CS630 Graduate Algorithms
November 25, 2024

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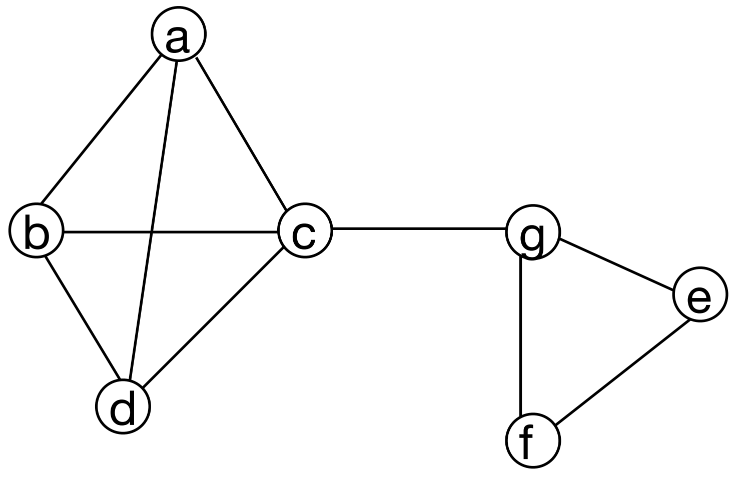
PageRank
Random walks on graphs

Slides by Dora Erdos

Graph adjacency matrix



M[i,j]=1 if there is a directed edge from i to j

x = [1,0,0,0,0,0,0] represents starting the walk at vertex a

Then:
xM = [0,1,1,1,0,0,0]

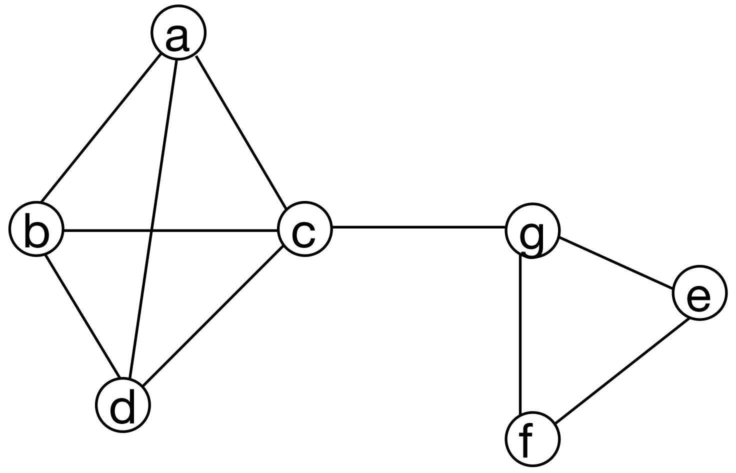
xM^2 = [3,2,2,2,0,0,1]

xM^3 = [6,7,8,7,1,1,2]

$$M = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix} \quad M^2 = \begin{bmatrix} 3 & 2 & 2 & 2 & 0 & 0 & 1 \\ 2 & 3 & 2 & 2 & 0 & 0 & 1 \\ 2 & 2 & 4 & 2 & 1 & 1 & 0 \\ 2 & 2 & 2 & 3 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 2 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 2 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 3 \end{bmatrix} \quad M^3 = \begin{bmatrix} 6 & 7 & 8 & 7 & 1 & 1 & 2 \\ 7 & 6 & 8 & 7 & 1 & 1 & 2 \\ 8 & 8 & 6 & 8 & 1 & 1 & 6 \\ 7 & 7 & 8 & 6 & 1 & 1 & 2 \\ 1 & 1 & 1 & 1 & 2 & 3 & 4 \\ 1 & 1 & 1 & 1 & 3 & 2 & 4 \\ 2 & 2 & 6 & 2 & 4 & 4 & 2 \end{bmatrix}$$

Graph adjacency matrix

M[i,j]=1 if there is a directed edge from i to j



Let x = [x_1,x_2,…,x_n] represent the starting vertices of a walk.

