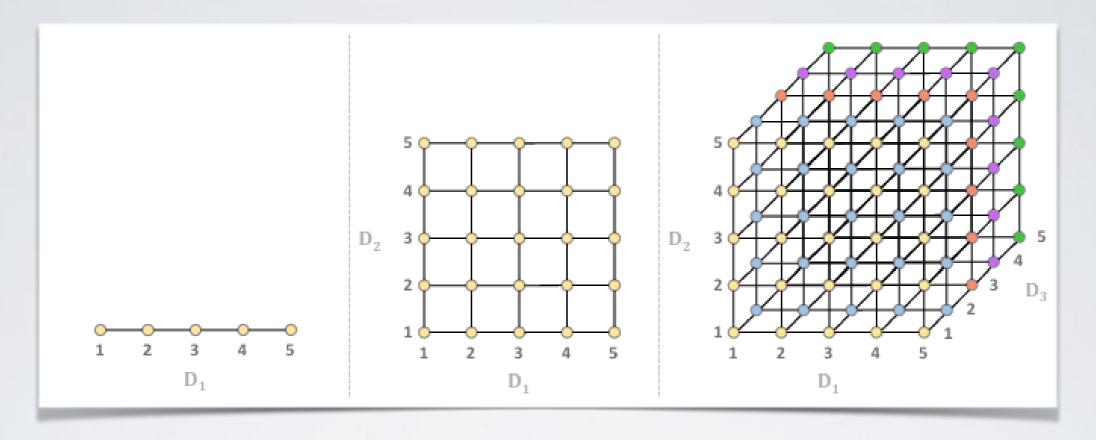
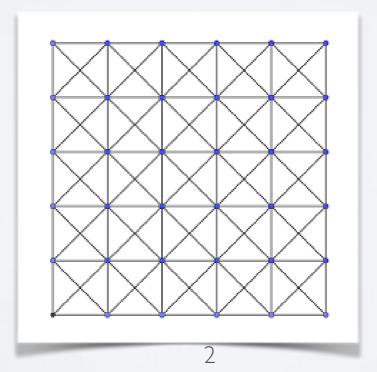
M2 TIW - M2 BIO-INFO

