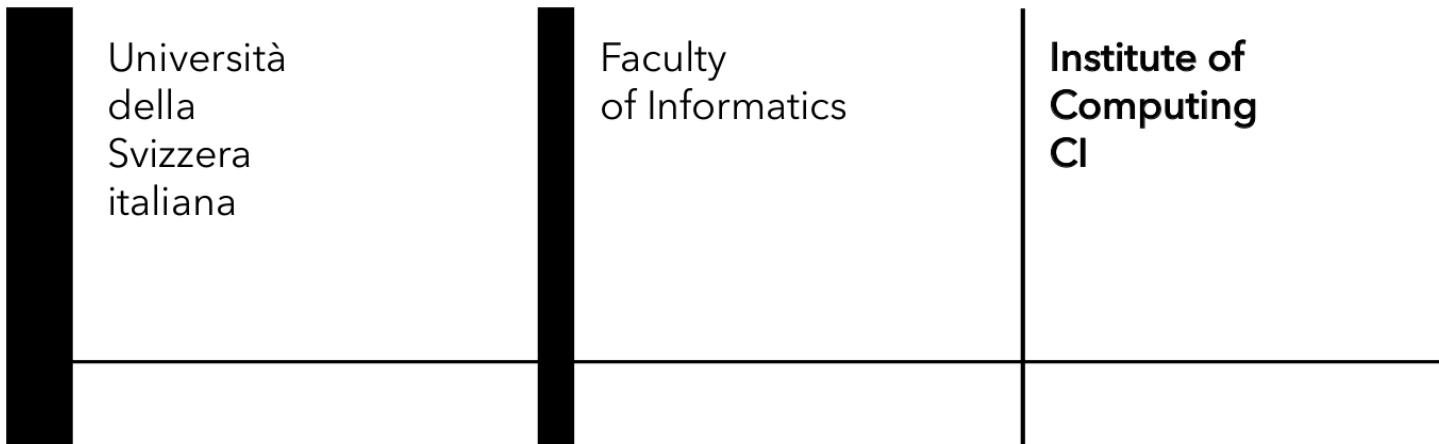


Analysis of large graphs with PageRank vectors

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Institute of Computing
Università della Svizzera italiana

September 26, 2023



Course calendar

Project 1



PagerRank and networks

26.09

Project 2



Graph partitioning

04.10

Project 3



Graph clustering

18.10

Project bonus



Linear least squares

08.11

Project 4



Image deblurring with CG

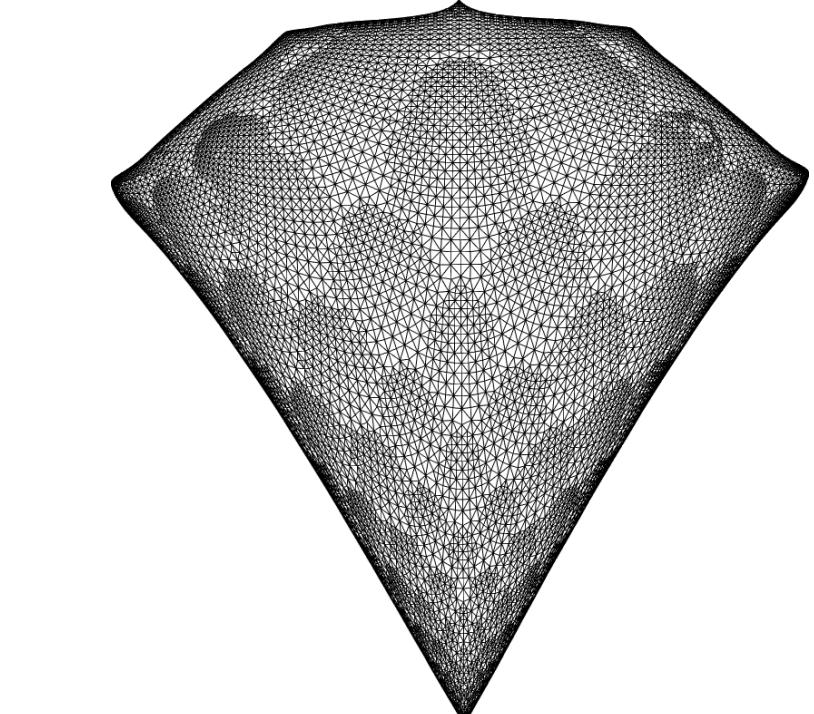
15.11

Today: PageRank and networks

Elements: directed networks, column stochastic matrices, teleportation

PageRank vector: Network structure + Iterative computation

Using: eigenvalue computations, linear system solution



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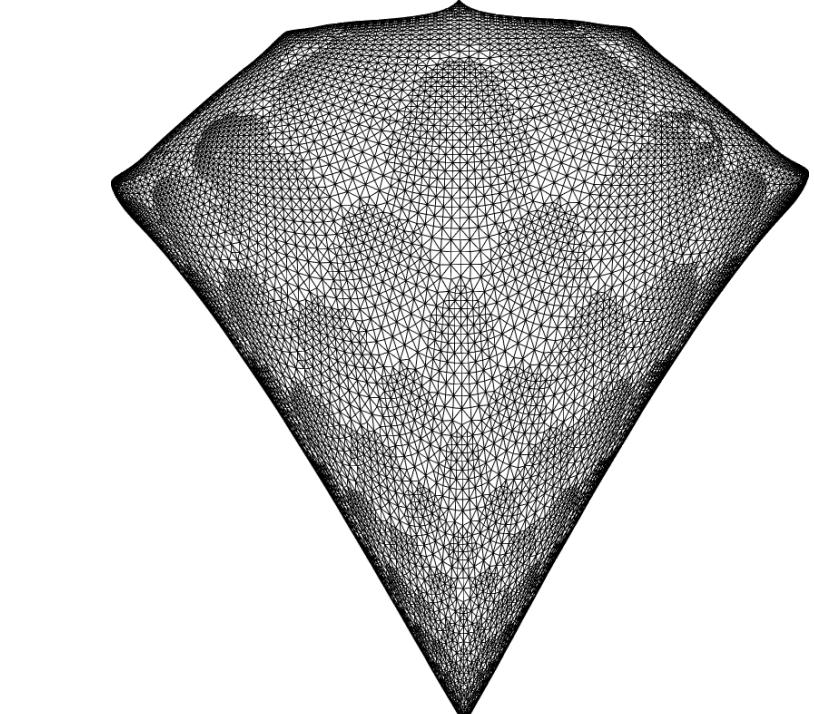
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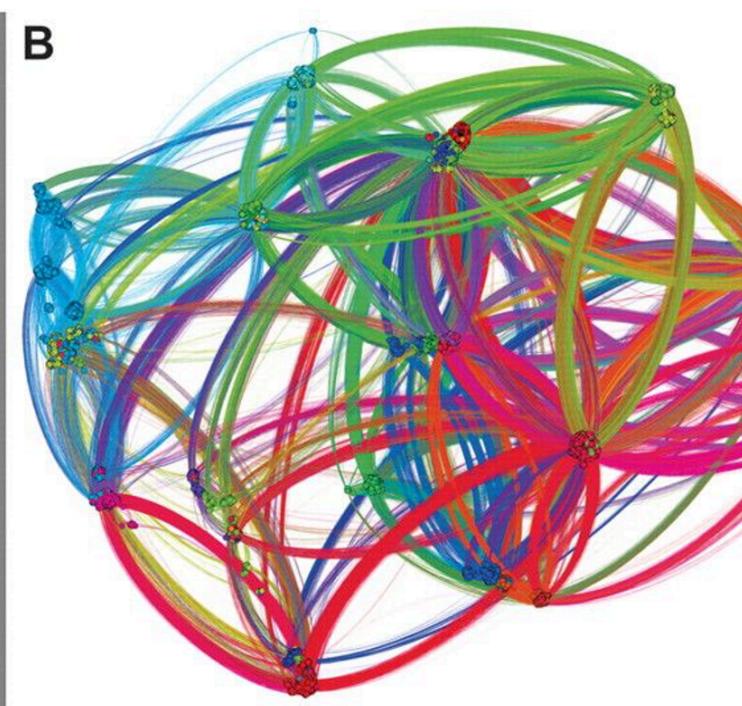
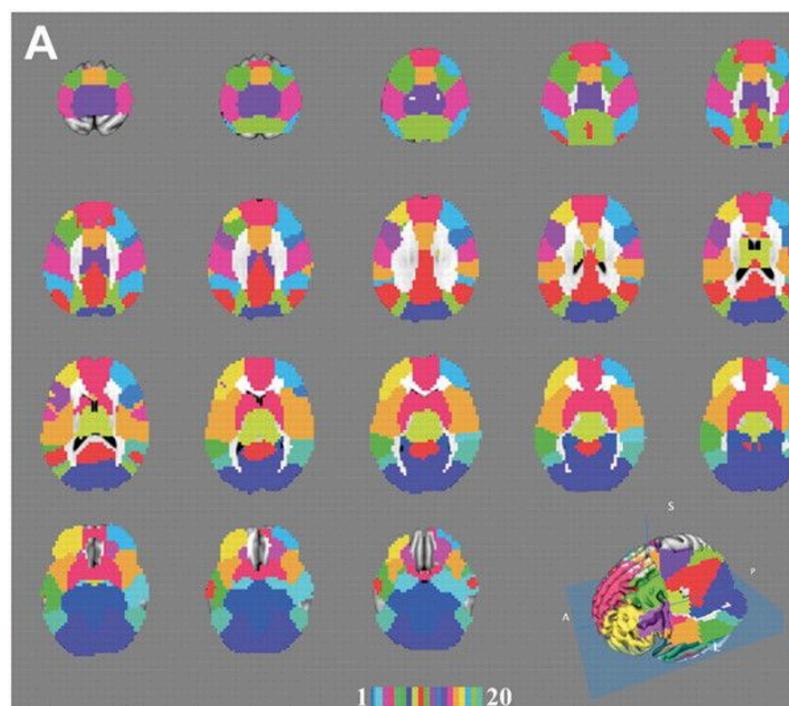
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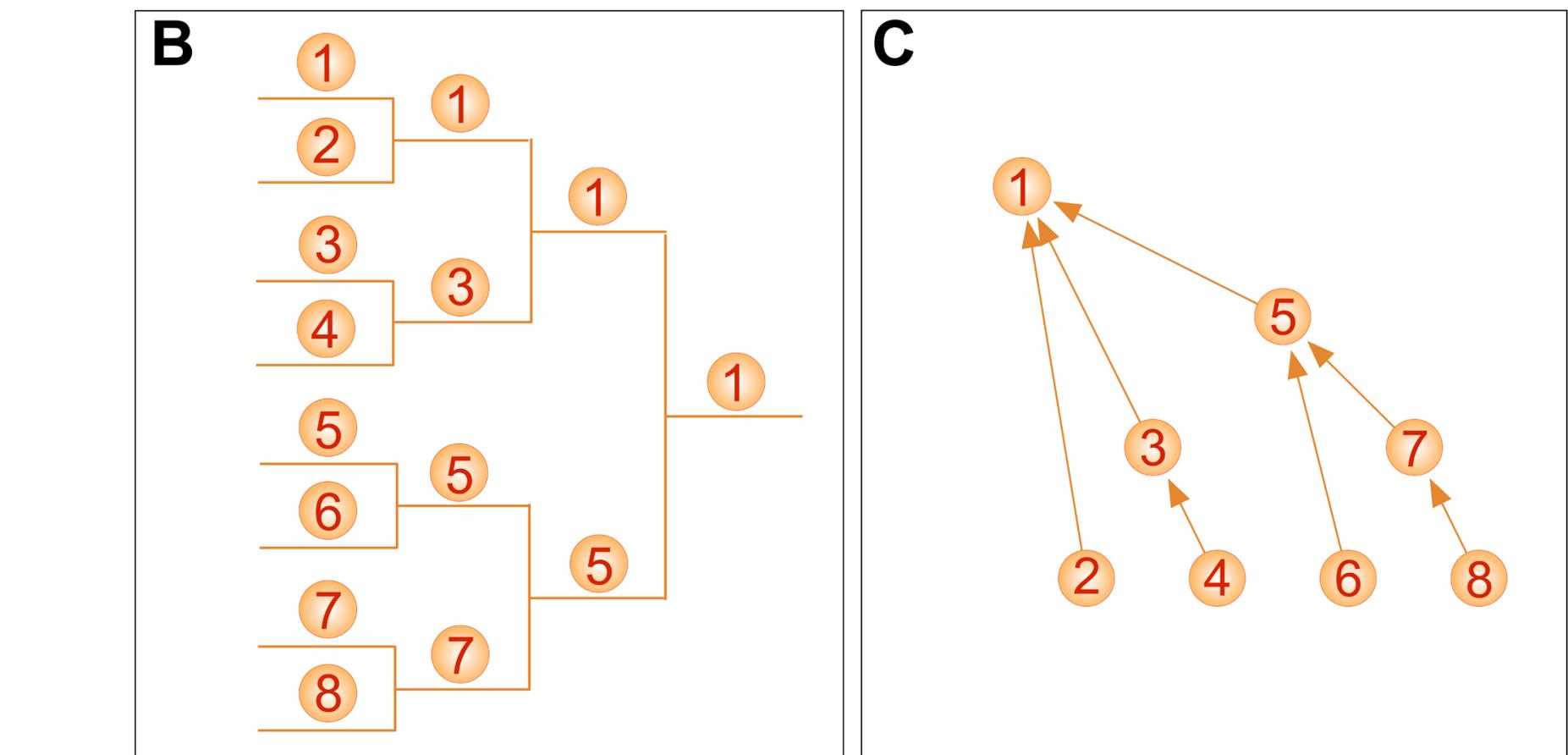
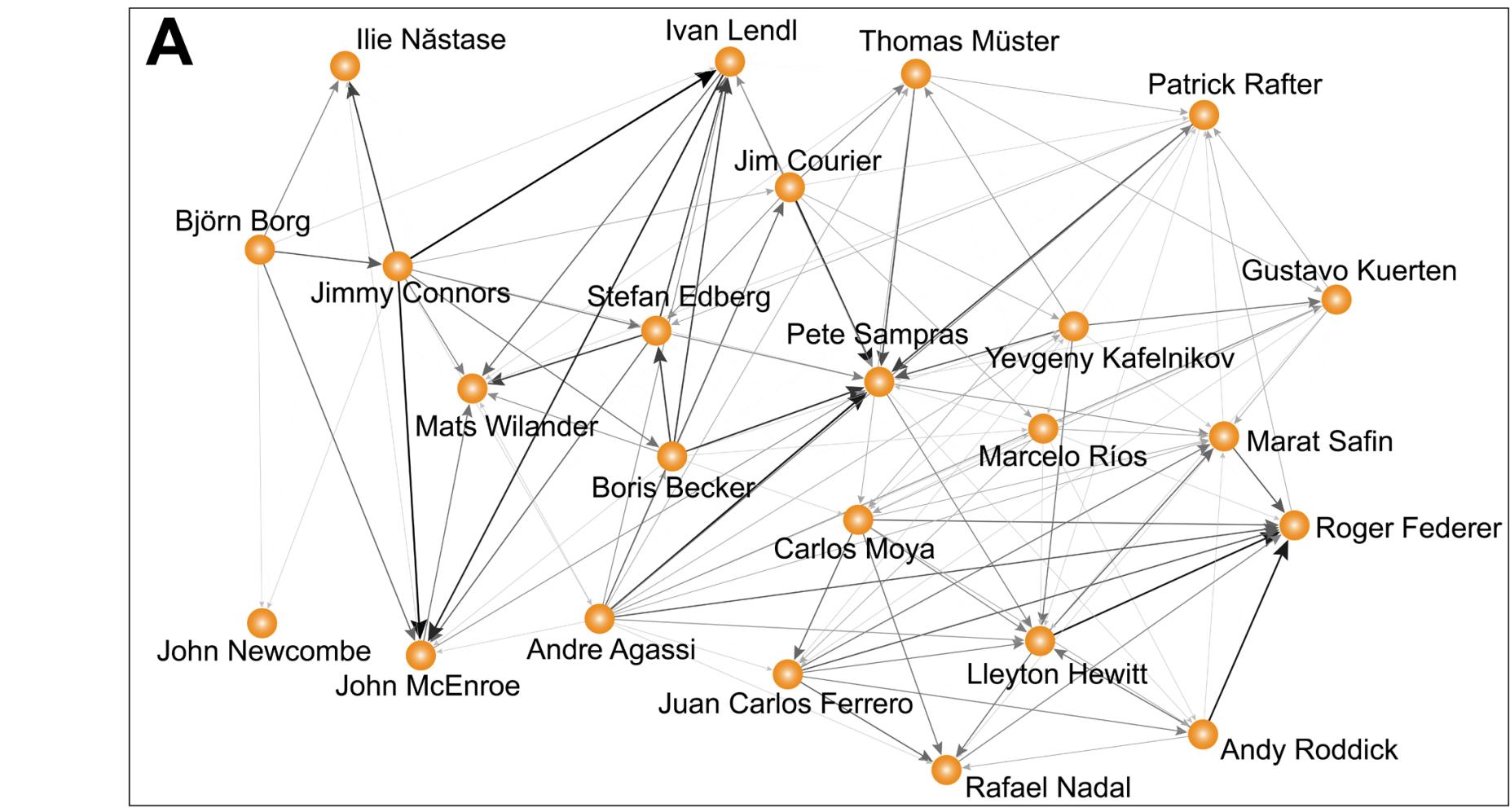
Applications

Rank the importance of graph nodes

- Biology
- Sports
- Local clustering
- ...
- Web search engines



- X.-N. Zuo, et al., Network centrality in the human functional connectome, Cerebral Cortex, 2012.