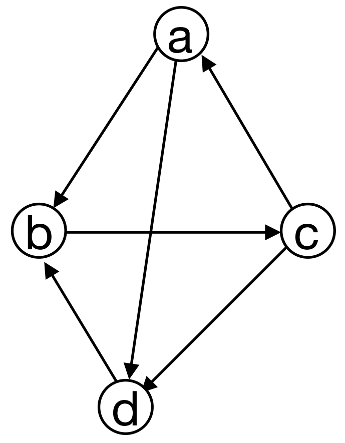
xi can be 0/1

xi can be a probability

$xM^k[j]$ = the number of ways we can reach j in k steps if we start based on x.

$$M = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix} \quad M^2 = \begin{bmatrix} 3 & 2 & 2 & 2 & 0 & 0 & 1 \\ 2 & 3 & 2 & 2 & 0 & 0 & 1 \\ 2 & 2 & 4 & 2 & 1 & 1 & 0 \\ 2 & 2 & 2 & 3 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 2 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 2 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 3 \end{bmatrix} \quad M^3 = \begin{bmatrix} 6 & 7 & 8 & 7 & 1 & 1 & 2 \\ 7 & 6 & 8 & 7 & 1 & 1 & 2 \\ 8 & 8 & 6 & 8 & 1 & 1 & 6 \\ 7 & 7 & 8 & 6 & 1 & 1 & 2 \\ 1 & 1 & 1 & 1 & 2 & 3 & 4 \\ 1 & 1 & 1 & 1 & 3 & 2 & 4 \\ 2 & 2 & 6 & 2 & 4 & 4 & 2 \end{bmatrix}$$

Graph adjacency matrix



D[i,j]=1 iff there is a directed edge from i to j.

$$D = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \quad D^2 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 2 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad D^3 = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 2 & 0 & 1 \\ 0 & 1 & 2 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

- D^2[i,j] contains the number of length-2 directed path from i to j.
- D^k[i,j] contains the length-k paths.
- The sum of column i in D^k is the total number of ways we can get to i in k steps.

Let x = [x_1,x_2,…,x_n] be a vector that represents the probability that we start in each node

Then xD^k tells us where the walk is after k steps if we start based on x.

“status” as centrality measure

- vertices have a status (importance) score
- vertices have ‘high’ status if they are connected to vertices with ‘high’ status (this is a circular definition ;))

Centrality x_i of a node i is the sum of the centrality of its neighbors, scaled by some constant.

$$x_i = \frac{1}{\lambda} \sum_{(i,j) \in E} x_j$$

λ is a constant that we chose in a clever way

Eigenvector centrality

Centrality x_i of a node i is the sum of the centrality of its neighbors, scaled by some constant.

$$x_i = \frac{1}{\lambda} \sum_{(i,j) \in E} x_j = \frac{1}{\lambda} \sum_{A[i,j]==1} x_j$$

Arrange the centrality values in a vector x = [x_1,x_2,....,x_n].

