

Network science / Graph mining

Metrics for analyzing a connected world of data

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- 1 Graphs and representations
- 2 Classical metrics
- 3 Three important graph models & a generative method
- 4 Exploring graphs
- 5 Importance metrics
- 6 Community metrics
- 7 Comparing graphs
- 8 TVGs: time varying graphs

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Graphs ?



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

An abstraction/representation for reasoning about characteristics of

- physical networks (computers, roads, circuits).
- relational data.

Focus on the structure rather than on the details of modeled objects

The omnipresence of graphs in applications

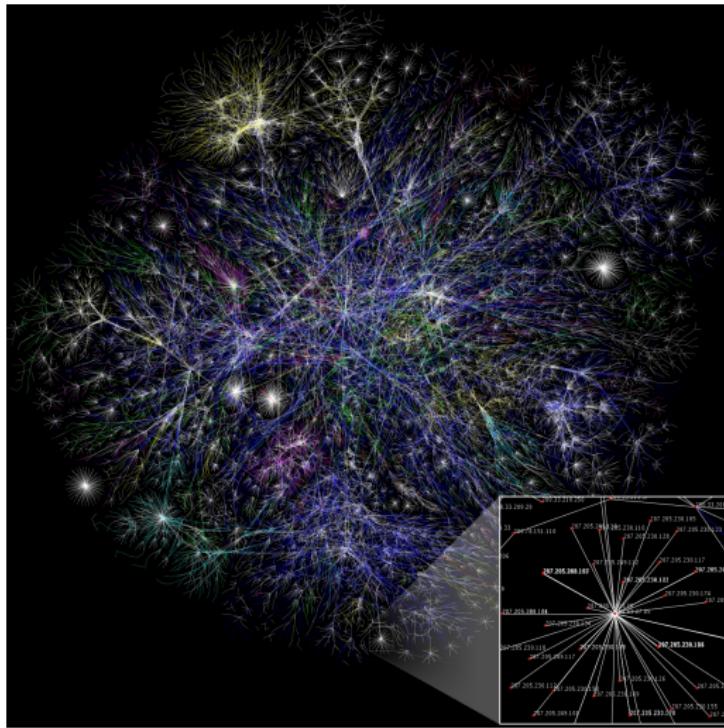


Figure: The Internet AS graph

The omnipresence of graphs in applications

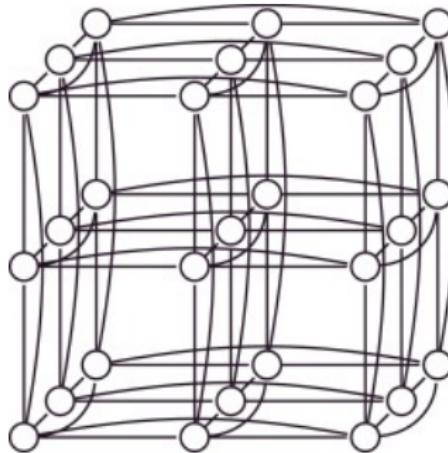


Figure: Interconnecting system-on-chips in a datacenter rack

The omnipresence of graphs in applications

- exemple use in social nets, epidemics...

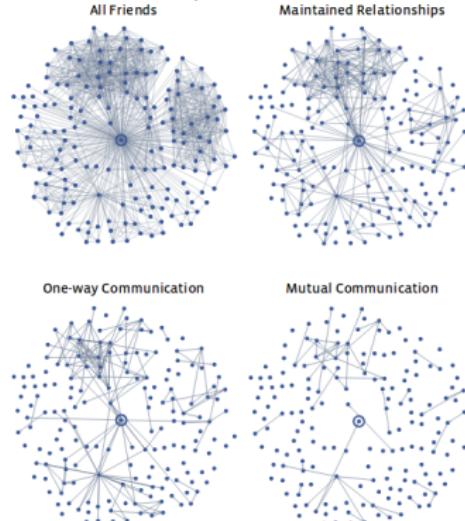


Figure 3.8: Four different views of a Facebook user's network neighborhood, showing the structure of links corresponding respectively to all declared friendships, maintained relationships, one-way communication, and reciprocal (i.e. mutual) communication. (Image from [286].)

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

e.g.: recommendations on YouTube

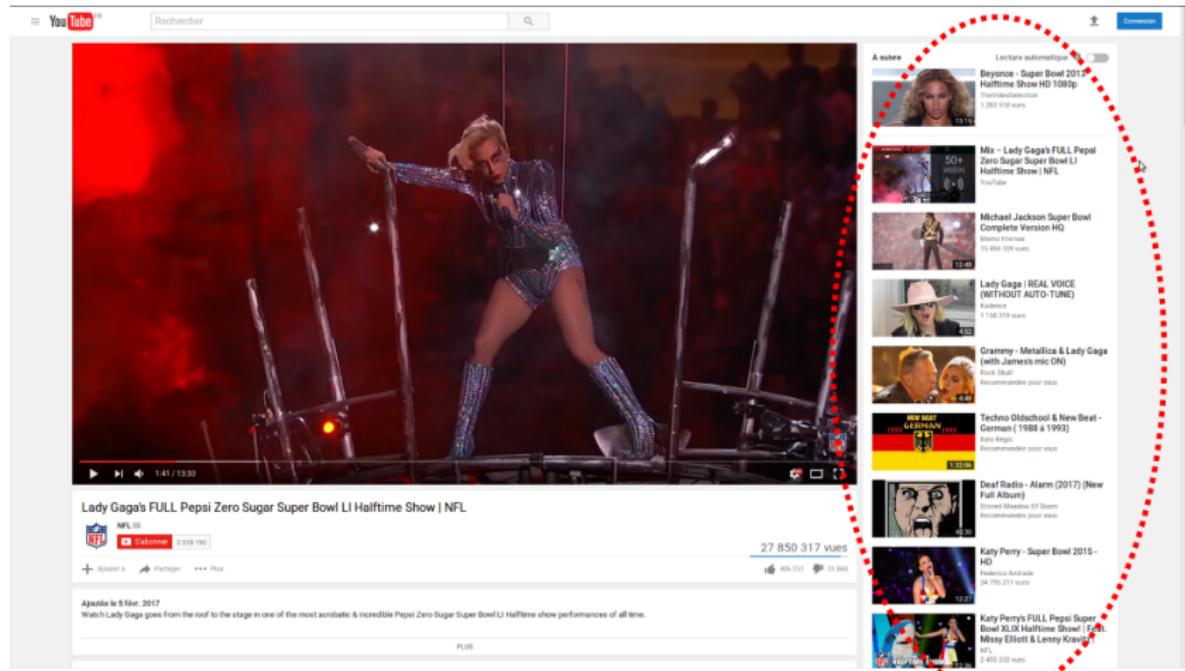
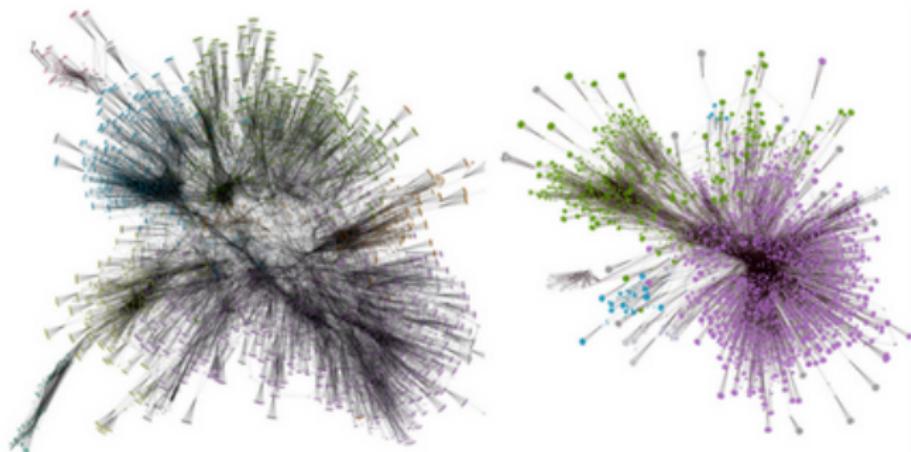


