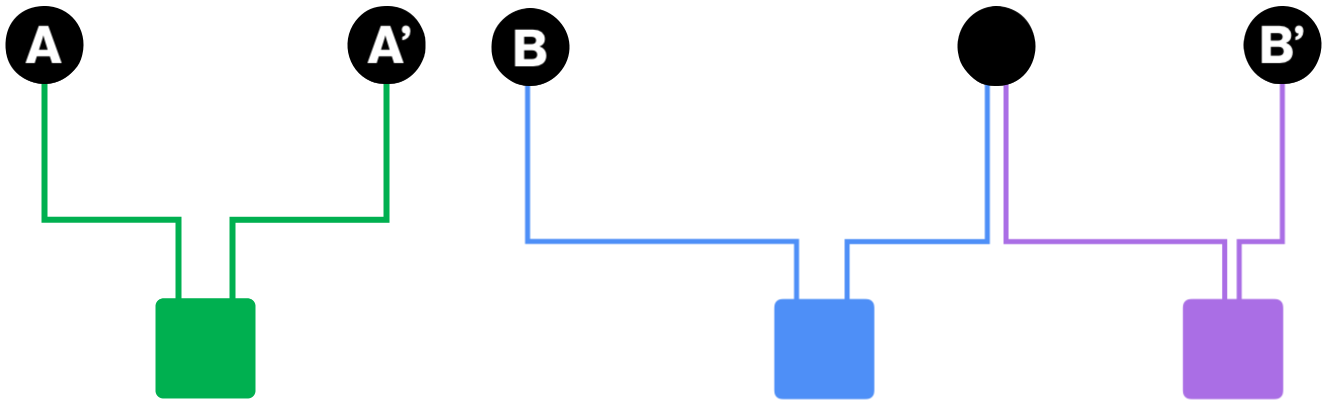
Bipartite User-to-Item Graph

- Which is more related A,A’ or B,B’?



Node proximity Measurements

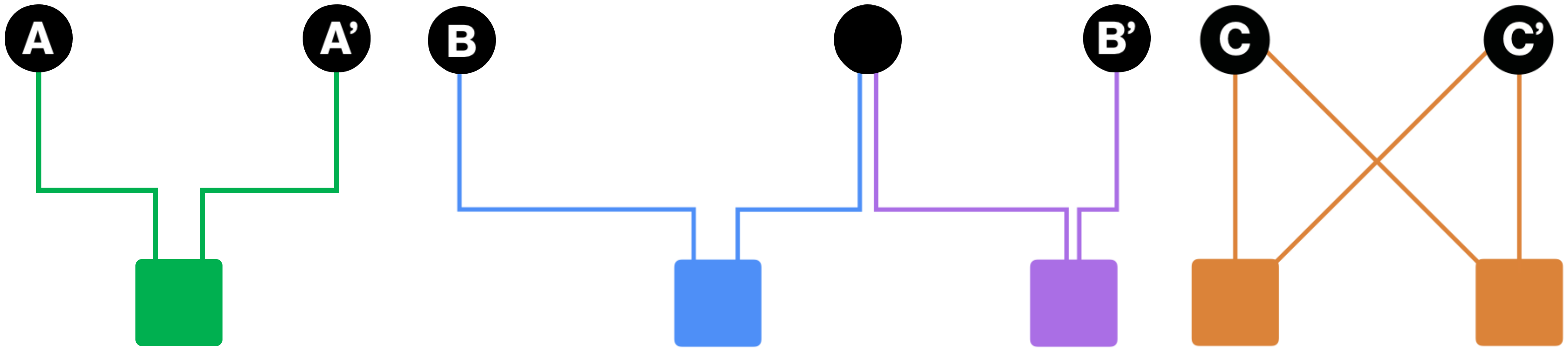
- Which is more related A,A', B,B' or C,C'?



Shortest path

Node proximity Measurements

- Which is more related A,A’, B,B’ or C,C’?