DATA ANALYSIS

Network Data Mining

NETWORKS/GRAPHS

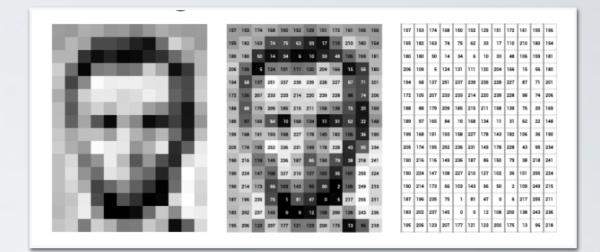




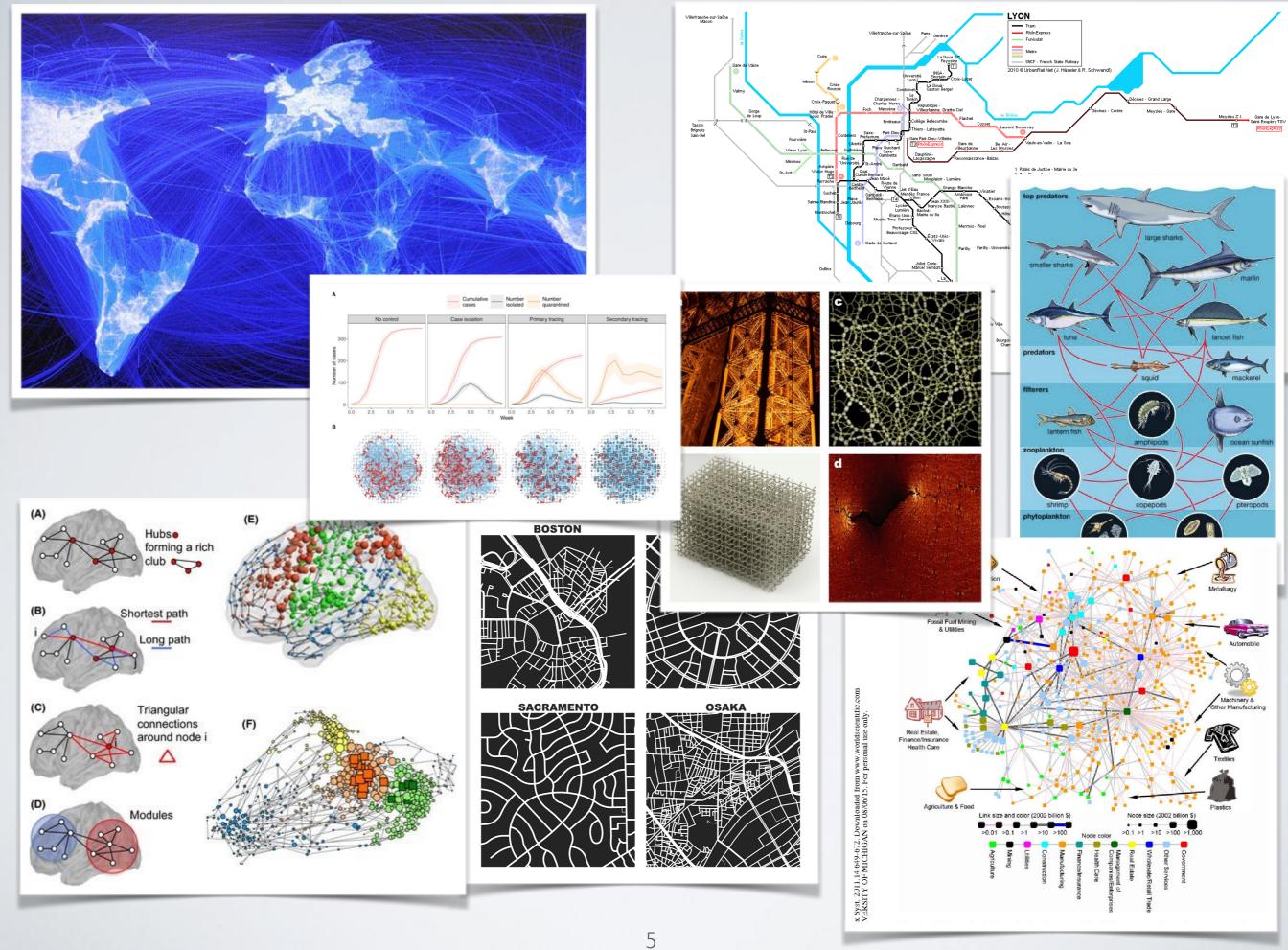
NETWORKS/GRAPHS

Structured data

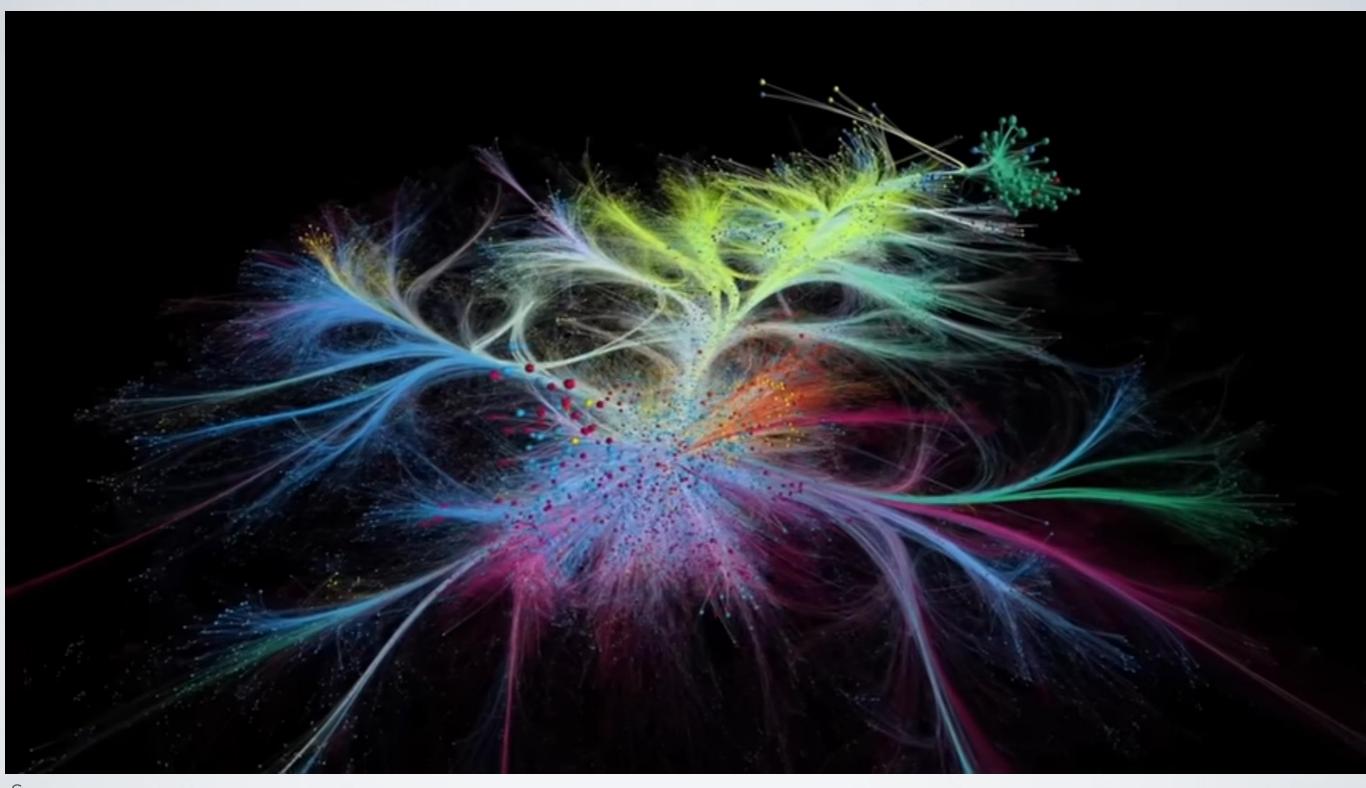
- Text
 - Sequence. Each item is **before** or **after** the other ones. And it is important
 - 1D organisation
- Images
 - Each pixel has a position in 2D grid, it is on the **left**, **right**, **top** or **bottom** compared with the other ones. And it is important
 - 2D organisation
- Variants: Video (3D), time series (1D continuous), spatial (2D/3D continuous), etc.
- Networks: Neighborhoods are not constrained. The graph is the structure
 - Generalization of discrete structures (text, images, videos)



NETWORKS ARE EVERYWHERE



150 YEARS OF PUBLICATIONS



Sources:

150 years of Nature: a data graphic charts our evolution

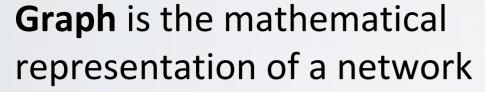
Nature 150 Interactive

Ce réseau décrypte 150 ans de découvertes scientifiques

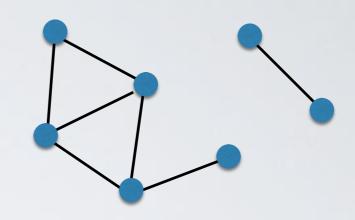
GRAPHS & NETWORKS

Networks often refers to real systems

- •WWW,
- social network
- metabolic network.
- Language: (Network, node, link)



Language: (Graph, vertex, edge)



Vertex	Edge		
person	friendship		
neuron	synapse		
Website	hyperlink		
company	ownership		
gene	regulation		

In most cases we will use the two terms interchangeably.

NETWORK REPRESENTATIONS

Networks: Graph notation

```
Graph notation : G = (V, E)
```

V _

Ε

 $u \in V$

set of vertices/nodes.

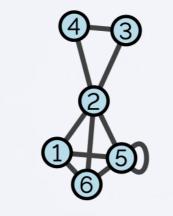
set of edges/links.

a node.

 $(u,v) \in E$ an edge.

Network - Graph notation

Graph



Graph notation

$$G = (V, E)$$

$$V = \{1, 2, 3, 4, 5, 6\}$$

$$E = \{(1, 2), (1, 6), (1, 5), (2, 4), (2, 3), (2, 5), (2, 6), (6, 5), (5, 5), (4, 3)\}$$

GRAPH REPRESENTATION

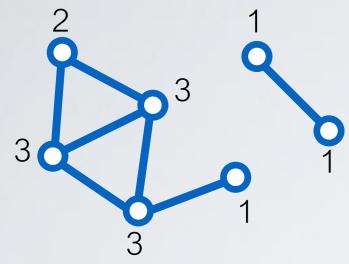
Node-Edge description

ı							
	N_u	N_u Neighbourhood of u , nodes sharing a link with u .					
	k_u	k_u Degree of u , number of neighbors $ N_u $.					
	N_u^{out} Successors of u , nodes such as $(u,v) \in E$ in a directed						
ı		graph					
	N_u^{in}	Predecessors of u , nodes such as $(v, u) \in E$ in a directed					
		graph					
	k_u^{out}	Out-degree of u , number of outgoing edges $ N_u^{out} $.					
	k_u^{out} Out-degree of u , number of outgoing edges $ N_u^{out} $. k_u^{in} In-degree of u , number of incoming edges $ N_u^{in} $						
	$\overline{w_{u,v}}$	Weight of edge (u, v) .					
	s_u	Strength of u , sum of weights of adjacent edges, $s_u =$					
		$\sum_{v} w_{uv}$.					

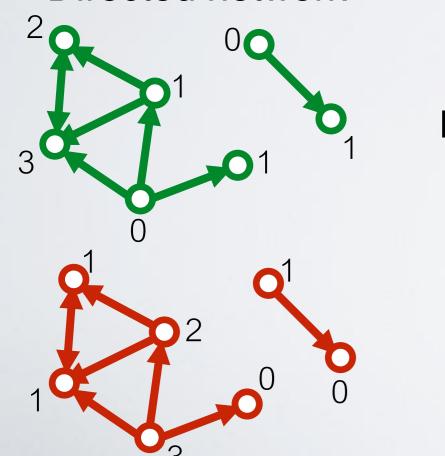
Node degree

Number of connections of a node

Undirected network



Directed network



In degree

Out degree

SIZE

Counting nodes and edges

 $N/n \ L/m \ L_{max}$

size: number of nodes |V|. number of edges |E| Maximum number of links

Undirected network:
$${N \choose 2} = N(N-1)/2$$

Directed network:
$$\binom{N}{2} = N(N-1)$$

DENSITY

Network descriptors 1 - Nodes/Edges

Average degree: Real networks are sparse, i.e., typically $\langle k \rangle \ll n$. Increases slowly with network size, e.g., $d \sim \log(m)$

$$\langle k \rangle = \frac{2m}{n}$$

Density: Fraction of pairs of nodes connected by an edge in G.

