Analysis of large graphs with PageRank vectors

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Course calendar

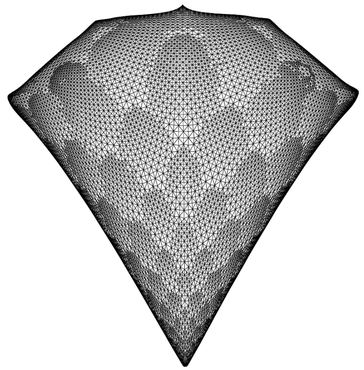
Project 1	Project 2	Project 3	Project bonus	Project 4
PagerRank and networks	Graph partitioning	Graph clustering	Linear least squares	Image deblurring with CG
26.09	04.10	18.10	08.11	15.11

Today: PageRank and networks

Elements: directed networks, columm stochastic matrices, teleportation

PageRank vector: Network structure + Iterative computation

Using: eigenvalue computations, linear system solution



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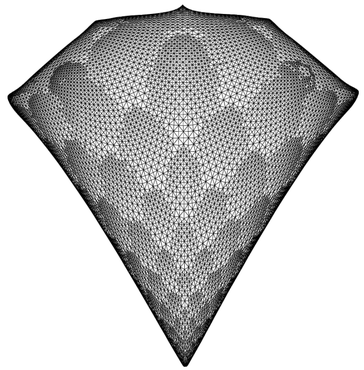
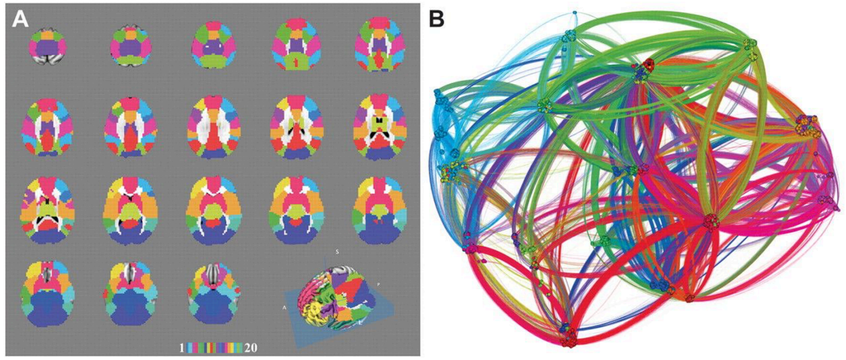


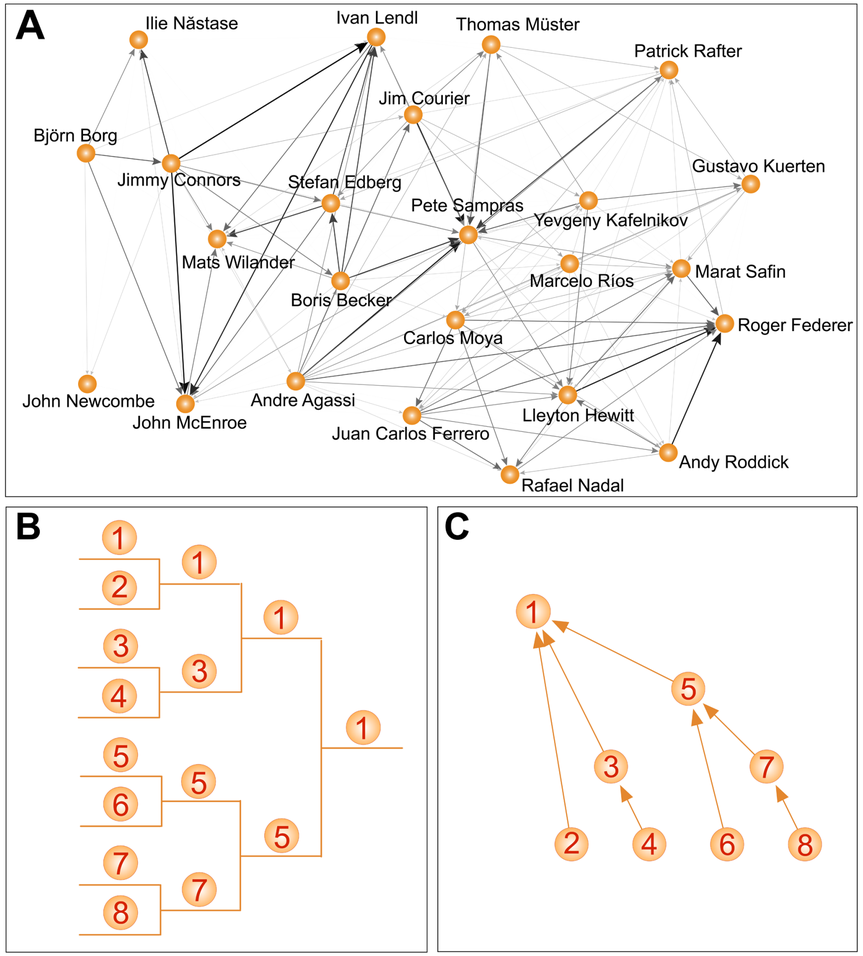
Applications

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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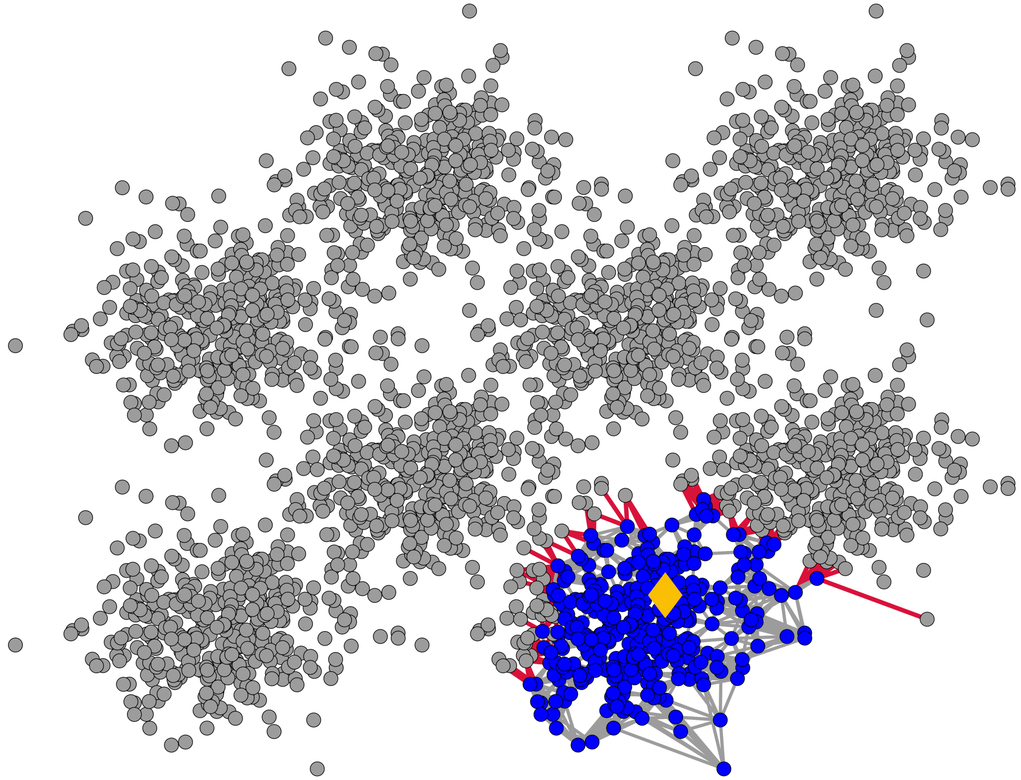