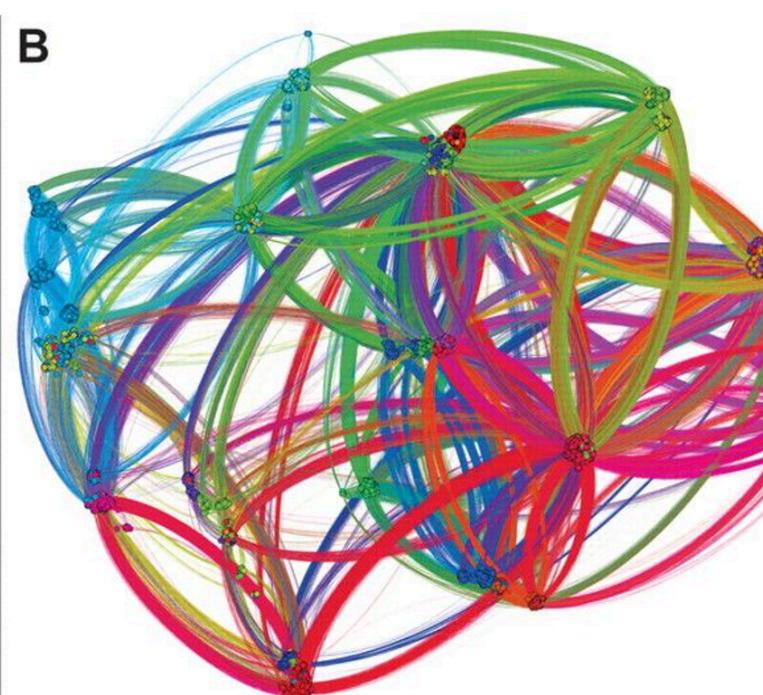
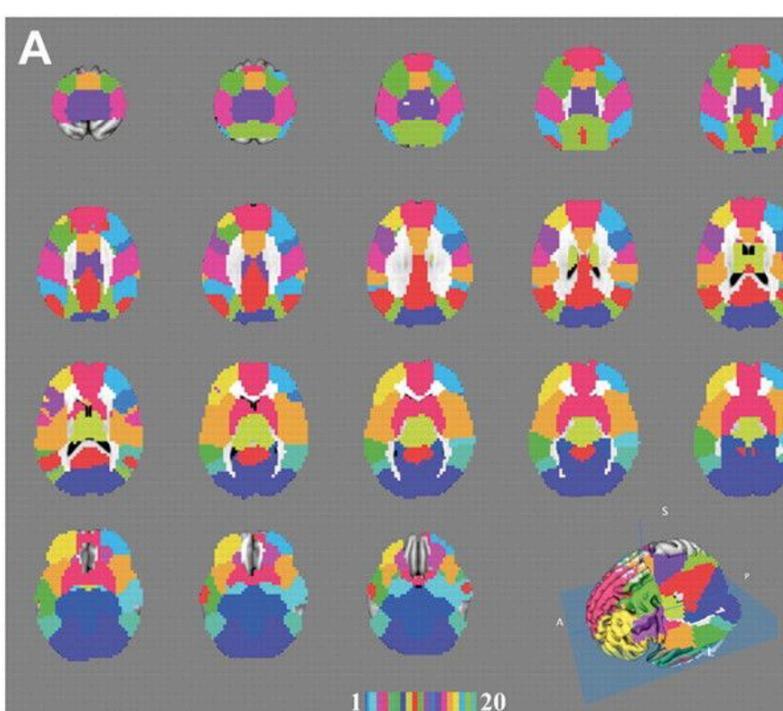


- F. Radicchi, Who is the best player ever? A complex network analysis of the history of professional tennis, PLoS ONE, 2011.

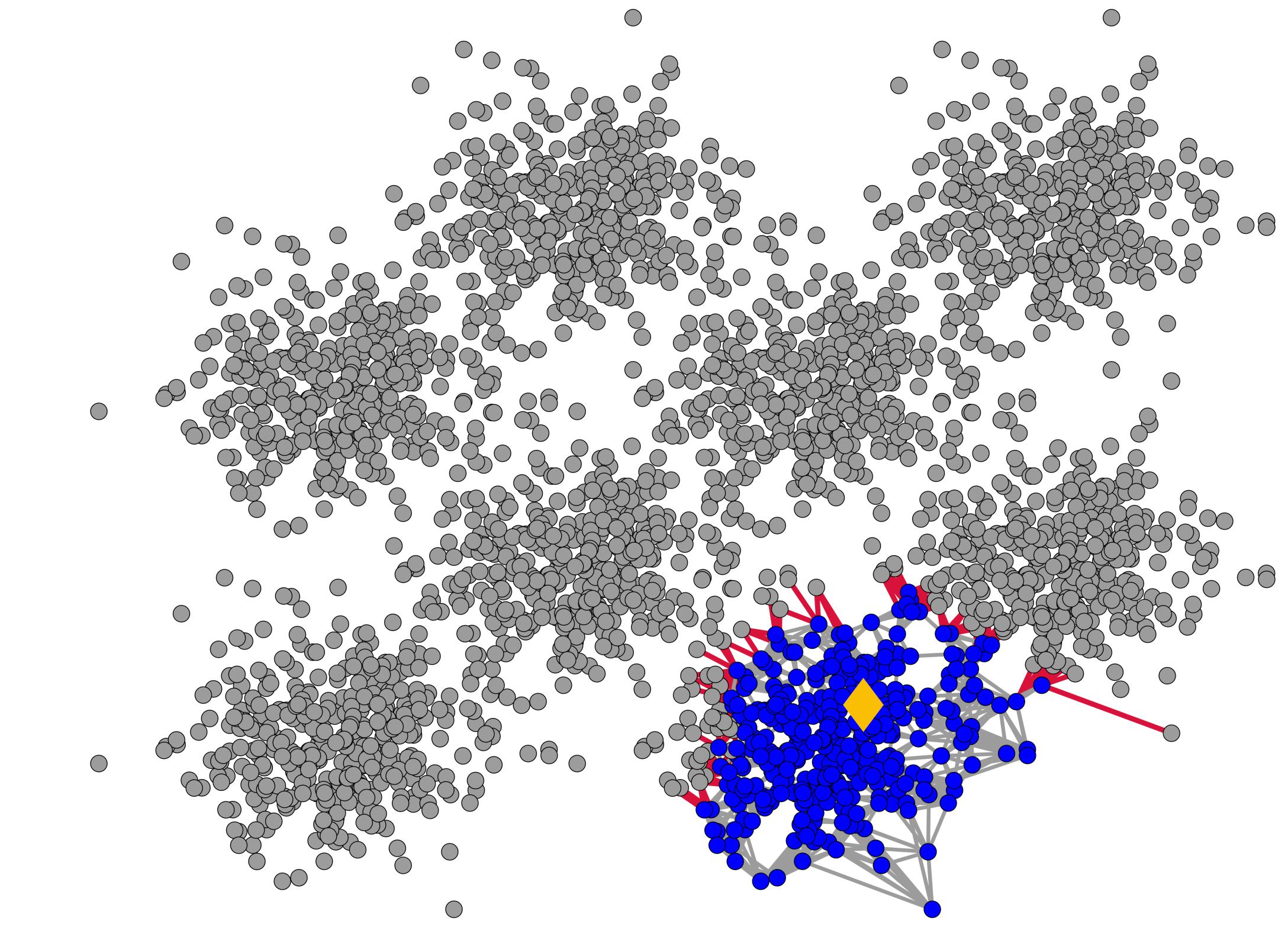
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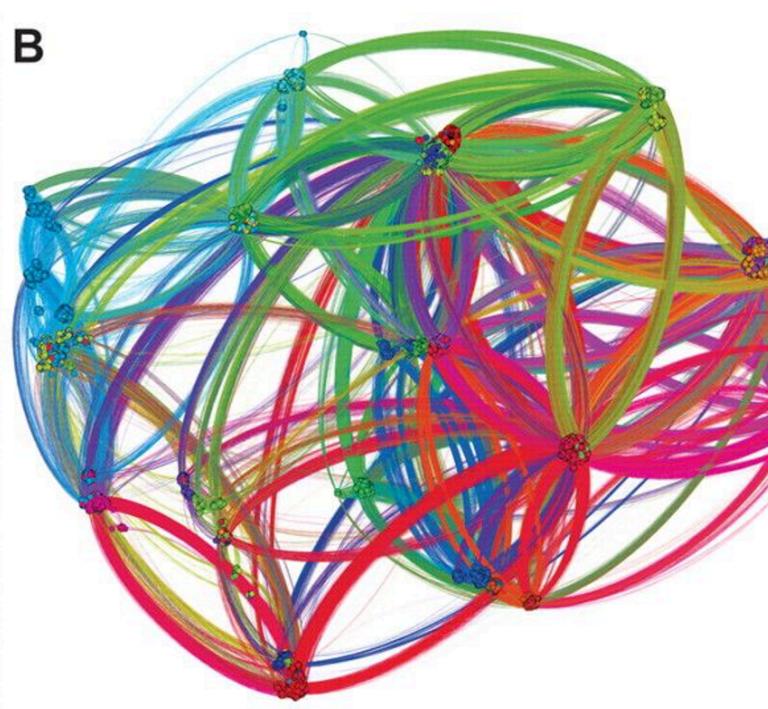
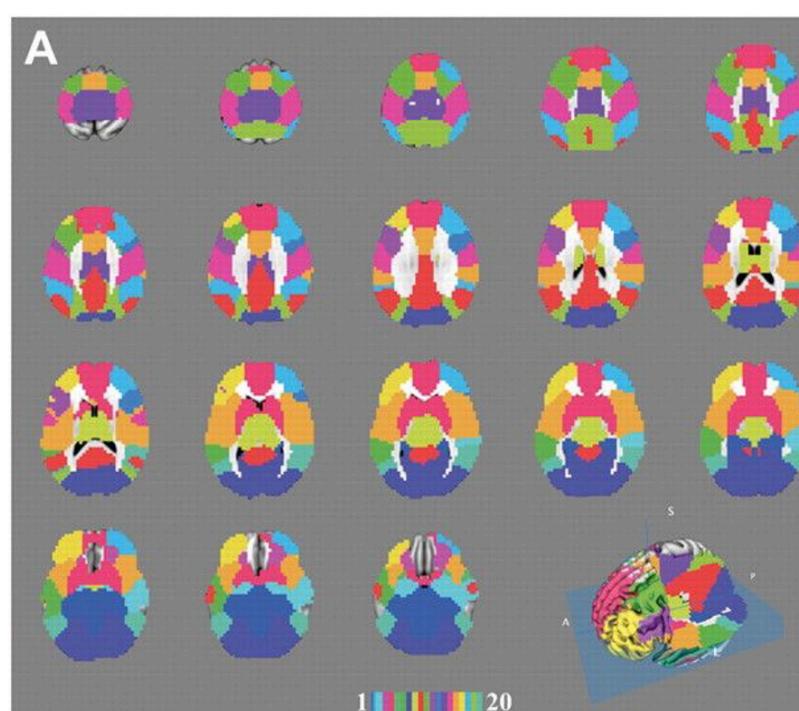


- C. Kodsi, and D. Pasadakis, Nonlinear PageRank for local graph partitioning, *in preparation*, 2023.

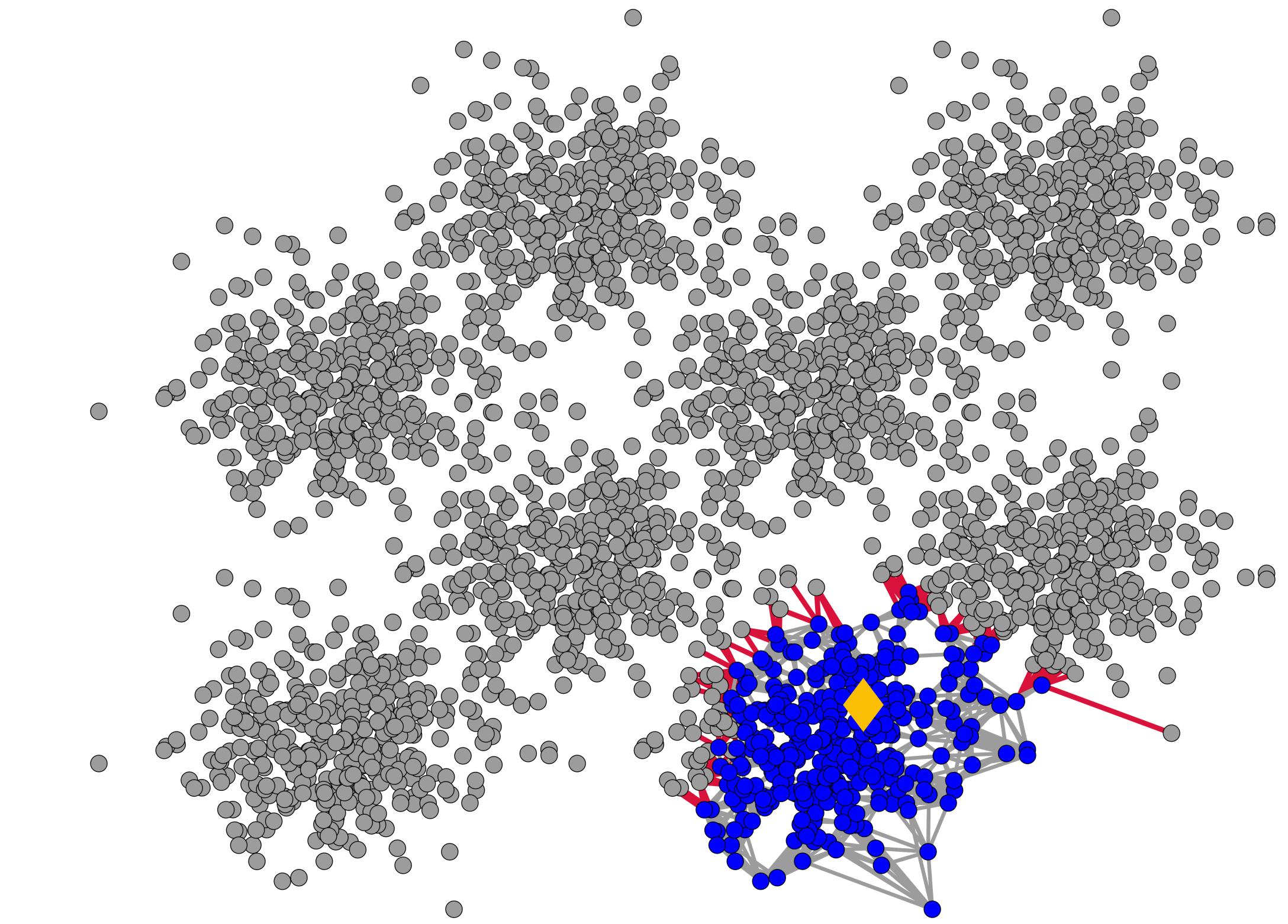
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Rank the importance of graph nodes

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Bringing order to the web

Search engines and users' queries

- ① Text processing to find all documents using the query terms.
 - Look-up into an inverted file, with a vector space method, or
 - query expander that uses a thesaurus.
- ✖ Massive size of the web, thousands of results.
- ➔ Rank this list based on some ranking criterion.