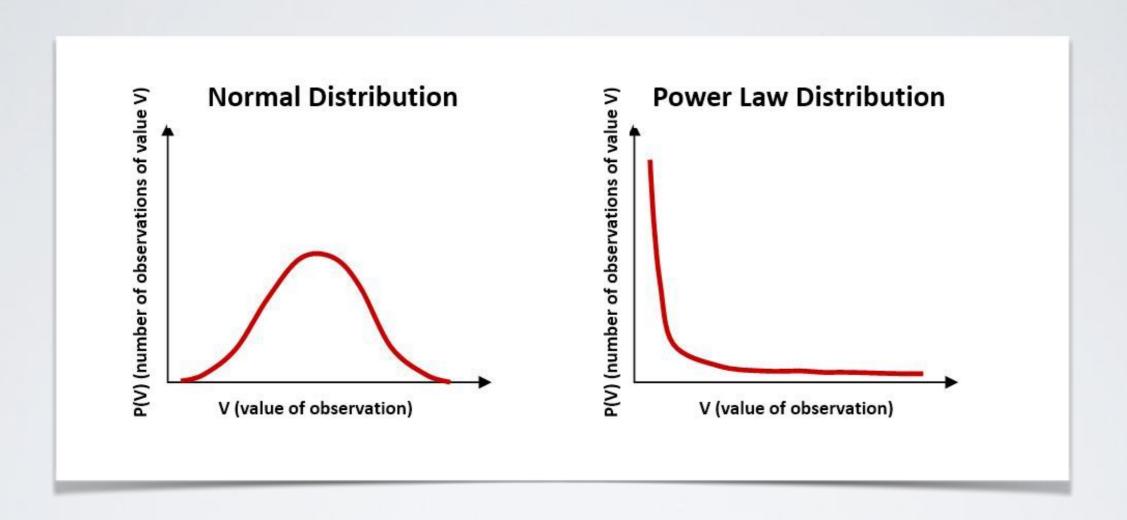
$$d = L/L_{\rm max}$$

DENSITY

	#nodes	#edges	Densité	Deg. Moyen	
Wikipedia HL	2M	30M	1.5x10 ⁻⁵	30	
Twitter 2015	288M	60B	1.4x10 ⁻⁶	416	
Facebook 2015	1.4B	400B	4x10 ⁻⁹	570	
Brain c. Elegans	280	6393	0,16	46	
Roads Calif.	2M	2.7M	6x10 ⁻⁷	2,7	
Airport traffic	3k	31k	0,007	21	

Attention: It's difficult to compare density of graphs with different sizes

DEGREE DISTRIBUTION



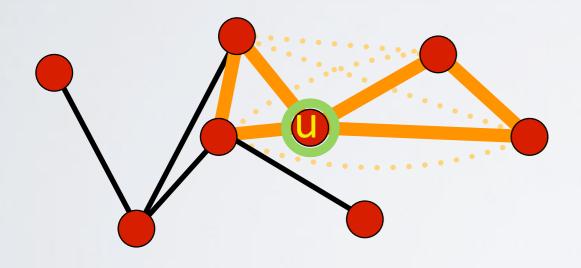
PDF (Probability Distribution Function)

DEGREE DISTRIBUTION

- In a fully random graph (Erdos-Renyi), degree distribution is (close to) a normal distribution centered on the average degree
- · In real graphs, in general, it is not the case:
 - A high majority of small degree nodes
 - A small minority of nodes with very high degree (Hubs)
- · Often modeled by a power law
 - More details later in the course

- Clustering coefficient or triadic closure
- Triangles are considered important in real networks
 - ► Think of social networks: *friends of friends are my friends*
 - # triangles is a big difference between real and random networks

 C_u - **Node clustering coefficient:** density of the subgraph induced by the neighborhood of u, $C_u=d(H(N_u))$. Also interpreted as the fraction of all possible triangles in N_u that exist, $\frac{\delta_u}{\delta_u^{\max}}$



Edges: 2

Max edges: 4*3/2=6

 $C_u = 2/6 = 1/3$

Triangles=2
Possible triangles=
$$\binom{4}{2}$$
=6
$$C_u$$
=2/6=1/3

SUBGRAPHS

Subgraphs

Subgraph H(W) (induced subgraph): subset of nodes W of a graph G = (V, E) and edges connecting them in G, i.e., subgraph H(W) = $(W, E'), W \subset V, (u, v) \in E' \iff u, v \in W \land (u, v) \in E$

Clique: subgraph with d=1

Triangle: clique of size 3

Connected component: a subgraph in which any two vertices are connected to each other by paths, and which is connected to no additional vertices in the supergraph

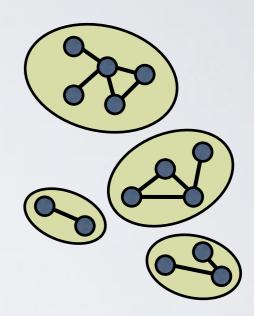
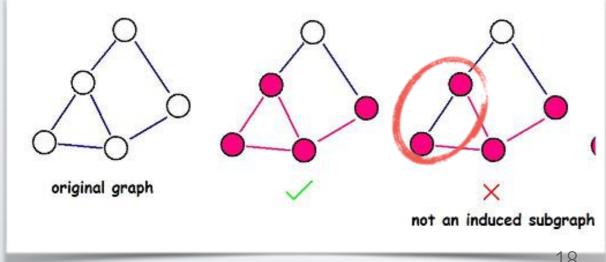


Figure after Newman, 2010





Nodes/Edges in the subgraph

 $\langle C \rangle$ - Average clustering coefficient: Average clustering coefficient of all nodes in the graph, $\bar{C}=\frac{1}{N}\sum_{u\in V}C_u$.

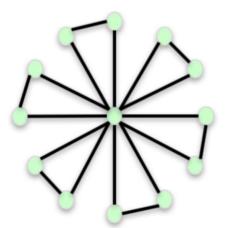
Be careful when interpreting this value, since all nodes contributes equally, irrespectively of their degree, and that low degree nodes tend to be much more frequent than hubs, and their C value is very sensitive, i.e., for a node u of degree 2, $C_u \in 0, 1$, while nodes of higher degrees tend to have more contrasted scores.

 C^g - **Global clustering coefficient:** Fraction of all possible triangles in the graph that do exist, $C^g=rac{3\Delta}{\Delta^{max}}$

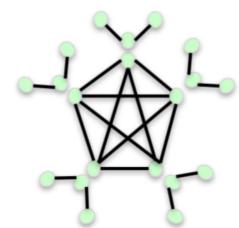
Global CC = Transitivity

Transitivity vs. Average Clustering Coefficient

Both measure the tendency for edges to form triangles. Transitivity weights nodes with large degree higher.



- Most nodes have high LCC
- The high degree node has low LCC



- Most nodes have low LCC
- High degree node have high LCC

Ave. clustering coeff. = 0.93 Transitivity = 0.23 Ave. clustering coeff. = 0.25 Transitivity = 0.86

Global CC:

- ► In random networks, GCC = density
 - =>very small for large graphs

Network	Size	$\langle k \rangle$	С	C_{rand}	Reference
WWW, site level, undir.	153 127	35.21	0.1078	0.00023	Adamic, 1999
Internet, domain level	3015-6209	3.52-4.11	0.18-0.3	0.001	Yook et al., 2001a,
					Pastor-Satorras et al., 2001
Movie actors	225 226	61	0.79	0.00027	Watts and Strogatz, 1998
LANL co-authorship	52 909	9.7	0.43	1.8×10^{-4}	Newman, 2001a, 2001b, 2001c
MEDLINE co-authorship	1 520 251	18.1	0.066	1.1×10^{-5}	Newman, 2001a, 2001b, 2001c
SPIRES co-authorship	56 627	173	0.726	0.003	Newman, 2001a, 2001b, 2001c
NCSTRL co-authorship	11 994	3.59	0.496	3×10^{-4}	Newman, 2001a, 2001b, 2001c
Math. co-authorship	70 975	3.9	0.59	5.4×10^{-5}	Barabási et al., 2001
Neurosci. co-authorship	209 293	11.5	0.76	5.5×10^{-5}	Barabási et al., 2001
E. coli, substrate graph	282	7.35	0.32	0.026	Wagner and Fell, 2000
E. coli, reaction graph	315	28.3	0.59	0.09	Wagner and Fell, 2000
Ythan estuary food web	134	8.7	0.22	0.06	Montoya and Solé, 2000
Silwood Park food web	154	4.75	0.15	0.03	Montoya and Solé, 2000
Words, co-occurrence	460.902	70.13	0.437	0.0001	Ferrer i Cancho and Solé, 2003
Words, synonyms	22 311	13.48	0.7	0.0006	Yook et al., 2001b
Power grid	4941	2.67	0.08	0.005	Watts and Strogatz, 1998
C. Elegans	282	14	0.28	0.05	Watts and Strogatz, 1998

PATH RELATED SCORES

Paths - Walks - Distance

Walk: Sequences of adjacent edges or nodes (e.g., **1.2.1.6.5** is a valid walk)

Path: a walk in which each node is distinct.