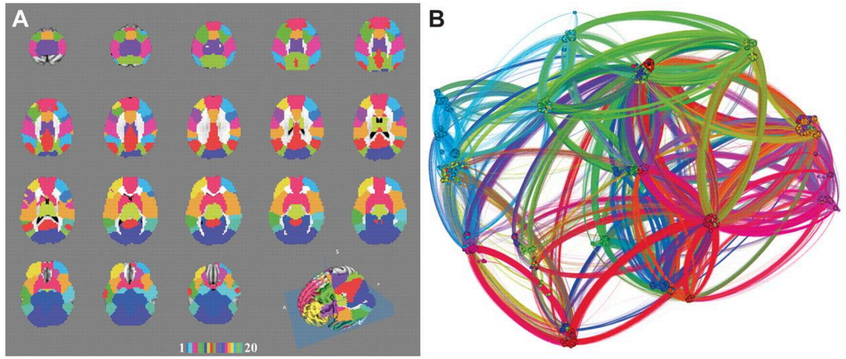

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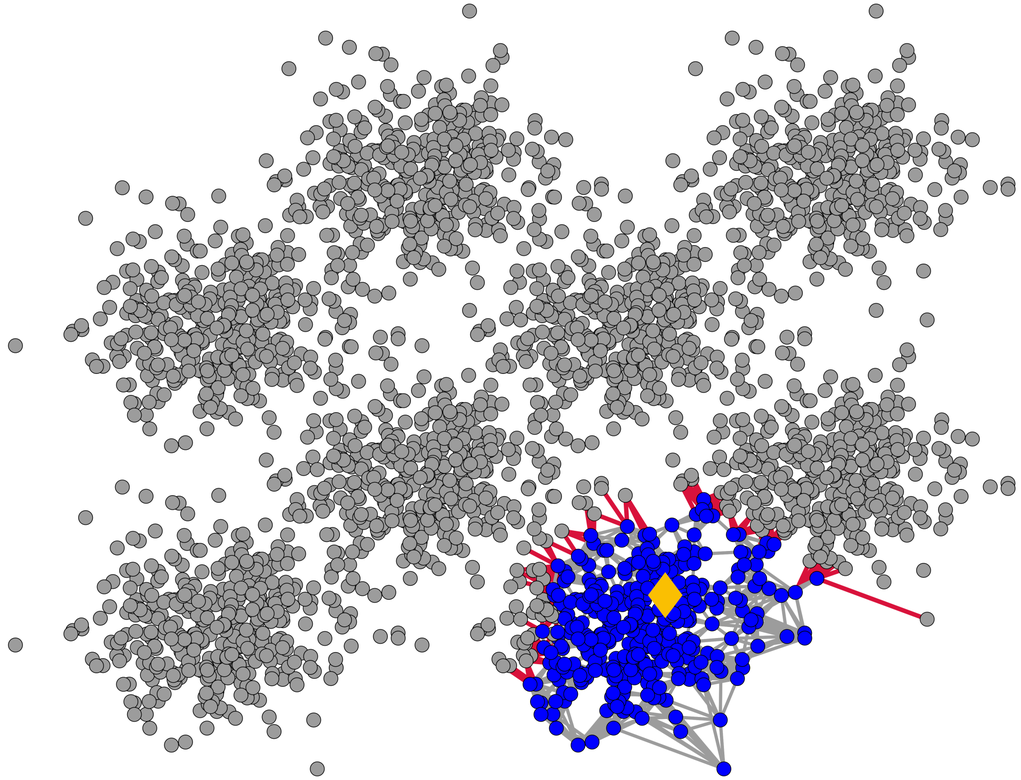

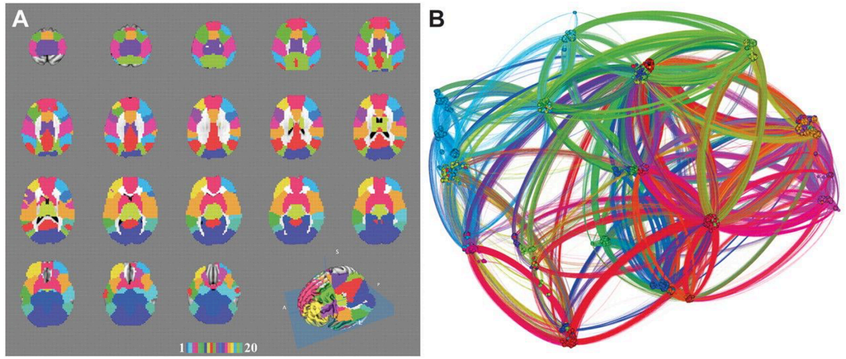

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Bringing order to the web

Search engines and users' queries

❶ 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

❷ 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.

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✔ **We will focus on the PR score in this class.**

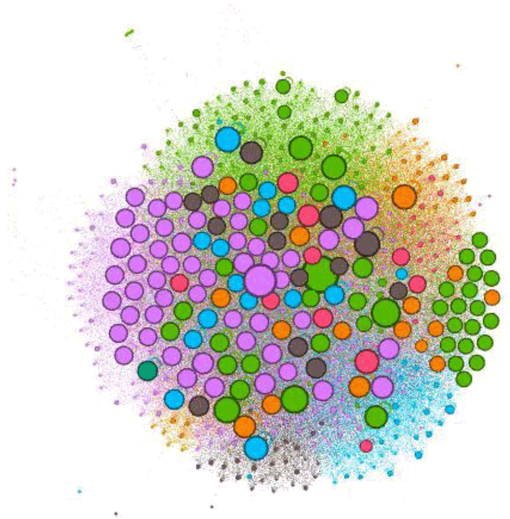
The web as a directed graph

Graphical structure

- Nodes: webpages ■
- Edges: hyperlinks →
- Not all web pages have the same importance (weight).
  www.usi.ch
  vs
  wikipedia.org/wiki/Empididae

Importance ∼ 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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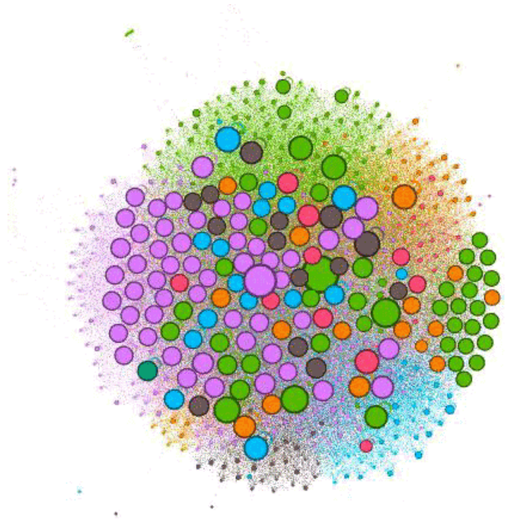