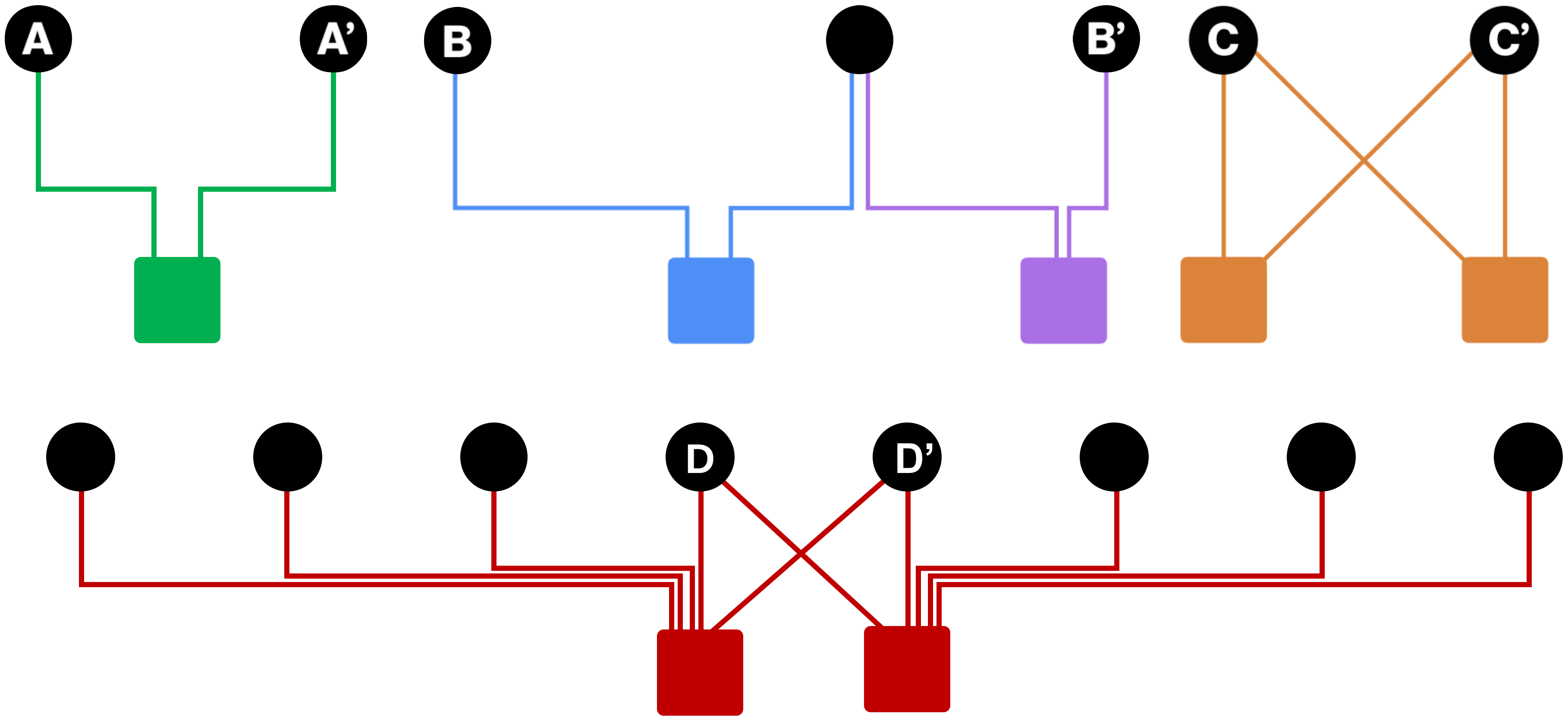


Shortest path

Common Neighbors

Node proximity Measurements

- Which is more related A,A', B,B' or C,C'?