Martin Grandjean. A social network analysis of Twitter: Mapping the digital humanities community. Cogent Arts & Humanities, 3(1), apr 2016.

Bringing order to the web

Search engines and users' queries

② Exploit additional information to rank the results

- The web has a hyperlink structure → link analysis.
- The **Google** search engine uses
 - IR (Information Retrieval) score, combined with,
 - PR (PageRank) score.



✓ We will focus on the PR score in this class.

Martin Grandjean. A social network analysis of Twitter: Mapping the digital humanities community. Cogent Arts & Humanities, 3(1), apr 2016.

The web as a directed graph

Graphical structure

- Nodes: webpages ■
- Edges: hyperlinks →
- Not all web pages have the same importance (weight).

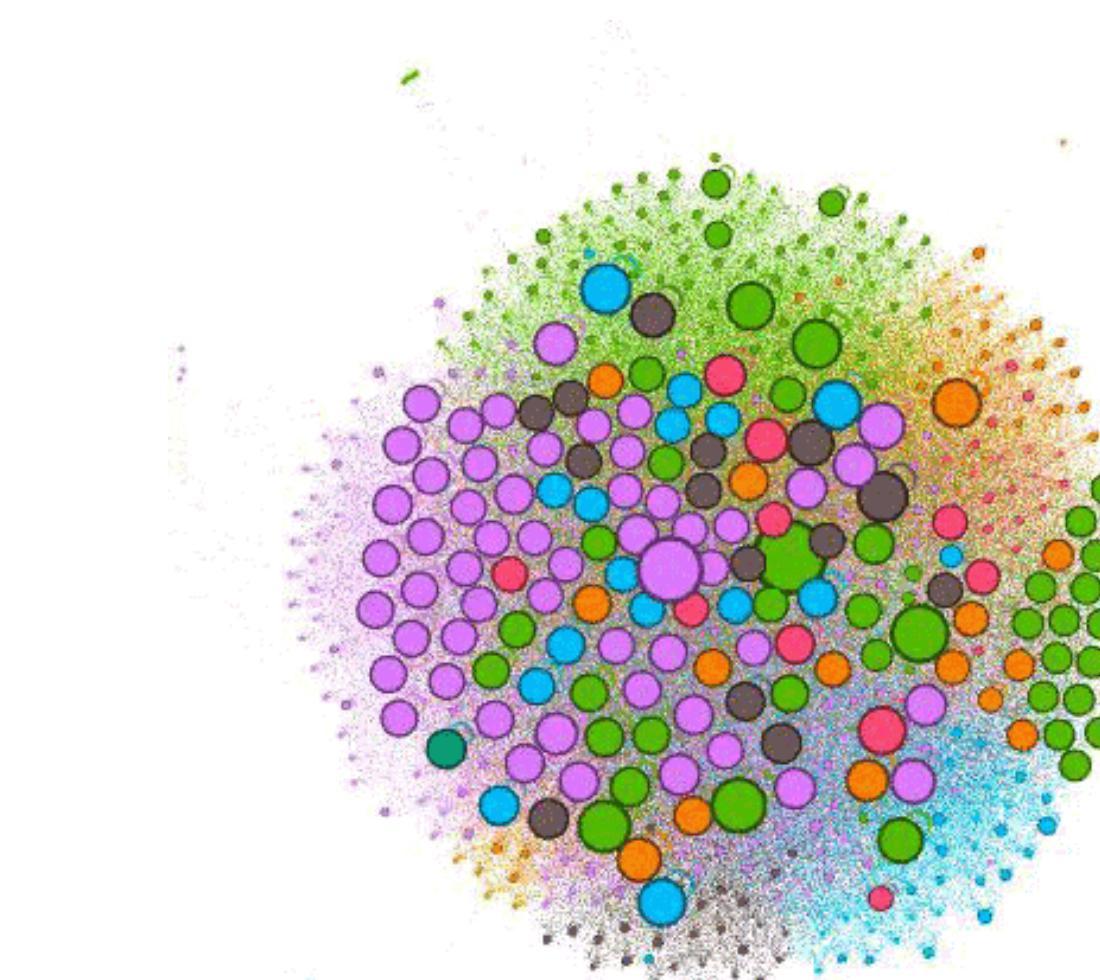
www.usi.ch

vs

[wikipedia.org/wiki/Empididae](https://en.wikipedia.org/wiki/Empididae)

Importance \sim number of links

- In-coming links → ■
- Out-going links ■ →
- Links from important pages
➡ more gravity.



We will rank the pages based on the link structure.

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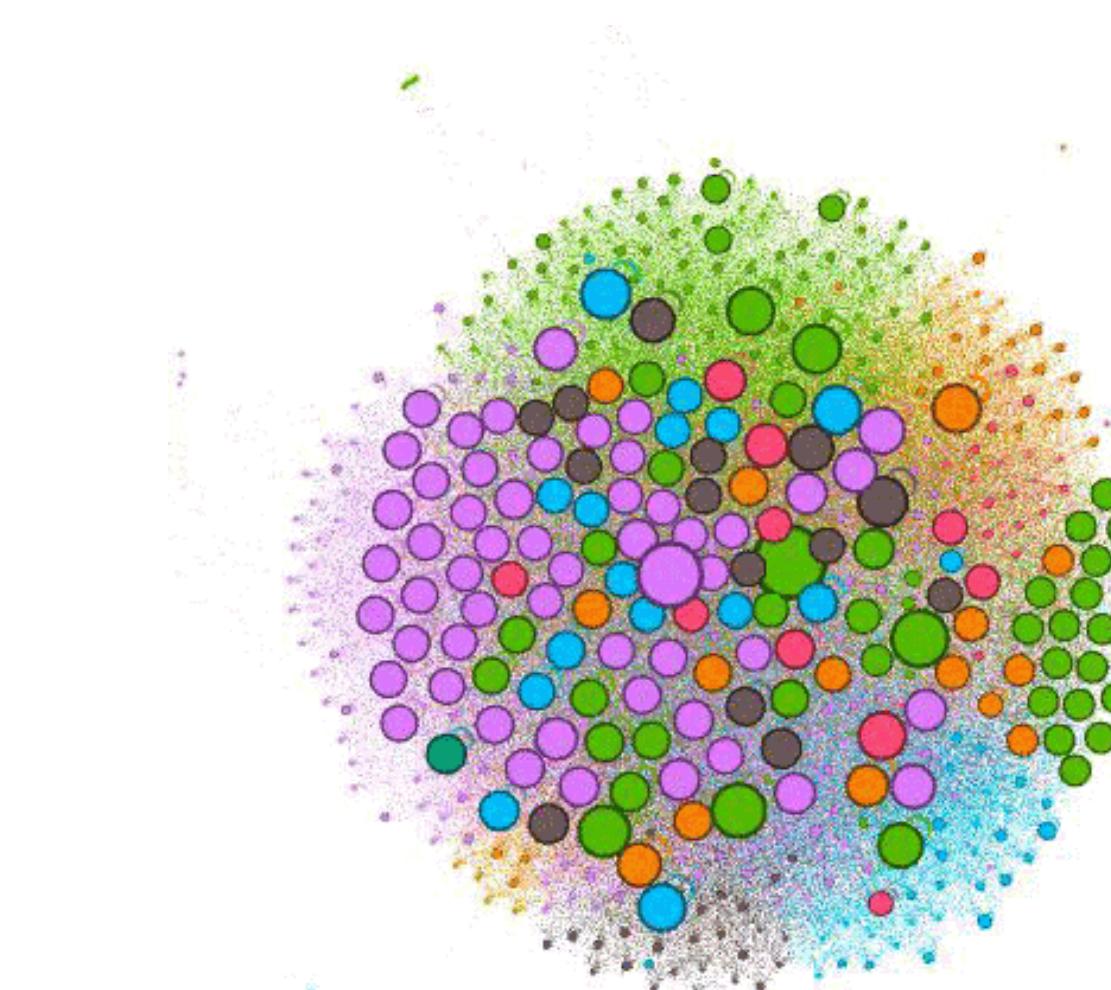
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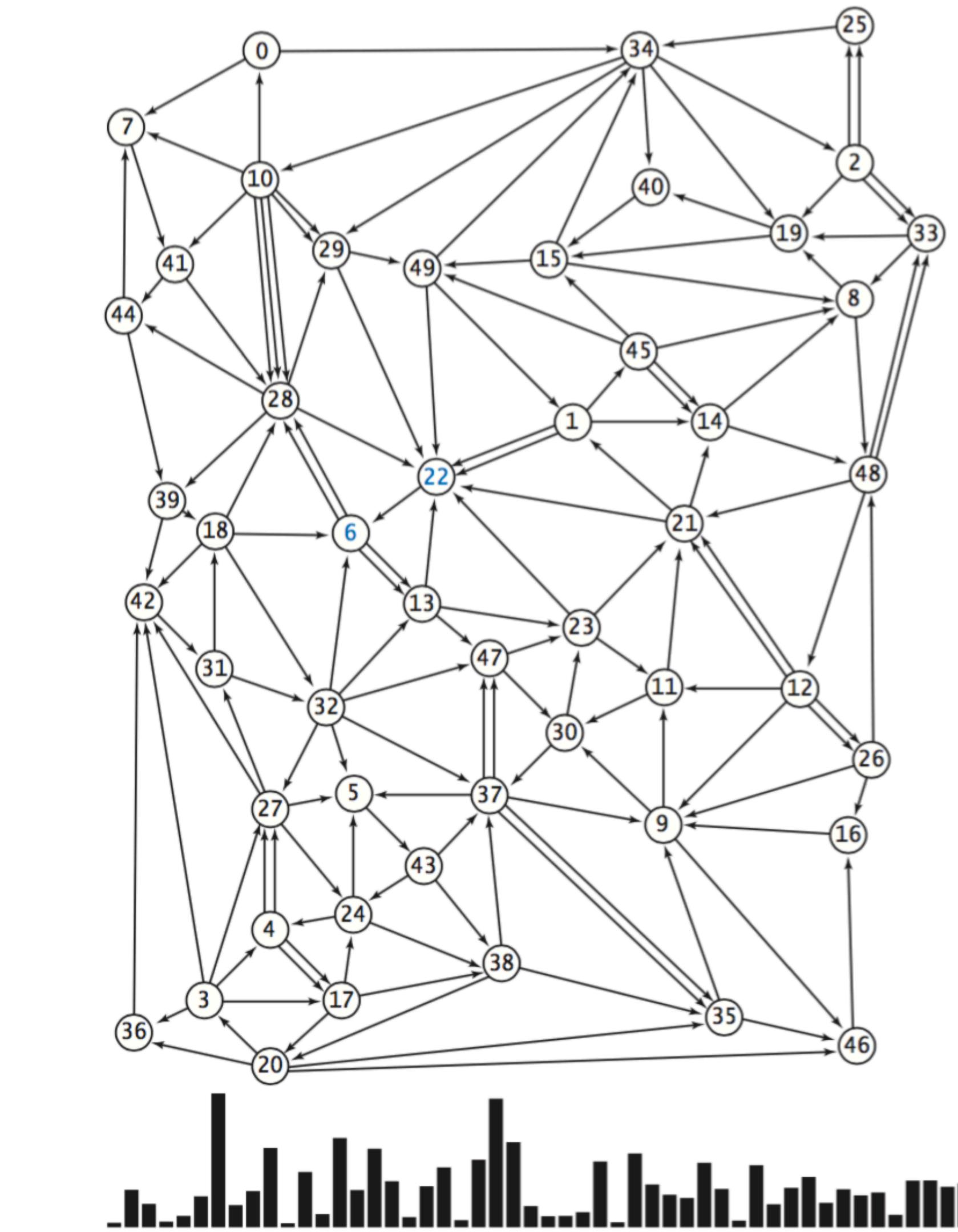


We will rank the pages based on the link structure.

Random surfing

Upon visiting a page on the web, our random surfer tosses a coin.

- ▲ Heads: randomly click a link on the current page and transition.
- ▼ Tails: teleport to a possibly random page.
- Pages where more likely to be visited (based on the web's structure) are more important in a PR sense.
- Teleporting: designed also to model external influence on the importance of nodes, can be more than a random choice.



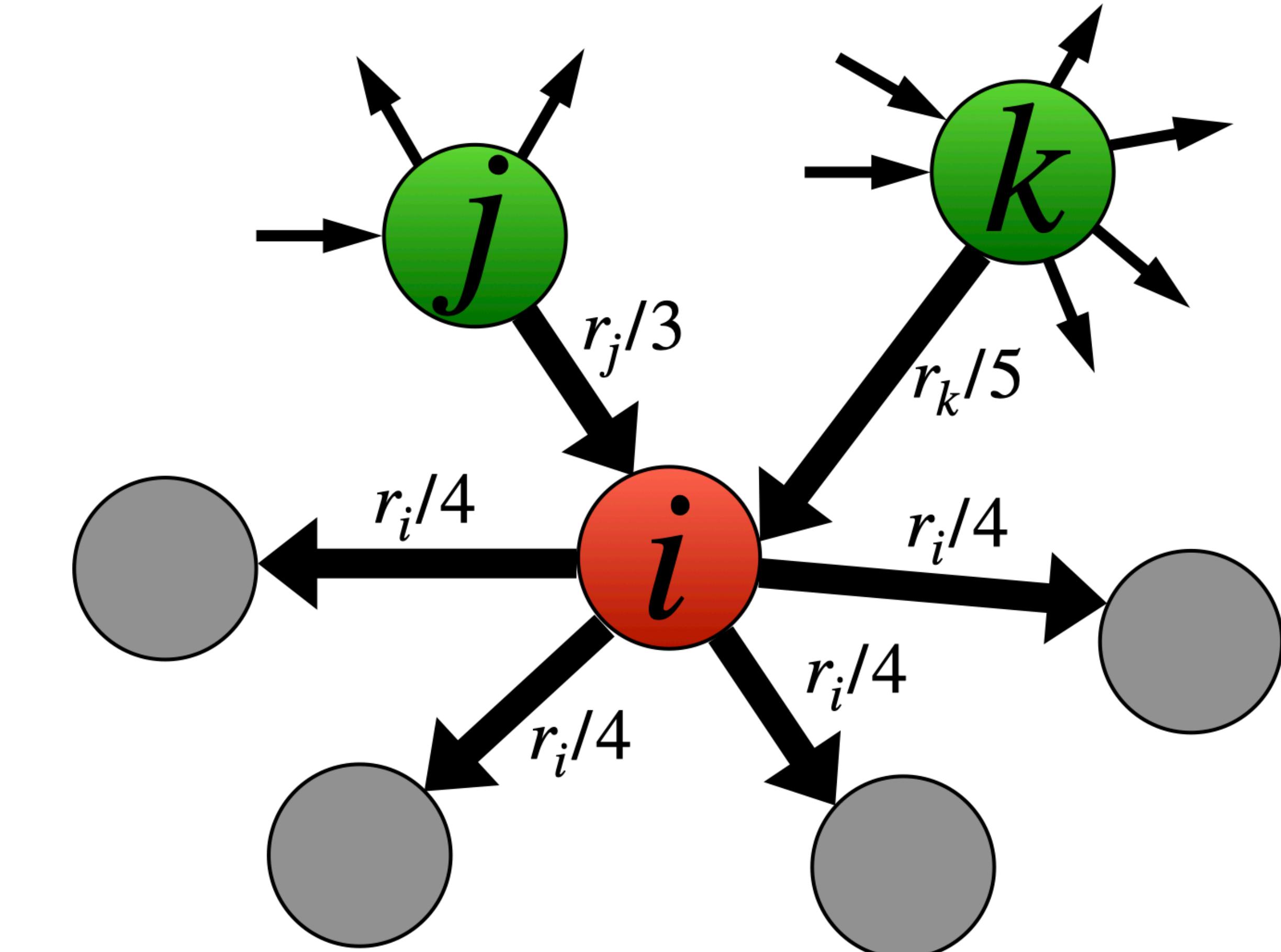
- <https://pi.math.cornell.edu/>, The Mathematics of Google Search.