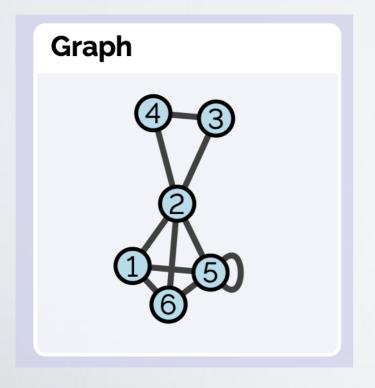
Path length: number of edges encountered in a path

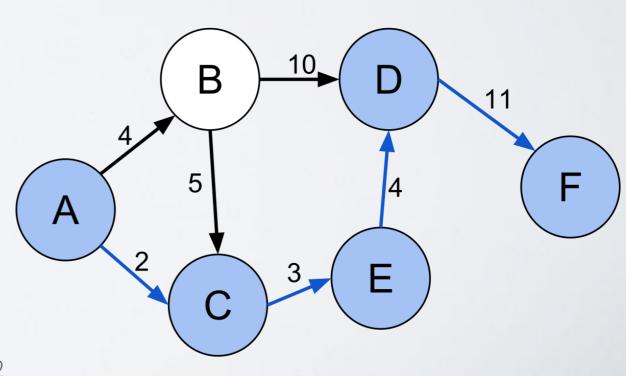
Weighted Path length: Sum of the weights of edges on a path

Shortest path: The shortest path between nodes u, v is a path of minimal path length. Often it is not unique.

Weighted Shortest path: path of minimal weighted path length.

 $\ell_{u,v}$: **Distance**: The distance between nodes u,v is the length of the shortest path





PATH RELATED SCORES

Network descriptors 2 - Paths

 $rac{\ell_{ ext{max}}}{\langle \ell
angle}$

Diameter: maximum *distance* between any pair of nodes. **Average distance**:

$$\langle \ell \rangle = \frac{1}{n(n-1)} \sum_{i \neq j} d_{ij}$$

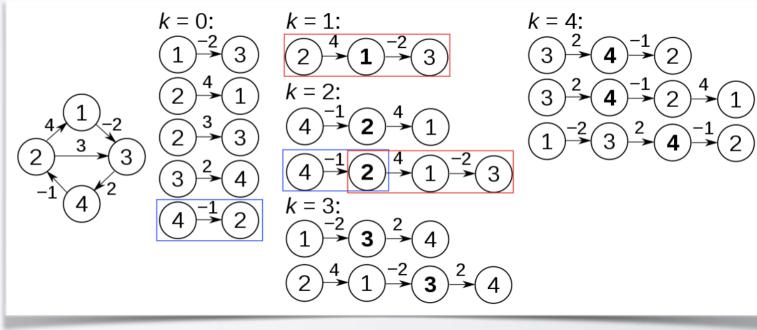
All shortest path algorithm

finding shortest paths in a weighted graph with positive or negative edge weights (but with no negative cycles)

Checking and updating all paths going through nodes k=1, 2, 3, ..., N by assuming that:

$$shp(i,j,k)=$$
 $min(shp(i,j,k-1)), shp(i,k,k-1)+shp(k,j,k-1))$

Complexity: $O(n^3)$



AVERAGE PATH LENGTH

- The famous 6 degrees of separation (Milgram experiment)
 - (More on that next slide)
- Not too sensible to noise
- · Tells you if the network is "stretched" or "hairball" like

SIDE-STORY: MILGRAM EXPERIMENT

- Small world experiment (60's)
 - Give a (physical) mail to random people
 - Ask them to send to someone they don't know
 - They know his city, job
 - They send to their most relevant contact
- · Results: In average, 6 hops to arrive

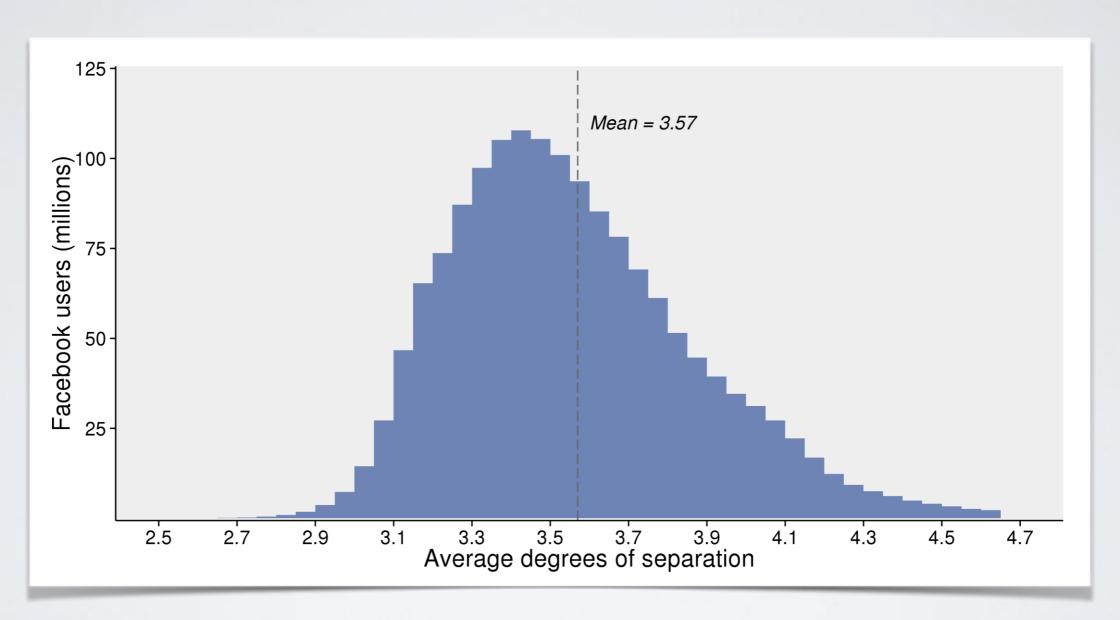


SIDE-STORY: MILGRAM EXPERIMENT

- Many criticism on the experiment itself:
 - Some mails did not arrive
 - Small sample
 - **•** ...
- · Checked on "real" complete graphs (giant component):
 - MSN messenger
 - Facebook
 - The world wide web

. . . .

SIDE-STORY: MILGRAM EXPERIMENT



Facebook

SMALL WORLD

Small World Network

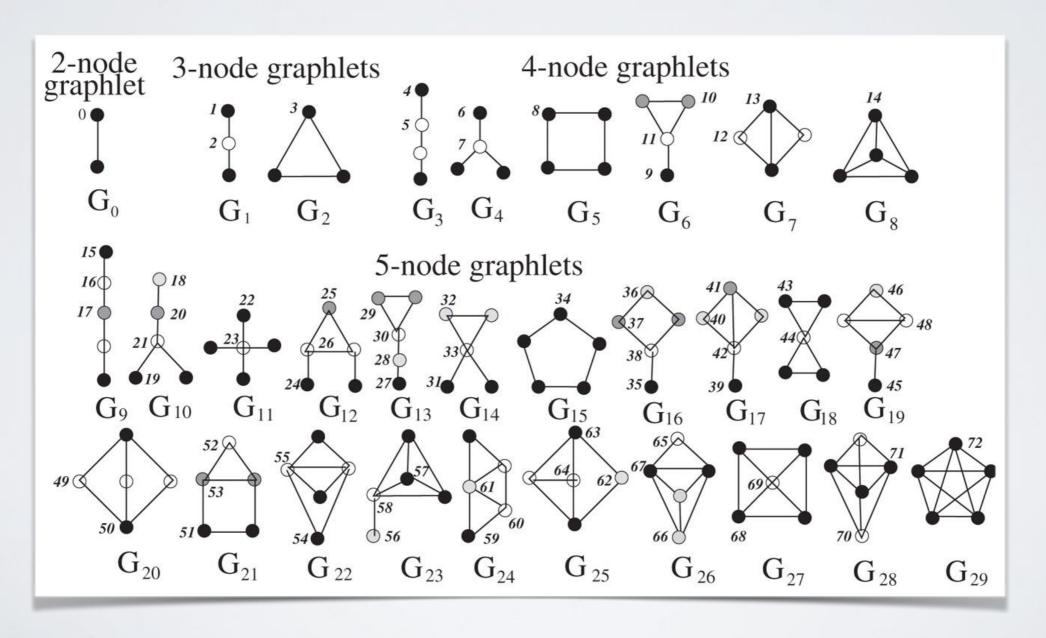
A network is said to have the **small world** property when it has some structural properties. The notion is not quantitatively defined, but two properties are required:

- Average distance must be short, i.e., $\langle \ell \rangle \approx \log(N)$
- Clustering coefficient must be high, i.e., much larger than in a random network , e.g., $C^g\gg d$, with d the network density

NETWORK DESCRIPTORS

- Many other network descriptors exist:
 - Modularity (later in community detection class)
 - Centralization (comparing the centrality scores between most central and less central, see later)
 - Rich-club coefficient: tendency of high-degrees to connected to high-degrees, cf random network class
 - Motif profiles (how often do specific subgraphs appear)
 - Network Resilience (see practicals)
 - etc.

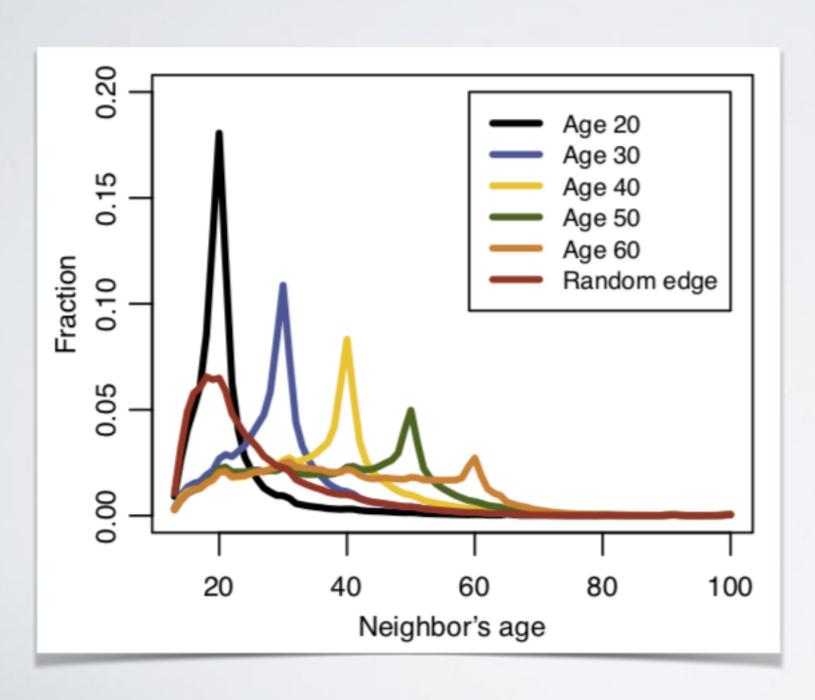
GRAPHLETS



EXEMPLE OF GRAPH ANALYSIS

- 721M users (nodes) (active in the last 28 days)
- 68B edges
- Average degree: 190 (average # friends)
- Median degree: 99
- Connected component: 99.91%

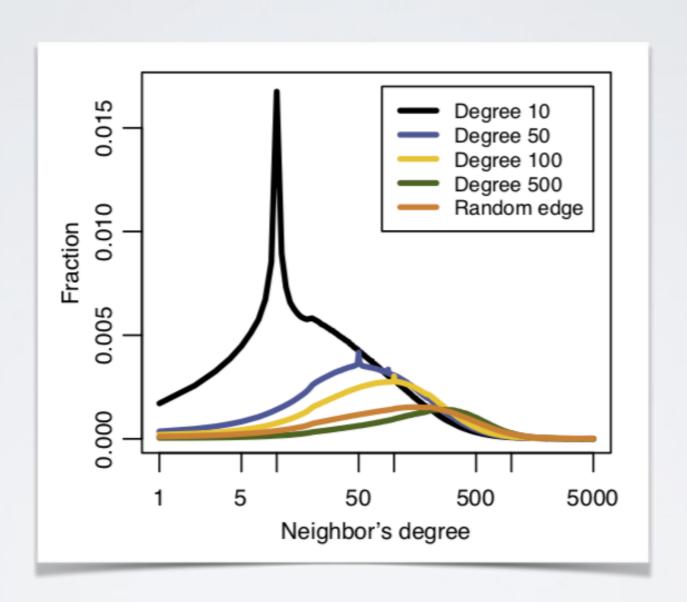
EXEMPLE OF GRAPH ANALYSIS



Age homophily

(More next class)

EXEMPLE OF GRAPH ANALYSIS



Many of my friends have the Same # of friends than me!

CENTRALITIES

Characterizing/Discovering important nodes

CENTRALITY

- We can measure nodes importance using so-called centrality.
- · Poor terminology: nothing to do with being central in general
- Usage:
 - Some centralities have straightforward interpretation
 - Centralities can be used as node features for machine learning on graph
 - (Classification, link prediction, ...)

NODE DEGREE

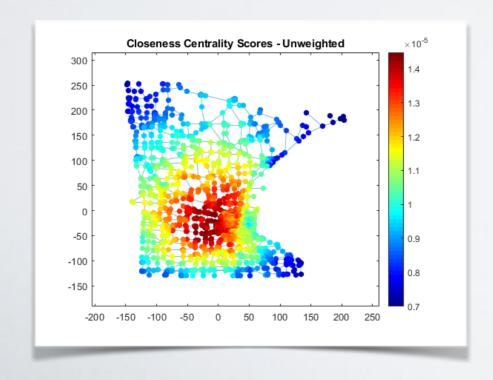
- Degree: how many neighbors
- Often enough to find important nodes
 - Main characters of a series talk with the more people
 - Largest airports have the most connections
 - **.** . . .
- But not always
 - Facebook users with the most friends are spam
 - Webpages/wikipedia pages with most links are simple lists of references

• ...

FARNESS, CLOSENESS HARMONIC CENTRALITY

FARNESS, CLOSENESS

- How close the node is to all other nodes
- Parallel with the center of a figure:
 - Center of a circle is the point of shorter average distance to any points in the circle





FARNESS, CLOSENESS

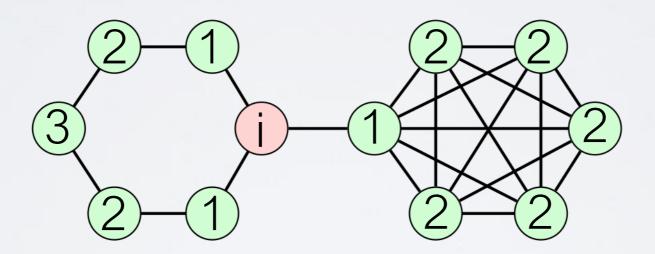
Farness: Average distance to all other nodes in the graph

$$\operatorname{Farness}(u) = \frac{1}{N-1} \sum_{v \in V \setminus u} \ell_{u,v}$$

CLOSENESS CENTRALITY

Closeness: Inverse of the farness, i.e., how close the node is to all other nodes in term of shortest paths.