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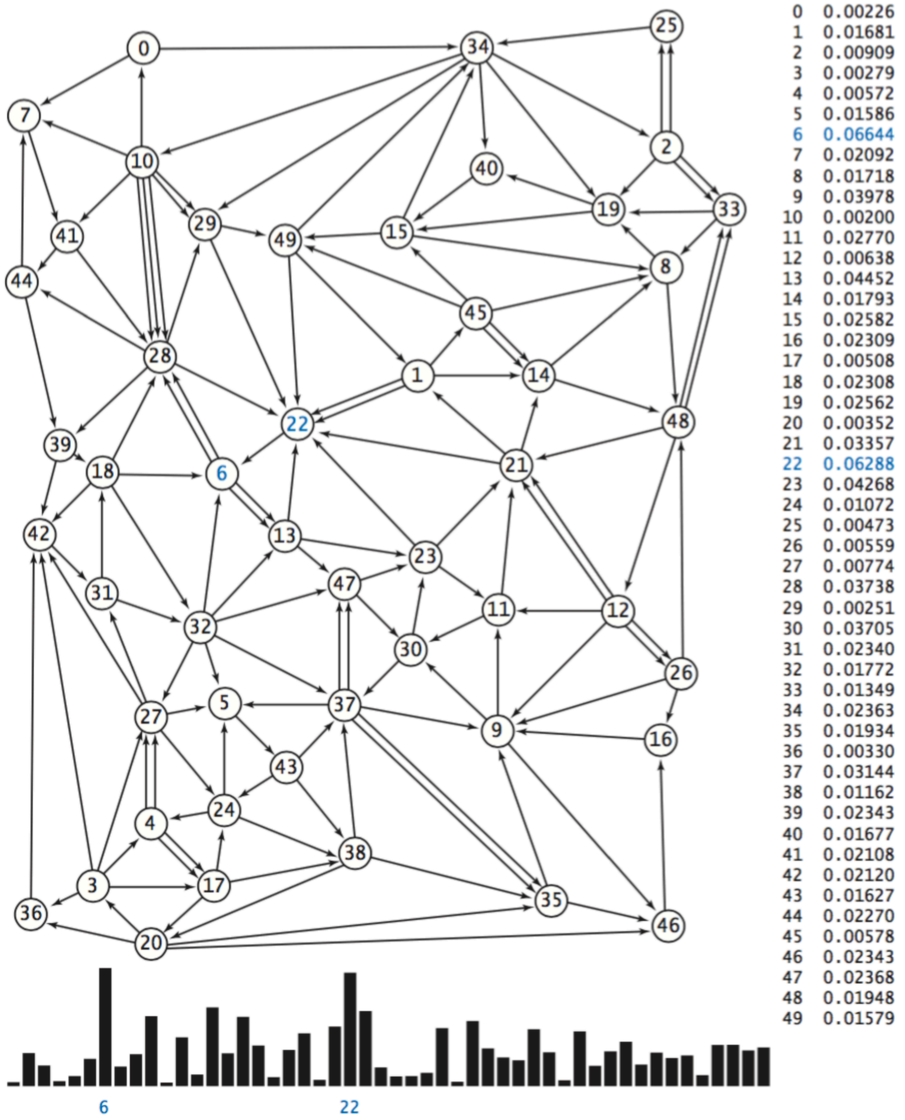
Random surfing

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.

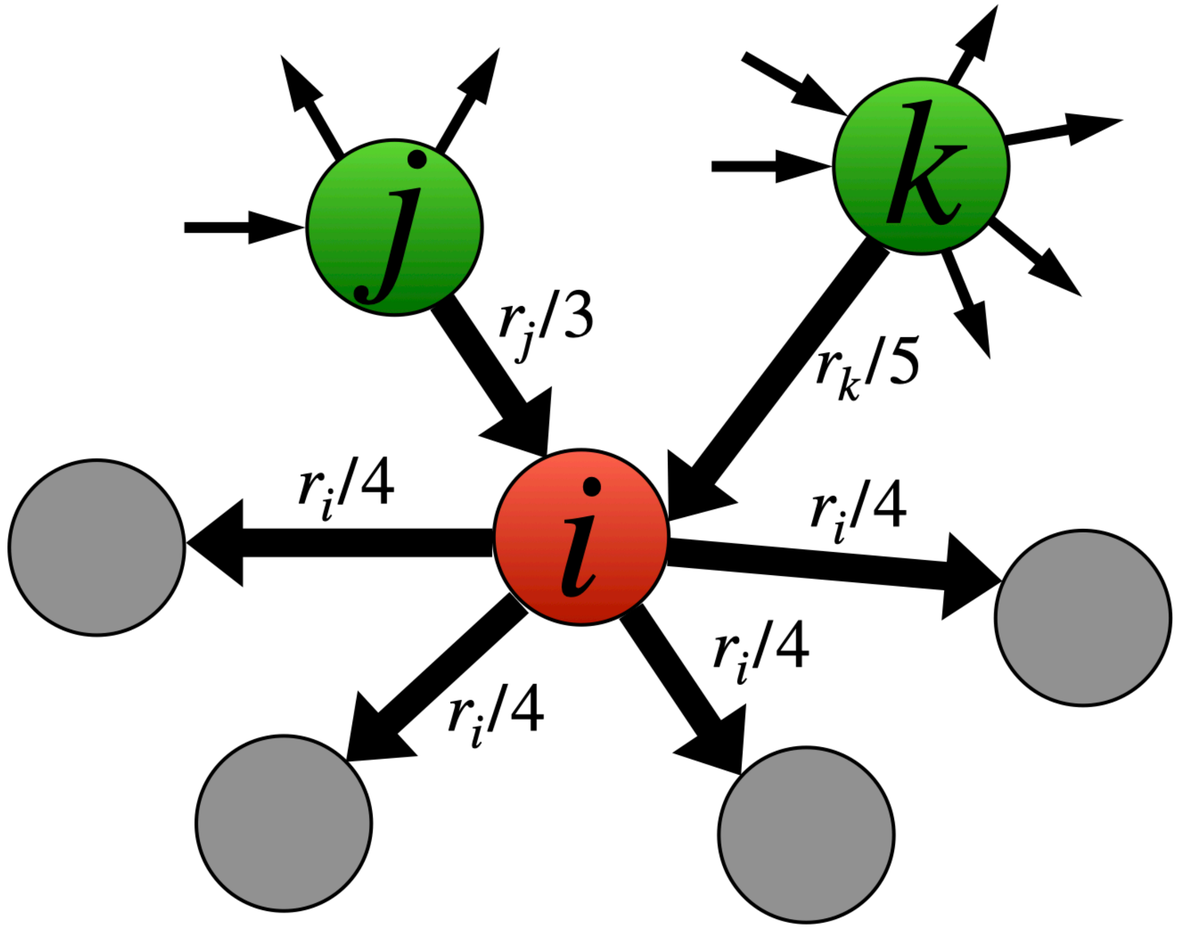


- https://pi.math.cornell.edu/, The Mathematics of Google Search.

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.