Figure: Recommendations: contextual, personalized?

e.g.: recommendations on YouTube

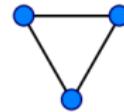
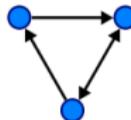


4-hops graphs from a YouTube video, new user (left) and returning user (right)

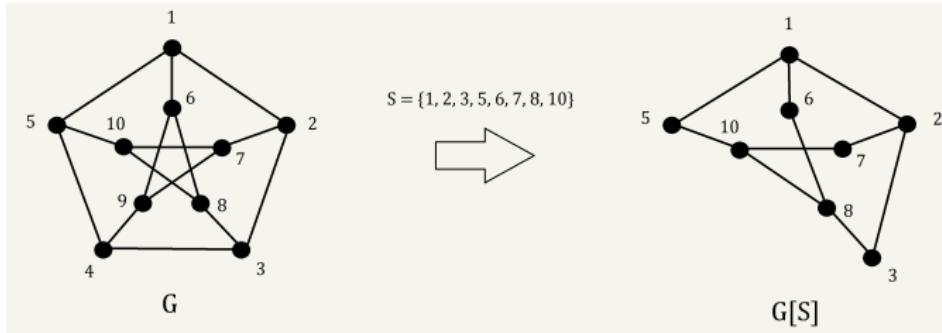
Figure: Blank profile vs. my recommendations

Core notions (1)

- *Directed* and *undirected* graphs:
 - in directed graphs, edges have orientation (arrow end)

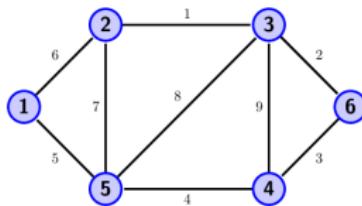


- A *subgraph* of G : formed by a subset of vertices and edges from G .

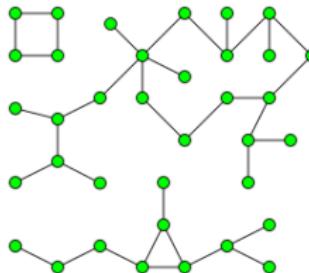


Core notions (2)

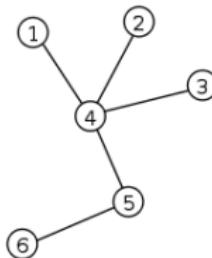
- Edge weight: value assigned as a label to an edge.
 - e.g., distance in km of a road from city 1 to 2.



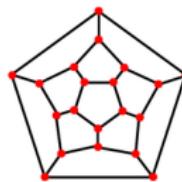
- Graph connectivity:
 - A graph is *connected* if there is a *path* btw any pair of vertices.
 - Otherwise, *connected components* are the subgraphs in which paths exist.



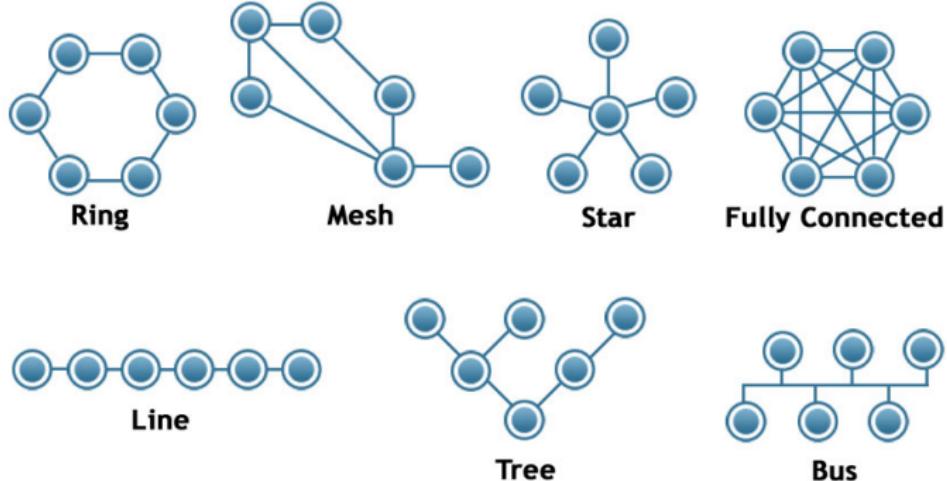
- A *cycle*: a path in which a vertex is reachable from itself.
 - Example of an *acyclic* connected graph: a *tree*



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



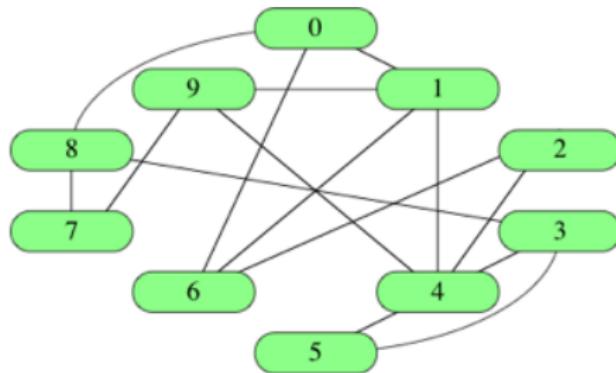
Special topologies



certiology.com

Figure: Graphs to remember, often used as illustrations

Adjacency list or edge list representations



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.¹

¹<https://www.khanacademy.org/computing/computer-science/algorithms/graph-representation/a/representing-graphs>

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



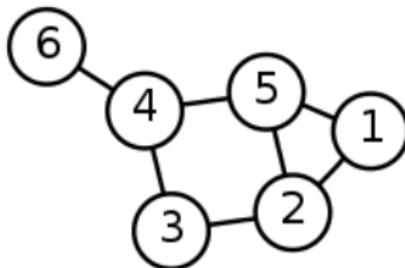
Figure: For a database-like handling of graphs

NetworkX

Figure: Prototyping in Python, lots of contributions

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- $G(V, E)$: 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: $0 \leq d_v \leq n - 1$ (if no self loops).
- *Degree distribution* $P(d)$ is the probability distribution of each degree in the current graph:

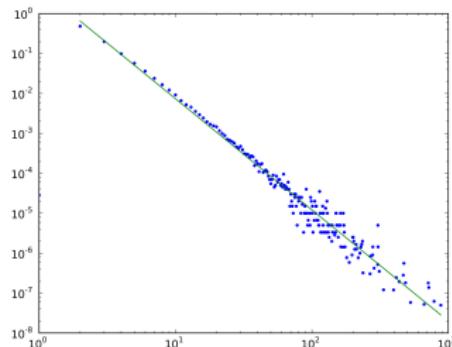


Figure: Degree distribution: x-axis is degree, y-axis is probability

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

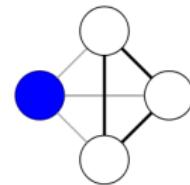
Clustering coefficient

- 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”:

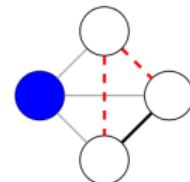
$$C_i = \frac{2|e_{jk} : v_j, v_k \in \Gamma(v_i), e_{jk} \in E|}{d_i(d_i - 1)}$$

- Average clustering coefficient:

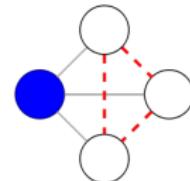
$$\bar{C} = \frac{1}{n} \sum_{i=1}^n C_i$$



$$c = 1$$

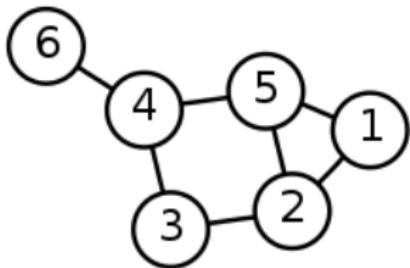


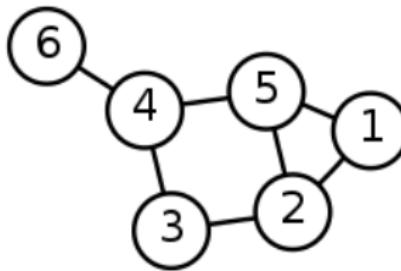
$$c = 1/3$$



$$c = 0$$

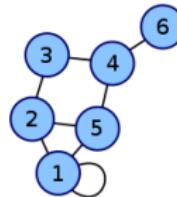
- *Path*: sequence of adjacent nodes connecting two nodes (if exists).
 - e.g., two paths btw 6 and 1: $(4,5,1)$ and $(4,3,2,5,1)$.
 - One *hop*: one transition from a node to another.
- *Shortest path*: path of minimal cardinality.
 - Distance $dist(6,1) = |(4,5,1)| = 3$
- *Single-source shortest path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





- *Average path length*: average of all-pair shortest distances in the graph.
- *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

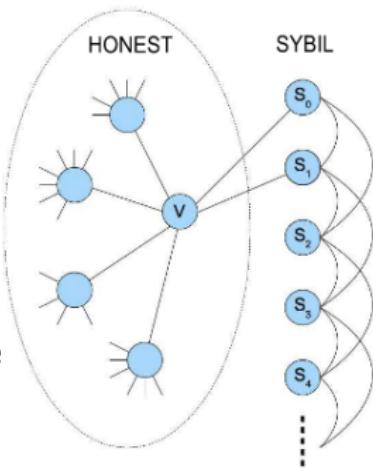
$$\begin{pmatrix} 2 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

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 .

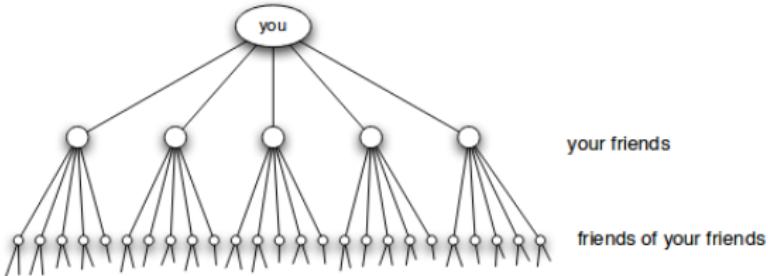


- *Expansion* of G : mean number of nodes that are reached in h hops from all nodes:

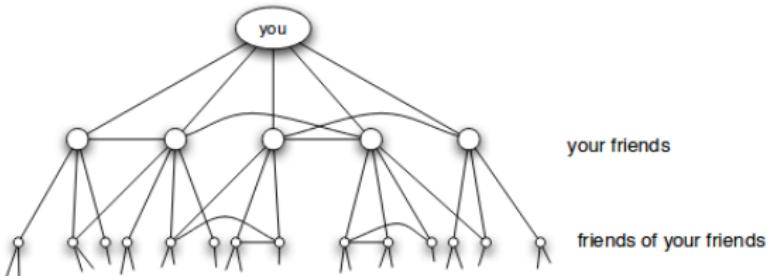
$$e_G(h) = \frac{1}{n^2} \sum_{v \in V} |C_v(h)|,$$

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 .

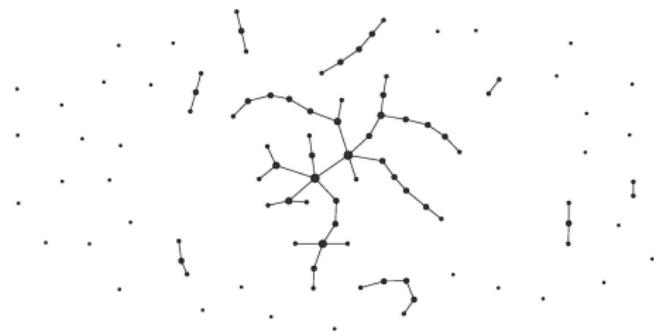


Figure: A random graph with $p = 0.01$.

- 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 Watts-Strogatz graph

- Graphs with high clustering (like regular graphs), and low path lengths (like a random graph).
 - Create a ring lattice of n nodes.
 - Replace every edge by a random edge, with probability p .

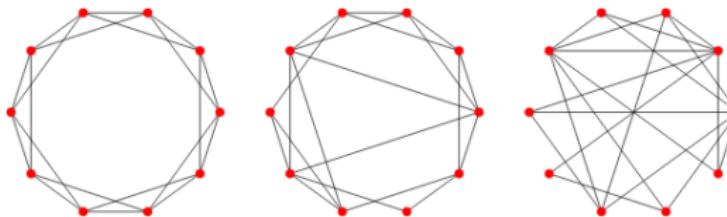


Figure 3.2: WS graphs with $n = 20$, $k = 4$, and $p = 0$ (left), $p = 0.2$ (middle), and $p = 1$ (right).

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).

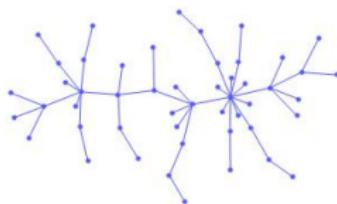


Figure: A Barabási-Albert graph with $n = 50$ and $m_0 = 1$.