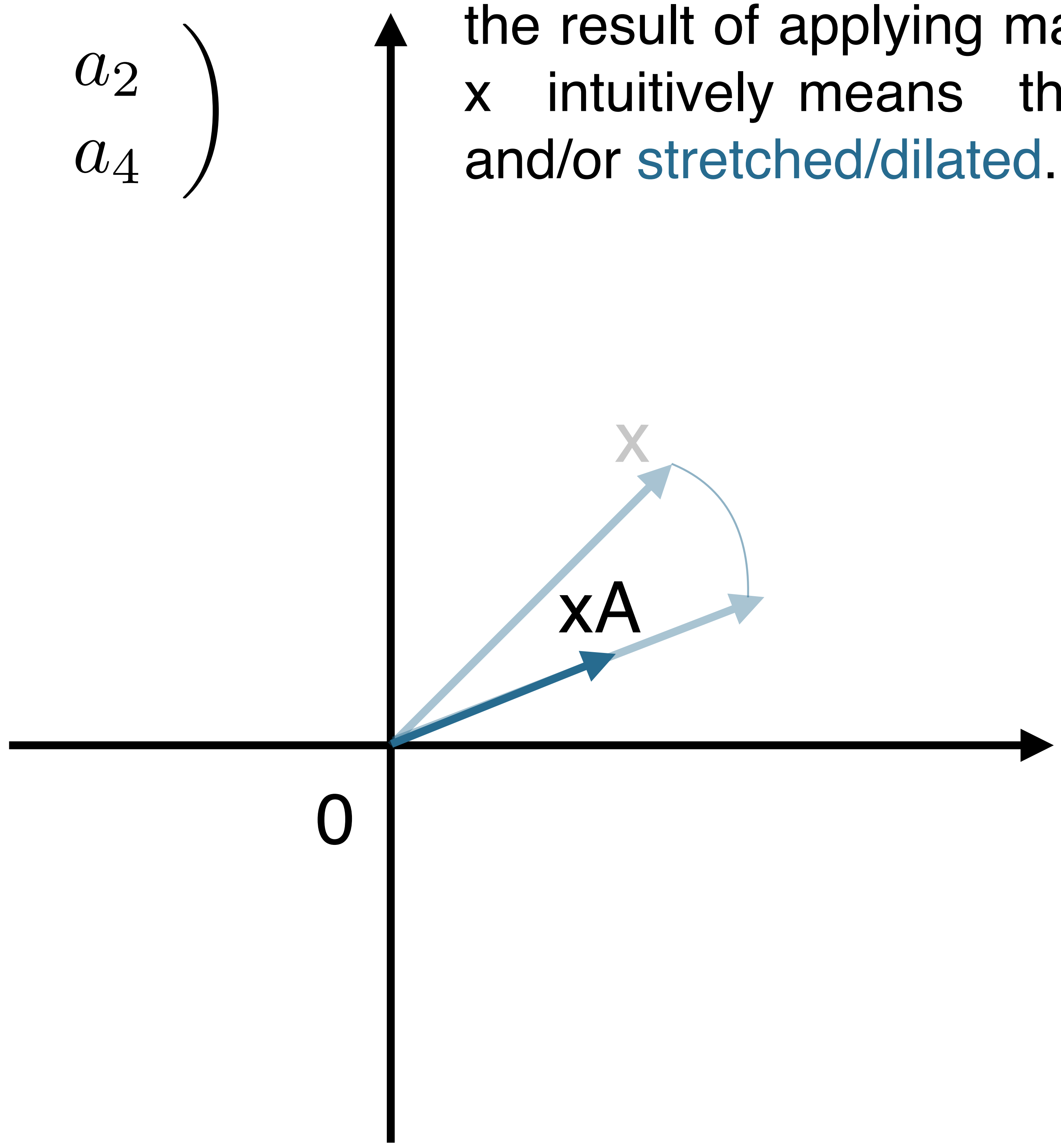
$$x = \tfrac{1}{\lambda} x A$$

Rearranging we get $x\lambda = xA$

x[i] is called the eigenvector centrality of node i.
if we choose λ to be the largest eigenvalue, than all x[i] are positive. (more on this later)

$$A = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}$$

the result of applying matrix A to a vector x intuitively means that x gets rotated and/or stretched/dilated.



Eigenvalue decomposition

Assume *A* is an *n x n* square matrix
u is an n-dim vector

$$v = uA = \sum_{j=1}^{n} u_j A[*, j]$$

You can think of *v* as a linear combination of the columns of *A*.

u is an eigenvector if applying *A* to it only changes its magnitude not its direction.

$$\lambda u = uA$$

If *A* has rank *n*, then there are *n* orthonormal eigenvectors and eigenvalues.

Eigenvalue decomposition of A

$$A = U \Lambda U^{-1}$$

U contains the eigenvectors as its columns
Λ is a diagonal matrix with the eigenvectors in its diagonal

Eigenvalue decomposition and powers of a matrix

eigenvalue decomposition $A = V \Lambda V^T$

- V is orthonormal $VV^T = V^T V = I$
- Λ is diagonal

compute A^k:

$$A = V \Lambda V^T$$

$$A^2 = V \Lambda V^T V \Lambda V^T = V \Lambda^2 V^T$$

$$A^k = V \lambda V^T V \lambda V^T \ldots V \Lambda V^T = V \Lambda^k V^T$$

Not sure how to use it yet, but there is definitely some kind of relationship between A^k and eigenvector centrality.

Path lengths

- degree centrality - length 1 path
- adjacency matrix = # of length-1 paths A
- # of length-k paths A^k
- # of paths of length at most k $\sum_{i=1}^{k} A^i$

- infinite paths?
    - define centrality as the relative fraction of paths passing through a vertex
    - equivalent to asking: starting from a random vertex and taking some number of steps along the edges, how likely are we to end up in vertex v?

Walking on the graph — power method

Let $x^{(0)} = [x_1, x_2, \ldots, x_n]$ correspond to some initial state of the vertices.

- The $^{(0)}$ in the notation corresponds to the 0th iteration, not an exponent.

