

Network science / Graph mining

Tools & metrics for analyzing a connected world of data

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Outline

1 Graphs and representations

- The graph abstraction
- Graph data-structures
- Tools for manipulating graphs

2 Loading a graph with networkx

3 Classical metrics

- Preliminaries
- Metrics

4 Two important graph models & the web

5 Exploring graphs

6 Importance metrics

7 Community metrics

8 TVGs: time varying graphs

9 Comparing graphs

10 Playing with graphs and Gephi

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Graphs ?



Figure: A graph: entities (nodes) and connections (edges)

- An abstraction for reasoning about core characteristics of a structure.
- Sometimes called “network science”; concept from 1800!
- This class: structural properties of graphs, not node intrinsic values (labels...)

The omnipresence of graphs in applications

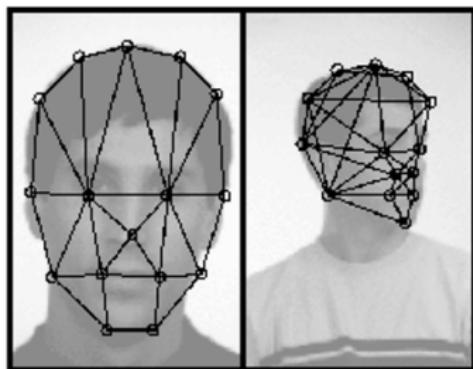
The Knowledge Graph is a database of facts about things in the world and the relationships between them. It's why you can do a search like "when was the wife of obama born" and get an answer about Michele Obama as below, without ever using her name:

A screenshot of a Google search results page. The search query is "when was the wife of obama born". The results are categorized by "Web", "News", "Images", "Shopping", "Videos", "More", and "Search tools". Below the categories, it says "About 87,300,000 results (0.57 seconds)". A "Knowledge Graph" card is displayed for Michelle Obama, showing her birth date and location: "January 17, 1964 (age 51 years), Chicago, IL". To the right of the text is a portrait photo of Michelle Obama. Below the card, there are three related entities with their names, birth dates, and relationships to Michelle Obama: Barack Obama (Spouse, August 4, 1961), Craig Robinson (Brother, April 21, 1962), and Hillary Rodham Clinton (October 26, 1947).

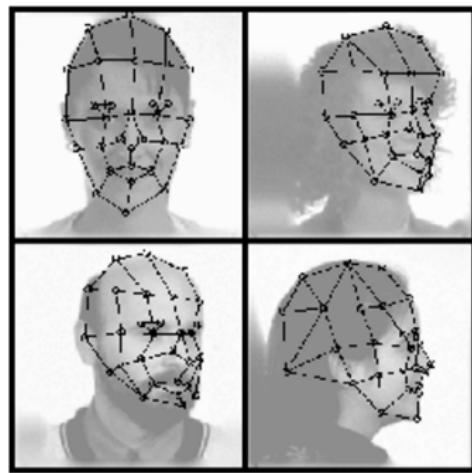
Entity	Relationship to Michelle Obama	Born
Barack Obama	Spouse	August 4, 1961
Craig Robinson	Brother	April 21, 1962
Hillary Rodham Clinton		October 26, 1947

Figure: Google's knowledge graph

The omnipresence of graphs in applications



grids for face finding



grids for face recognition

Figure: Graphs in computer vision

The omnipresence of graphs in applications

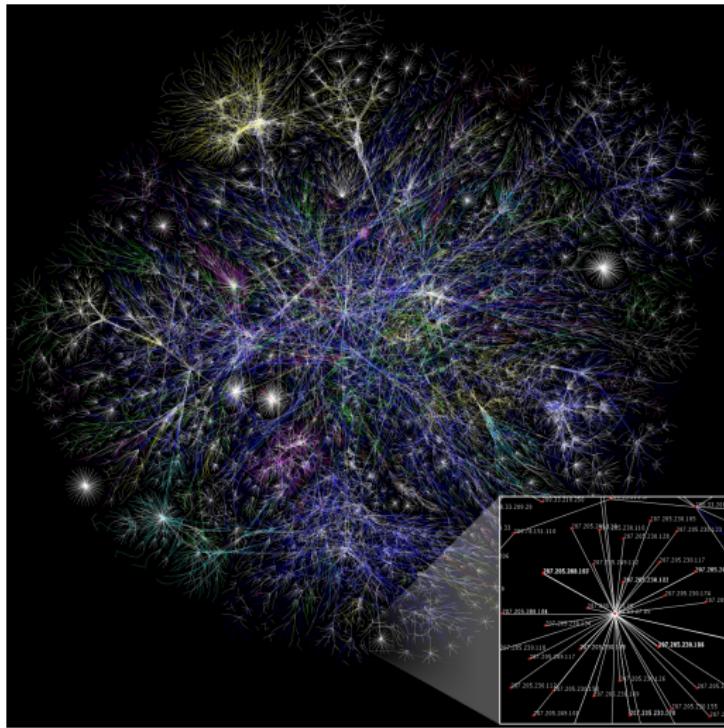


Figure: The Internet AS graph

The omnipresence of graphs in applications

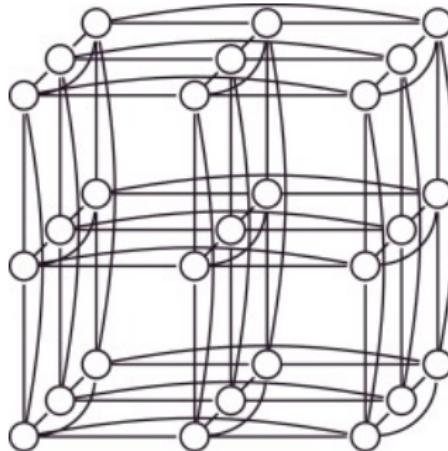
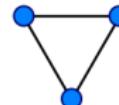
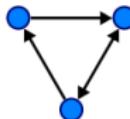


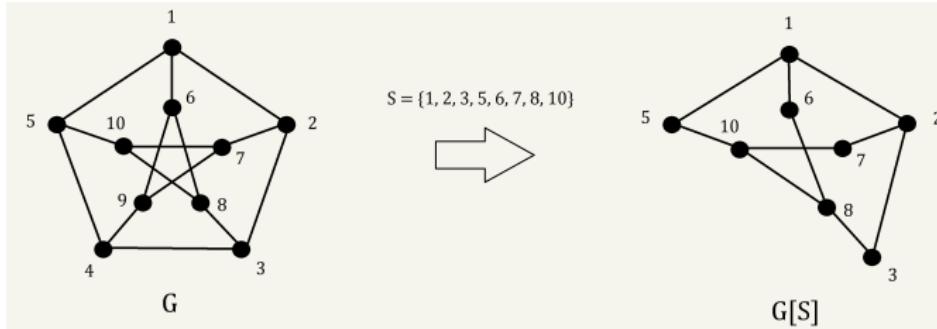
Figure: Interconnecting system-on-chips in a datacenter rack

Most important notions

- *Vertex*: a graph node, or entity.
- *Edge*: a link connecting two vertices.
- *Directed and undirected graphs*:
 - in directed graphs, edges have orientation (arrow end)

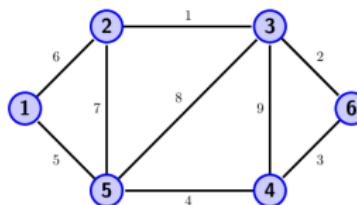


- A *subgraph* of G : formed by a subset of vertices and edges from G .