$$\mathsf{Closeness}(u) = \frac{N-1}{\sum_{v \in V \setminus u} \ell_{u,v}}$$



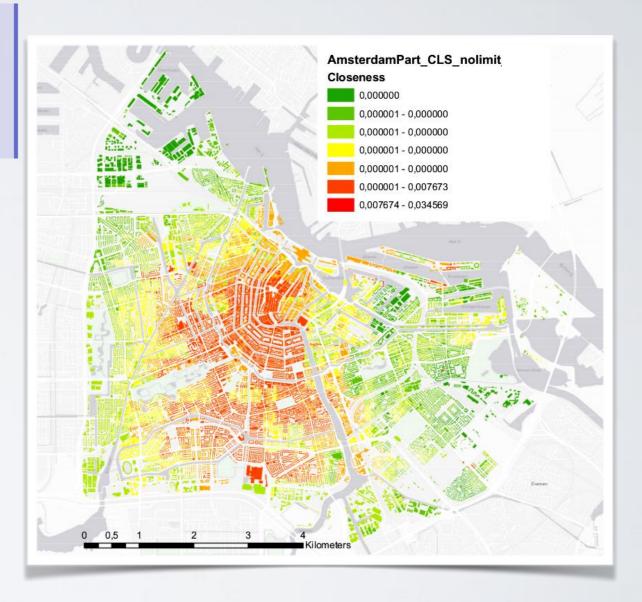
$$C_{cl}(i) = \frac{12-1}{(3\times1+7\times2+1\times3)} = \frac{11}{20} = 0.55$$

CLOSENESS CENTRALITY

Closeness: Inverse of the farness, i.e., how close the node is to all other nodes in term of shortest paths.

$$\mathsf{Closeness}(u) = \frac{N-1}{\sum_{v \in V \setminus u} \ell_{u,v}}$$

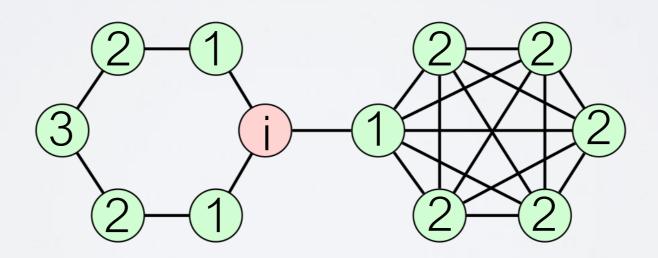
1=all nodes are at distance one



Harmonic Centrality

Harmonic centrality: A variant of the closeness defined as the average of the inverse of distance to all other nodes (Harmonic mean). Well defined on disconnected network with $\frac{1}{\infty} = 0$. Its interpretation is the same as the closeness.

$$\mathsf{Harmonic}(u) = \frac{1}{N-1} \sum_{v \in V \setminus u} \frac{1}{\ell_{u,v}}$$



$$C_h(i) = \frac{1}{12 - 1} \left(3 \times \frac{1}{1} + 7 \times \frac{1}{2} + 1 \times \frac{1}{3} \right) = \frac{41}{66} = 0.6212$$

BETWEENNESS CENTRALITY

- · Measure how much the node plays the role of a bridge
- Betweenness of u: fraction of all the shortest paths between all the pairs of nodes going through u.

$$C_B(v) = \sum_{s \neq v \neq t \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

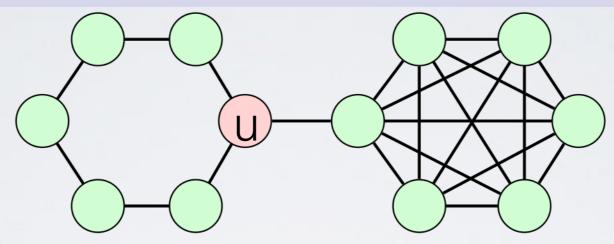
with σ_{st} the number of shortest paths between nodes s and t and $\sigma_{st}(v)$ the number of those paths passing through v.

The betweenness tends to grow with the network size. A normalized version can be obtained by dividing by the number of pairs of nodes, i.e., for a directed graph: $C_B^{\text{norm}}(v) = \frac{C_B(v)}{(N-1)(N-2)}$.

Betweenness Centrality

$$C_B(v) = \sum_{s \neq v \neq t \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

directed graph: $C_B^{\mathsf{norm}}(v) = \frac{C_B(v)}{(N-1)(N-2)}$.



$$C_B(u) = 2\frac{5*6+1+\frac{1}{2}+\frac{1}{2}}{11*10} = \frac{64}{110}$$

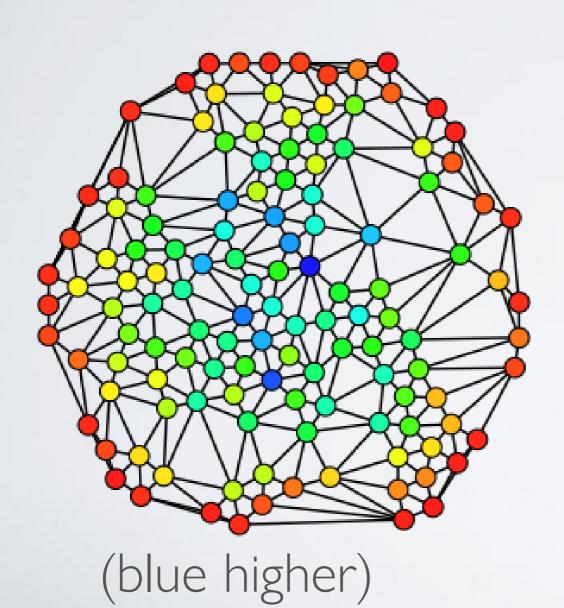
Exact computation:

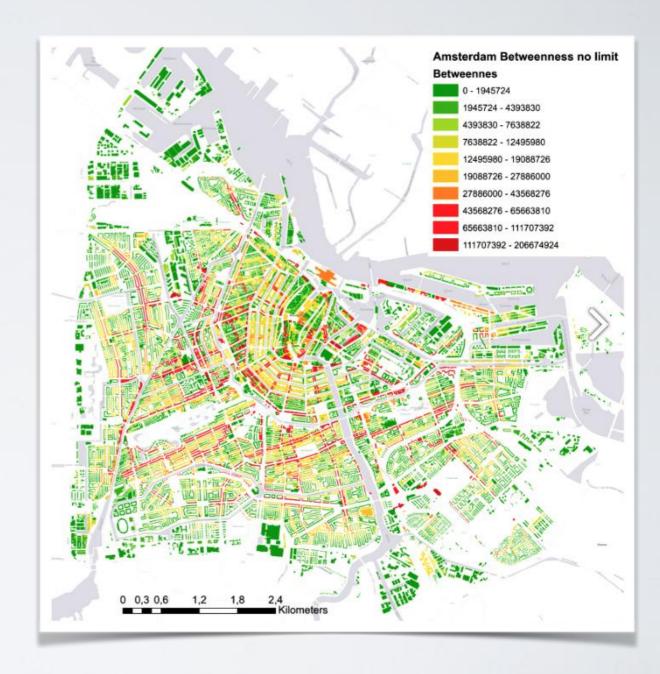
Floyd-Warshall: $O(n^3)$ time complexity $O(n^2)$ space complexity

Approximate computation

Dijskstra: $O(n(m+n \log n))$ time complexity

BETWEENNESS CENTRALITY





(red higher)

EDGE - BETWEENNESS

Same definition as for nodes

Can you guess the edge of highest betweenness in the European rail network?



RECURSIVE DEFINITIONS

RECURSIVE DEFINITIONS

- Recursive importance:
 - Important nodes are those connected to important nodes
- · Several centralities based on this idea:
 - Eigenvector centrality
 - PageRank
 - **.** . . .