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

A real structure example

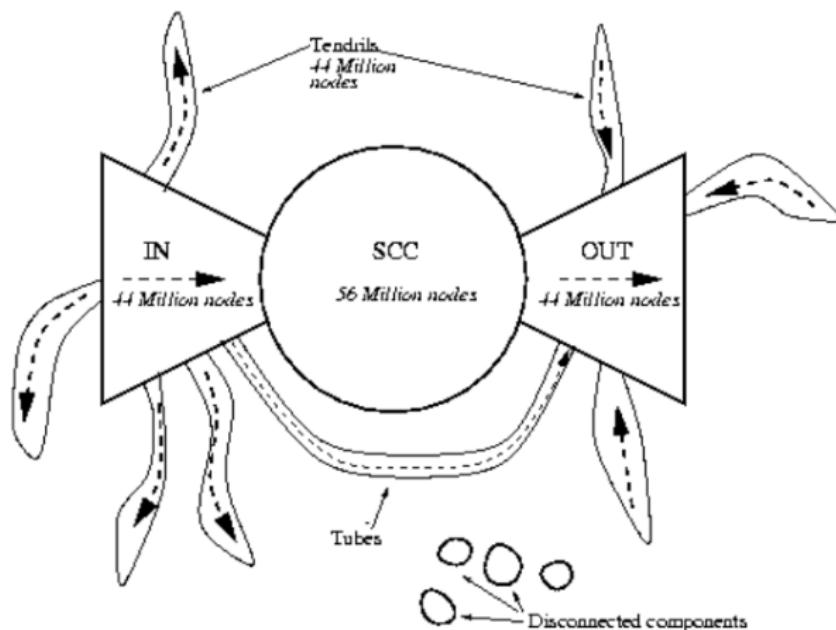
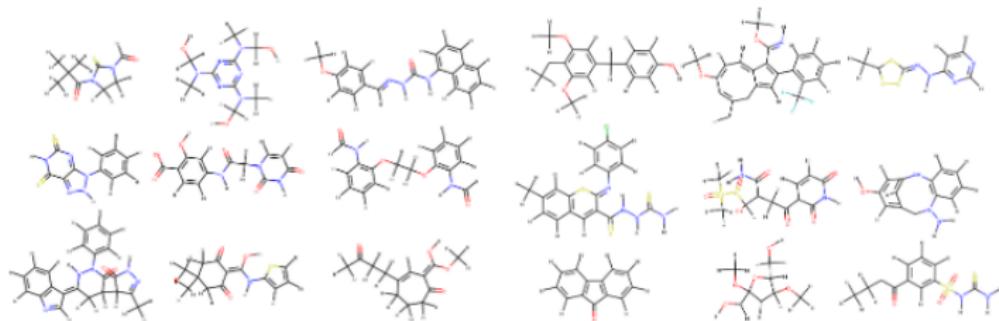


Figure: Bow-tie structure of the web

Generating graphs with neural nets: GraphGen (1)

- How to generate graphs from an unknown generative process?



(a) Real graphs

(b) GraphGen

Generating graphs with neural nets: GraphGen (2)

- Instances of graphs in a categorie → learn → generate others [8]
- Converting a graph to a sequence

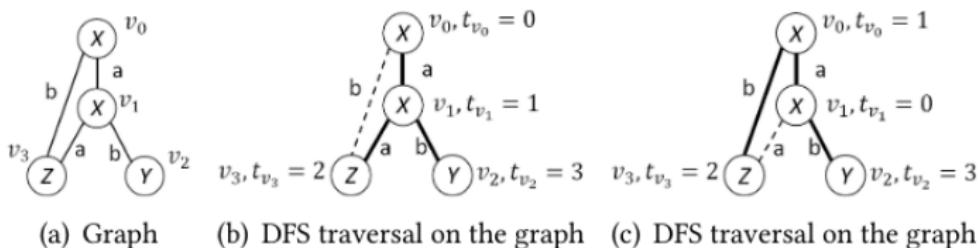


Figure: Extracting DFS "codes" from a graph to learn from.

- 5-tuples $(t_u, t_v, L_u, L_{(u,v)}, L_v)$, with L the label. Fig (b): $(0, 1, X, a, X), (1, 2, X, a, Z), (2, 0, Z, b, X), (1, 3, X, b, Y)$.

Generating graphs with neural nets: GraphGen (3)

- A recurrent neural network (RNN) learns a DFS sequence S
 $p(S) = \prod_{i=1}^{m+1} p(s_i | s_1, \dots, s_{i-1})$ (i.e., conditional distribution over the elements.)
- Generation from $m = 1$ to $m = |E|$, one single edge at a time

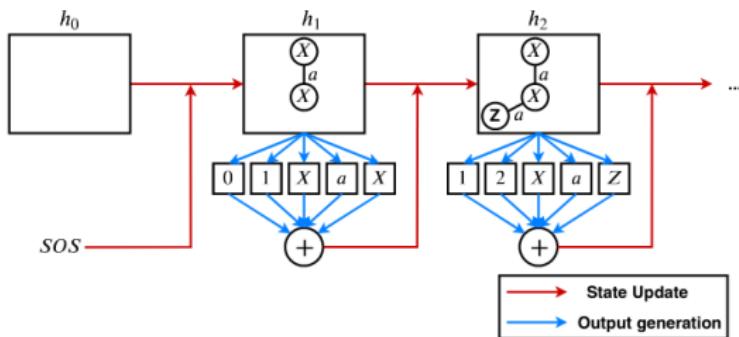
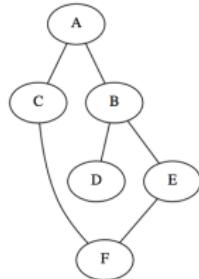


Figure 3: Architecture of GRAPHGEN. Red arrows indicate data flow in the RNN whose hidden state h_i captures the state of the graph generated so far. Blue arrows show the information flow to generate the new edge tuple s_i .

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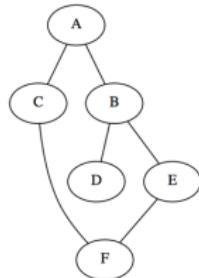
Depth first search



- 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
```

Breadth first search

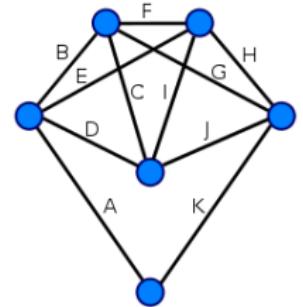


- *breadth first:*