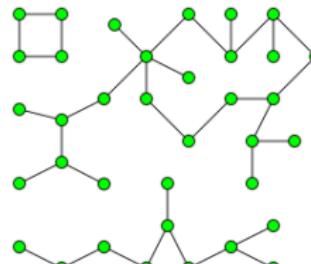


Most important notions (cont'd)

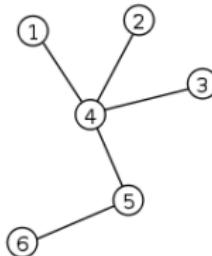
- Edge weight: value assigned as a label to an edge.
 - e.g., distance in km of a road from city 1 to 2.



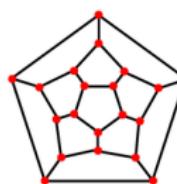
- Graph connectivity:
 - A graph is *connected* if there is a *path* btw any pair of vertices.
 - Otherwise, *connected components* are the subgraphs in which paths exist.



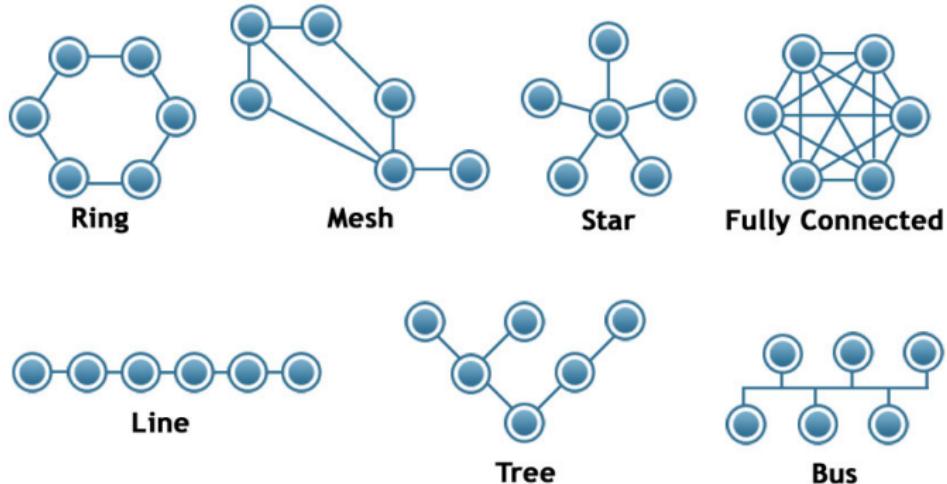
- A *cycle*: a path in which a vertex is reachable from itself.
 - Example of an *acyclic* connected graph: a *tree*



- A *planar* graph: can be drawn without any edges crossing each other.



Special topologies



certiology.com

Figure: Graphs to remember, often used as illustrations

Adjacency list or edge list representations

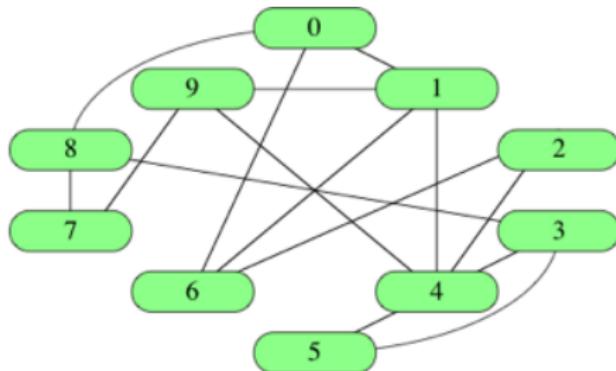


Figure: A graph, to represent for integration in programs

Edge list:

```
[ [0,1], [0,6], [0,8], [1,4], [1,6], [1,9], [2,4], [2,6], [3,4], [3,5], [3,8], [4,5], [4,9], [7,8], [7,9] ]
```

$O(|V|)$ access time to find an edge, but $O(|E|)$ space in memory.

Adjacency list:

```
[ [1, 6, 8], [0, 4, 6, 9], [4, 6], [4, 5, 8], [1, 2, 3, 5, 9], [3, 4], [0, 1, 2], [8, 9], [0, 3, 7], [1, 4, 7] ]
```

$O(1)$ access time to vertex , but $O(|V|)$ to access a given edge.

Image¹

Matrix representation

	0	1	2	3	4	5	6	7	8	9
0	0	1	0	0	0	0	1	0	1	0
1	1	0	0	0	1	0	1	0	0	1
2	0	0	0	0	1	0	1	0	0	0
3	0	0	0	0	1	1	0	0	1	0
4	0	1	1	1	0	1	0	0	0	1
5	0	0	0	1	1	0	0	0	0	0
6	1	1	1	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	1	1
8	1	0	0	1	0	0	0	1	0	0
9	0	1	0	0	1	0	0	1	0	0

Figure: Matrix representation of previous graph

Find edge presence in $O(1)$ time, but $\Theta(V^2)$ space in memory.
1's to be replaced by edge weights for weighted graphs.

Example tool families for manipulating graphs



Figure: For massive graphs (cannot fit into on server's memory)

X – Stream

Figure: Big graph processing on a single machine



Figure: For a database-like handling of graphs

NetworkX

Figure: Prototyping in Python, lots of contributions

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Graph repositories

Stanford Large Network Dataset Collection

- Social networks : online social networks, edges represent interactions between people
- Networks with ground-truth communities : ground-truth network communities in social and information networks
- Communication networks : email communication networks with edges representing communication
- Citation networks : nodes represent papers, edges represent citations
- Collaboration networks : nodes represent scientists, edges represent collaborations (co-authoring a paper)
- Web graphs : nodes represent webpages and edges are hyperlinks
- Amazon networks : nodes represent products and edges link commonly co-purchased products
- Internet networks : nodes represent computers and edges communication
- Road networks : nodes represent intersections and edges roads connecting the intersections
- Autonomous systems : graphs of the internet
- Signed networks : networks with positive and negative edges (friend/foe, trust/distrust)
- Location-based online social networks : Social networks with geographic check-ins
- Wikipedia networks, articles, and metadata : Talk, editing, voting, and article data from Wikipedia
- Temporal networks : networks where edges have timestamps
- Twitter and Memetracker : Memetracker phrases, links and 467 million Tweets
- Online communities : Data from online communities such as Reddit and Flickr
- Online reviews : Data from online review systems such as BeerAdvocate and Amazon

SNAP networks are also available from [UF Sparse Matrix collection](#). [Visualizations of SNAP networks](#) by Tim Davis.