RECURSIVE DEFINITION

- · We would like scores such as:
 - Each node has a score (centrality),
 - If every node "sends" its score to its neighbors, the sum of all scores received by each node will be equal to its original score

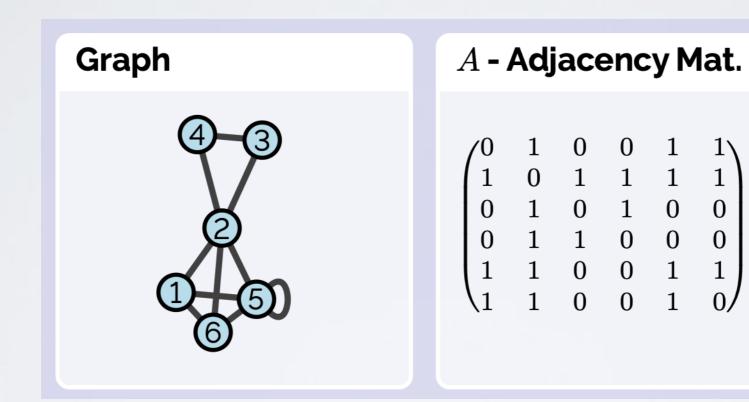
$$C_u^{t+1} = \frac{1}{\lambda} \sum_{v \in N_u^{in}} C_v^t \tag{1}$$

• With λ a normalisation constant

RECURSIVE DEFINITION

- This problem can be solved by what is called the power method:
 - ▶ 1) We initialize all scores to random values
 - 2) Each score is updated according to the desired rule, until reaching a stable point (after normalization)
- Why does it converge?
 - Perron-Frobenius theorem (see next slide)
 - =>True for undirected graphs with a single connected component

ADJACENCY MATRIX



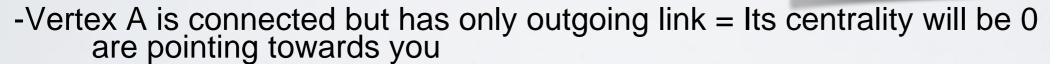
EIGENVECTOR CENTRALITY

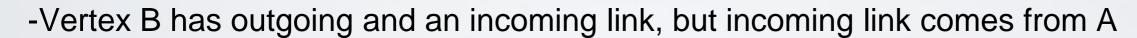
- · What we just described is called the Eigenvector centrality
- A couple eigenvector (x) and eigenvalue (λ) is defined by the following relation: $Ax = \lambda x$
 - $\rightarrow x$ is a column vector of size n, which can be interpreted as the scores of nodes
- What Perron-Frobenius algorithm says is that the power method will always converge to the *leading eigenvector*, i.e., the eigenvector associated with the highest eigenvalue

Eigenvector Centrality

Some problems in case of directed network:

- Adjacency matrix is asymmetric
- 2 sets of eigenvectors (Left & Right)
- 2 leading eigenvectors
 - Use right eigenvectors: consider nodes that



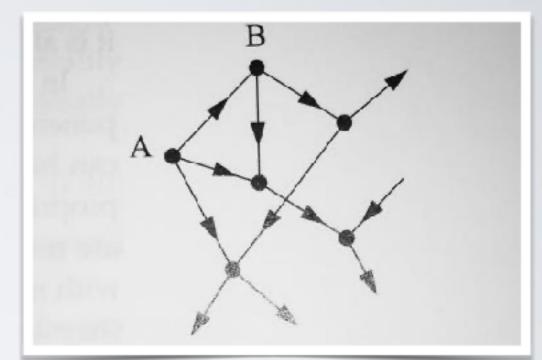


= Its centrality will be 0

-etc.

Solution: Only in strongly connected component

Note: Acyclic networks (citation network) do not have strongly connected component



PageRank Centrality

Eigenvector centrality generalised for directed networks

PageRank

The Anatomy of a Large-Scale Hypertextual Web Search Engine

Brin, S. and Page, L. (1998) The Anatomy of a Large-Scale Hypertextual Web Search Engine. In: Seventh International World-Wide Web Conference (WWW 1998), April 14-18, 1998, Brisbane, Australia.

Sergey Brin and Lawrence Page

Computer Science Department, Stanford University, Stanford, CA 94305, USA sergey@cs.stanford.edu and page@cs.stanford.edu

PageRank Centrality

Eigenvector centrality generalised for directed networks

PageRank

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Abstract

In this paper, we present Google, a prototype of a large-scale search engine which makes heavy use of the structure present in hypertext. Google is designed to crawl and index the Web efficiently and produce much more satisfying search results than existing systems. The prototype with a full text and hyperlink database of at least 24 million pages is available at http://google.stanford.edu/

PAGERANK

- 2 main improvements over eigenvector centrality:
 - In directed networks, problem of source nodes
 - => Add a constant centrality gain for every node
 - Nodes with very high centralities give very high centralities to all their neighbors (even if that is their only in-coming link)
 - => What each node "is worth" is divided equally among its neighbors (normalization by the degree)

$$C_u^{t+1} = \frac{1}{\lambda} \sum_{v \in N_u^{in}} C_v^t = \sum_{v \in N_u^{in}} \frac{C_v^t}{k_v^{out}} + \beta$$

With by convention β =1 and α a parameter (usually 0.85) controlling the relative importance of β

PAGERANK

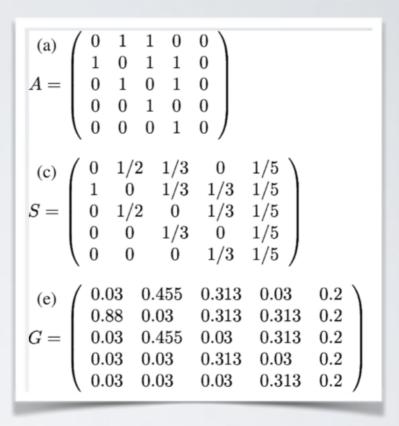
Matrix interpretation
Principal eigenvector of the "Google Matrix":

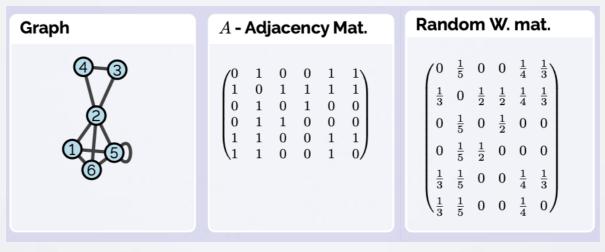
First, define matrix S as:

- -Normalization by columns of A
- -Columns with only 0 receives 1/n (dead end)

-Finally,
$$G_{ij} = \alpha S_{ij} + (1 - \alpha)/n$$

Removing some trip probability from out-link And distributing them at random among other nodes ((1-0.85)/5=0.03)





PageRank - as Random Walk

Main idea: The PageRank computation can be interpreted as a Random Walk process with restart

Teleportation probability: the parameter α gives the probability that in the next step of the RW will follow a Markov process or with probability $1-\alpha$ it will jump to a random node

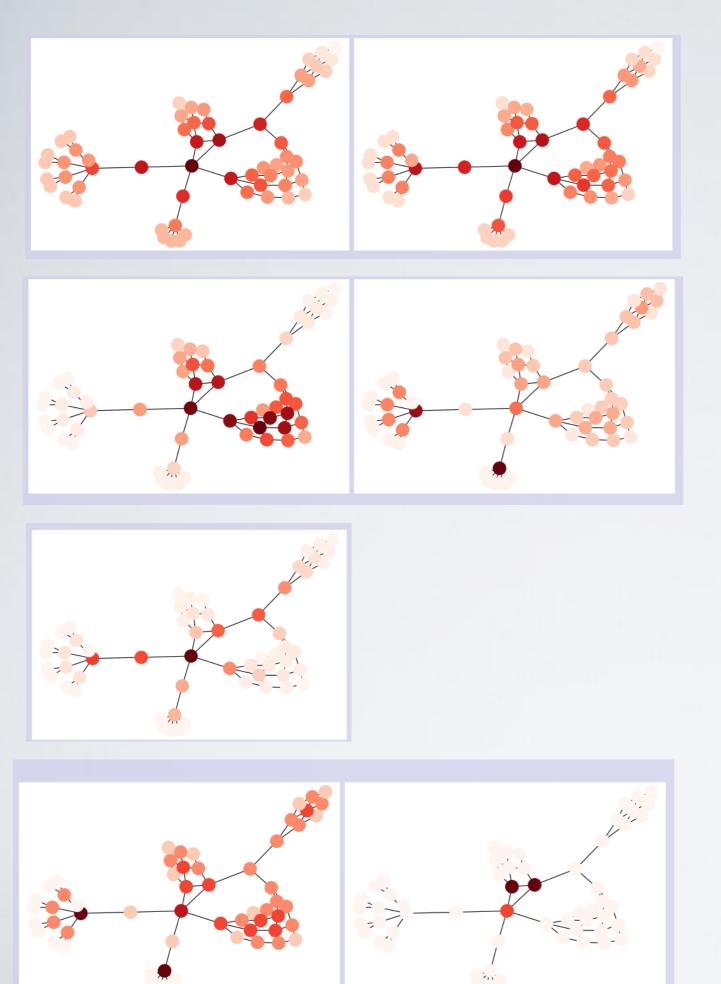
Pagerank score of a node thus corresponds to the probability of this random walker to be on this node after an infinite number of hops.