Now take a step

$$x^{(1)} = x^{(0)} A$$

$x_i^{(1)}$ is the weight-scaled notion of being in node i.

Another step, then many more

$$x^{(2)} = x^{(1)} A = x^{(0)} A^2$$

$$x^{(k)} = x^{(k-1)} A = x^{(0)} A^k$$

Walking on the graph — power method

Let $x^{(0)} = [x_1, x_2, \ldots, x_n]$ correspond to some initial state of the vertices.

- The $^{(0)}$ in the notation corresponds to the 0th iteration, not an exponent.

In summary we have

$$x^{(1)} = x^{(0)}A$$

$$x^{(k)} = x^{(0)}A^k$$

If x can be any kind of weight, then these would be really large numbers. So let's normalize in each iteration.

$$\text{Assume } \|x^{(0)}\|_2 == 1 \text{ (or take } x^{(0)} = \frac{x^{(0)}}{\|x^{(0)}\|_2}\text{)}$$

$$x^{(1)} = x^{(0)}A$$

$$x^{(1)} = \frac{x^{(1)}}{\|x^{(1)}\|_2}$$

After k iterations

$$x^{(k)} = x^{(k-1)}A = x^{(0)}A^k$$

$$x^{(k)} = \frac{x^{(k)}}{\|x^{(k)}\|_2}$$

Walking on the graph — power method

$$x^{(0)} = \frac{x^{(0)}}{\|x^{(0)}\|_2}$$

$$x^{(k)} = x^{(k-1)}A = x^{(0)}A^k$$

$$x^{(k)} = \frac{x^{(k)}}{\|x^{(k)}\|_2} = \frac{x^{(0)}A^k}{\|x^{(0)}A^k\|_2}$$

Power method: instead of computing $x^{(k)}$ directly from A^k we perform the k iterations to get there.

Now we can think of $x_i^{(k)}$ as some kind of probability of being in node i after k steps (since x sums to 1).

- this is in fact not quite the proper probability distribution, but very similar

Search engines on the web

In the mid 90s there were dozens of search engines. Then, after 1998 Google emerged as the engine and the others mostly disappeared.

How did search engines work?

- submit a query , e.g. “personal 737 jet”
- first step: basic text processing is done to find the pages containing the term
  - thousands of pages are retrieved
- second step: show the results to the user
  - Google turned out to be the best at finding the most relevant ones
  - they used PageRank to decide relevance
-

Brin, S.; Page, L. (1998). "The anatomy of a large-scale hypertextual Web search engine" (PDF). *Computer Networks and ISDN Systems*. **30** (1–7): 107–117.

PageRank centrality — random walks

Setting:

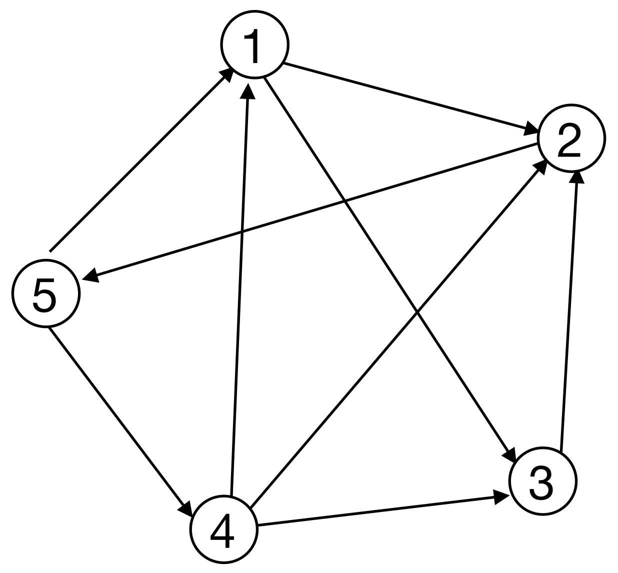
- on the Web there are sites and hyperlinks directing from one page to an other.
- remember the status score?
  - high status nodes (sites) are the ones pointed (linked) by high status nodes.
  - here links are endorsements by the author
- we are still on a quest to assign the “status” score to nodes

Random surfer:

- we start on a random page
- at each step we follow one of the outgoing links at random
- sometimes we get bored (e.g. quit browsing), and start over at some random page
- if we were to walk for a looooong time, then our starting page doesn’t matter anymore
- we should find the probability that at any given time we are in any given page
- it turns out that after many steps this probability is independent of the walk itself
- this probability distribution (called stationary distribution) is Pagerank
  - is related to Markov Chains

Random walks on graphs — PageRank

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



The transition matrix P represents the probability of traversing from one node to its neighbor.
The (row) vector q$^{(t)}$ contains the probability that we are in each node after t steps.
Then q$^{(t+1)}$ = q$^{(t)}$P

$$P = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

$$q_1^{(t+1)} = \tfrac{1}{3} q_4^{(t)} + \tfrac{1}{2} q_5^{(t)}$$

$$q_2^{(t+1)} = \tfrac{1}{2} q_1^{(t)} + q_3^{(t)} + \tfrac{1}{3} q_4^{(t)}$$

$$q_3^{(t+1)} = \tfrac{1}{2} q_1^{(t)} + \tfrac{1}{3} q_4^{(t)}$$

$$q_4^{(t+1)} = \tfrac{1}{2} q_5^{(t)}$$

$$q_5^{(t+1)} = q_2^{(t)}$$

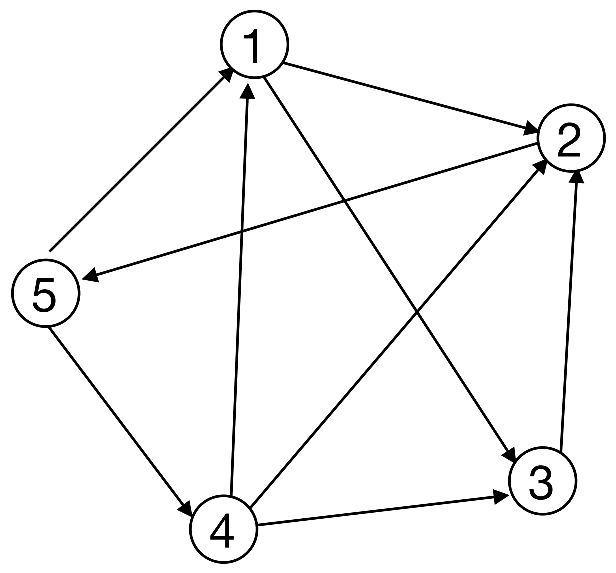
general formula:

$$q^{(t+1)} = q^{(t-1)} P = q^{(0)} P^t$$

$$q^{(t+1)} = q^{(0)} P^t$$

Random walks on graphs — PageRank

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



Incorporating the random restart (often referred as random jump):
In each iteration with some probability we jump to any of the nodes uniformly at random.

$$P = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix} \qquad J = \begin{bmatrix} \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{bmatrix}$$

$$P' = \alpha P + (1-\alpha)J \text{ where } \alpha \in [0,1]$$

general formula:

$$q^{(t+1)} = q^{(0)}(P')^t$$

Random walks on graphs — PageRank

$$P = \begin{bmatrix} P_{11} & P_{12} & \dots & P_{in} \\ P_{21} & \dots & & p_{2n} \\ \vdots & \ddots & & \vdots \\ P_{n1} & P_{n2} & \dots & P_{nn} \end{bmatrix} \qquad J = \begin{bmatrix} \frac{1}{n} & \frac{1}{n} & \dots & \frac{1}{n} \\ \frac{1}{n} & \dots & & \frac{1}{n} \\ \vdots & \ddots & & \vdots \\ \frac{1}{n} & \frac{1}{n} & \dots & \frac{1}{n} \end{bmatrix}$$