Social networks

Name	Type	Nodes	Edges	Description
ego-Facebook	Undirected	4,039	88,234	Social circles from Facebook (anonymized)
ego-Gplus	Directed	107,614	13,673,453	Social circles from Google+
ego-Twitter	Directed	81,306	1,768,149	Social circles from Twitter
soc-Epinions1	Directed	75,879	508,837	Who-trusts-whom network of Epinions.com

Figure: Stanford Large Network Dataset Collection,
<https://snap.stanford.edu/data/>

Also: Koblenz Network Collection, <http://konect.uni-koblenz.de/>
Network Repository, <http://networkrepository.com>

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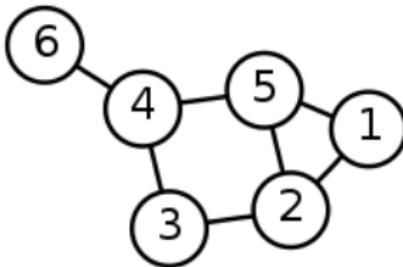
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- $G(V, E)$: graph G with node set V , connected by edge set E .
 - $V = \{1, 2, 3, 4, 5, 6\}$;
 $E = [[1, 5], [1, 2], [2, 3], [2, 5], [3, 4], [4, 5], [4, 6]]$
- Number of nodes is $n = |V|$, edges is $m = |E|$.
- Neighbors of node i are set $\Gamma(i)$.
 - $\Gamma(1) = \{2, 5\}$

Degree of a node

- The degree d_v of node v is equal to $|\Gamma(v)|$ (its number of neighbors).
- Degree span: $0 \leq d_v \leq n - 1$.
- *Degree distribution* $P(d)$ is the probability distribution of each degree in the current graph:

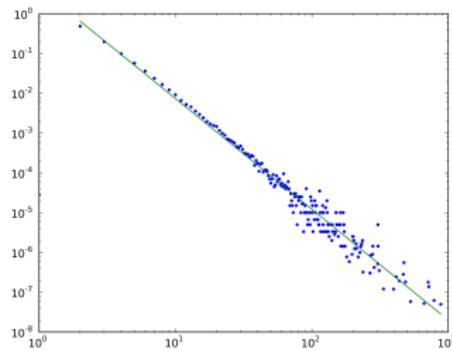


Figure: Degree distribution: x-axis is degree, y-axis is probability

- In(out)-degree of v : counts incoming(outgoing) edges only.

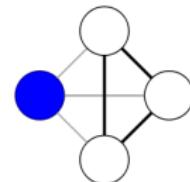
Clustering coefficient

- Every two nodes in a *clique* are neighbors.
- *Local clustering coefficient of a node i measures “how close are $\Gamma(i)$ from being a clique”:*

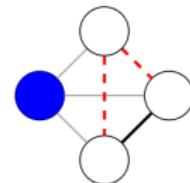
$$C_i = \frac{2|e_{jk} : v_j, v_k \in \Gamma(v_i), e_{jk} \in E|}{d_i(d_i - 1)}$$

- Network average clustering coefficient:

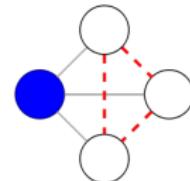
$$\bar{C} = \frac{1}{n} \sum_{i=1}^n C_i$$



$$c = 1$$

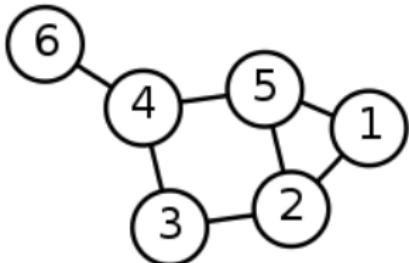


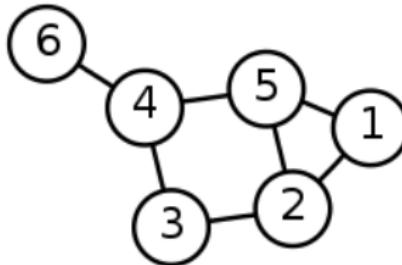
$$c = 1/3$$



$$c = 0$$

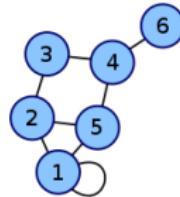
- *Path*: sequence of adjacent nodes connecting two nodes (if exists).
 - e.g., two paths btw 6 and 1: $(4,5,1)$ and $(4,3,2,5,1)$.
 - One *hop*: one transition from a node to another.
- *Shortest path*: path of minimal cardinality.
 - Distance $dist(6,1) = |(4,5,1)| = 3$
- *Single-source shortest path (SSSP)*: shortest paths from node i to all other graph nodes ($V \setminus i$).
- *Average path length*: average of all-pair shortest distances in the graph.





- All-pairs shortest paths (APSP): SSSP from $\forall i \in V$.
- Diameter: longest path of the APSP, i.e., greatest distance between any pair of vertices.
 - $diam(G) = |(4, 5, 1)| = 3$, starting at node 6.

Algebraic connectivity



- *Degree matrix D*: diagonal matrix containing the degree of each vertex.
- *Adjacency matrix A*: 1 if edge exists (2 for self-loop), 0 otherwise.
- *Laplacian matrix*: $L = D - A$.
- *Algebraic connectivity*: second-smallest eigenvalue of L .
 - $> 0 \iff$ graph is connected.
- Number of 0s as eigenvalues equals number of connected components.

$$\begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Figure: D

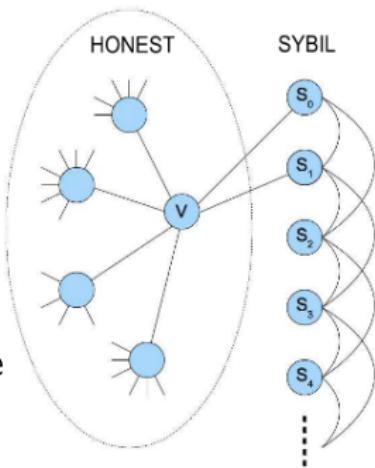
$$\begin{pmatrix} 2 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Figure: A

- The conductance $\Phi(C)$ of a set C of vertices in a given graph G is the ratio between the number of edges going out from C and the number of edges inside C :

$$\Phi(C) = \frac{|cut(C)|}{vol(C)},$$

where $vol(C)$, is the sum of the degrees of the vertices in C .

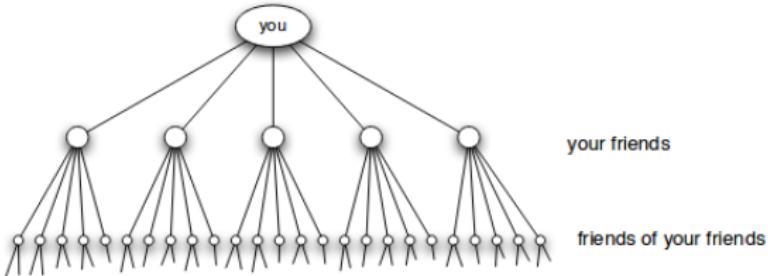


- *Expansion* of G : mean number of nodes that are reached in h hops from a node i :

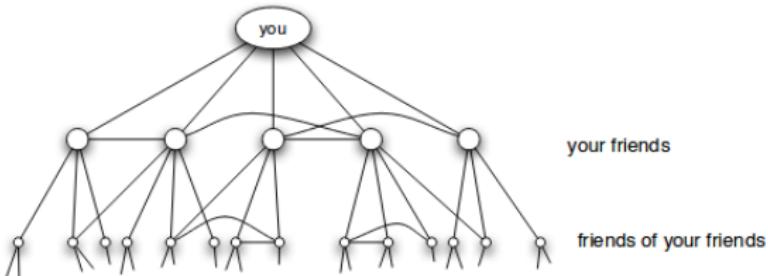
$$e_G(h) = \frac{1}{n^2} \sum_{v \in V} |C_v(h)|,$$

with $C_v(h)$ the set of reachable nodes from v in h hops.