PAGERANK

- Then how do Google rank when we do a research?
- Compute pagerank (using the power method for scalability)
- Create a subgraph of documents related to our topic
- Of course now it is certainly much more complex, but we don't really know: "Most search engine development has gone on at companies with little publication of technical details. This causes search engine technology to remain largely a black art" [Page, Brin, 1997]

OTHERS

- Many other centralities have been proposed
 - ► 50+ (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4646361/)
- The problem is how to interpret them?
- · Can be used as supervised tool:
 - Compute many centralities on all nodes
 - Learn how to combine them to find chosen nodes
 - Discover new similar nodes
 - (roles in social networks, key elements in an infrastructure, ...)

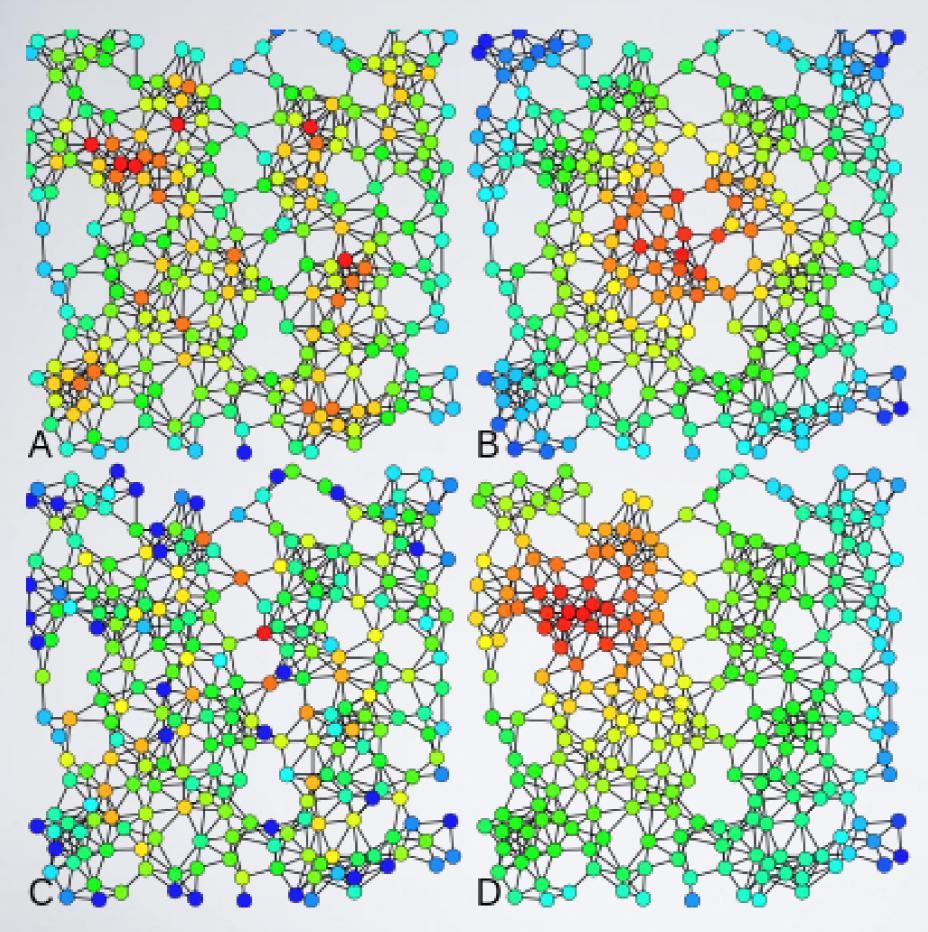


Which is which?

Degree
Clustering coefficient
Closeness
Harmonic Centrality
Betweenness
Eigenvector
PageRank

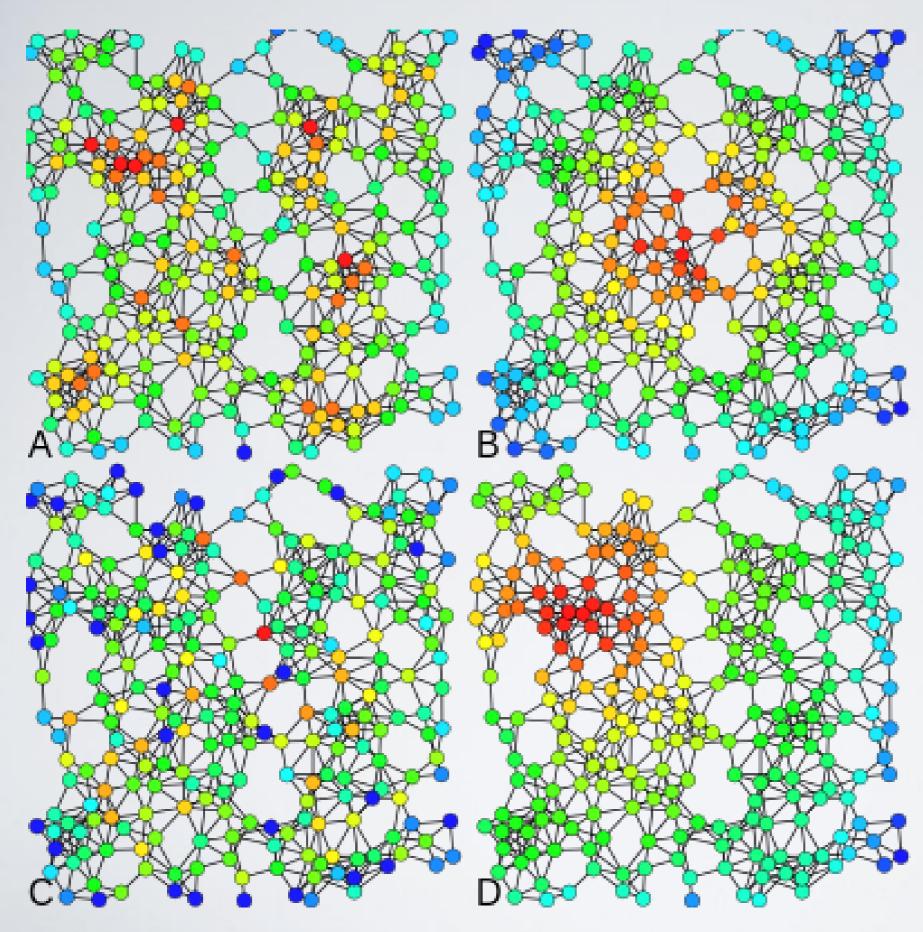
Which is which?

Degree
Clustering coefficient
Closeness
Harmonic Centrality
Betweenness
Eigenvector
PageRank



Try again:)

Degree
Betweenness
Closeness
Eigenvector



Try again:)

Degree: A
Betweenness: C
Closeness: B

Eigenvector: D