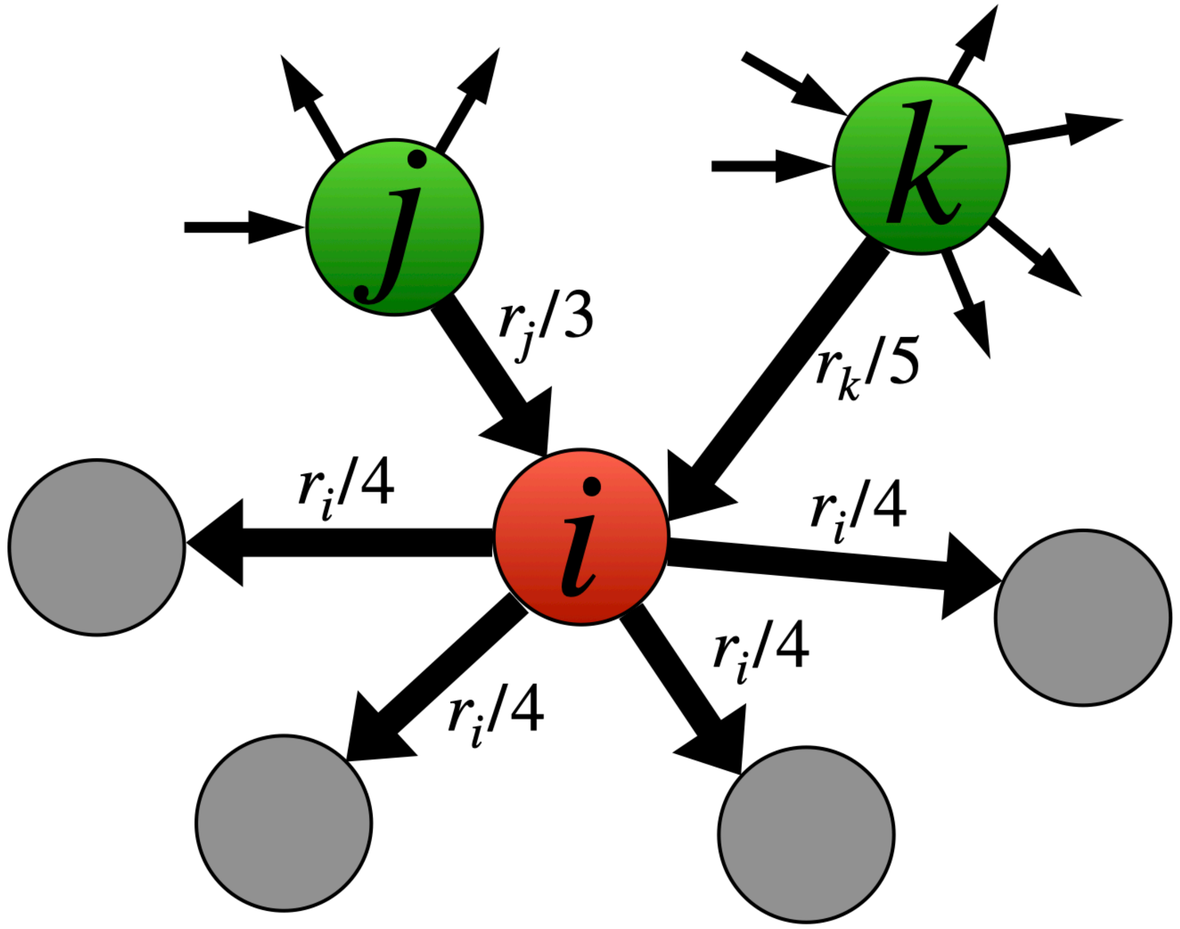
$$r_i = r_j/3 + r_k/5$$

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

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

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



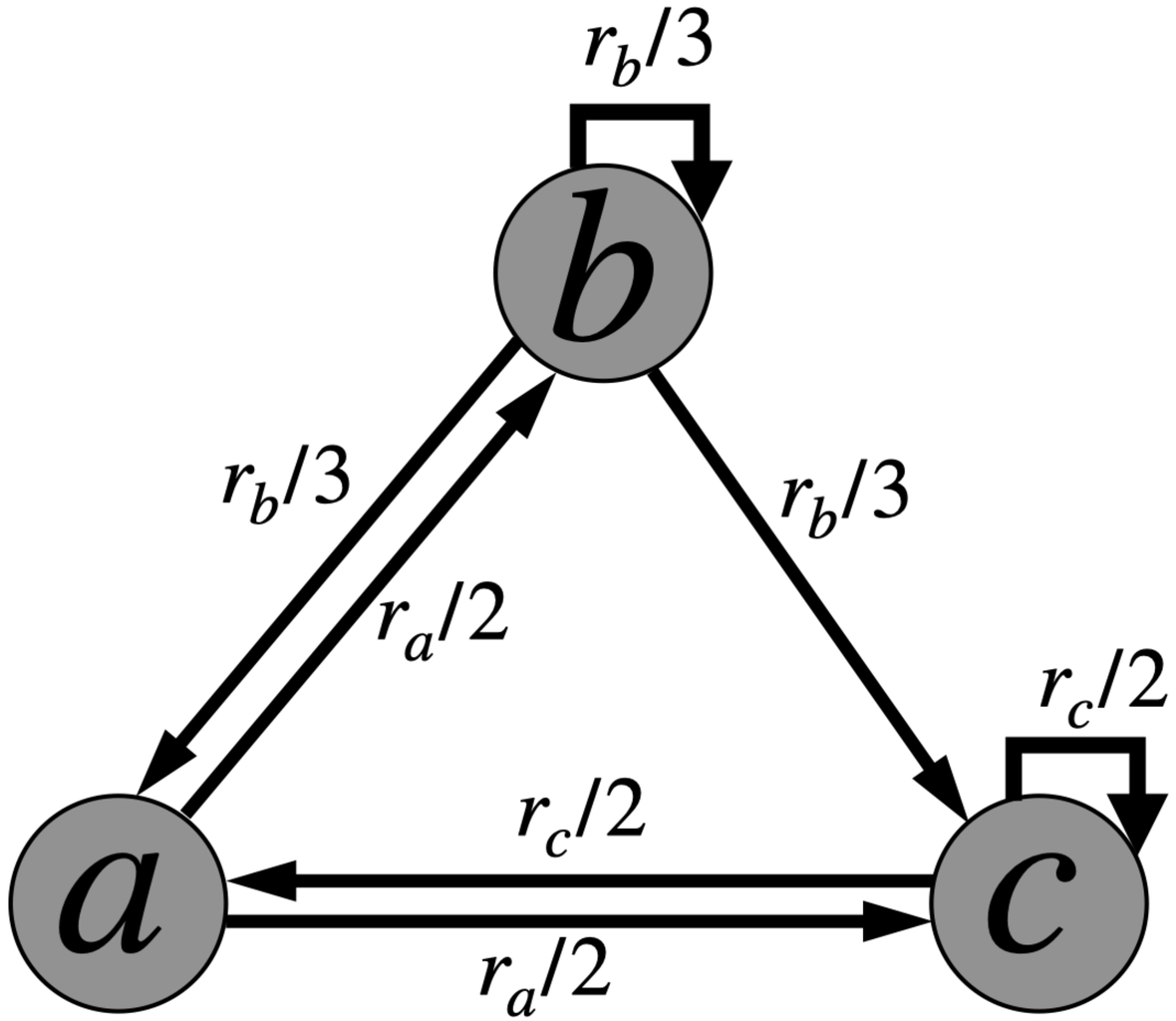
A small example

The flow equations

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

- 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

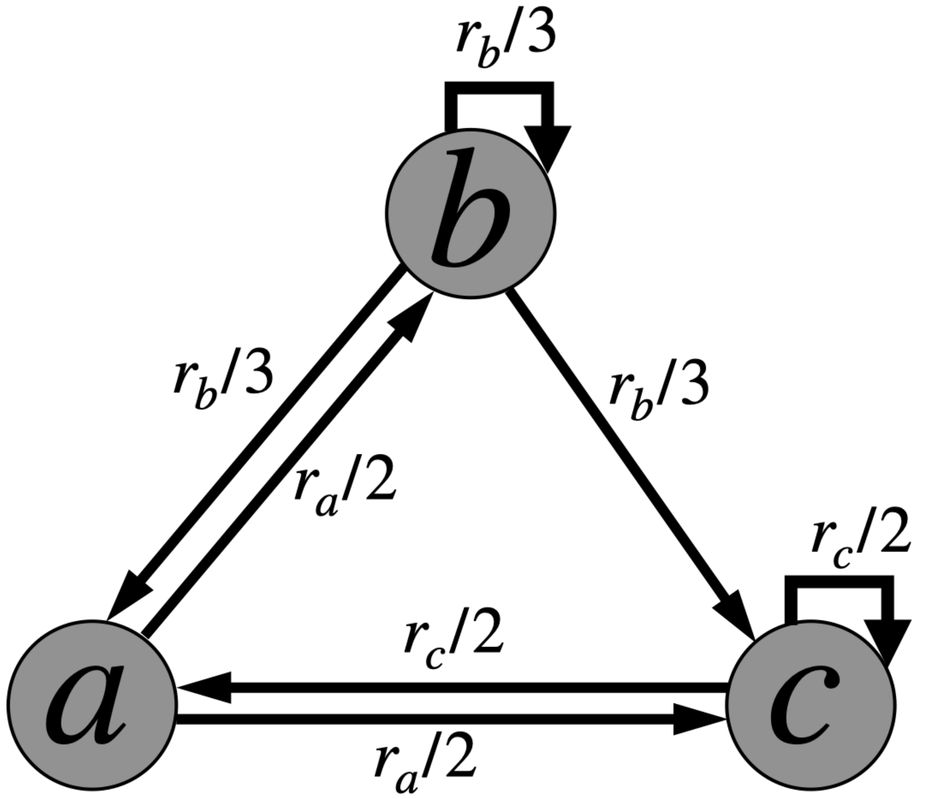
$$r_j = \sum_{i \to j} \frac{r_i}{d_i} \Rightarrow \mathbf{r} = \mathbf{M}\mathbf{r}.$$