```
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
```

- Queue → search in vertices breadth (FIFO)

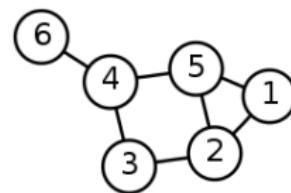
Eulerian path



- An Eulerian path visits every edge exactly once (allowing for revisiting vertices).
- Euler's Theorem: A connected graph has an Euler cycle if and only if every vertex has even degree.

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)

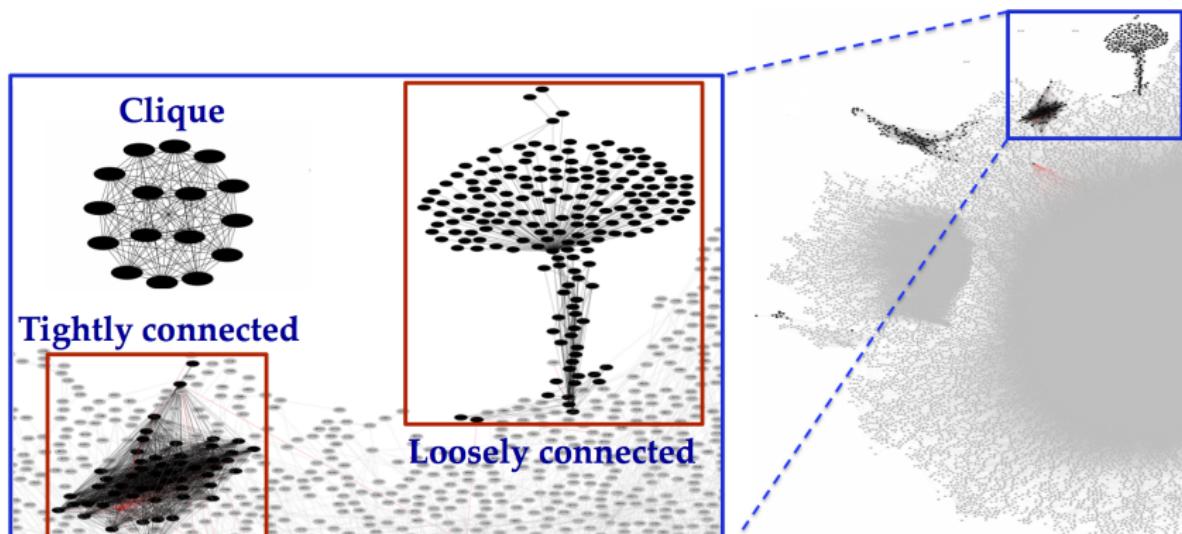
- Select a random node in the graph (but biased).
- Given a graph, a *start* node, and a “large” h use a simple random walk:
 - selects uniformly a neighbor; jump on it; $h \leftarrow h - 1$
 - loop until $h \leq 0$
- Results in probability of node j to be selected: $P_j = \frac{d_j}{\sum_{i=0}^n d_i}$

- 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: $P_j = \frac{1}{\sum_{i=0}^n d_i}$

- Distributed computation of n ; 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.



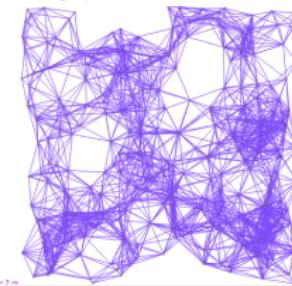
Spanner

- A spanner H 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 $G \iff \forall(u, v): dist_H((u, v)) \leq \alpha \times dist_G((u, v)) + \beta$, with α : multiplicative stretch, β : additive stretch.

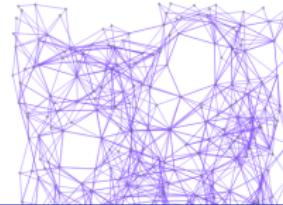
```
H := []
For each edge (u, v) in E do
  If dist_H((u, v)) > 2k-1 do
    add (u, v) to H
```

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

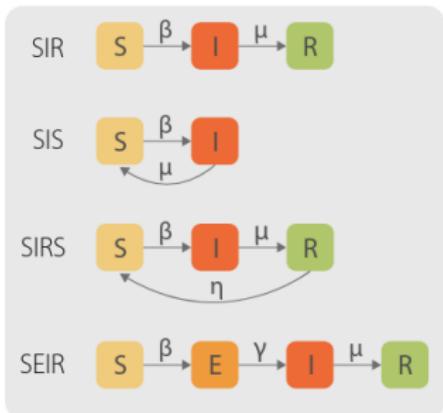
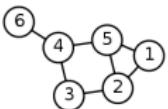
From a graph G



Compute a subgraph H spanning G

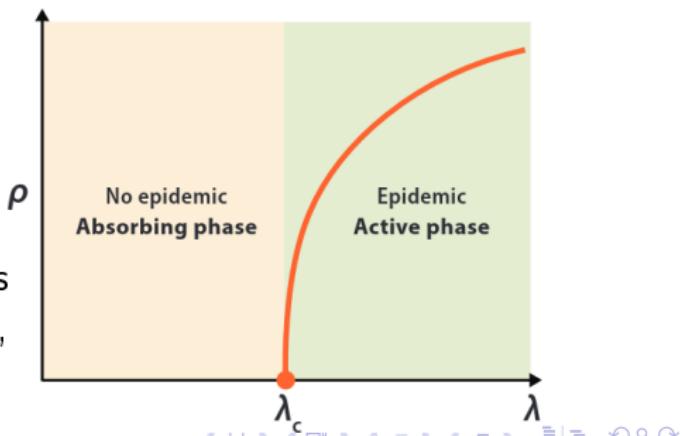


Epidemics on graphs (1)