Expansion - example



(a) *Pure exponential growth produces a small world*



(b) *Triadic closure reduces the growth rate*

Figure: Expansion in a social network

- Measures the robustness of a graph:

$$r_G(h) = \frac{1}{|E|} \sum_{v \in V} I(v, |C_v(h)|),$$

with $I(v, |C_v(h)|)$ the number of edges that need to be removed to split $C_v(h)$ into 2 sets (of roughly the same size). h : distance (hops).

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The Erdős–Rényi random graph

- Model $G(n, p)$ for generating a canonical random graph.
 - Create n nodes.
 - Every pair of nodes connected with independant probability p .



Figure: A random graph with $p = 0.01$.

- If $np = 1$, G almost surely has a largest component of $n = O(n^{2/3})$.
- $p = \frac{\ln n}{n}$ is a threshold for G 's connectivity.
- ...

The Barabási–Albert scale-free graph

- Model to generate a graph with *power-law* degree-distribution.
 - Create m_0 nodes, as a connected graph.
 - Iteratively add one node, and connect it to $m < m_0$ nodes, with probability depending on the degree of existing nodes:
$$p_i = \frac{d_i}{\sum_j d_j}$$
 (method called preferential attachment).

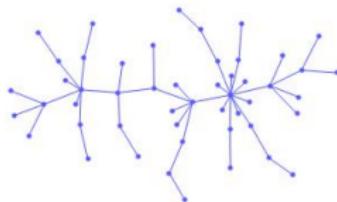


Figure: A B.A. graph with $n = 50$ and $m_0 = 1$.

- Well connected nodes “accumulate” incoming links: rich gets richer
- Resulting degree distribution is $P(d) \sim d^{-3}$.
- Average path length is $\frac{\ln n}{\ln \ln n}$.

Real structure example

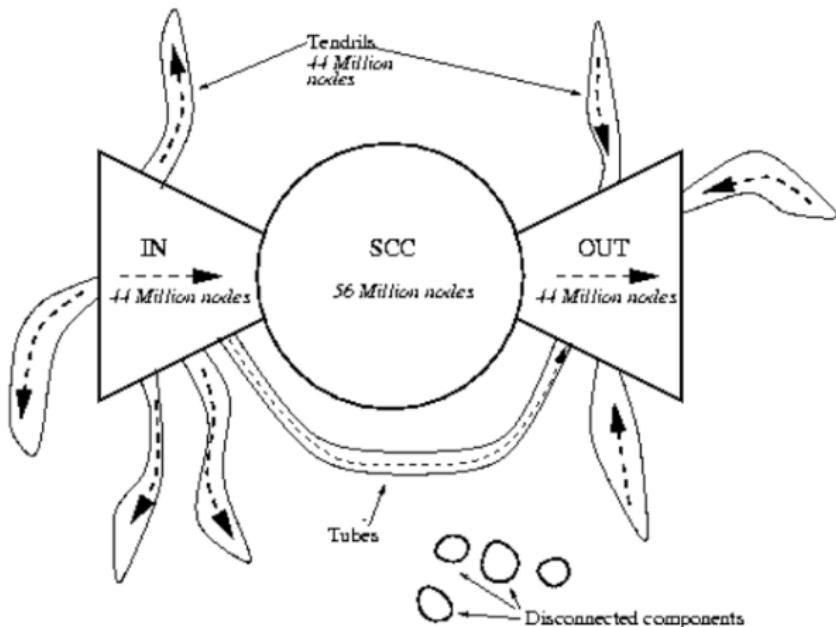


Figure: Box-tie structure of the web

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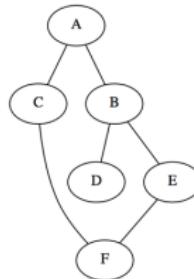
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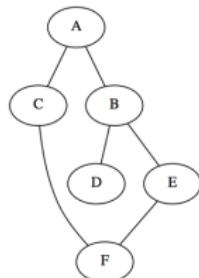
Depth first search



- Graph exploration, from a given start node, *depth first*:

```
def dfs(graph, start):  
    visited, stack = set(), [start]  
    while stack:  
        vertex = stack.pop()  
        if vertex not in visited:  
            visited.add(vertex)  
            stack.extend(graph[vertex] - visited)  
    return visited  
  
dfs(graph, 'A') # {'E', 'D', 'F', 'A', 'C', 'B'}
```

Breadth first search



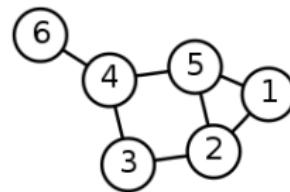
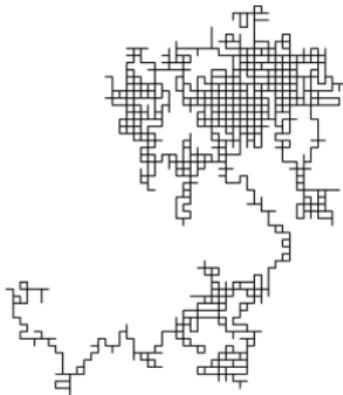
- *breadth first:*

```
def bfs(graph, start):  
    visited, queue = set(), [start]  
    while queue:  
        vertex = queue.pop(0)  
        if vertex not in visited:  
            visited.add(vertex)  
            queue.extend(graph[vertex] - visited)  
    return visited  
  
---  
> bfs(graph, 'A') # {'B', 'C', 'A', 'F', 'D', 'E'}
```

- Queue → search in vertices breadth (FIFO)

Random walk

- Randomized exploration.
- Given a graph and a *start* node, a simple random walk[1] proceeds by random steps:
 - selects uniformly at random a neighbor from walk position
 - jump on it
 - loop process



$$\text{RDW}(6,7\text{hops}) = (6,4,3,4,5,4,3,2)$$

Figure: Random walk on a grid (i.e., 4 neighbors per node)