The PageRank score

A recursive calculation

- Each link's gravity is proportional to the importance of its source page.
- A page i with importance r_i has n out-links. Each link gets r_i/n weight.
- The importance of page i is the sum of the weights on its in-links.

$$r_i = r_j/3 + r_k/5$$

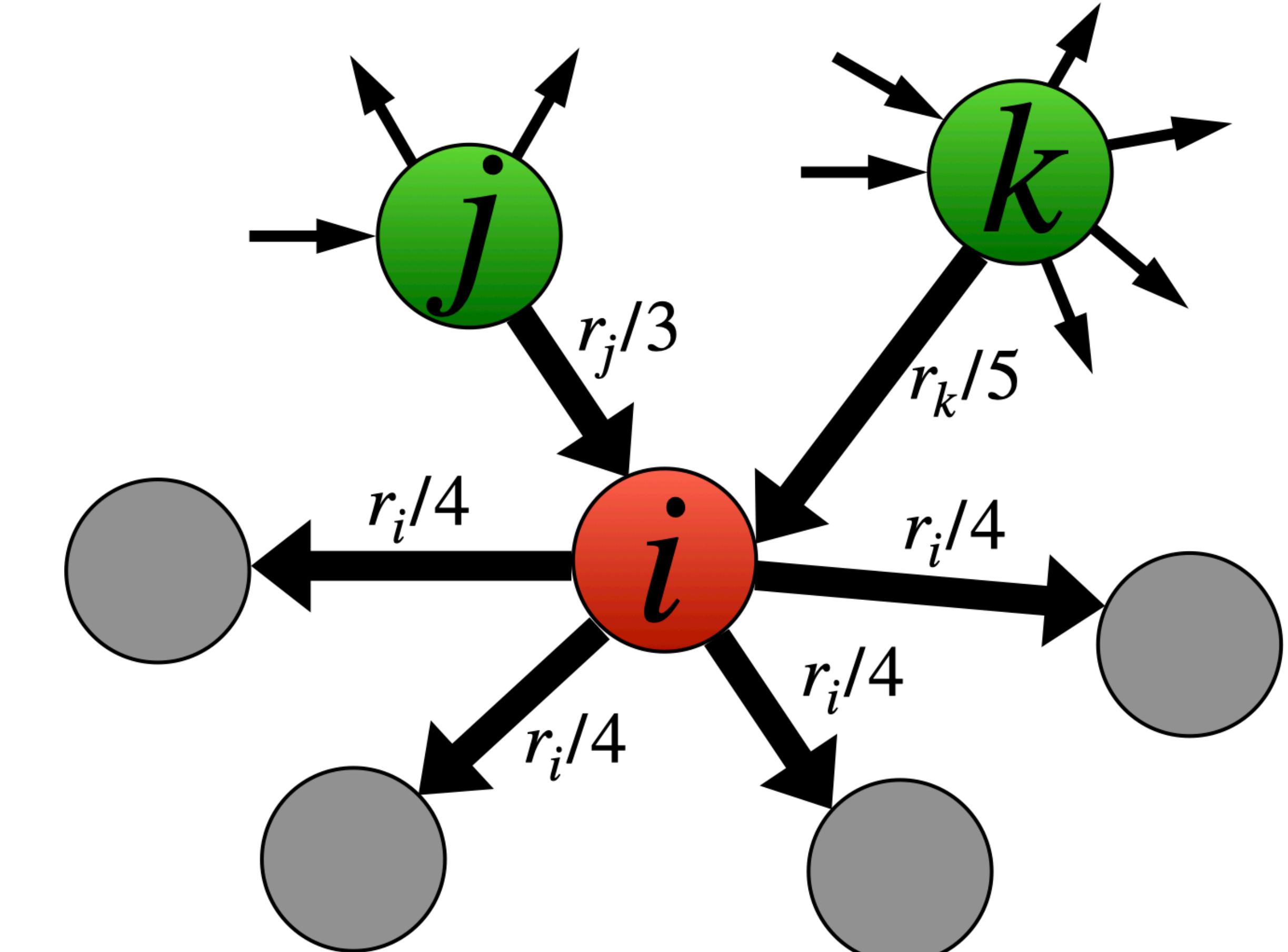


PageRank as a flow model

- The weight of an important page is higher.
- A page is important if other important pages → to it.
- The rank r_i of a page i is defined as

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

where d_i is the out-degree of node i , and r_j the solutions to the flow equation.



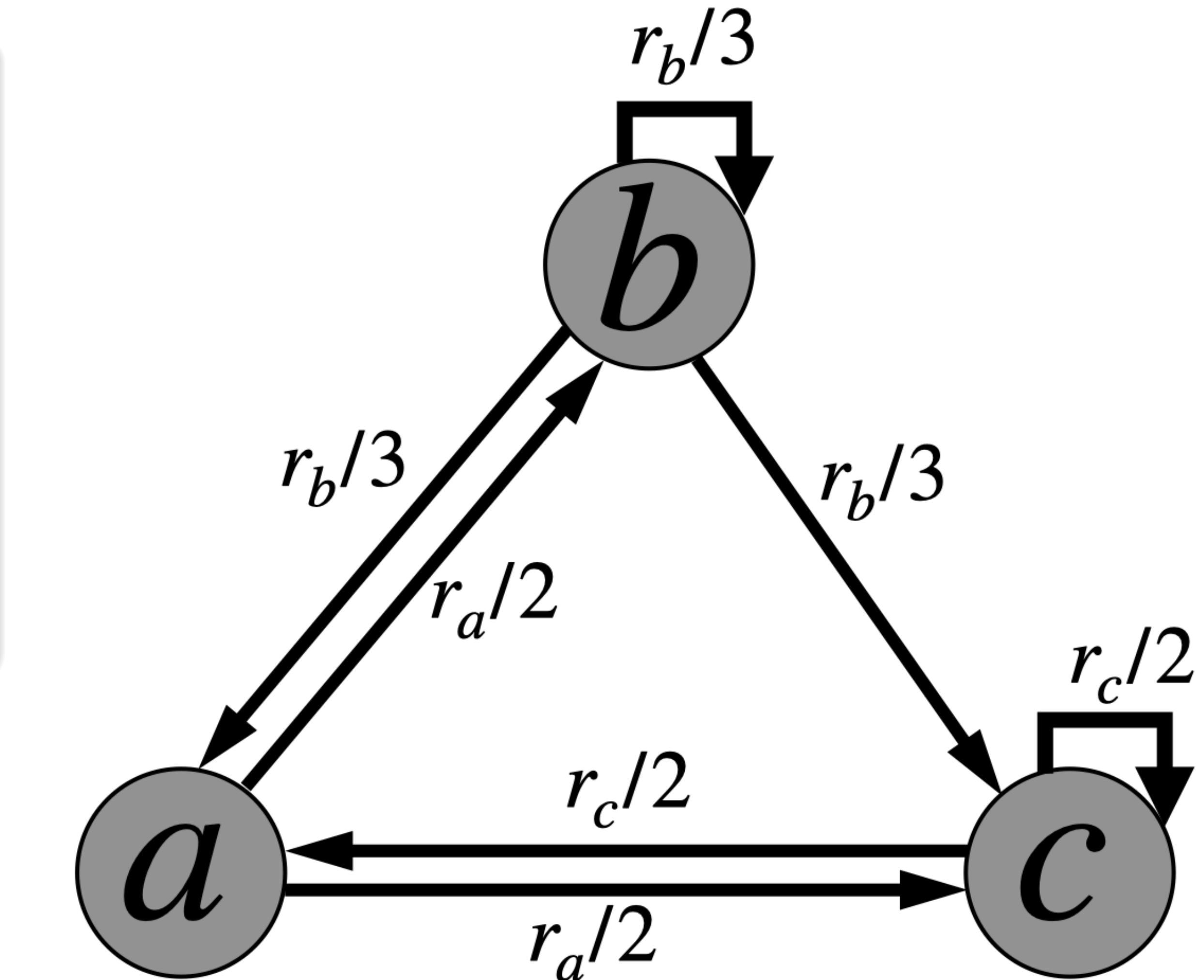
A small example

The flow equations

$$\begin{aligned}r_a &= r_b/3 + r_c/2, \\r_b &= r_a/2 + r_b/3, \\r_c &= r_a/2 + r_b/3 + r_c/2.\end{aligned}$$

- Enforce $r_a + r_b + r_c = 1$ to guarantee uniqueness.
- Gaussian elimination can solve this.

We need a better/faster method, and a new formulation for web-size graphs.



A new formulation

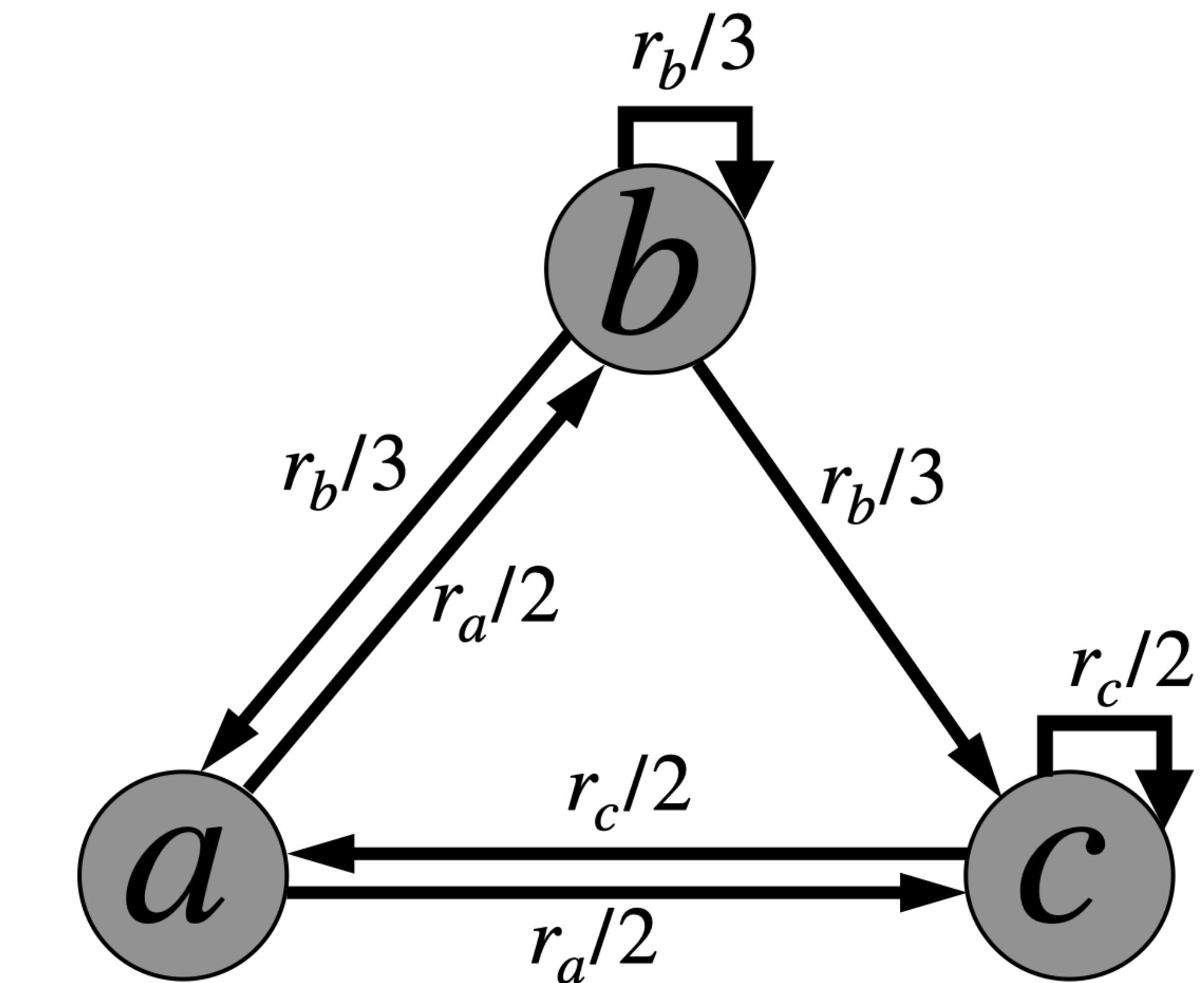
Matrix formulation

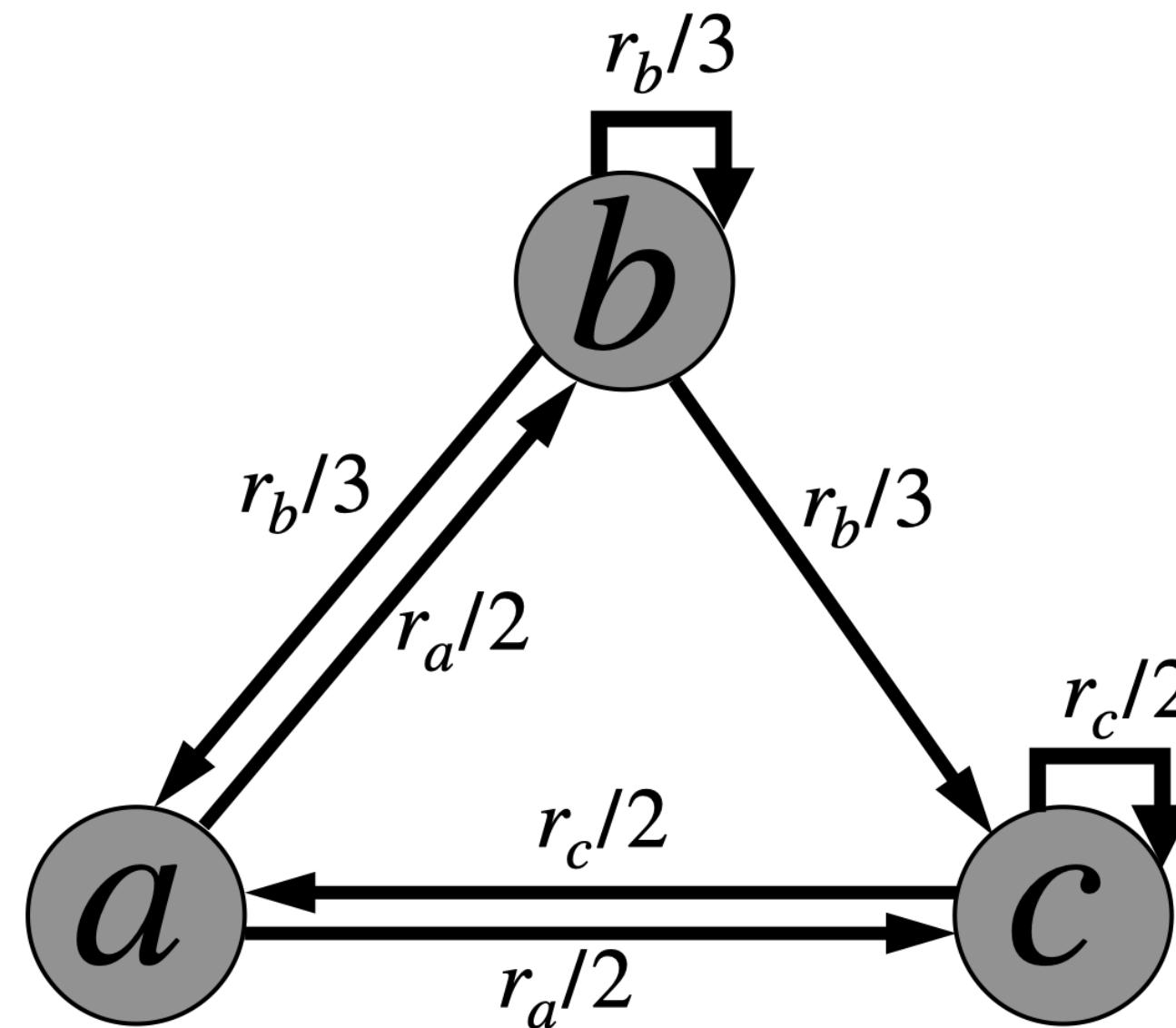
- Define the column stochastic adjacency matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$.
- $\sum_i \mathbf{M}_{ij} = 1$.
- Page i has d_i out-links.
- If $i \rightarrow j$, then $\mathbf{M}_{ji} = \frac{1}{d_i}$, else $\mathbf{M}_{ji} = 0$.
- The rank vector \mathbf{r} has one entry per page \rightarrow importance of the page.