$$P' = \alpha P + (1-\alpha)J \text{ where } \alpha \in [0,1]$$

$$q^{(t+1)} = q^{(0)}(P')^t$$

We get Pagerank as $t \to \infty$

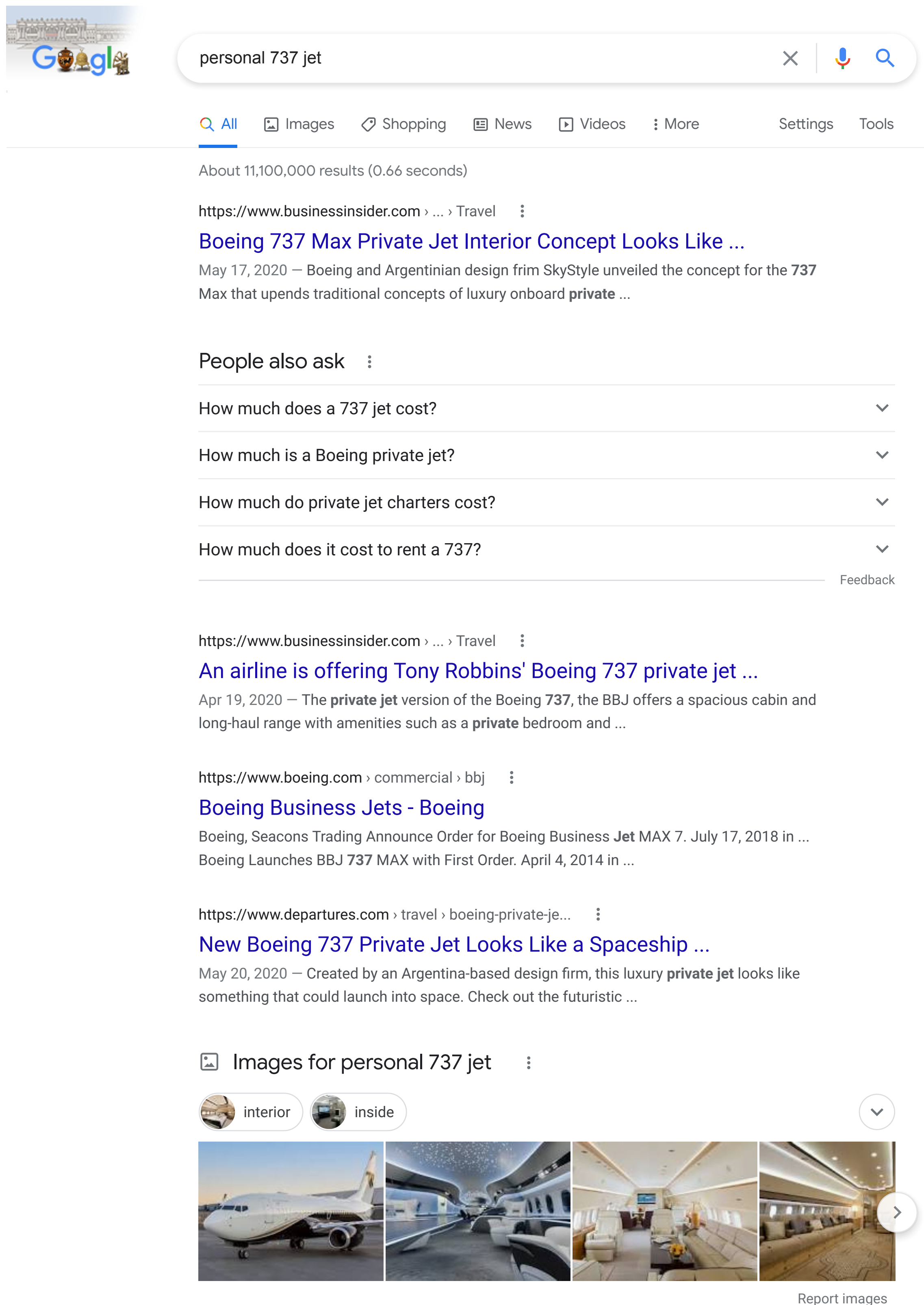
α controls the rate of convergence

variant: personalized PageRank

- instead if jumping to a uniform random location, we jump back to some specific starting node.

Pagerank and the power method

Remember? we said that computing (P')^t is inefficient, hence we use an iterative approach.



personal 737 jet

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To compute (P')^t

$$(P')^t = V\Lambda^t V^T$$

For this we need to compute the eigenvalue decomposition of P'

- Remember, that takes computing the inverse matrix (say, for the largest eigenvalue)
- using Gaussian elimination that takes $O(\frac{2}{3}n^3)$

$$(P' - \lambda I)^{-1} v = 0$$

There are 11 million hits! lots of flops…

$$O(\frac{2}{3}n^3) \approx 11^{18} \cdot 10^{18} \approx 10^{36}$$

That takes 10^{27} seconds, is measured in months….

conclusion: use the power method instead….