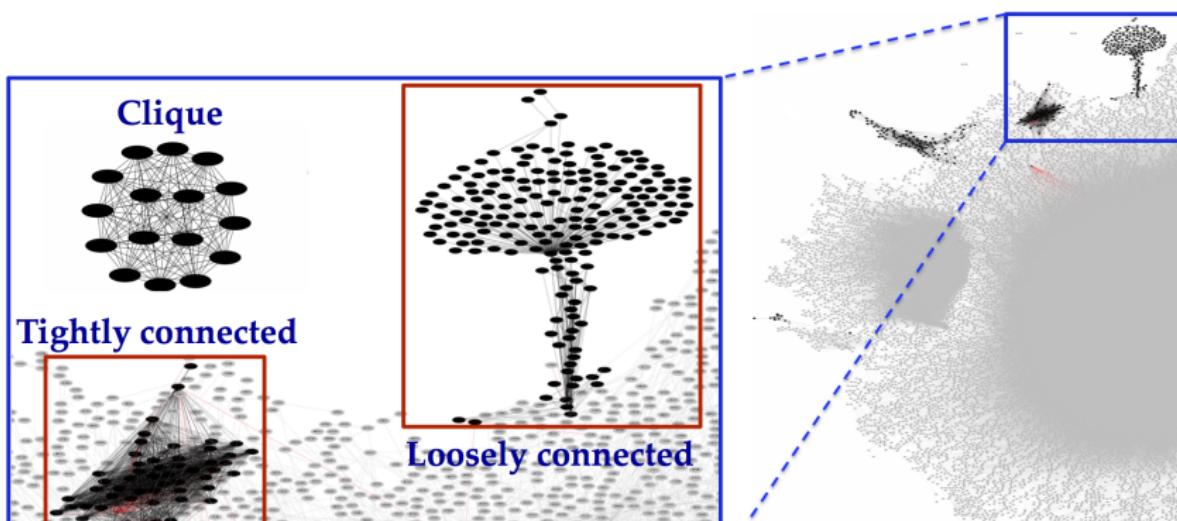
- Select a random node in the graph (but biased).
- Given a graph, a *start* node, and a “large” h use a simple random walk:
 - selects uniformly a neighbor; jump on it; $h \leftarrow h - 1$
 - loop until $h \leq 0$
- Results in probability of node j to be selected: $P_j = \frac{d_j}{\sum_{i=0}^n d_i}$

- Select a random node in the graph uniformly (Metropolis-Hastings method).
- Same as for biased except that, from current node i :
 - generate $p \sim U(0,1)$
 - selects uniformly a neighbor j ; jump on it if $p \leq \min\{1, \frac{d_i}{d_j}\}$, else stay on i
- Results in probability of node j to be selected: $P_j = \frac{1}{\sum_{i=0}^n d_i}$

- Estimate n in a distributed fashion; based on the *birthday paradox* [6].
 - Sample uniformly nodes: $X_{t+1} \leftarrow X_t \cup j$
 - Stop when “collision” after l samples, i.e., when a node j appears twice in X_t
 - $\hat{n} = \sqrt{l^2/2}$

Random walks - app3: sybil detection

- “Early-terminated random walk starting from a non-Sybil node in a social network has a higher degree-normalized (divided by the degree) landing probability to land at a non-Sybil node than a Sybil node”. [7]
 - observation holds because the limited number of attack edges forms a narrow passage from the non-Sybil region to the Sybil region in a social network.



- A spanner S of a graph G : subgraph of G with *few edges* and *short distances*.²
 - Tradeoff between number of edges and distance stretch.
- (α, β) -spanner of $G \iff \forall(u, v):$

$$dist_H((u, v)) \leq \alpha \times dist_G((u, v)) + \beta$$

- α : multiplicative stretch, β : additive stretch.

```
S := []
For each edge (u, v) in E do
  If dist_H((u, v)) > 2k-1 do
    add (u, v) to S
```

- S is a $(2k - 1, 0)$ -spanner of G .
- $|V_S| < n_G^{1+1/k}$.

²Graph spanners, Viennot, 2010.

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Measuring the importance of individual nodes

- *Importance* has to be defined precisely, generally based on the application using the extracted importance metrics.
- Here, *centrality* metrics target *individual* importance, with regards to the rest of nodes in the graph.

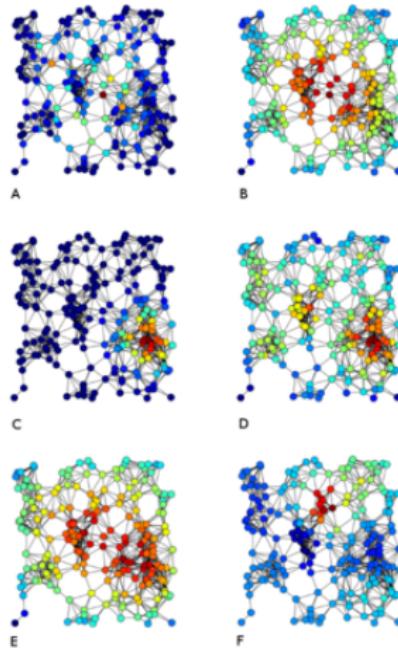
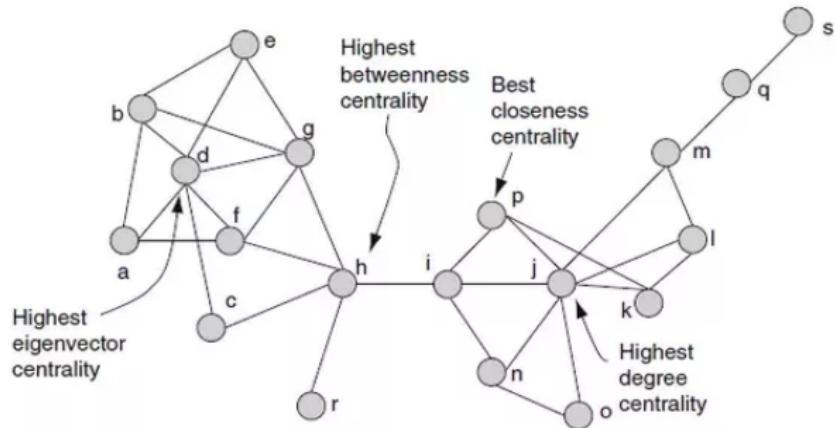


Figure: Various importance results

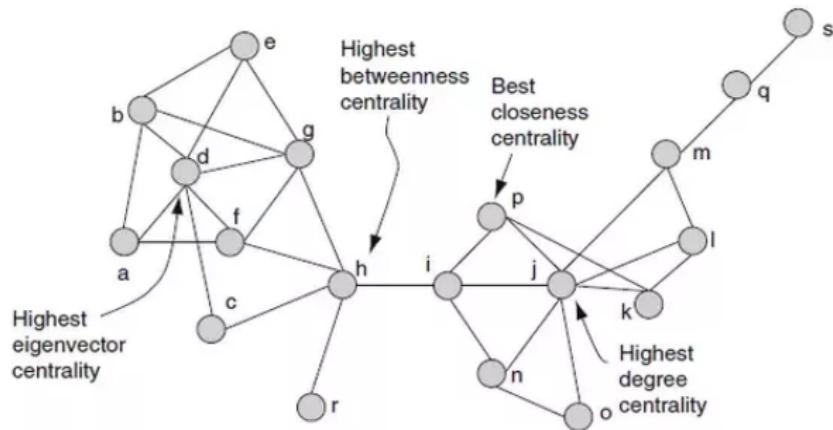
Degree centrality



An important node is a node that has *many* neighbors

$$C_d(i) = \frac{d(i)}{n - 1}$$

Eigenvector Centrality



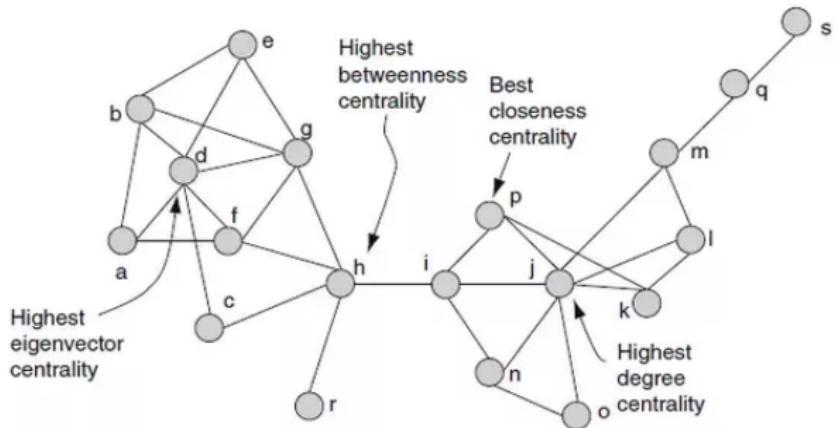
An important node is a node that has *important* neighbors