Matrix formulation

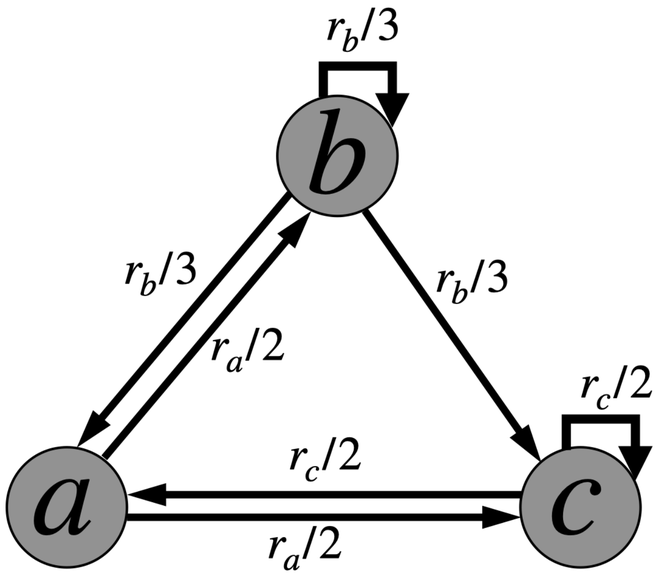
- Define the column stochastic adjacency matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$.
- $\sum_i \mathbf{M}_{ij} = 1$.
- Page i has d_i out-links.
- If $i \to j$, then $\mathbf{M}_{ji} = \frac{1}{d_i}$, else $\mathbf{M}_{ji} = 0$.
- The rank vector $\mathbf{r}$ has one entry per page ➜ importance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

$$\mathbf{r}_i = \text{importance of page } i$$

$$\sum_i \mathbf{r}_i = 1$$



The same small example



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$$r_a = r_b/3 + r_c/2,$$
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In matrix form

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

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

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

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 $\mathbf{M}$:

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

ALGORITHM: Power iteration method

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

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

Eigenvector formulation

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

- $\mathbf{x}$ is an eigenvector with corresponging 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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2: **Initialize**: $\mathbf{r}_0 = [1/n, \ldots, 1/n]^\intercal$
3: **while** $|\mathbf{r}_k - \mathbf{r}_{k-1}|_1 \geq \epsilon$ **do**
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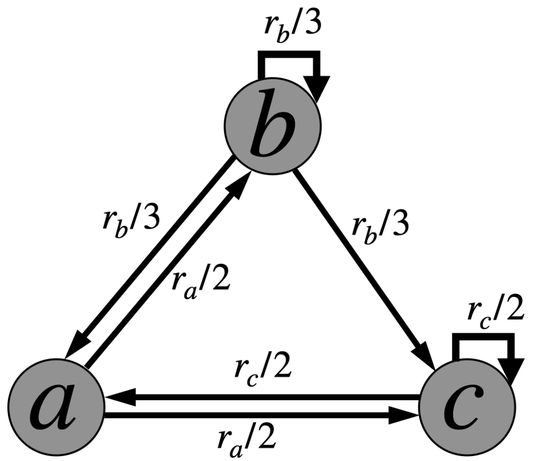
5: $\quad \mathbf{r}_k = \tilde{\mathbf{r}}/\|\tilde{\mathbf{r}}\|$
6: **end while**

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

The same small example



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

❶ $\mathbf{M}$ 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 $\mathbf{v}_1 \in \mathbb{R}^n$.

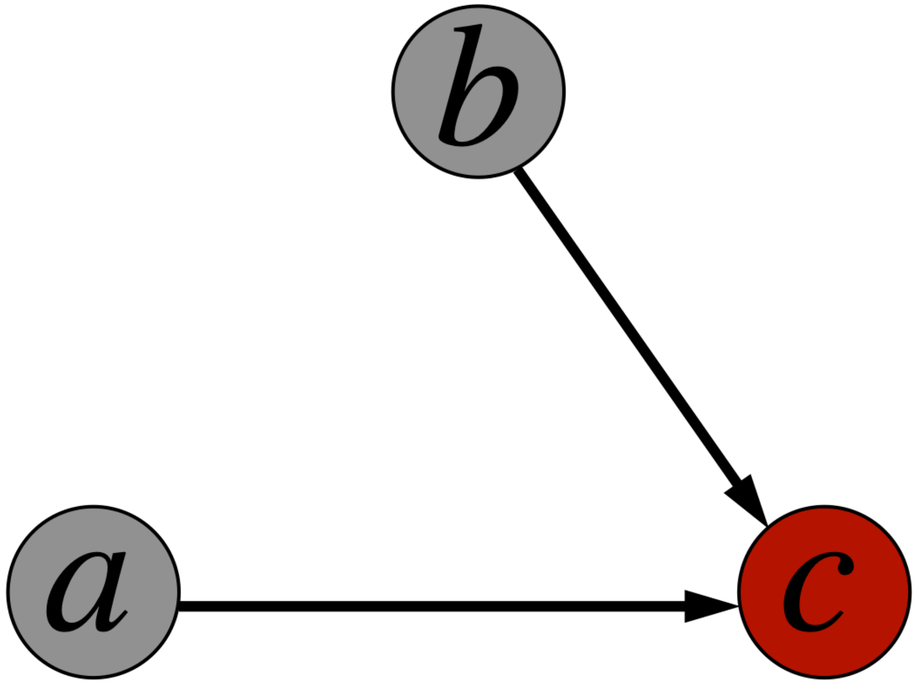
➠ Initial unbiased guess $\mathbf{r}_0 = [1/3, 1/3, 1/3]^\intercal$

❷ Converges to $\mathbf{r} = \mathbf{M}^8 * \mathbf{r}_0 = [0.3077, 0.2308, 0.4615]^\intercal$, so $\mathrm{rank} = [2, 3, 1]$.

$$\mathbf{r}_1 = \mathbf{M} \cdot \mathbf{r}_0,$$
$$\mathbf{r}_2 = \mathbf{M} \cdot \mathbf{r}_1 = \mathbf{M}(\mathbf{M}\mathbf{r}_0) = \mathbf{M}^2 \cdot \mathbf{r}_0,$$
$$\mathbf{r}_3 = \mathbf{M} \cdot \mathbf{r}_2 = \mathbf{M}(\mathbf{M}^2\mathbf{r}_0) = \mathbf{M}^3 \cdot \mathbf{r}_0,$$
$$\mathbf{r}_4 = \dots$$

Adapting to real-world (1)

Col stochastic assumption violated.



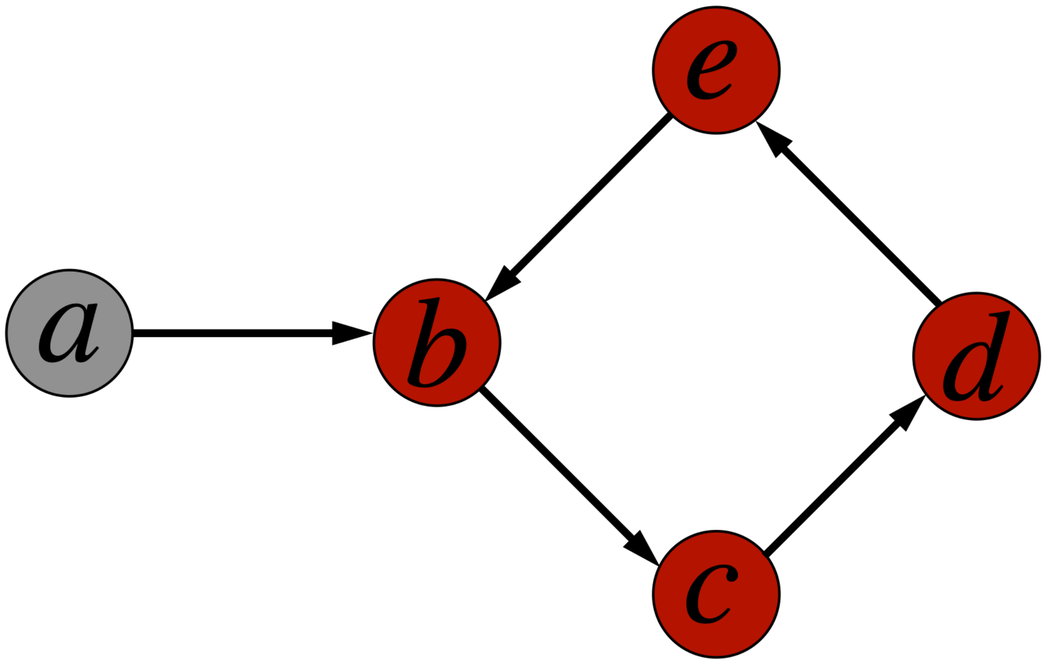
Dangling nodes

- 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.
- Propabilistically 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

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

d_i: the out-degree of node i.