Personalized Page Rank/Random Walk with Restarts

Proximity on Graphs

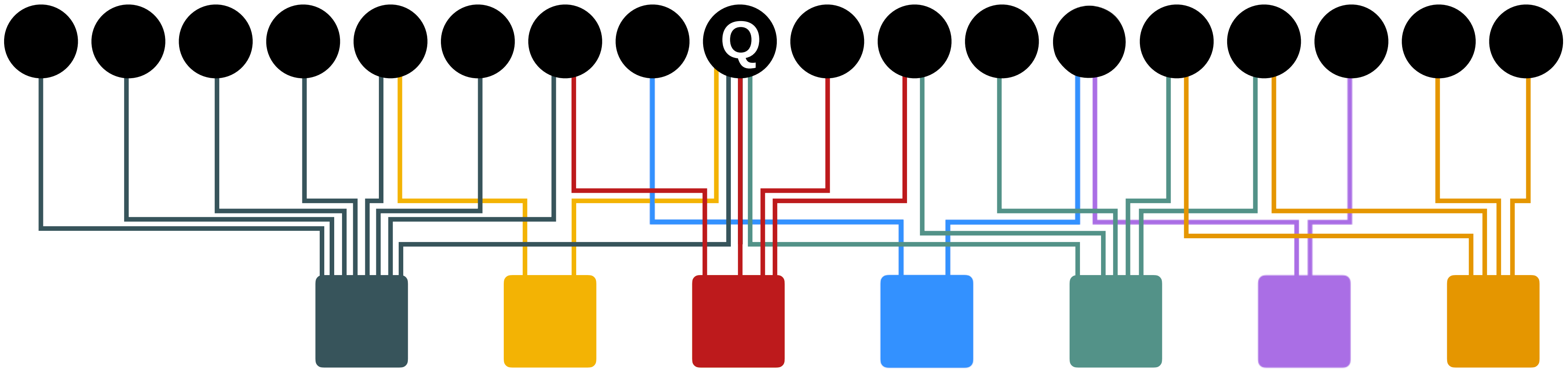
- **PageRank:**
  - Ranks nodes by "importance"
  - Teleports with uniform probability to any node in the network
- **Personalized PageRank:**
  - Ranks proximity of nodes to the teleport nodes $\boldsymbol{S}$
- **Proximity on graphs:**
  - **Q:** What is most related item to **Item Q**?
  - **Random Walks with Restarts**
    - Teleport back to the starting node: $\boldsymbol{S} = \{\boldsymbol{Q}\}$

Idea: Random Walks

- **Idea**
  - Every node has some importance
  - Importance gets evenly split among all edges and pushed to the neighbors:
- **Given a set of QUERY_NODES, we simulate a random walk:**
  - Make a step to a random neighbor and record the visit (visit count)
  - With probability ALPHA, restart the walk at one of the QUERY_NODES
  - The nodes with the highest visit count have highest proximity to the QUERY_NODES

Random Walks

- **Idea:**
  - Every node has some importance
  - Importance gets evenly split among all edges and pushed to the neighbors
- Given a set of **QUERY NODES Q**, simulate a random walk:

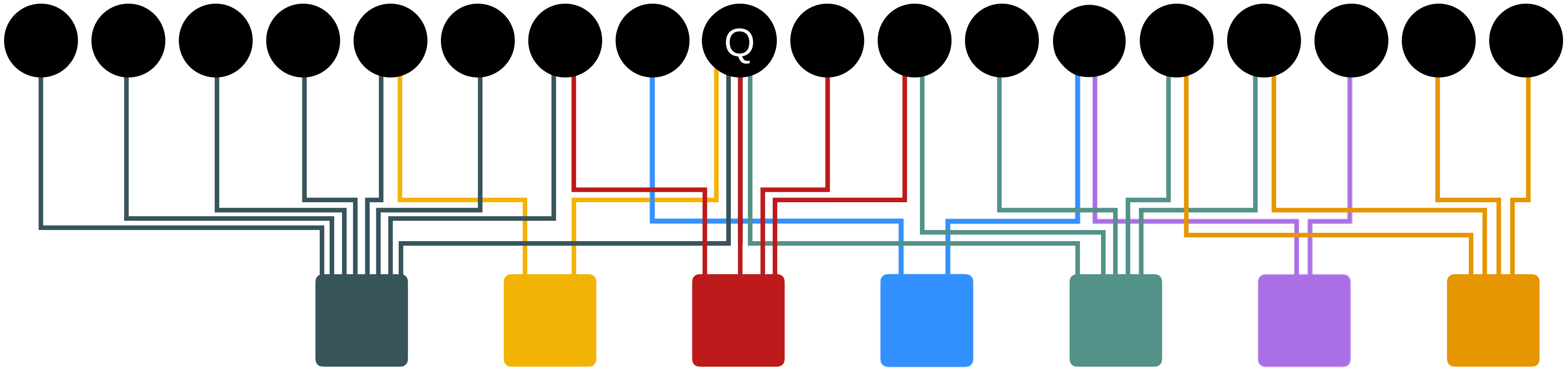


Random Walk Algorithm

- Proximity to query node(s) ***Q***:

```
ALPHA = 0.5
QUERY_NODES = { Q }
```

```
item = QUERY_NODES.sample_by_weight( )
for i in range( N_STEPS ):
    user = item.get_random_neighbor( )
    item = user.get_random_neighbor( )
    item.visit_count += 1
    if random( ) < ALPHA:
        item = QUERY_NODES.sample.by_weight ( )
```



Random Walk Algorithm

- Proximity to query node(s) ***Q***:

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ALPHA = 0.5
QUERY_NODES = { Q }
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```
item = QUERY_NODES.sample_by_weight( )
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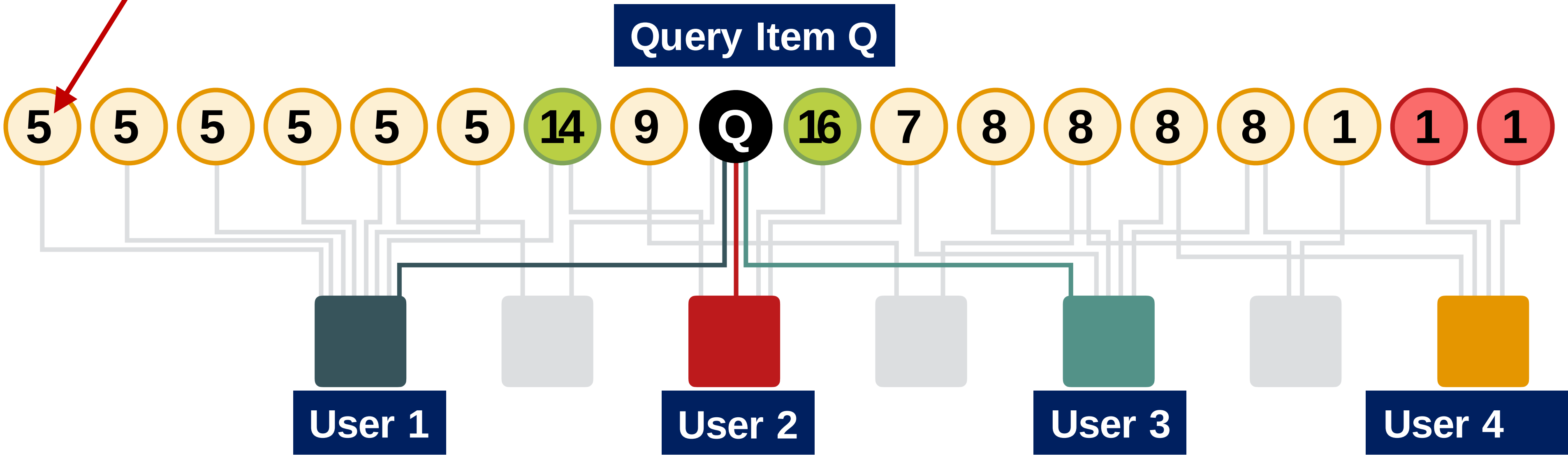
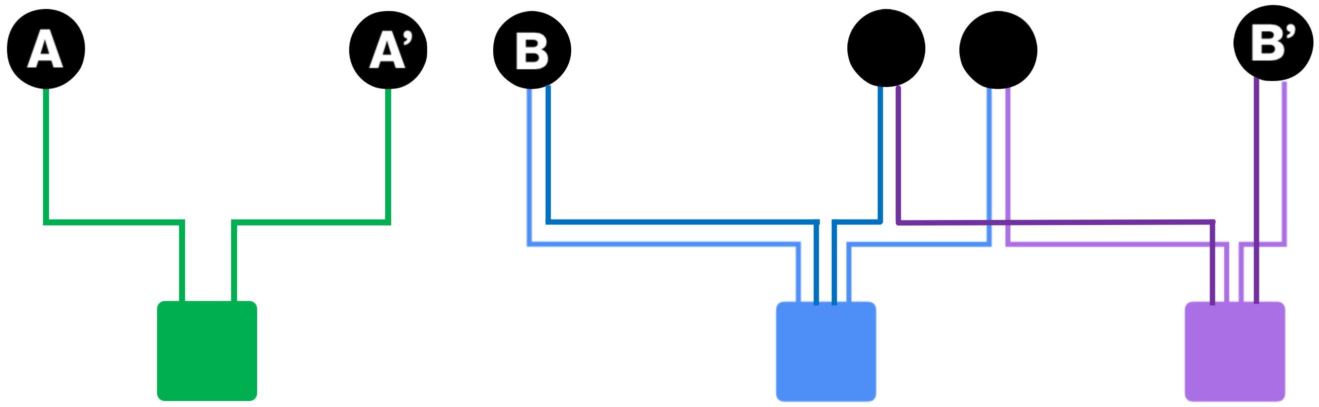