$$C_\lambda(i) = \sum_{j \in \Gamma(i)} C_\lambda(j)$$

- In a network with n nodes, we assign all nodes the same initial PageRank, set to be $1/n$
- Choose a number of steps k
- Perform a sequence of k updates to the PageRank values, with following rule for each update:
 - Each page divides its current PageRank equally across its out-going links, and passes these equal shares to the pages it points to. Each page updates its new PageRank to be the sum of the shares it receives.

The probability of being at a page i after k steps of this random walk is precisely the PageRank of i after k applications of the update Rule.

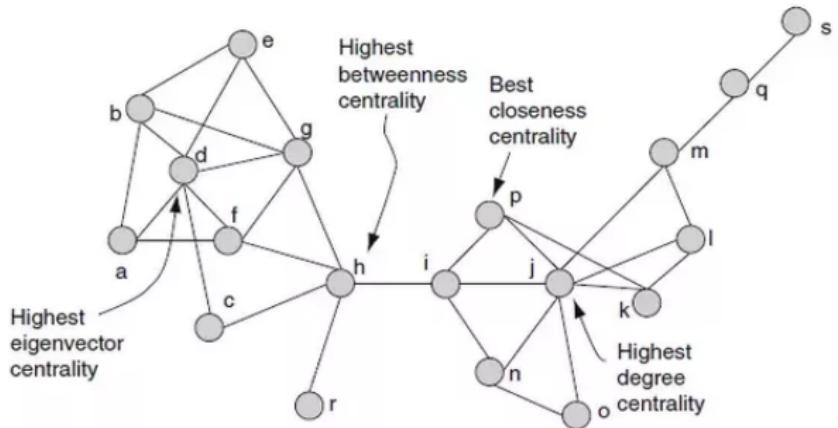
Closeness centrality



An important node is *close* from all other nodes in the graph

$$C_c(i) = \frac{1}{\sum_{j \in V} d(i,j)}$$

Betweenness centrality



An important node is a node that lies on many *shortest paths*

$$C_b(i) = \sum_{j \neq k \neq i} \frac{\sigma_{jk}(i)}{\sigma_{jk}},$$

where $\sigma_{jk}(i)$ the number of s.p. from j to k passing through i

An important node is not *eccentered*

$$C_e(i) = \frac{1}{\max_{j \in V} dist(i,j)}$$

An important node is a node that is on many *potential* paths
 $\forall j, k \in V$, j sends a random walk (r.w.) that stops on k ;
each node i on the r.w. path earns a point

An important node see *regularly* random data flows

- Let an unbiased³ random walk running on the graph
- Each node records *return time* of the walk in Ξ_i
- After N visits on a node i , its standard deviation is:

$$C_{\sigma_i}(N) = \sqrt{\frac{1}{N-1} \sum_{k=1}^N \Xi_i(k)^2 - [\frac{1}{N-1} \sum_{k=1}^N \Xi_i(k)]^2},$$

Important nodes have a low standard deviation of those return times

³jumps on neighbors regardless of its in-degree

Importance non-agreement

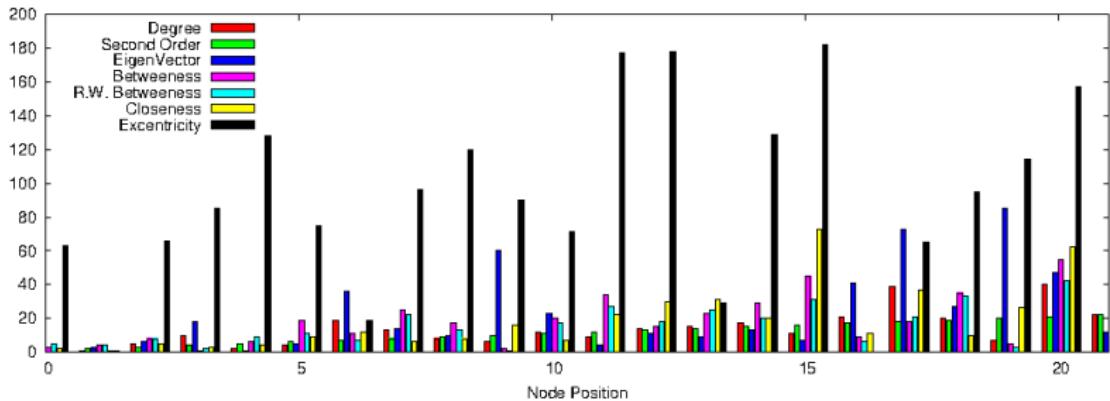
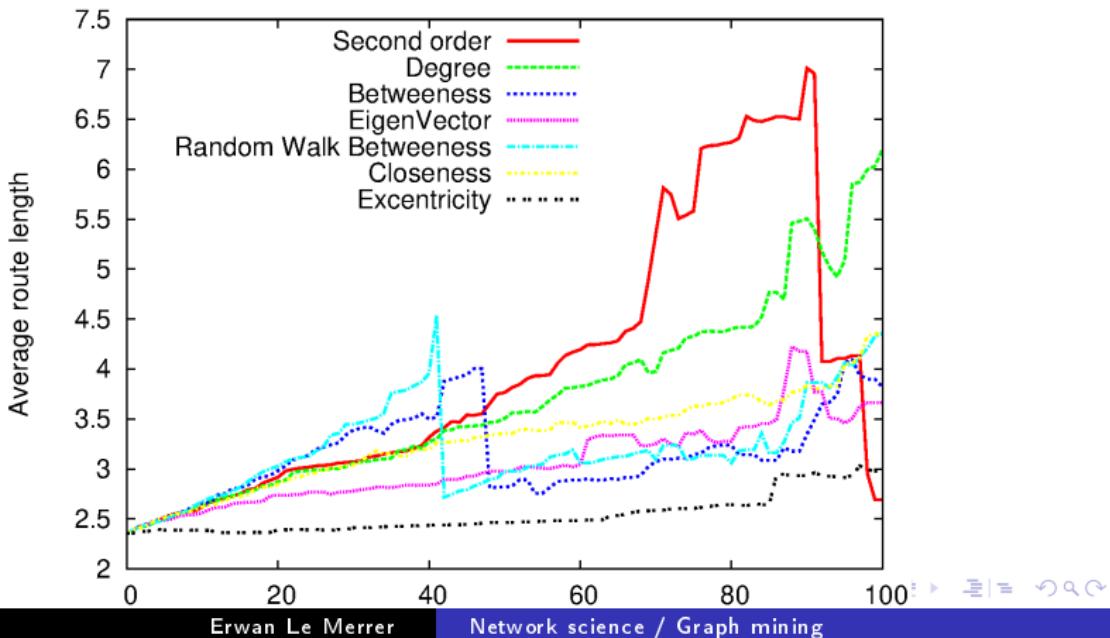
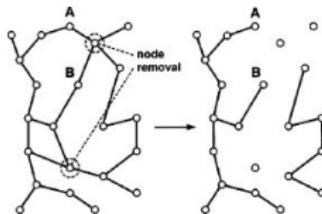


Figure: Importance is indeed totally definition dependant

Removal impact on path lengths



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Study of complex networks

- exemple use in social nets, epidemics...