Epidemic on graph nodes: models with states Susceptible, Infected, Recovered, Exposed.[9]

- SIS-like: $\lambda = \beta/\mu$
- Order parameter ρ : transition point λ_c , s.t. for $\lambda > \lambda_c \rightarrow \rho > 0$, while for $\lambda \leq \lambda_c \rightarrow \rho = 0$



Epidemics on graphs (2)

- Application to marketing: which initial node for best spread?

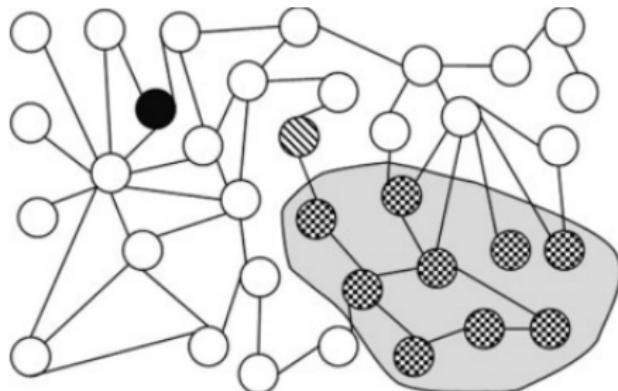


Fig. 1. Example of a social network. Black node denotes the globally central node; chequered nodes denote the potential market; hatched node denotes the node central w.r.t. the potential market.

Figure: cf “A targeted approach to viral marketing”

Outline

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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.

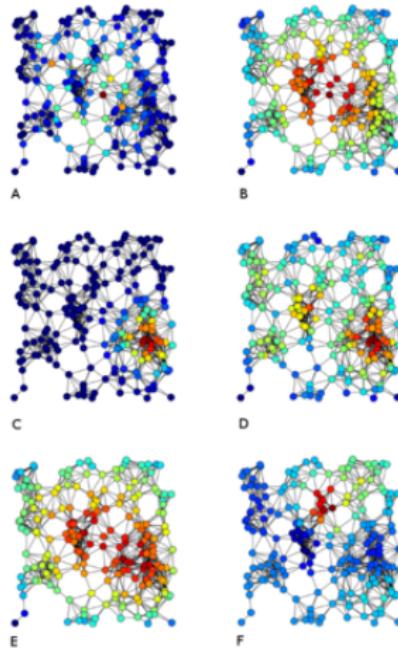
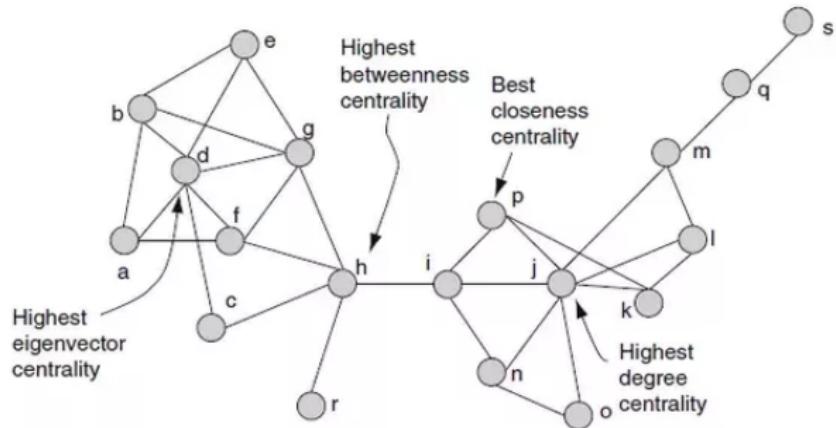


Figure: Various importance results

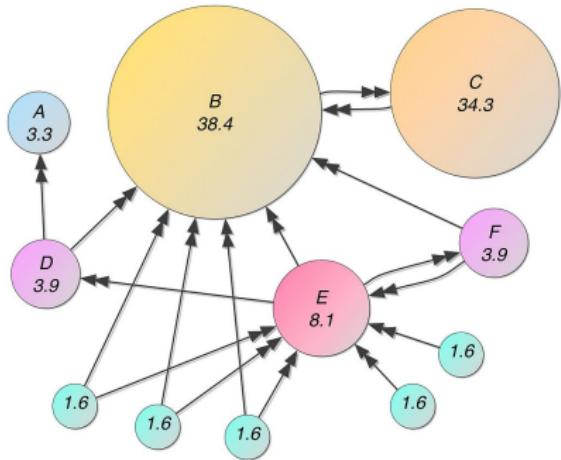
Degree centrality



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

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

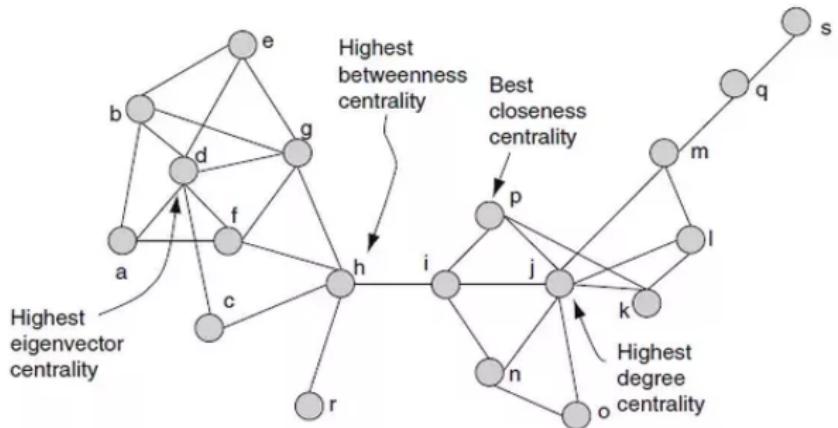
Pagerank basic computation



- assign all nodes the same initial PageRank: $1/n$
- perform k updates of the PR values, as follows:
 - Each node divides its current PR equally across its out-going links, and passes these equal shares to the nodes it points to. Nodes update PRs to be the sum of the shares they receive.

$$PR(i) = \sum_{j \in \Gamma(i)} \frac{PR(j)}{|\Gamma_{out}(j)|}$$

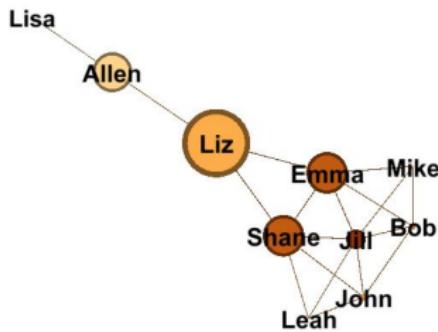
Closeness centrality



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

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