Benefits

- **Why is this a good solution?**
- **Because the “similarity” considers:**
  - Multiple connections
  - Multiple paths
  - Direct and indirect connections
  - Degree of the node



Summary: Page Rank Variants

- **PageRank:**
  - Teleports to any node
  - Nodes can have the same probability of the surfer landing:
    $$\boldsymbol{S} = [0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1, 0.1]$$
- **Topic-Specific PageRank** aka **Personalized PageRank:**
  - Teleports to a specific set of nodes
  - Nodes can have different probabilities of the surfer landing there:
    $$\boldsymbol{S} = [0.1, 0, 0, 0.2, 0, 0, 0.5, 0, 0, 0.2]$$
- **Random Walk with Restarts:**
  - Topic-Specific PageRank where teleport is always to the same node:
    $$\boldsymbol{S} = [0, 0, 0, 0, \mathbf{1}, 0, 0, 0, 0, 0, 0]$$

Summary

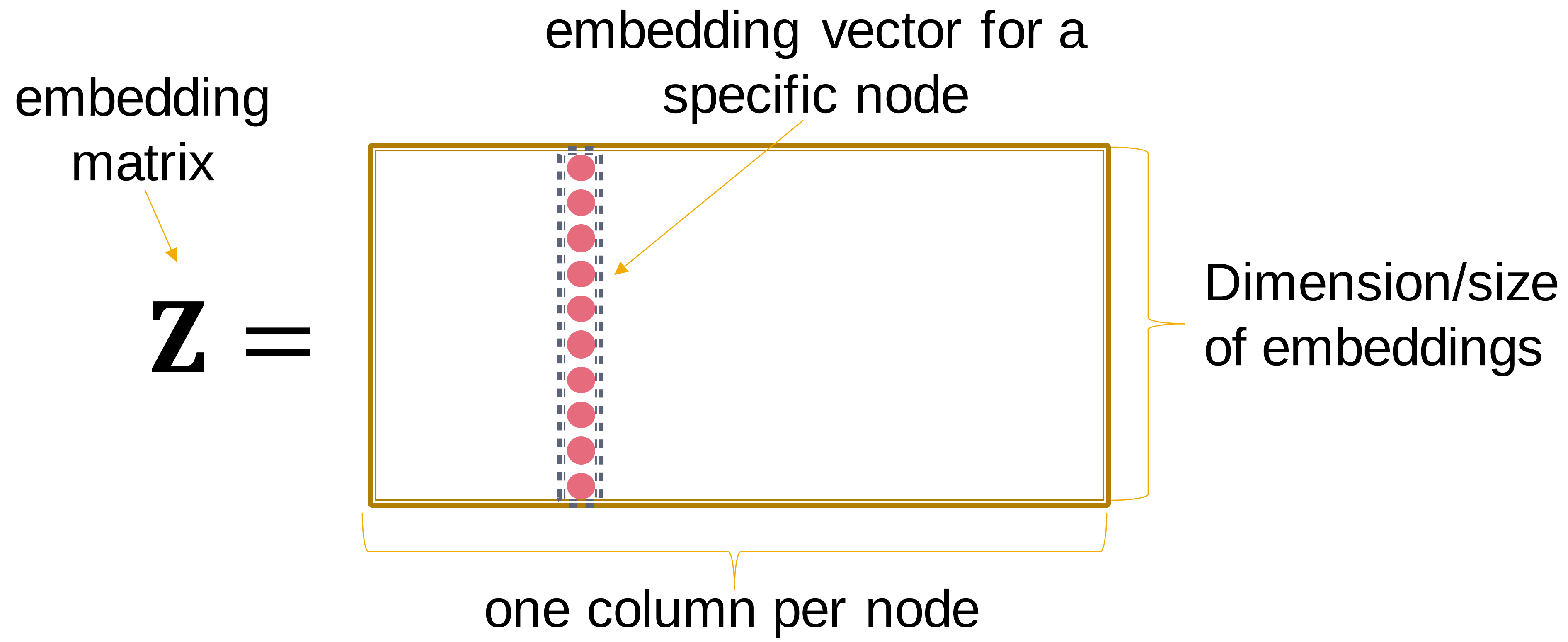
- A graph is naturally represented as a matrix
- We defined a random walk process over the graph
  - Random surfer moving across the links and with random teleportation
  - Stochastic adjacency matrix M
- PageRank = Limiting distribution of the surfer location represented node importance
  - Corresponds to the leading eigenvector of transformed adjacency matrix M.