Markov Chains

- A Markov chain describes a discrete time stochastic process over a set of states

according to a transition probability matrix

$$S = \{s_1, s_2, \dots s_n\}$$

  - P_{ij} = probability of moving to state j when at state i
    - $\sum_j P_{ij} = 1$ (stochastic matrix)

$$P = \{P_{ij}\}$$

- Memorylessness property: The next state of the chain depends only at the current state and not on the past of the process (first order MC)
  - higher order MCs are also possible

Random Walk

- Random walks on graphs correspond to Markov Chains
  - The set of states S is the set of nodes of the graph G
  - The transition probability matrix P is the probability that we follow an edge from one node to another

State probability

- The vector $q^0 = (q^0_1, q^0_2, \dots, q^0_n)$ that stores the probability of being at state i at the start of the random walk
- $q^1 = q^0 P$ is the probability of being in each node after one random step
- $q^t = q^{t-1} P$ is the probability of being at node i after t steps
- Can we generalize this?

Stationary Distribution

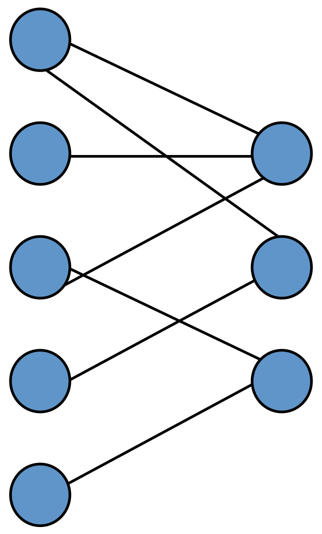
- $q^t = q^{t-1}P$ is the probability of being at node i after t steps
- The stationary distribution is the probability of being in any given node = the fraction of time spent in each node
- as $t \longrightarrow \infty$ this doesn't change by taking another step: $q=qP$

Stationary Distribution

- A stationary distribution for a MC with transition matrix P, is a probability distribution π, such that $\pi = \pi P$
- π is the eigenvector corresponding to eigenvalue 1
  - since P is stochastic 1 is its largest eigenvalue
- The stationary distribution exists if the MC is irreducible and aperiodic.
  - The underlying graph is strong connected and not bipartite

Undirected graphs — stationary distribution not very informative

- connected undirected graph is always irreducible
- why not bipartite?
  - every other step the walker is not in a node with probability 1 (periodic)

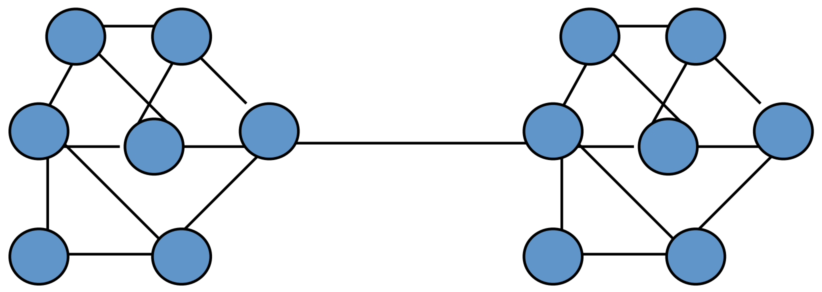


Undirected graphs — stationary distribution not very informative

- connected undirected graph is always irreducible
- why not bipartite?
- In a connected and non-bipartite graph the stationary distribution is proportional to the degrees of the nodes

Undirected graphs — stationary distribution not very informative

- connected undirected graph is always irreducible
- why not bipartite?
- In a connected and non-bipartite graph the stationary distribution is proportional to the degrees of the nodes
- mixing time: the rate of convergence



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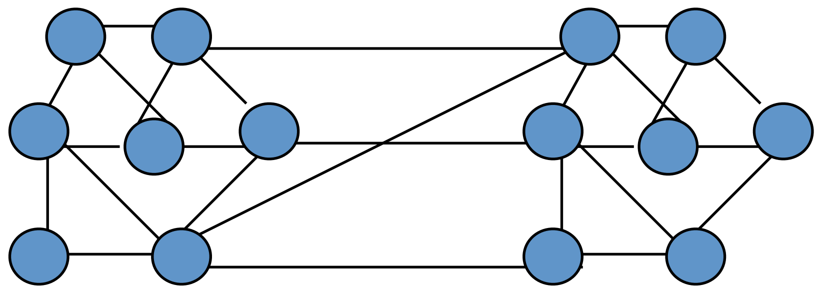

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