- The Google matrix $\mathbf{A}$ reads

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

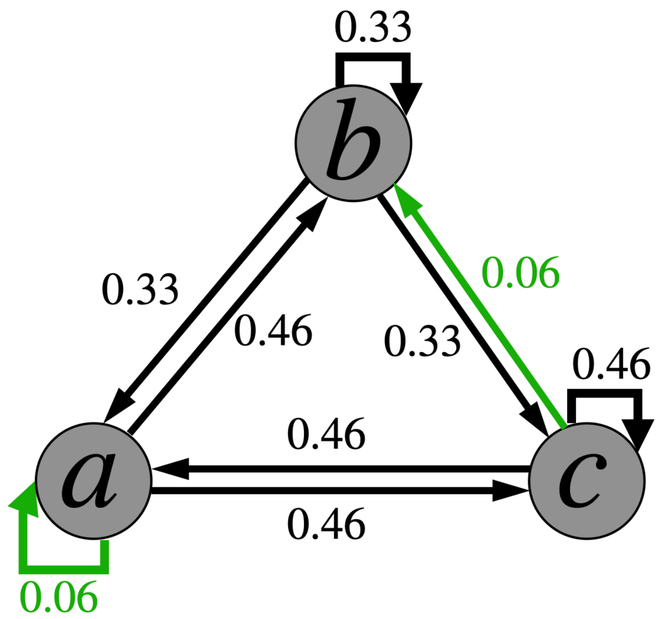
$\mathbf{u} = \frac{1}{n}\mathbf{e}$: unbiased personalization vector.

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



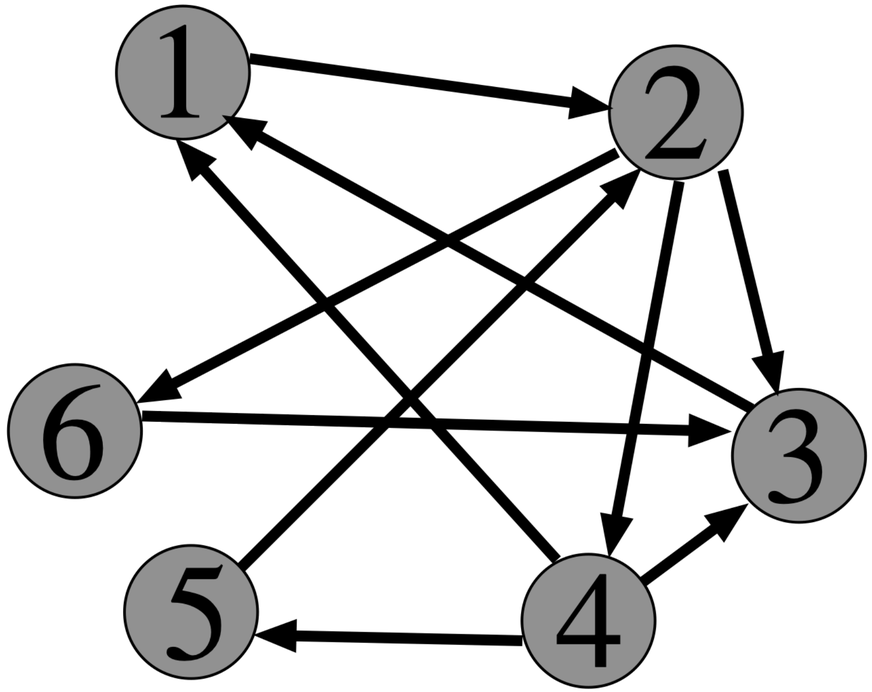
- If the personalization vector $\mathbf{u}$ contains zeros, then the random jump is done only to the nodes of the graph that has a corr. $u_i \neq 0, i \in \{1, n\}$.

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

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

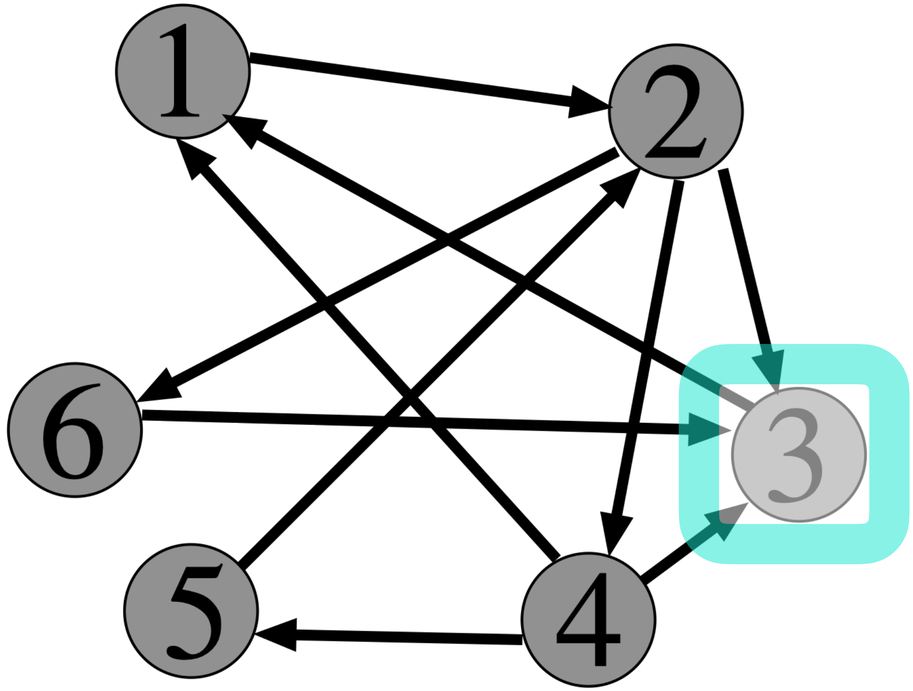
$$\mathbf{A} = p\mathbf{M} + (1-p)\mathbf{u}\mathbf{e}^\intercal = 0.8 \cdot \begin{pmatrix} 0 & 1/3 & 1/2 \\ 1/2 & 1/3 & 0 \\ 1/2 & 1/3 & 1/2 \end{pmatrix} + 0.2 \cdot \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} = \begin{pmatrix} 0.0667 & 0.3333 & 0.4667 \\ 0.4667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

Degree $\neq$ PageRank



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

Degree $\neq$ PageRank



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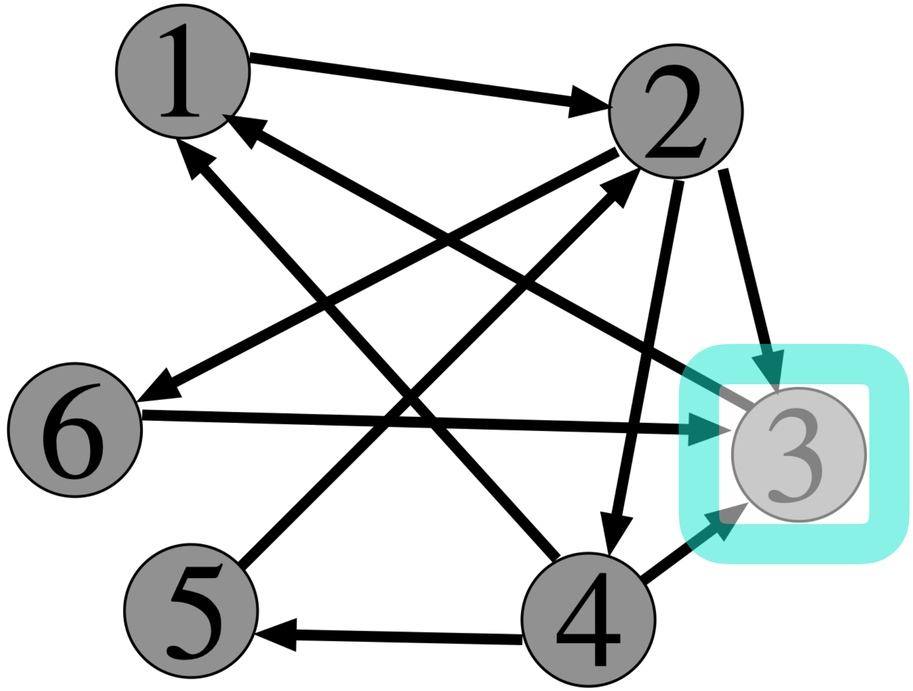