Stanford CS224W: Matrix Factorization and Node Embeddings

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Embeddings & Matrix Factorization

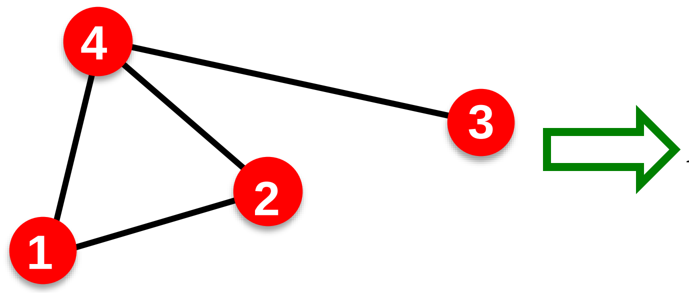
- **Recall:** encoder as an embedding lookup


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

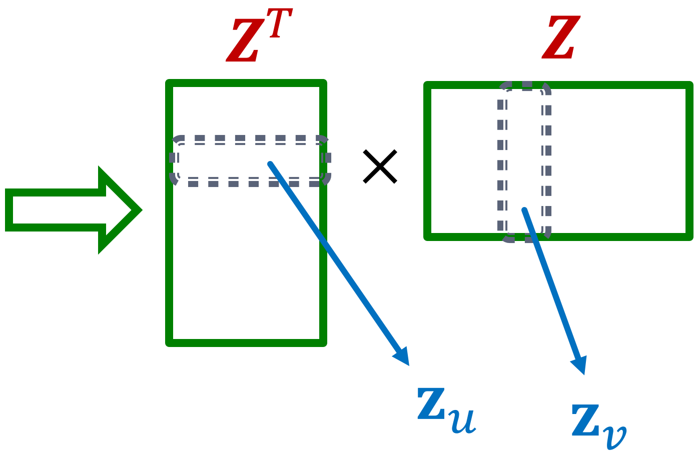
Objective: maximize $\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u$ for node pairs (u, v) that are **similar**

Connection to Matrix Factorization

- Simplest **node similarity**: Nodes u, v are similar if they are connected by an edge
- This means: $\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u = A_{u,v}$ which is the (u, v) entry of the graph adjacency matrix A
- Therefore, $\boldsymbol{Z}^T \boldsymbol{Z} = A$



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



Matrix Factorization

- The embedding dimension d (number of rows in $\boldsymbol{Z}$) is much smaller than number of nodes n.
- Exact factorization $A = \boldsymbol{Z}^T\boldsymbol{Z}$ is generally not possible
- However, we can learn $\boldsymbol{Z}$ approximately
- **Objective:** $\min_{\mathbf{Z}} \parallel \mathrm{A} - \boldsymbol{Z}^T\boldsymbol{Z} \parallel_2$
  - We optimize $\boldsymbol{Z}$ such that it minimizes the L2 norm (Frobenius norm) of $\mathrm{A} - \boldsymbol{Z}^T\boldsymbol{Z}$
  - Note in Lecture 3 we used softmax instead of L2. But the goal to approximate A with $\boldsymbol{Z}^T\boldsymbol{Z}$ 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:

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

  - 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

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

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

See Lec 3 slide 30:

$T = |N_R(u)|$

Power of normalized adjacency matrix

Number of negative samples

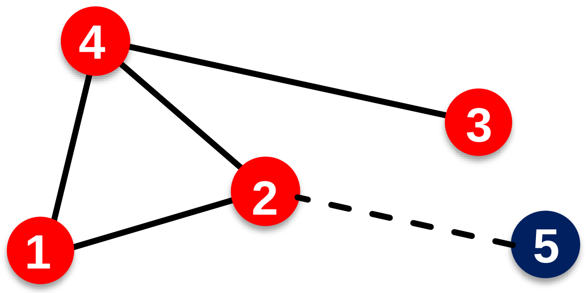
- **Node2vec** can also be formulated as a matrix factorization (albeit a more complex matrix)
- Refer to the paper for more details:

Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec, WSDM 18

Limitations (1)

Limitations of node embeddings via matrix factorization and random walks

- Cannot obtain embeddings for nodes not in the training set



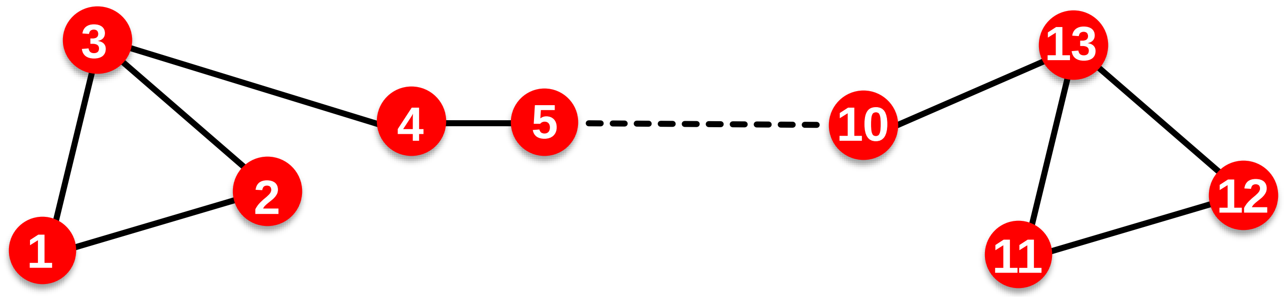
Training set

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**:

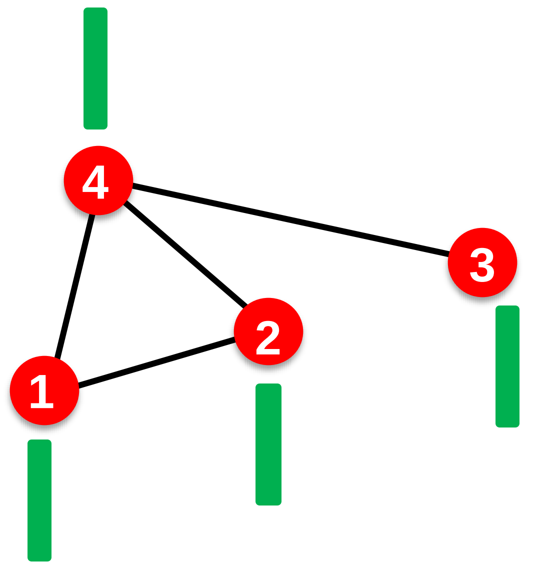


- Node 1 and 11 are **structurally similar** – part of one triangle, degree 2, …
- However, they have very **different** embeddings.
  - It's unlikely that a random walk will reach node 11 from node 1.

- **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 week)

Summary

- **PageRank**
  - Measures importance of nodes in graph
  - Can be efficiently computed by **power iteration of adjacency matrix**
- **Personalized PageRank (PPR)**
  - Measures importance of nodes with respect to a particular node or set of nodes
  - Can be efficiently computed by **random walk**
- **Node embeddings** based on random walks can be expressed as **matrix factorization**
- **Viewing graphs as matrices plays a key role in all above algorithms!**