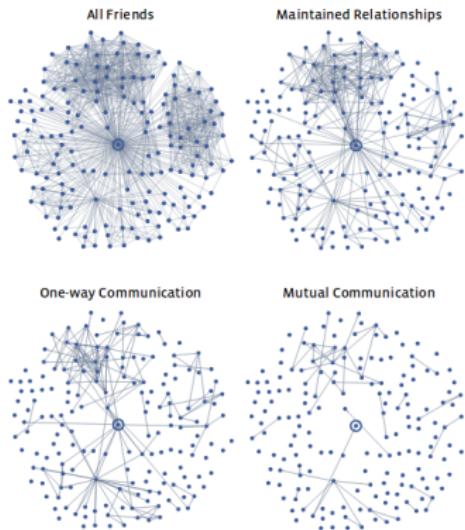
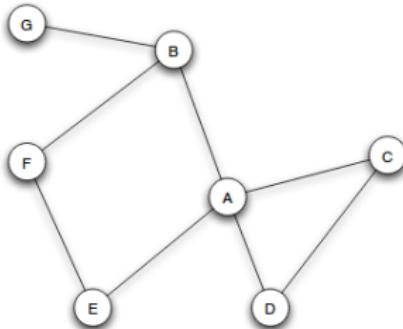


Figure 3.8: Four different views of a Facebook user's network neighborhood, showing the structure of links corresponding respectively to all declared friendships, maintained relationships, one-way communication, and reciprocal (i.e. mutual) communication. (Image from [286].)

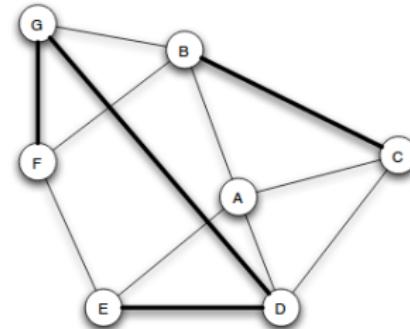
Figure: From Networks, Crowds, and Markets: Reasoning about a Highly Connected World . By David Easley and Jon Kleinberg. Cambridge University Press, 2010.

Triadic closure

- “If two people in a social network have a friend in common, then there is an increased likelihood that they will become friends themselves at some point in the future”.



(a) Before new edges form.



(b) After new edges form.

- $\{G, B, F\}$ form a new triangle, which might have been predicted.

- *Mixing*: tendency of nodes to connect preferentially to other nodes with either similar or opposite properties.
- $\rho_D > 0$: the graph possesses *assortative mixing*, a preference of high-degree nodes to connect to other high-degree nodes.
- $\rho_D < 0$: the graph possesses *disassortative mixing*, a preference of high-degree nodes to connect to low-degree nodes.

- *Modularity*: fraction of the edges that fall within the given communities, minus the expected fraction if edges were distributed at random.
 - *Louvain modularity*: measures the density of links inside communities compared to links between communities, $\in [-1, 1]$:

$$LM(G) = \frac{1}{2m} \sum_{ij} \left[A_{ij} - \frac{k_i k_j}{2m} \right] \delta(c_i, c_j),$$

with:

- c_v the community hosting node v
- k_v the sum of the weights of the edges attached to node v
- $\delta(c_i, c_j)$ the Kronecker delta function (i.e., zero if $c_i \neq c_j$)

Node removal and k-core

- Removing node sequentially, to obtain a *dendrogram*⁴

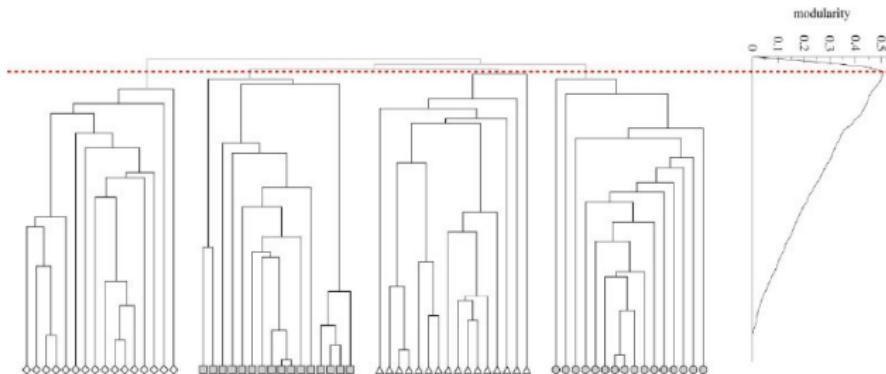


Fig.: A network dendrogram (aka hierarchical tree)

- A k -core of G is a maximal connected subgraph of G in which all vertices have degree at least k
 $(\forall v \in \text{subgraph}(G), d(v) \geq k)$.
 - Component obtained deleting all vertices with degree $< k$.

⁴<http://perso.crans.org/aynaud/communities/api.html>

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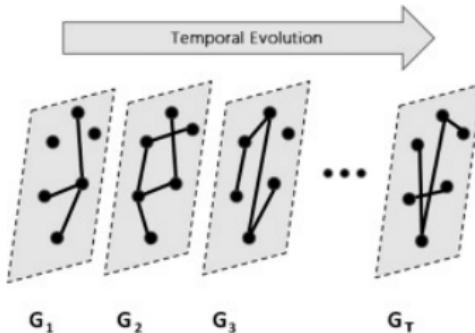
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The time dimension

- When e.g., observed at runtime, some graphs are dynamic (arriving/departing nodes, edge creation/deletion).



- The time dimension is not classically used in graph analysis (focus on one single “snapshot”), while of obvious value.