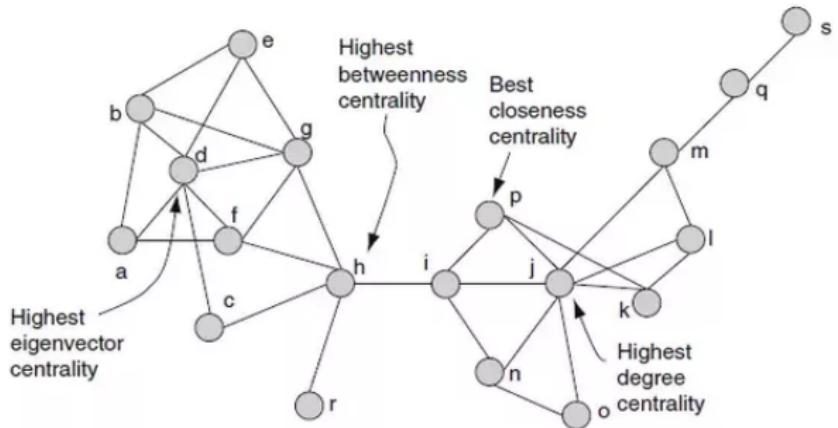
Eccentricity



An important node is not *eccentered*

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

Betweenness centrality

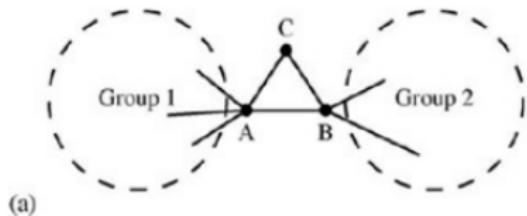


An important node is a node that lies on many *shortest paths*

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

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

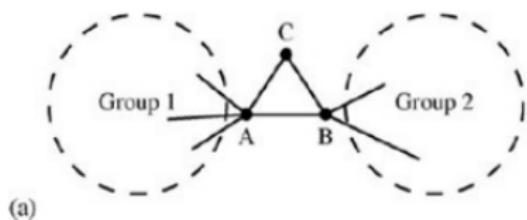
Random walk betweenness centrality



Vertices A and B have high (shortest-path) betweenness in this configuration, while vertex C does not.

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

Second Order centrality



Vertices A and B have high (shortest-path) betweenness in this configuration, while vertex C does not.

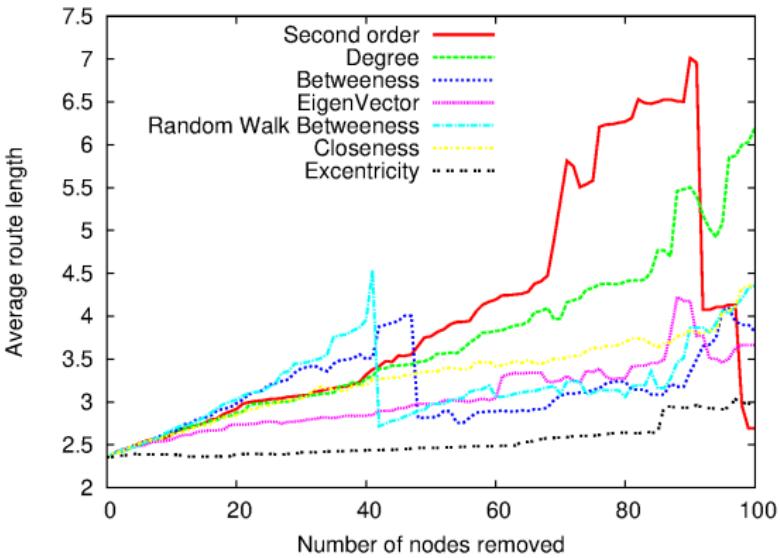
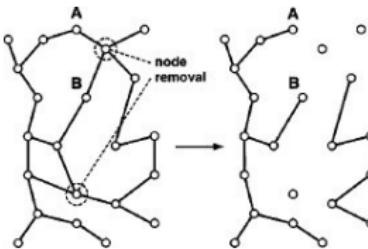
An important node see *regularly* random data flows

- Let an unbiased 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

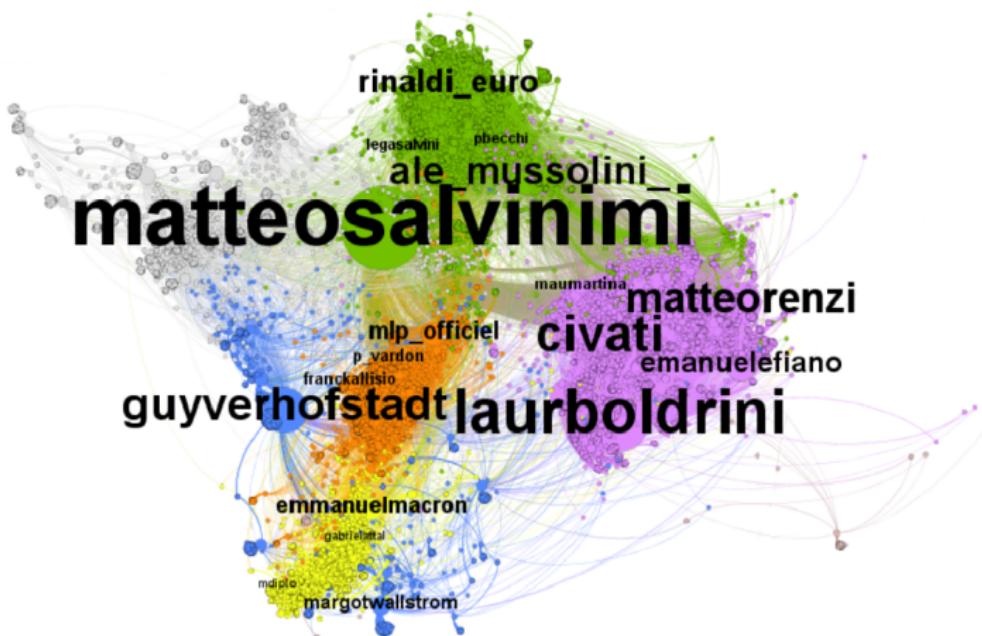
Removal impact on path lengths



Outline

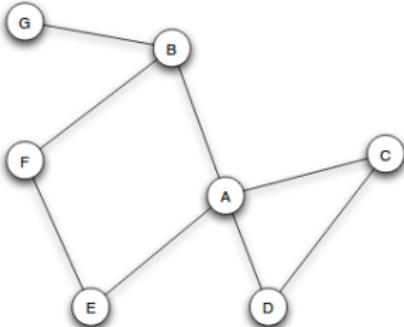
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Detecting communities in graphs

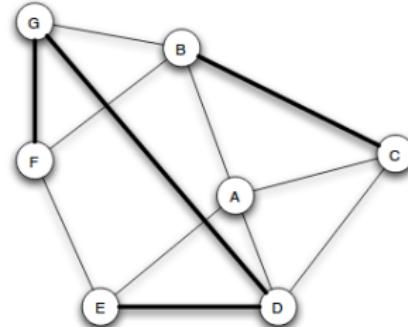


Triadic closure

- “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.



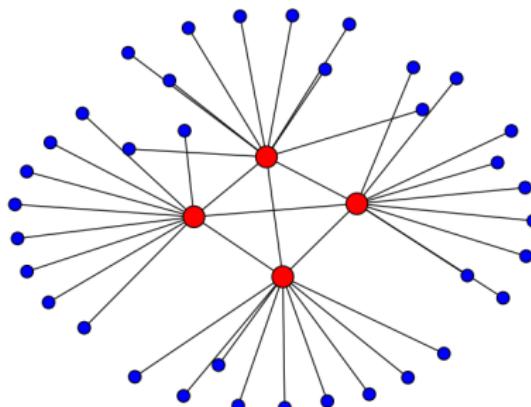
(b) After new edges form.

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

Assortativity

- *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.

e.g., the “rich club”:



- Removing nodes or edges sequentially, to obtain a *dendrogram*³