r_i = importance of page i

$$\sum_i r_i = 1$$

$$r_j = \sum_{i \rightarrow j} \frac{r_i}{d_i} \Rightarrow \mathbf{r} = \mathbf{M}\mathbf{r}.$$



The same small example

The flow equations

$$r_a = r_b/3 + r_c/2,$$

$$r_b = r_a/2 + r_b/3,$$

$$r_c = r_a/2 + r_b/3 + r_c/2.$$

In matrix form

$$\mathbf{M} = \begin{pmatrix} a & b & c \\ 0 & 1/3 & 1/2 \\ 1/2 & 1/3 & 0 \\ 1/2 & 1/3 & 1/2 \end{pmatrix} \begin{matrix} a \\ b \\ c \end{matrix}$$

$$\mathbf{r} = \mathbf{M} \cdot \mathbf{r}$$

$$\begin{bmatrix} r_a \\ r_b \\ r_c \end{bmatrix} = \begin{pmatrix} 0 & 1/3 & 1/2 \\ 1/2 & 1/3 & 0 \\ 1/2 & 1/3 & 1/2 \end{pmatrix} \cdot \begin{bmatrix} r_a \\ r_b \\ r_c \end{bmatrix}$$

Is this a familiar equation?

Eigenvector approximation

The power iteration

- An approximation method for computing the eigenvectors of a matrix. It uses the following recursive formula to find the principal eigenvector \mathbf{r} of a matrix \mathbf{M} :

$$\mathbf{r}^{n+1} = \frac{\mathbf{M} \cdot \mathbf{r}^n}{\|\mathbf{M} \cdot \mathbf{r}^n\|}$$

ALGORITHM: Power iteration method

```
1: Input: Graph  $\mathbf{M}$  with  $n$  nodes and  $m$  links
2: Initialize:  $\mathbf{r}_0 = [1/n, \dots, 1/n]^\top$ 
3: while  $|\mathbf{r}_k - \mathbf{r}_{k-1}|_1 \geq \epsilon$  do
4:    $\tilde{\mathbf{r}} = \mathbf{M} \cdot \mathbf{r}_{k-1}$ 
5:    $\mathbf{r}_k = \tilde{\mathbf{r}} / \|\tilde{\mathbf{r}}\|$ 
6: end while
```

A simplification

- In the case of PR, \mathbf{M} is col.-stochastic, and \mathbf{r} is a probability vector, therefore $\|\mathbf{M} \cdot \mathbf{r}\| = 1$, and we reduce the power iteration to

$$\mathbf{r}^{n+1} = \mathbf{M} \cdot \mathbf{r}^n$$

Eigenvector formulation

Flow equations in matrix form $\mathbf{r} = \mathbf{M} \cdot \mathbf{r}$

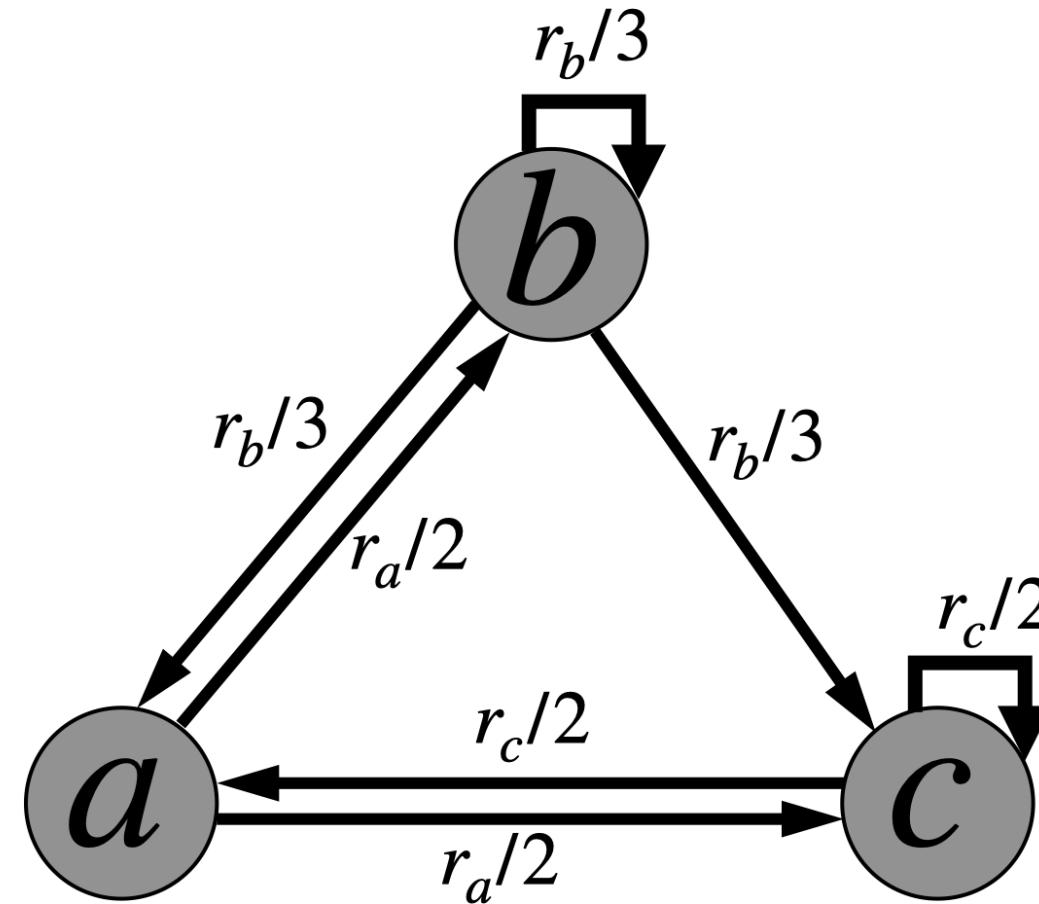
- ↪ \mathbf{x} is an eigenvector with corresponding eigenvalue λ if: $\mathbf{Ax} = \lambda\mathbf{x}$.
- ↪ \mathbf{r} (the rank vector) is an eigenvector of the col. stochastic web adjacency matrix \mathbf{M} .
- ↪ Starting from any stochastic \mathbf{u} , the rank \mathbf{r} is the limit of $\mathbf{M} \cdot \mathbf{M} \cdots \mathbf{Mu}$.
- ↪ The associated eigenvalue $\lambda = 1$.
- ↪ We can efficiently solve for \mathbf{r} .

(Power method or Shift and inverse)