The time dimension for community analysis

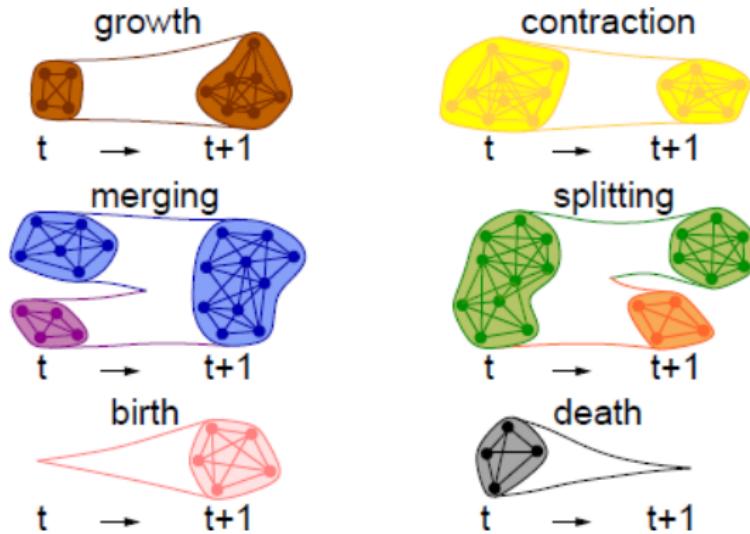


Figure: The fate of communities, observation possible through the time dimension

- A *time-varying* graph (TVG) defined as[5]:

$$\mathcal{G} = (V, E, T, \rho, \varsigma),$$

with:

- $T \subseteq \mathcal{T}$ the lifetime of the system captured as a graph
- $\rho : E \times T \rightarrow \{0, 1\}$ the *presence function*, returning the edge presence at a given time
- $\varsigma : E \times T \rightarrow \mathcal{T}$ the *latency function*, returning the time needed to cross that edge, if starting at a given time

A journey in a TVG

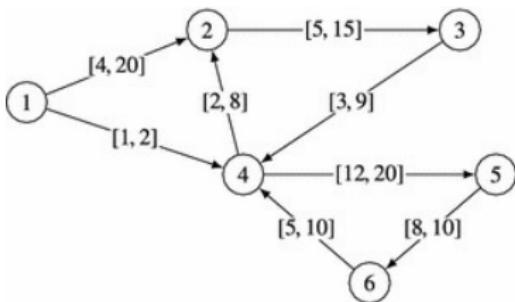


Figure: A directed TVG, with fix nodes, but dynamic edges

- A *journey*: temporal extension of the notion of path.
- A sequence of tuples $\mathcal{J} = \{(e_1, t_1), (e_2, t_2), \dots, (e_k, t_k)\}$, with e_i a given edge in \mathcal{G} , is a journey if $\forall i, 1 \leq i < k, \rho(e_i, t_i) = 1$ and $t_{i+1} \geq t_i$.
 - i.e., \mathcal{J} is a path over time in \mathcal{G} (set of all journeys is \mathcal{J}^*).
- *Shortest distance* starting at t from u to v is

$$dist^t(u, v) = \min\{|\mathcal{J}| : \mathcal{J} \in \mathcal{J}^*(u, v) \wedge \text{departure}(\mathcal{J}) > t\}$$

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Graph edit distance

- *Edit distance*: measure graph dissimilarity from the number as well as the strength of the distortions that have to be applied to transform a source pattern into a target pattern [2].
- Let G_1 and G_2 two graphs to compare, edit distance is:

$$ed_{\lambda_{min}(G_1, G_2)} = \min_{\lambda \in \gamma(G_1, G_2)} \sum_{e_i \in \lambda} c(e_i),$$

with:

- $\gamma(G_1, G_2)$ the set of edit paths from G_1 to G_2
- $c(e_i)$ the cost of edit operation e_i

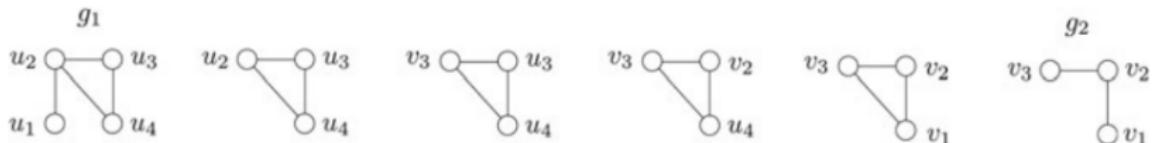


Figure: An edit path λ between to graphs G_1 and G_2

- Graph edit distance is computationnally expansive...
- A *kernel* $k(G_1, G_2)$ is a measure of similarity for those two graphs, with properties that $k(G_1, G_2) = k(G_2, G_1)$, and that it is *positive semi-definite*.
- *Random walk graph kernel* [4]:
 - Run random walks on both graphs
 - Count the number of *matching* walks
 - This number is used as a similarity metric
 - Fast C++ implementation here: <https://github.com/BorgwardtLab/random-walk-graph-kernels>

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The Open Graph Viz Platform

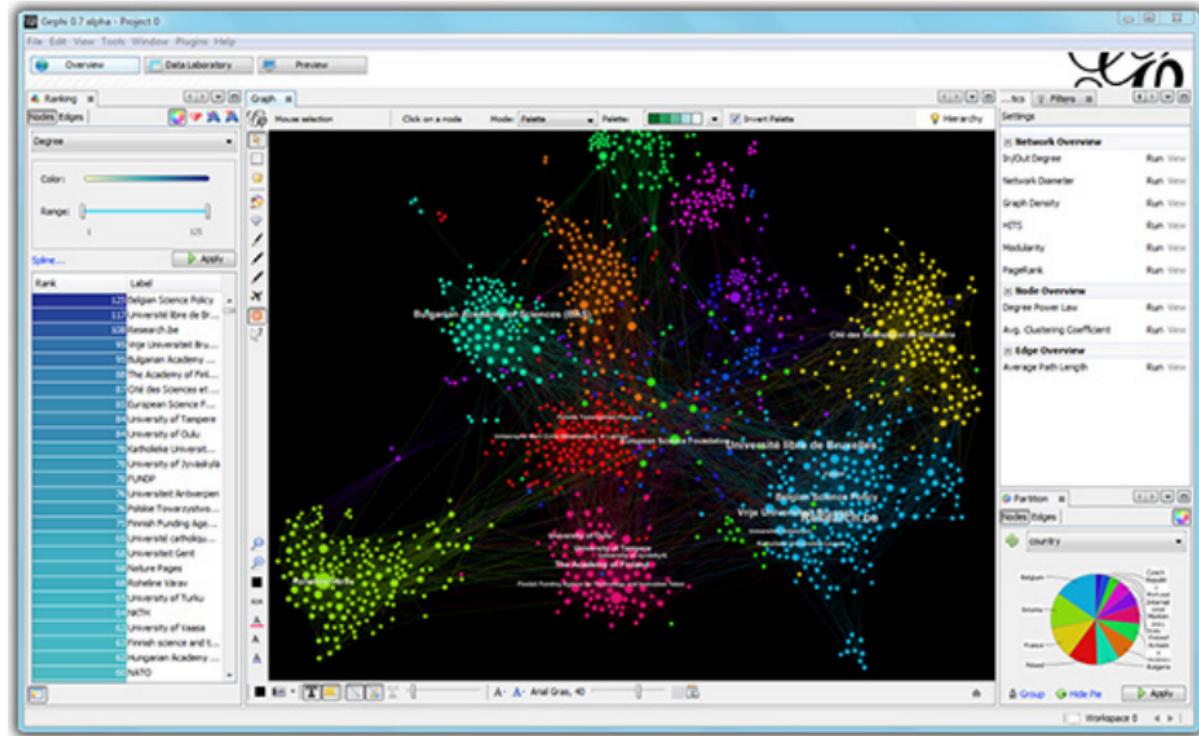


Figure: Gephi, <https://gephi.org/>

Erwan Le Merrer

Network science / Graph mining

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