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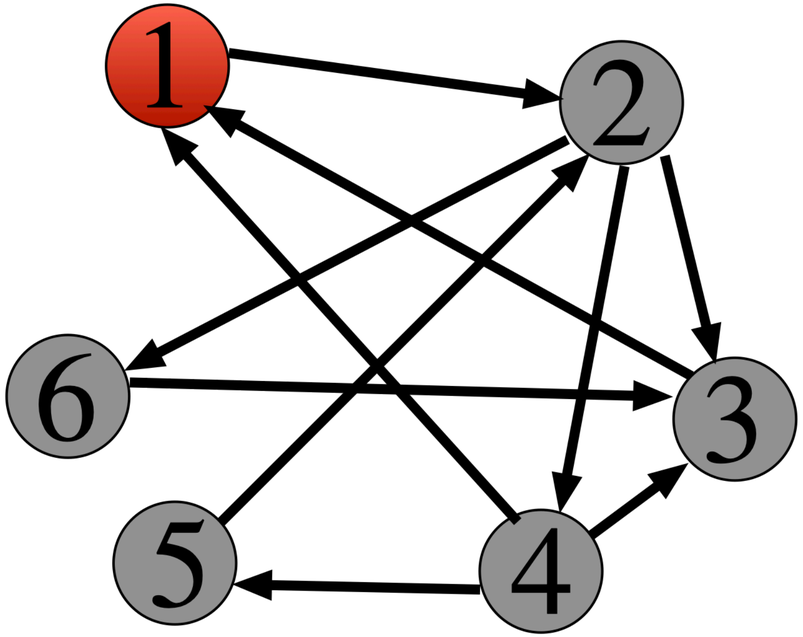
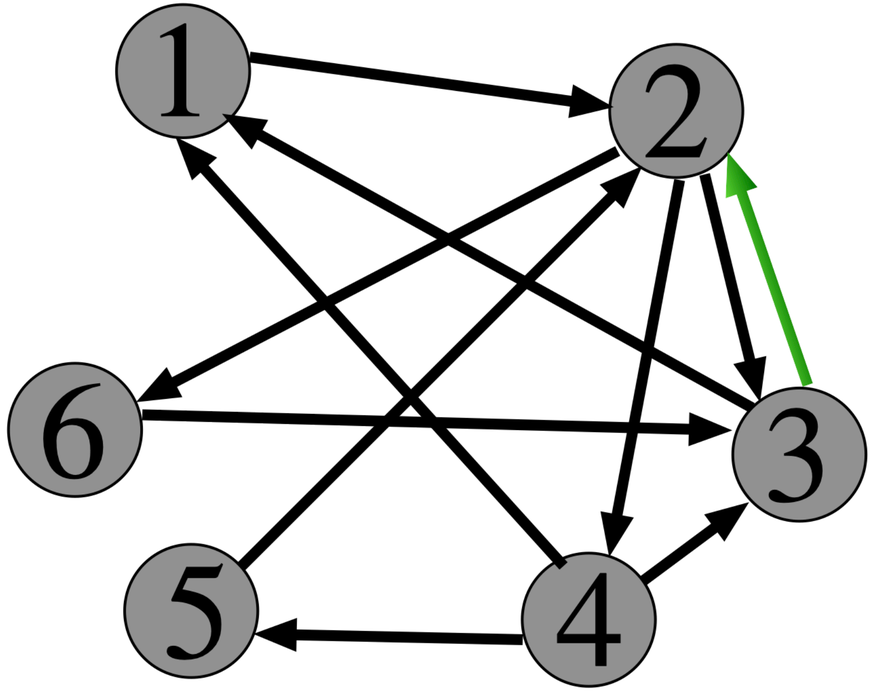


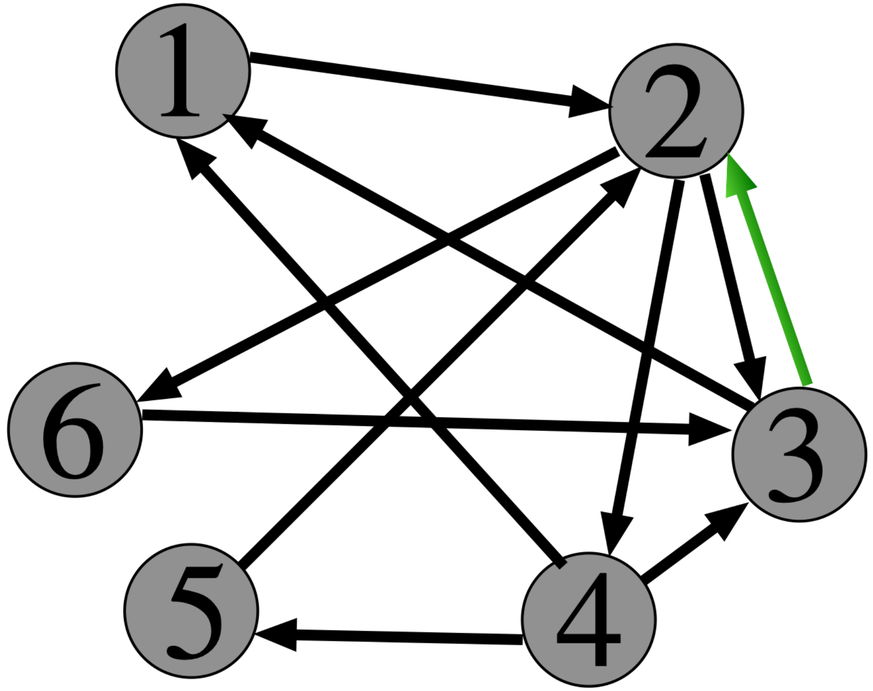
The PageRank ranking does not always correspond to the degree ranking.

Degree $\neq$ PageRank

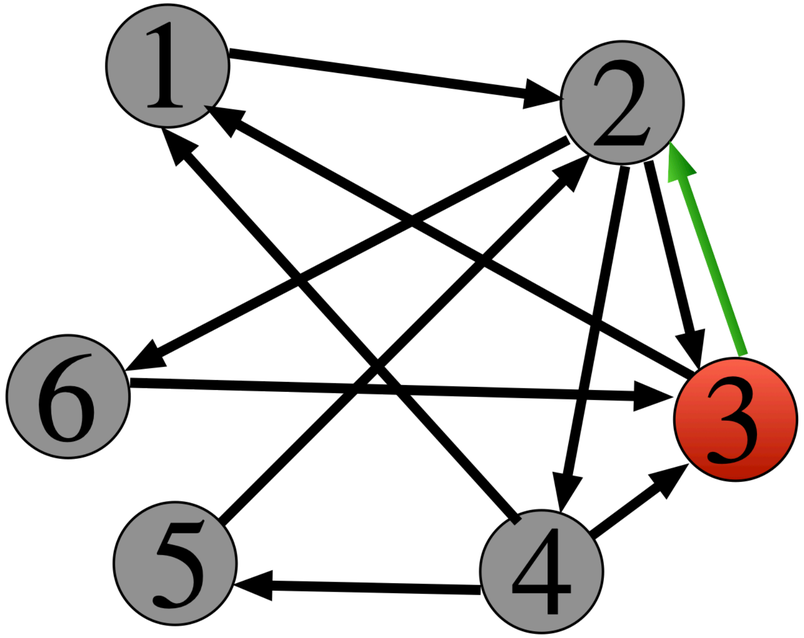


Let's perturb the graph slightly.