ALGORITHM: Power iteration method

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6: end while
```

★ L1 norm (Manhattan distance/Taxicab norm)
 $|\mathbf{r}|_1 = \sum_{1 \leq i \leq n} |r_i|$.

The same small example

$$\mathbf{M} = \begin{pmatrix} a & b & c \\ 0 & 1/3 & 1/2 \\ 1/2 & 1/3 & 0 \\ 1/2 & 1/3 & 1/2 \end{pmatrix}$$

- ① \mathbf{M} is col. stoch., and $\mathbf{M}_{ij} \geq 0$.
 - ⇒ Perron-Frobenius: A unique $\lambda = 1$ exists, $|\lambda_1| = 1 > |\lambda_2| \geq |\dots| \geq |\lambda_n|$, and $\mathbf{v}_1 \in \mathbb{R}^n$.
 - ⇒ Initial unbiased guess
 $\mathbf{r}_0 = [1/3, 1/3, 1/3]^\top$
- ② Converges to
 $\mathbf{r} = \mathbf{M}^8 * \mathbf{r}_0 = [0.3077, 0.2308, 0.4615]^\top$, so rank = [2, 3, 1].

$$\mathbf{r}_1 = \mathbf{M} \cdot \mathbf{r}_0,$$

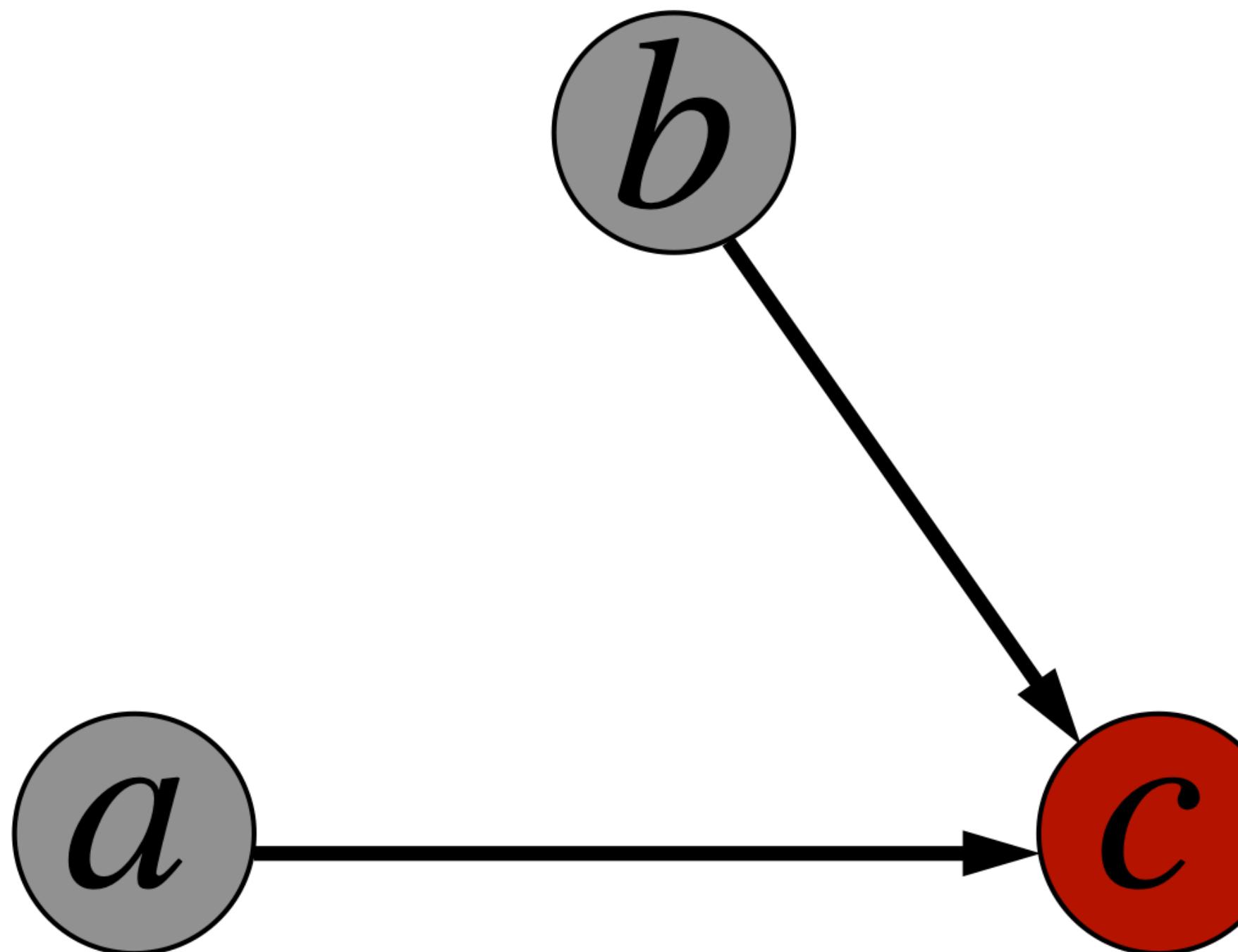
$$\mathbf{r}_2 = \mathbf{M} \cdot \mathbf{r}_1 = \mathbf{M}(\mathbf{M}\mathbf{r}_0) = \mathbf{M}^2 \cdot \mathbf{r}_0,$$

$$\mathbf{r}_3 = \mathbf{M} \cdot \mathbf{r}_2 = \mathbf{M}(\mathbf{M}^2\mathbf{r}_0) = \mathbf{M}^3 \cdot \mathbf{r}_0,$$

$$\mathbf{r}_4 = \dots$$

Adapting to real-world (1)

Col stochastic assumption violated.



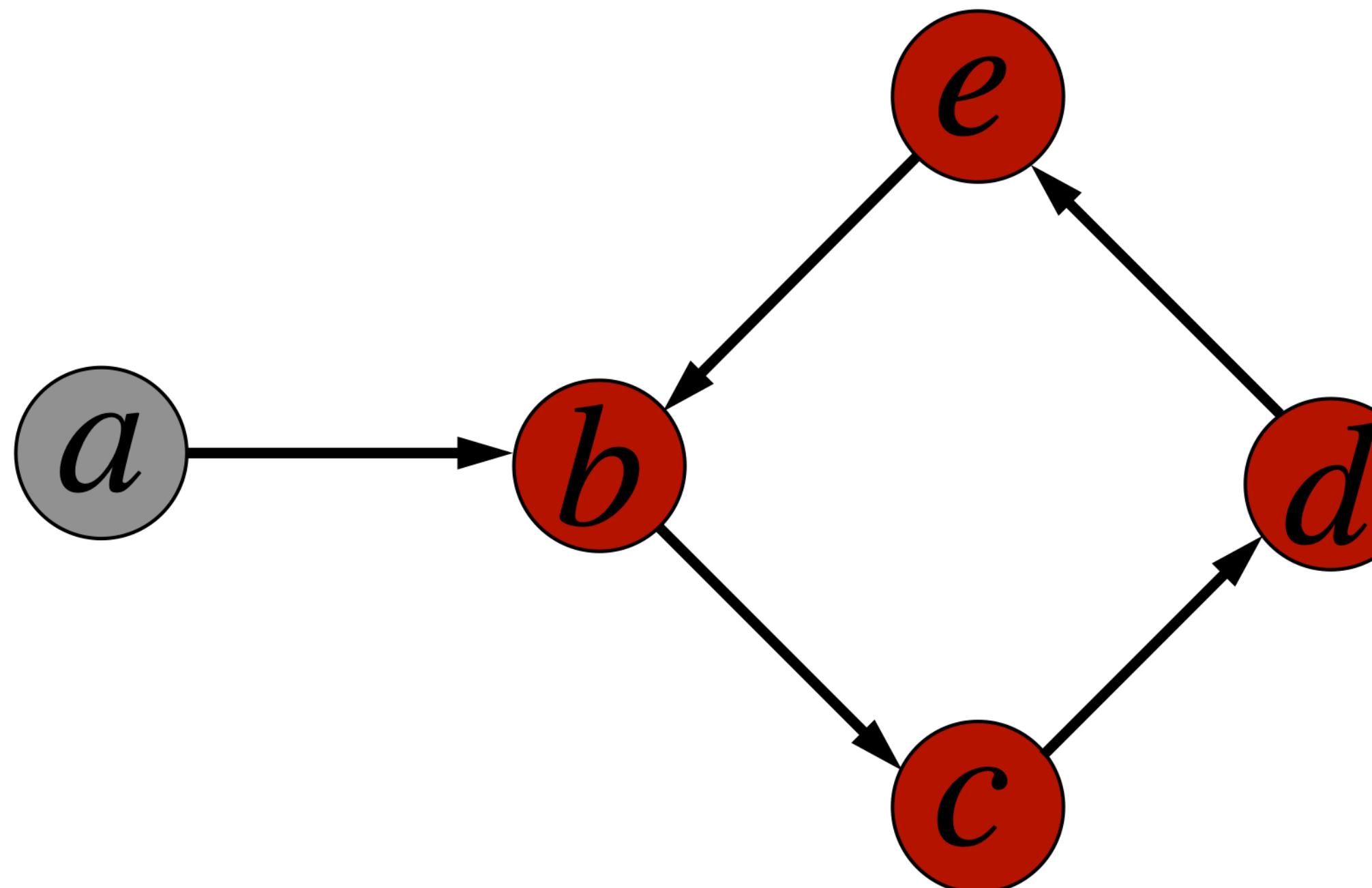
Dangling nodes

- No outlinks from a certain webpage.
- The corresponding column in A is zero.
- At node c , we are “stuck”.
- Change the whole column from zeros to entries $1/n$.
- If surfers follow links and arrive at a webpage without outlinks, they can jump out to any webpage with equal probability.
- M is now col. stochastic.

Always teleport!

Adapting to real-world (2)

The trap absorbs all importance.



Probabilistically teleport!

Spider traps

- Cyclic path with no way out.
- Iteratively, the trap will absorb all importance.
- Probabilistically teleport
- With probability p follow a link at random (follow the edges structure).
- With probability $1 - p$ jump to a random page. $(1 - p)/n$ for a specific jump.
- Teleport out of the trap in a finite number of steps.
- Typically $p \in [0.8, 0.9]$, jump every 5 steps on avg.

The Google matrix

- Preprocess matrix \mathbf{M} to remove dangling nodes.
- PageRank equation reads

$$r_j = \sum_{i \rightarrow j} p \frac{r_i}{d_i} + (1 - p) \frac{1}{n},$$

d_i : the out-degree of node i .

- The Google matrix \mathbf{A} reads

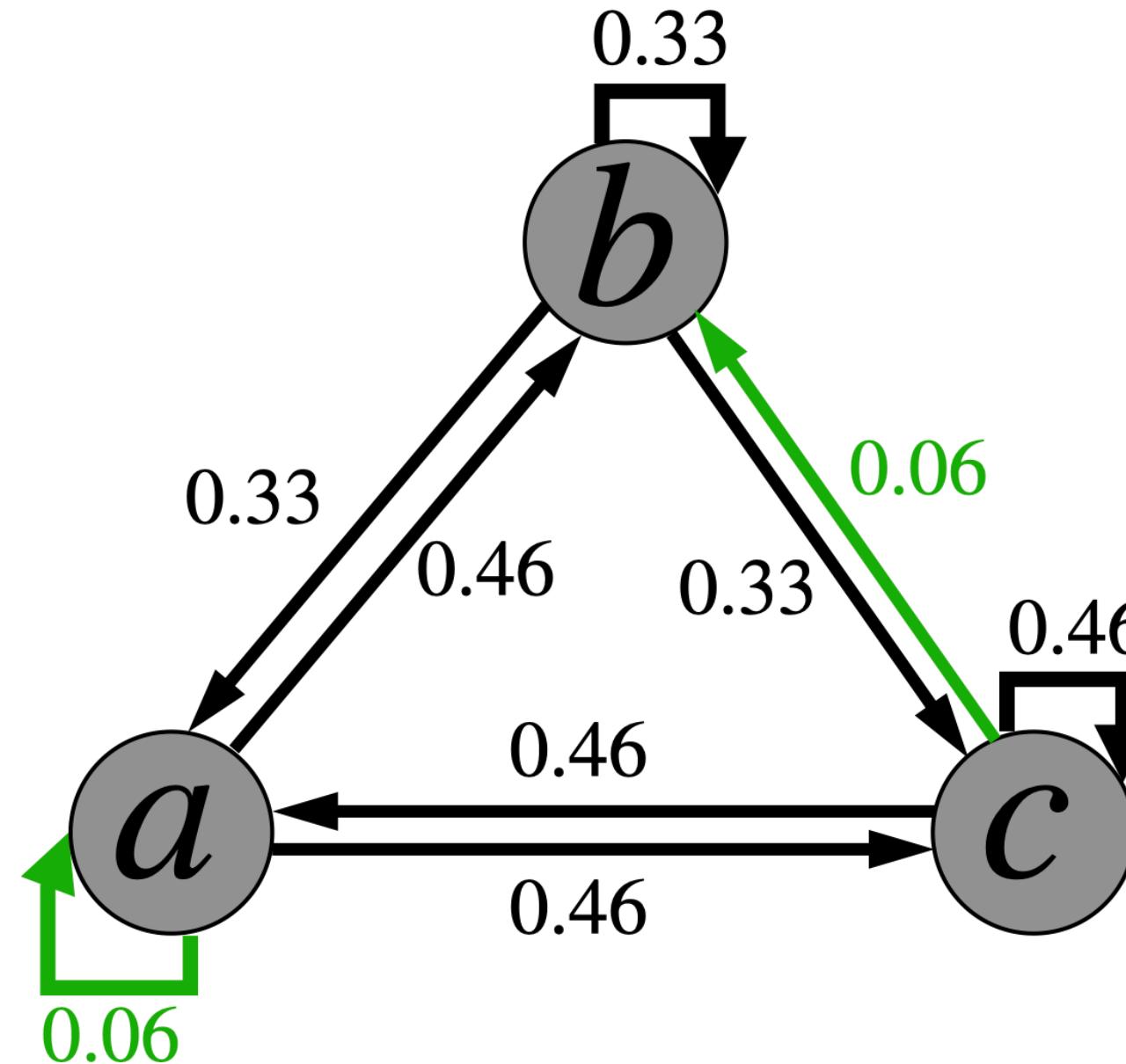
$$\begin{aligned}\mathbf{A} &= p\mathbf{M} + (1 - p) \left[\frac{1}{N} \right]_{n \times n}, \\ &= p\mathbf{M} + (1 - p)\mathbf{u}\mathbf{e}^T,\end{aligned}$$

$\mathbf{u} = \frac{1}{n}\mathbf{e}$: unbiased personalization vector.

Dominant eigenvector computation

- Recursive problem $\mathbf{r} = \mathbf{A} \cdot \mathbf{r}$.
 - Dominant eigenvalue $\lambda = 1$.
- We will employ the power iteration.

The Google matrix - computation



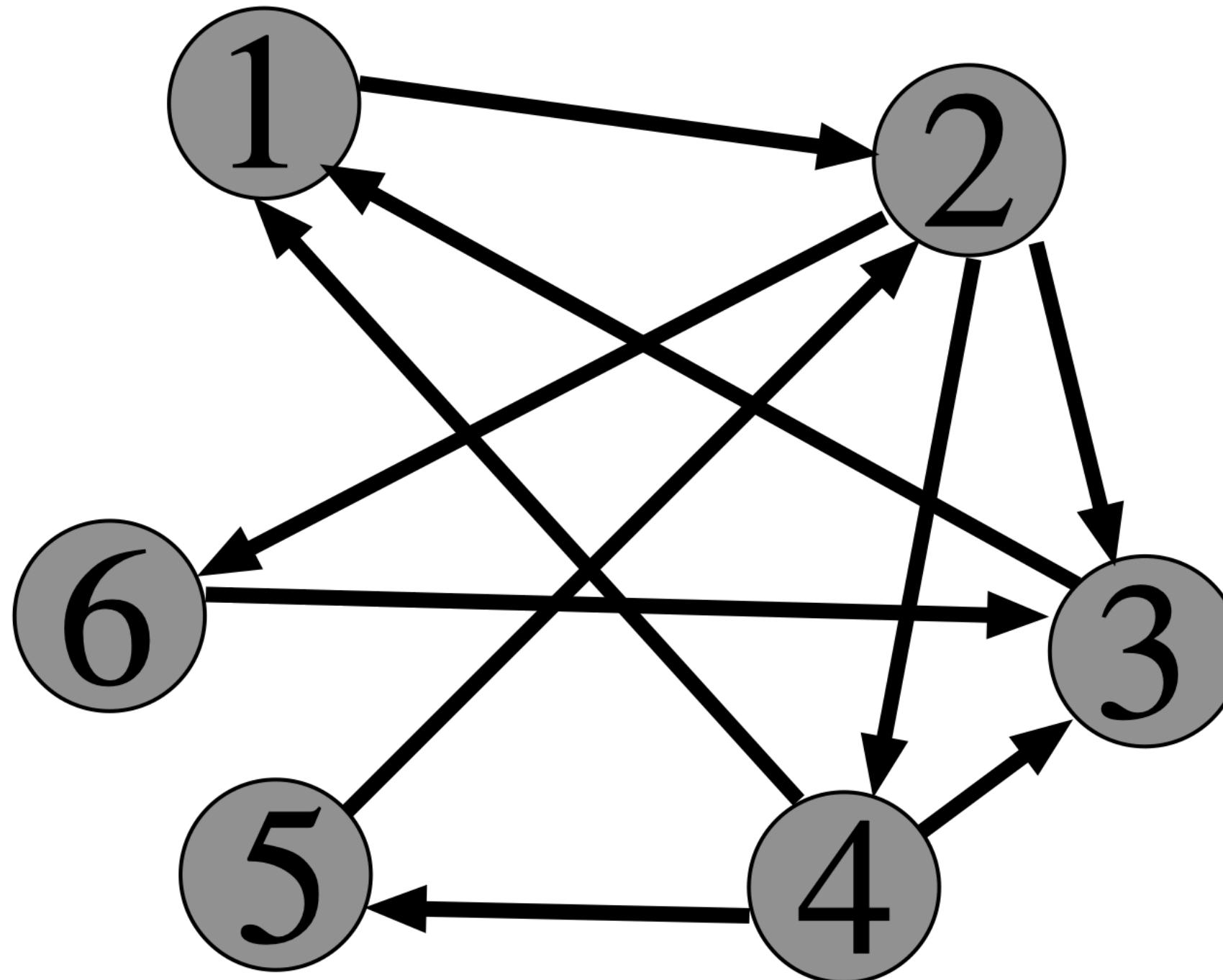
- If the personalization vector \mathbf{u} contains zeros, then the random jump is done only to the nodes of the graph that has a corr. $u_i \neq 0, i \in \{1, n\}$.

$$\mathbf{r} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{array}{ccccc} \mathbf{Ar}_0 & \mathbf{A}^2\mathbf{r}_0 & \mathbf{A}^3\mathbf{r}_0 & \mathbf{A}^k\mathbf{r}_0 & \mathbf{A}^7\mathbf{r}_0 \\ \hline 1/3 & 0.2889 & 0.3126 & \cdots & 0.3085 \\ 1/3 & 0.2889 & 0.2593 & \cdots & 0.2594 \\ 1/3 & 0.4222 & 0.4281 & \cdots & 0.4321 \end{array}$$

Let $p = 0.8, \mathbf{u} = \frac{1}{n}\mathbf{e}$.

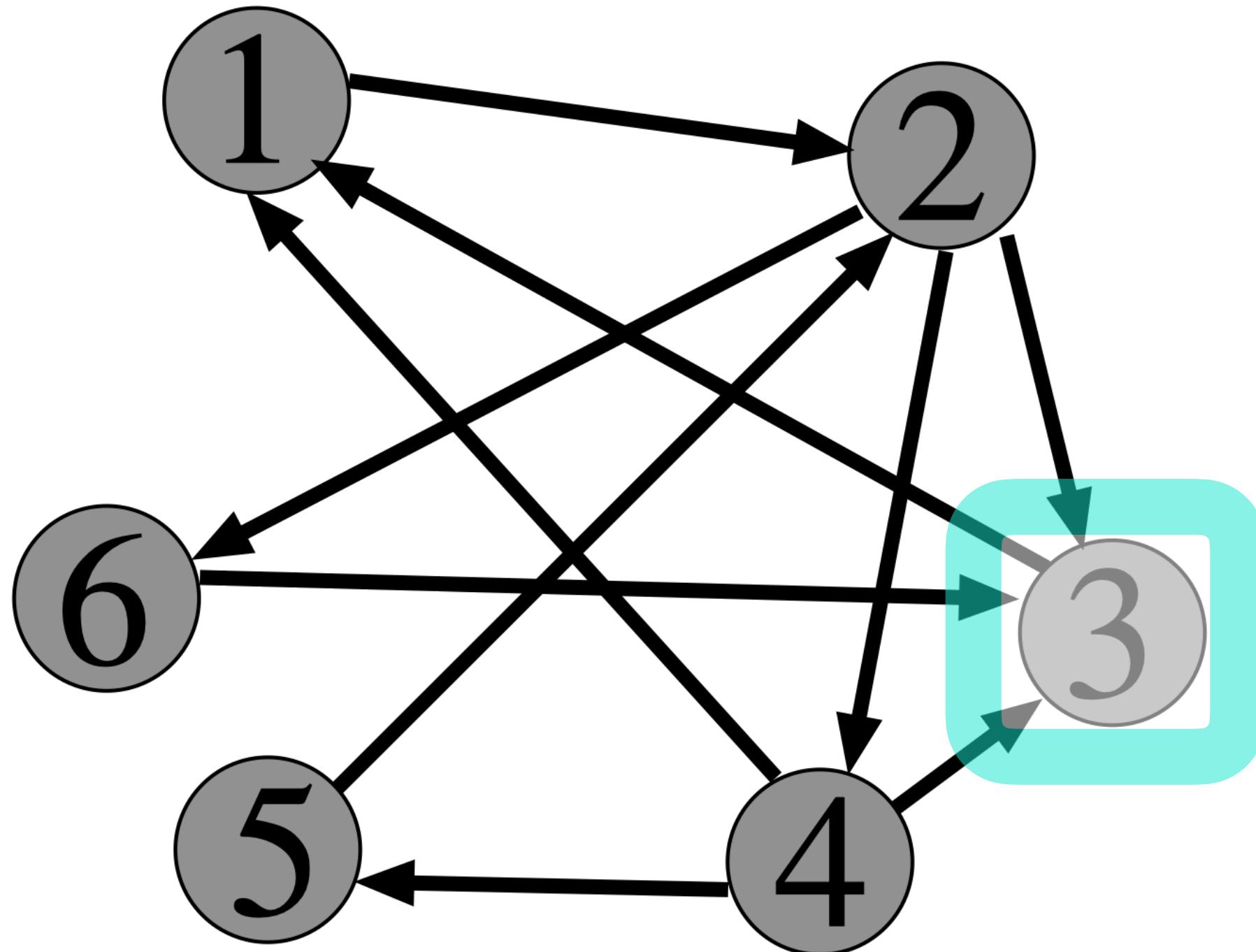
$$\mathbf{A} = p\mathbf{M} + (1 - p)\mathbf{u}\mathbf{e}^\top = 0.8 \cdot \begin{pmatrix} 0 & 1/3 & 1/2 \\ 1/2 & 1/3 & 0 \\ 1/2 & 1/3 & 1/2 \end{pmatrix} + 0.2 \cdot \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} = \begin{pmatrix} 0.0667 & 0.3333 & 0.4667 \\ 0.4667 & 0.3333 & 0.0667 \\ 0.4667 & 0.3333 & 0.4667 \end{pmatrix}$$

Degree \neq PageRank



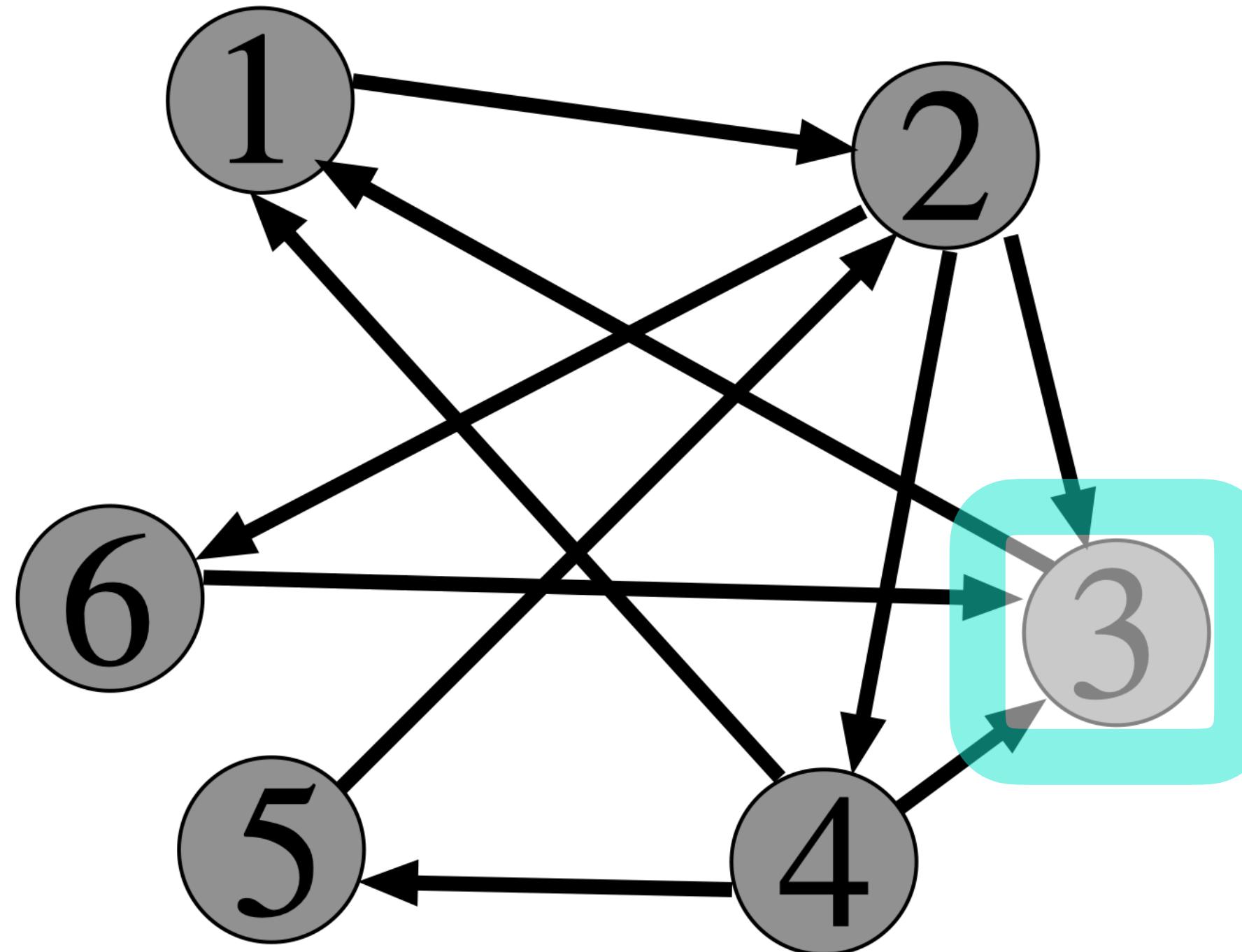
Can you identify the node with the highest in-degree?

Degree \neq PageRank

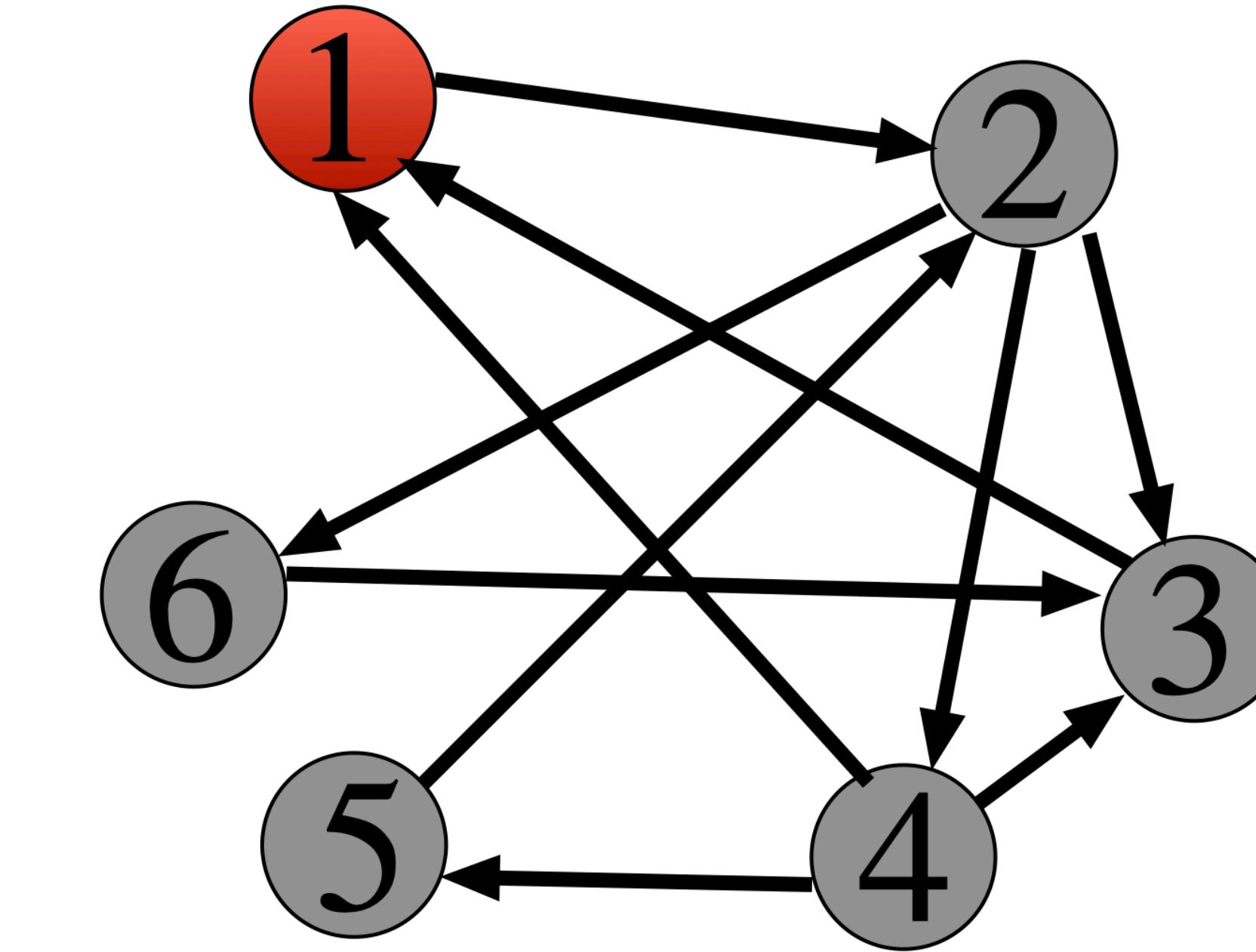


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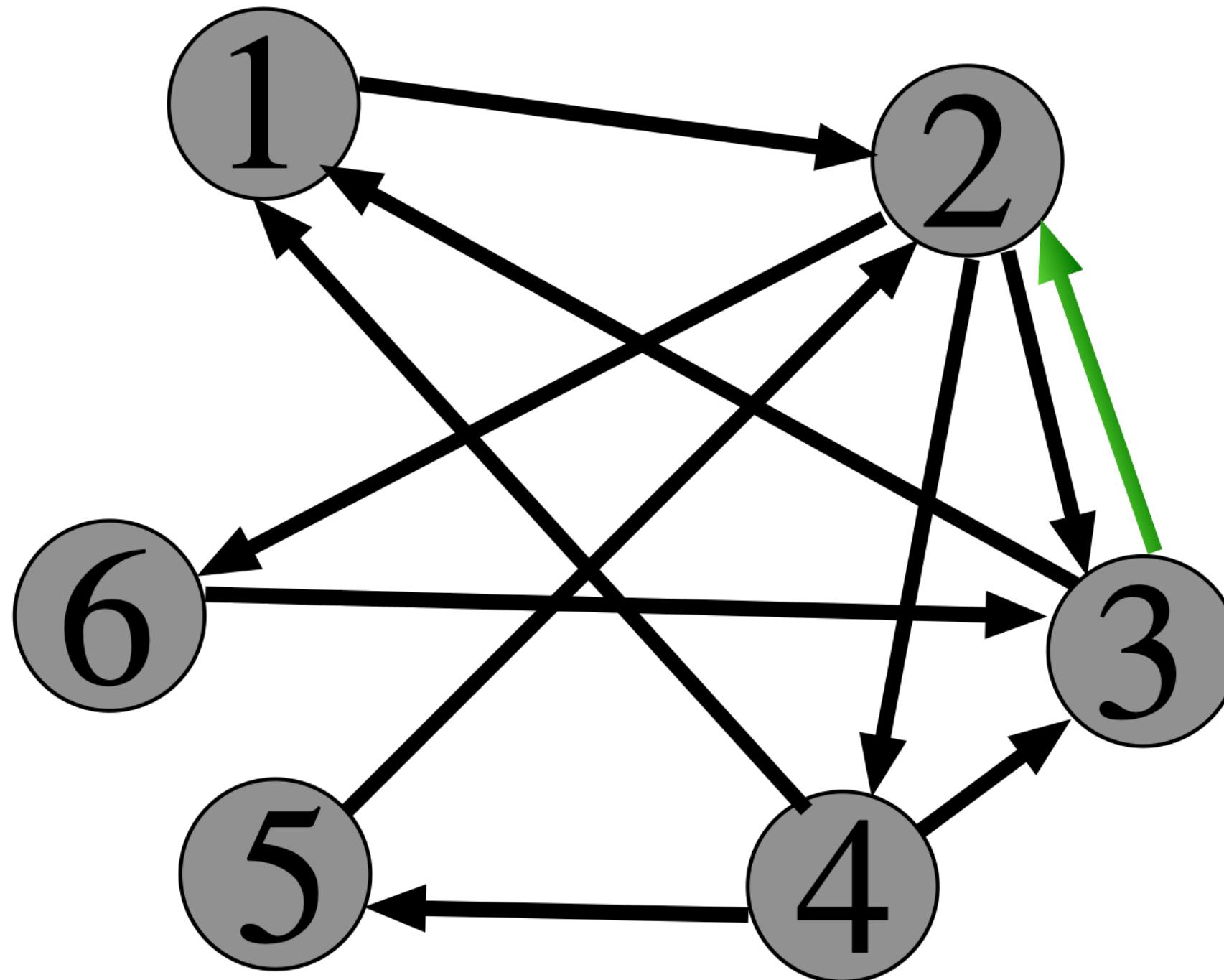


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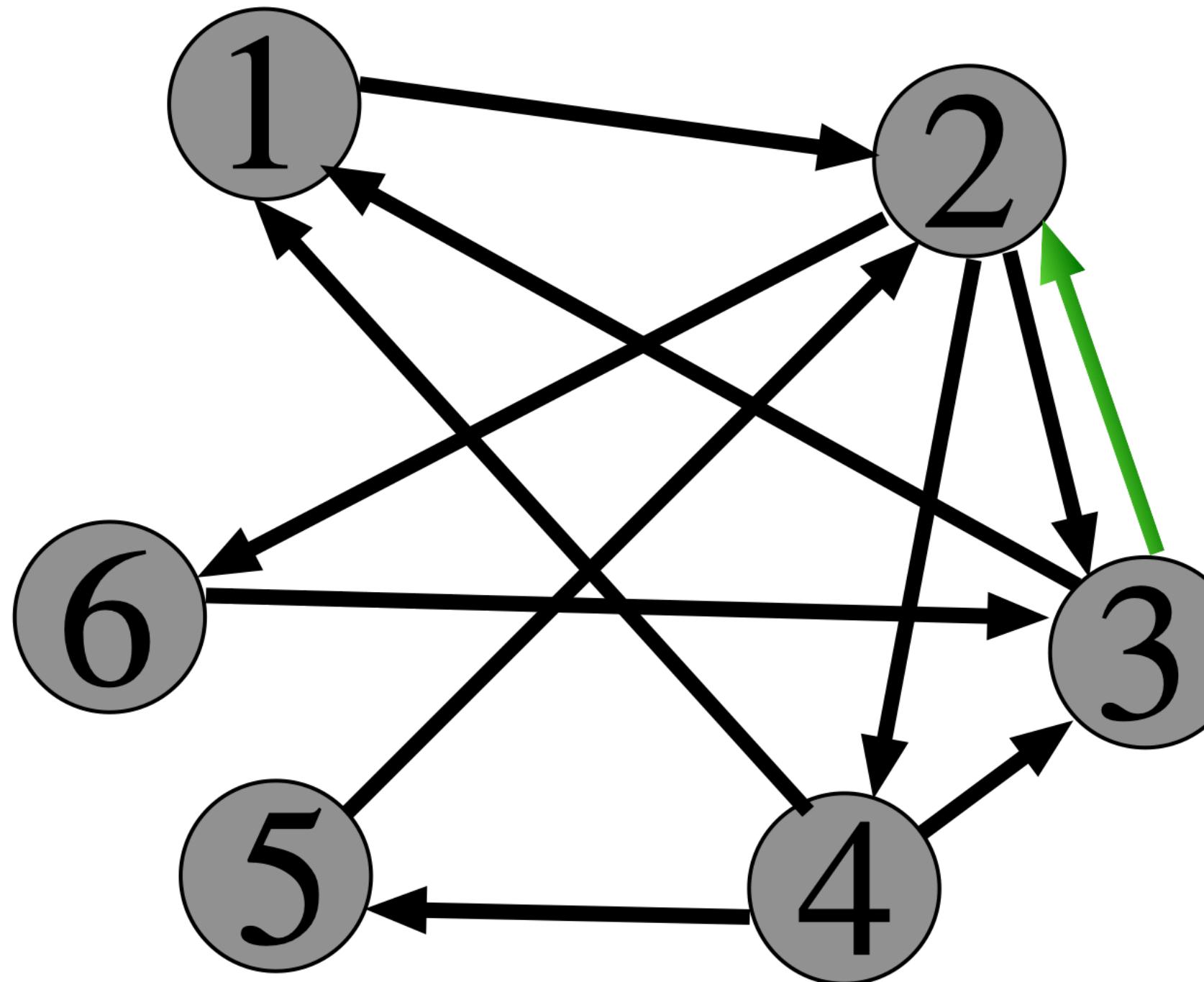


The PageRank ranking does not always correspond to the degree ranking.

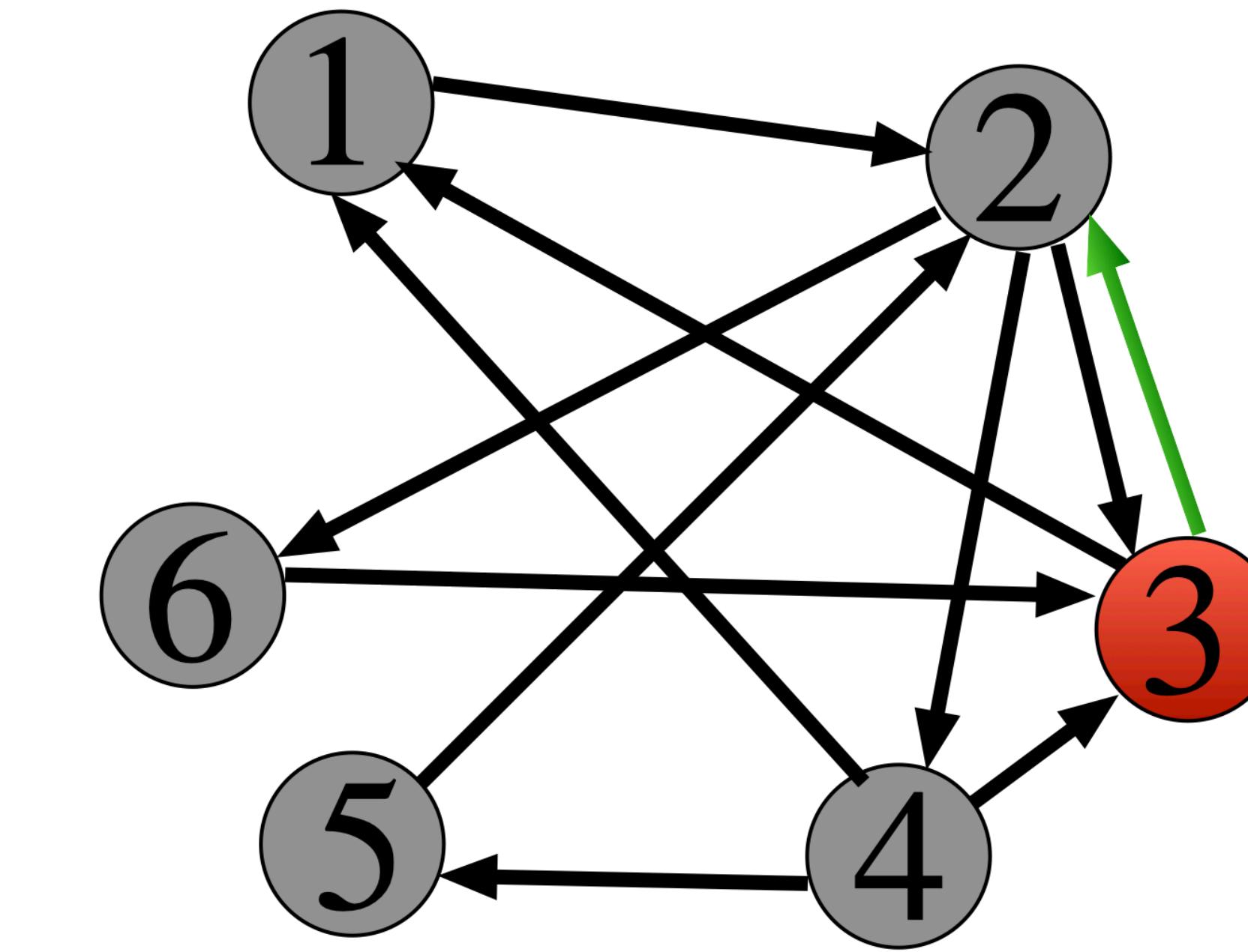
Degree \neq PageRank



Let's perturb the graph slightly.

Degree \neq PageRank

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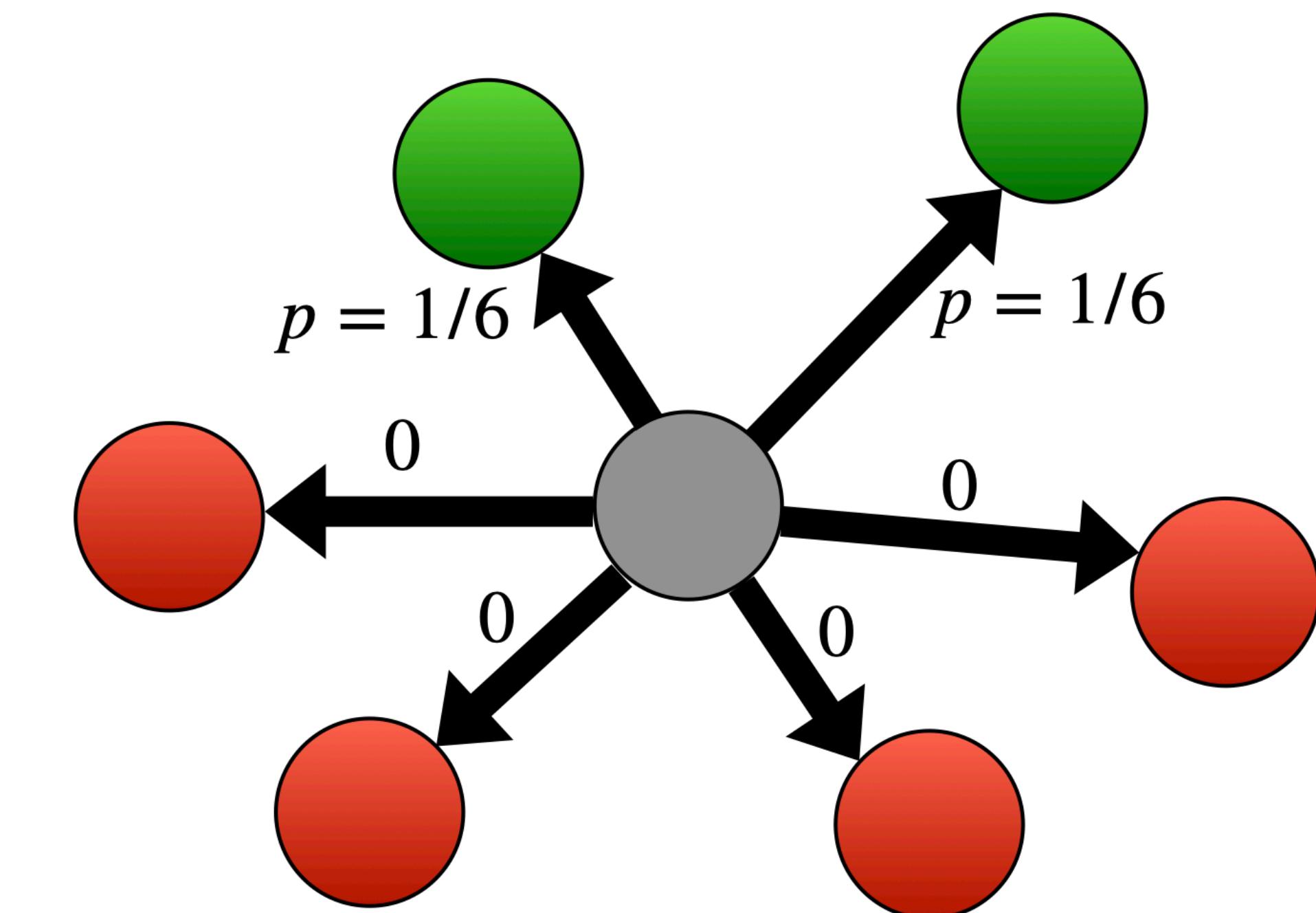
Small changes in the (small) graph structure change the PR drastically.

The picture today

Does Google still use it?

- ⇒ Over 200 types of ranking metrics to determine the final order.
S. Levy (2010), How Google's algorithm rules the web, Wired Magazine, 17, www.wired.com.
- ⇒ Unclear to what extend PR is used.
- ⇒ Using a full substochastic matrix to handle spam url links.
M. Cutts (2009), PageRank sculpting, Matt Cutts: Gadgets, Google, and SEO blog.
www.mattcutts.com/blog/pagerank-sculpting.

Google's PageRank computation is a pseudo-PageRank problem now.



Equivalent formulations for PageRank (1)

Let \mathbf{M} be a col. stochastic matrix with nonnegative entries, and the sum of entries in each column is 1. Let \mathbf{v} be a col. stochastic vector ($\mathbf{e}^T \mathbf{v} = 1$), and let $0 < p < 1$ be the teleportation parameter. Then the PR problem is to find the solution to the linear system

$$(\mathbf{I} - p\mathbf{M}) \mathbf{x} = (1 - p) \mathbf{v},$$

where the solution \mathbf{x} is called the PageRank vector.

Equivalent formulations for PageRank (2)

The eigenvector and linear system formulations are equivalent if we seek an eigenvector \mathbf{x} with $\mathbf{x} \geq 0$ and $\mathbf{e}^T \mathbf{x} = 1$, in which case

$$\begin{aligned}\mathbf{x} &= p\mathbf{M}\mathbf{x} + (1 - p)\mathbf{v} \mathbf{e}^T \mathbf{x} = p\mathbf{M}\mathbf{x} + (1 - p)\mathbf{v} \\ &\iff (\mathbf{I} - p\mathbf{M})\mathbf{x} = (1 - p)\mathbf{v}.\end{aligned}$$

- The matrix $\mathbf{I} - p\mathbf{M}$ is a diagonally dominant M-matrix.
 - ⇒ Existence and uniqueness of \mathbf{x} .
 - ⇒ \mathbf{x} is nonnegative.