Degree $\neq$ PageRank



Let's perturb the graph slightly.



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

The picture today

Does Google still use it?

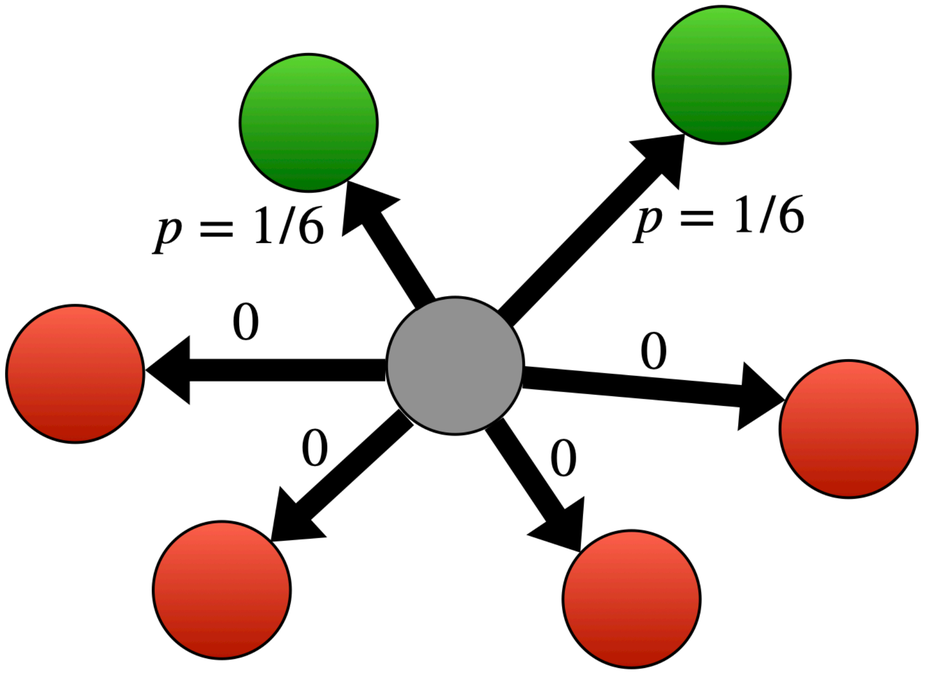
- ⇛ Over 200 types of ranking metrics to determine the final order.

  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 $\mathbf{e}^\mathsf{T}\mathbf{x} = 1$, in which case

$$\mathbf{x} = p\mathbf{M}\mathbf{x} + (1-p)\mathbf{v}\mathbf{e}^\mathsf{T}\mathbf{x} = p\mathbf{M}\mathbf{x} + (1-p)\mathbf{v}$$

$$\Longleftrightarrow$$

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

- 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 $\lambda_1 > \lambda_2 > \cdots > \lambda_n$ 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

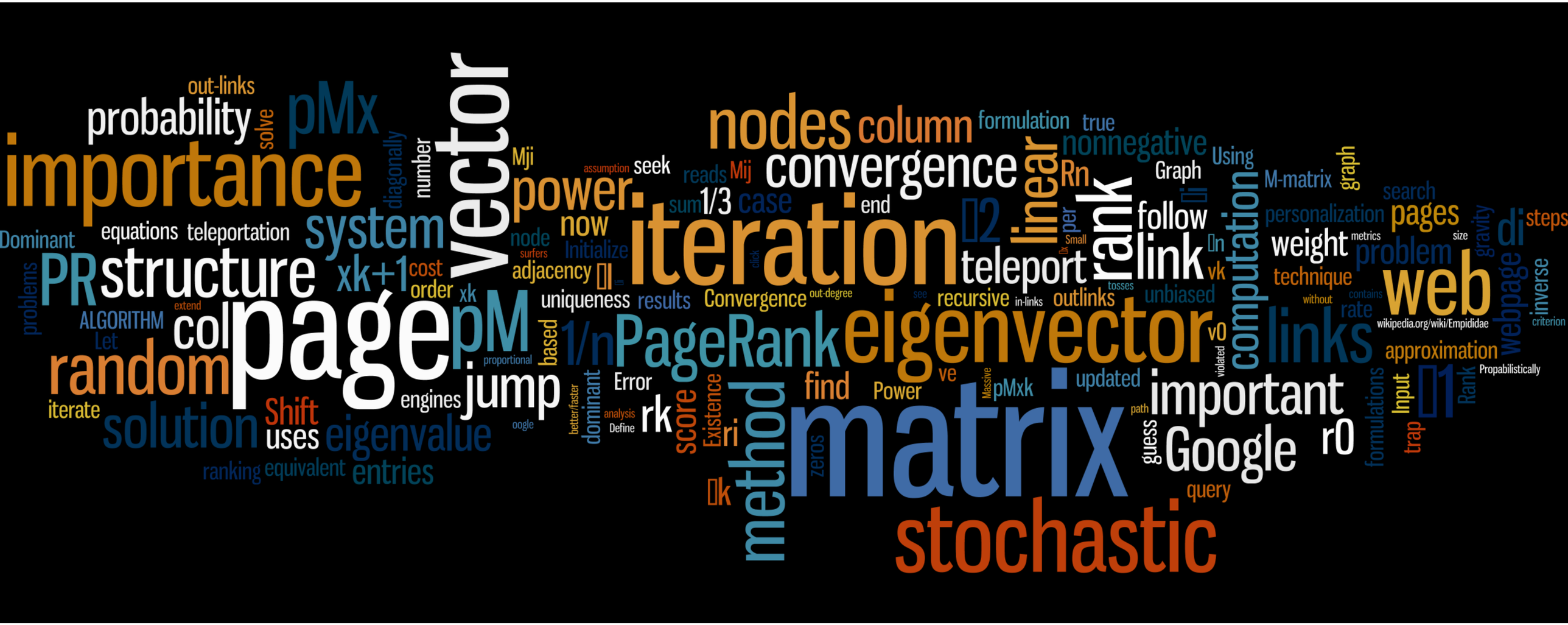
- λ_i: eigvals of $\mathbf{A}$, then $\lambda_i - \alpha$: of $\mathbf{A} - \alpha\mathbf{I}$, and $\mu_i = \frac{1}{\lambda_i - \alpha}$: of $\mathbf{B} = (\mathbf{A} - \alpha\mathbf{I})^{-1}$.
- ➠ Imagine applying the power method on $\mathbf{B}$
- Convergence rate now is $|\frac{\mu_2}{\mu_1}| = |\frac{\lambda_1 - \alpha}{\lambda_2 - \alpha}|$. If $\alpha \approx \lambda_1$ ➜ 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**: $\mathbf{r}_0 = [1/n, \ldots, 1/n]^\intercal$
3: **for** $k = 1, 2, \ldots,$ until termination criteria **do**
4: Solve $(\mathbf{A} - \alpha\mathbf{I})\tilde{\mathbf{v}} = \mathbf{v}_{k-1}$
5: $\mathbf{v}_k = \tilde{\mathbf{v}}/\|\mathbf{v}\|$
6: $\lambda^k = \mathbf{v}_k^\intercal \mathbf{A} \mathbf{v}_k$
7: **end for**

- If $\mathbf{v}_0$ normalized, $\lambda^0 = \mathbf{v}_0^\intercal \mathbf{A} \mathbf{v}_0$, and $\alpha = \lambda^{k-1}$, the Rayleight quotient is approximated.
- $\lambda(\mathbf{v}) = \frac{\mathbf{v}^\intercal \mathbf{A} \mathbf{v}}{\mathbf{v}^\intercal \mathbf{v}}$
- 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