- Error after an iteration $\mathbf{x} - \mathbf{x}^{k+1} = \underbrace{p\mathbf{M}\mathbf{x} + (1 - p)\mathbf{v}}_{\text{the true solution } \mathbf{x}} - \underbrace{p\mathbf{M}\mathbf{x}^k + (1 - p)\mathbf{v}}_{\text{the updated iterate } \mathbf{x}^{k+1}} = p\mathbf{M}(\mathbf{x} - \mathbf{x}^k)$
 - ⇒ Good convergence properties when p is not too close to 1.

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 - ⇒ Small values of p means that we teleport too often!

Shift and inverse technique

- The power iteration has cost $O(n^2)$ (matrix-vector product) per iteration.
- Convergence can be very slow if for eigenvalues $\lambda_1 > \lambda_2 > \dots > \lambda_n$ of the matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ we have $|\frac{\lambda_2}{\lambda_1}| \approx 1$.
 - ☞ Linear convergence with $|\frac{\lambda_2}{\lambda_1}|$ the asymptotic error constant (see proof in book).
- Shift and invert technique improves the convergence rate, but solves a linear system at each iteration with $O(n^3)$ cost.
 - ☞ Attractive for smaller problems, or problems that have a special structure that enable fast direct methods.

Shift and inverse technique - main idea

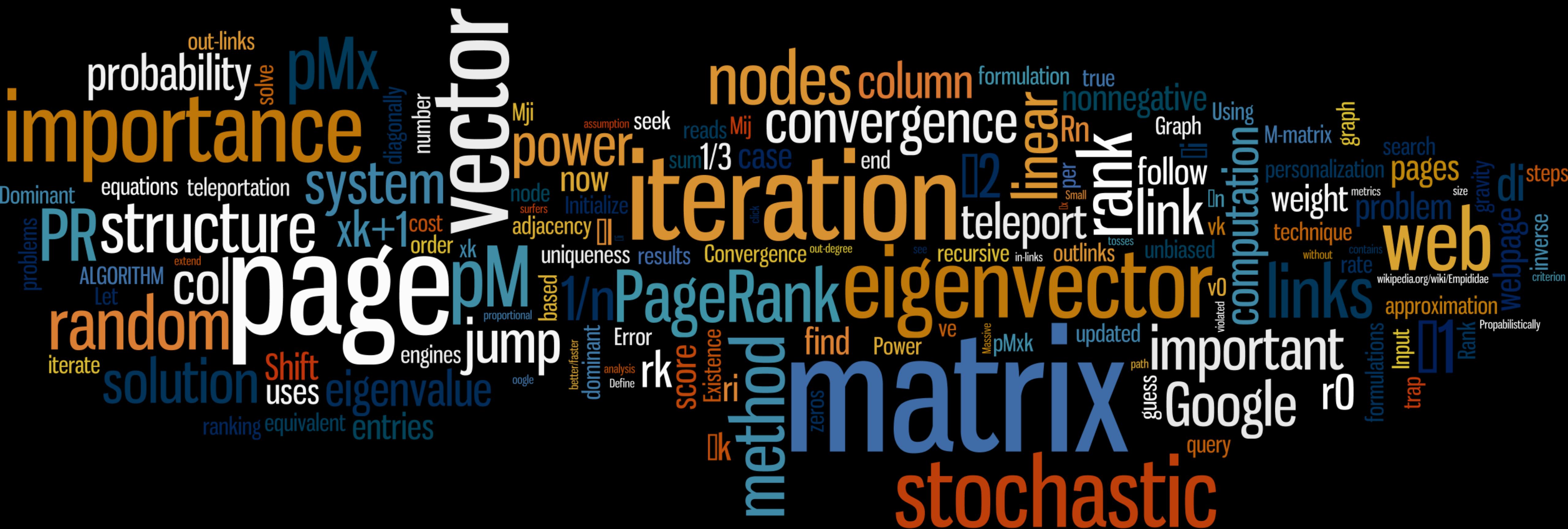
- λ_i : eigvals of \mathbf{A} , then $\lambda_i - \alpha$: of $\mathbf{A} - \alpha\mathbf{I}$, and $\mu_i = \frac{1}{\lambda_i - \alpha}$: of $\mathbf{B} = (\mathbf{A} - \alpha\mathbf{I})^{-1}$.
- ⇒ Imagine applying the power method on \mathbf{B}
- Convergence rate now is $|\frac{\mu_2}{\mu_1}| = |\frac{\lambda_1 - \alpha}{\lambda_2 - \alpha}|$. If $\alpha \approx \lambda_1 \rightarrow$ rapid convergence.
- ⇒ Popular choices for $\alpha = |\mathbf{A}|_1$, or $\alpha = \lambda^{k-1}$.
- If α fixed, inversion of \mathbf{B} takes place outside the for loop.

ALGORITHM: Inverse iteration

- 1: **Input:** Graph \mathbf{A} , initial guess \mathbf{v}_0 , shift α
- 2: **Initialize:** $\mathbf{r}_0 = [1/n, \dots, 1/n]^T$
- 3: **for** $k = 1, 2, \dots$, until termination criteria **do**
- 4: Solve $(\mathbf{A} - \alpha\mathbf{I})\tilde{\mathbf{v}} = \mathbf{v}_{k-1}$
- 5: $\mathbf{v}_k = \tilde{\mathbf{v}} / \|\tilde{\mathbf{v}}\|$
- 6: $\lambda^k = \mathbf{v}_k^T \mathbf{A} \mathbf{v}_k$
- 7: **end for**

- If \mathbf{v}_0 normalized, $\lambda^0 = \mathbf{v}_0^T \mathbf{A} \mathbf{v}_0$, and $\alpha = \lambda^{k-1}$, the Rayleigh quotient is approximated.
- $\lambda(\mathbf{v}) = \frac{\mathbf{v}^T \mathbf{A} \mathbf{v}}{\mathbf{v}^T \mathbf{v}}$
- Cubic convergence justifies increased cost/iteration.

Complementary reading



Complementary reading

- ① Amy N. Langville and Carl D. Meyer, Deeper Inside PageRank, Internet Math. 1 (3) 335 - 380, 2003/2004.
www.stat.uchicago.edu/~lekheng/meetings/mathofranking/ref/langville.pdf
- ② Cornell University blogs, The Academic Paper That Started Google, 2019.
<https://blogs.cornell.edu/info2040/2019/10/28/the-academic-paper-that-started-google>
- ③ David F. Gleich, PageRank Beyond the Web, SIAM Review, Vol. 57, Iss. 3, 2015.
<https://doi.org/10.1137/140976649>
- ④ Uri M. Ascher, Chen Greif, A First Course in Numerical Methods, Chapter 8: Eigenvalues and Singular Values. Book available at [icorsi](#)