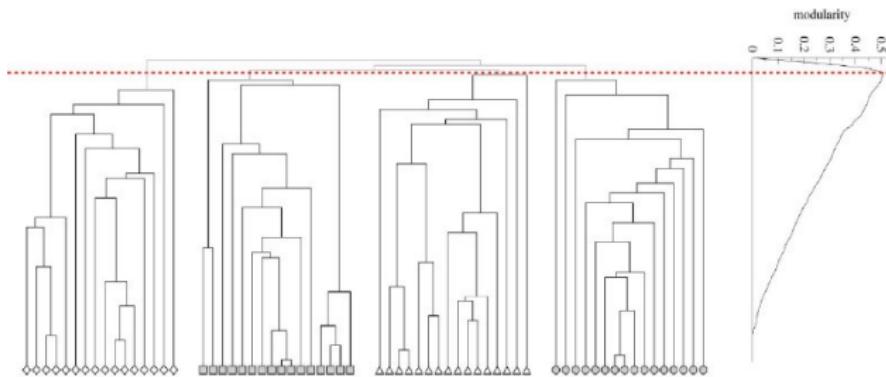
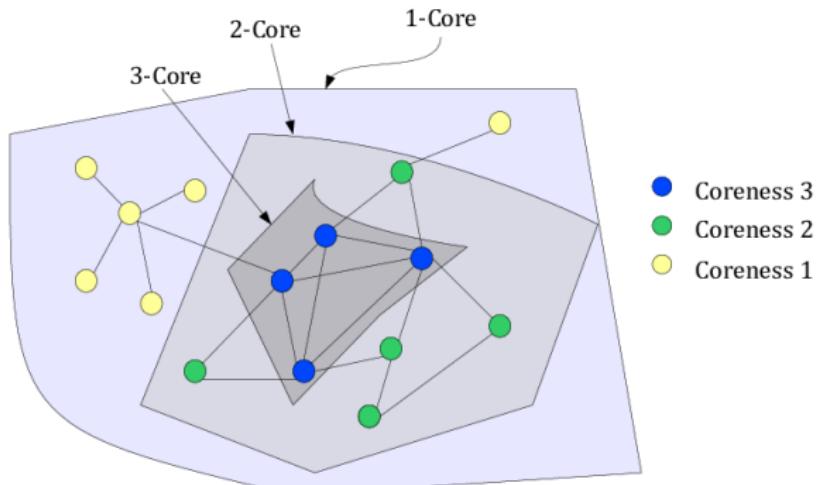


Fig.: A network dendrogram (aka hierarchical tree)

³<http://perso.crans.org/aynaud/communities/api.html>



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

- *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 $c_i \neq c_j$)

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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 editions from G_1 to G_2
- $c(e_i)$ the cost of edit operation e_i

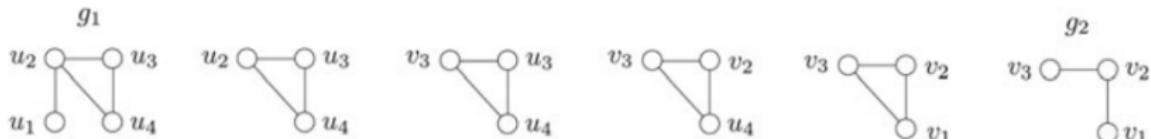
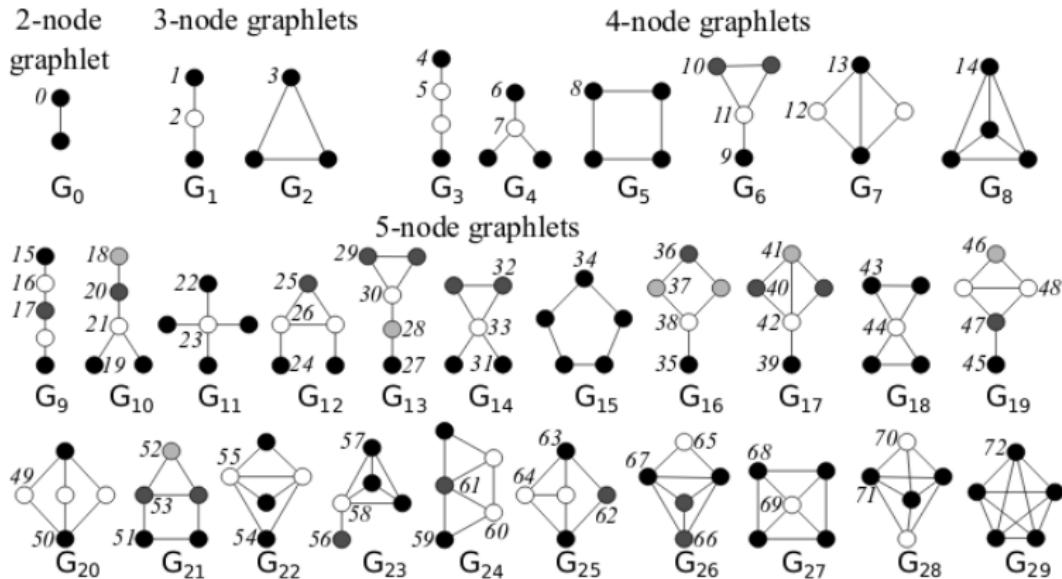


Figure: An edit path λ between to graphs G_1 and G_2

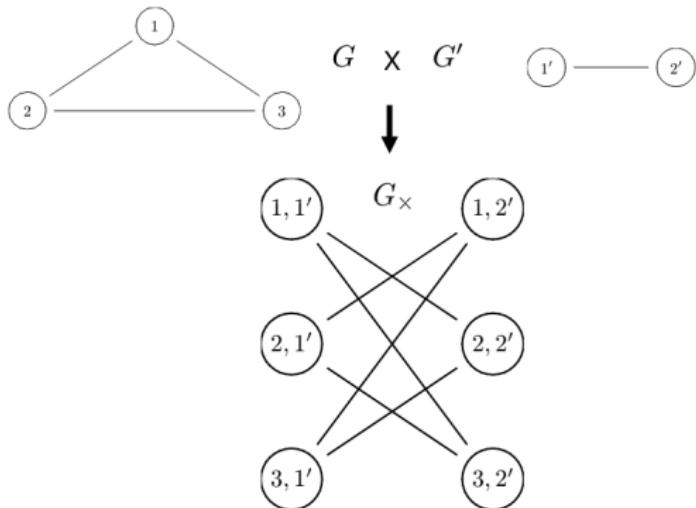
Graphlet frequencies

- Comparing graphs based on the frequency of graphlets they have in their structure
- Graphlets: small connected induced subgraphs of a graph



Graph kernels, e.g. the random walk kernel

- Similarity as the amount of unique walks on G_x the direct product of G and G'
- The larger, the more similar the two graphs [10]

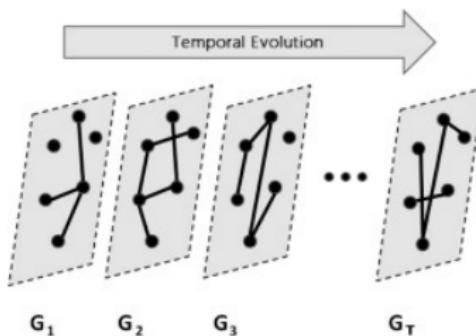


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The time dimension

- 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

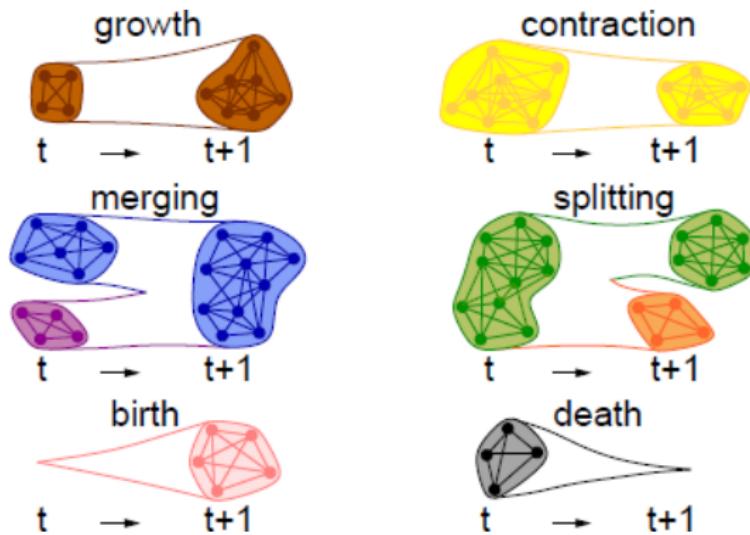


Figure: The fate of communities, observation possible through the time dimension

- 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

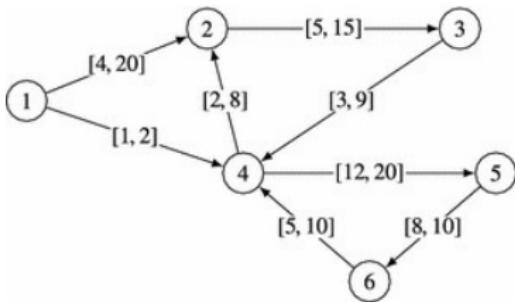


Figure: A directed TVG, with fix nodes, but dynamic edges

- 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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9 Playing with graphs and Gephi

The Open Graph Viz Platform

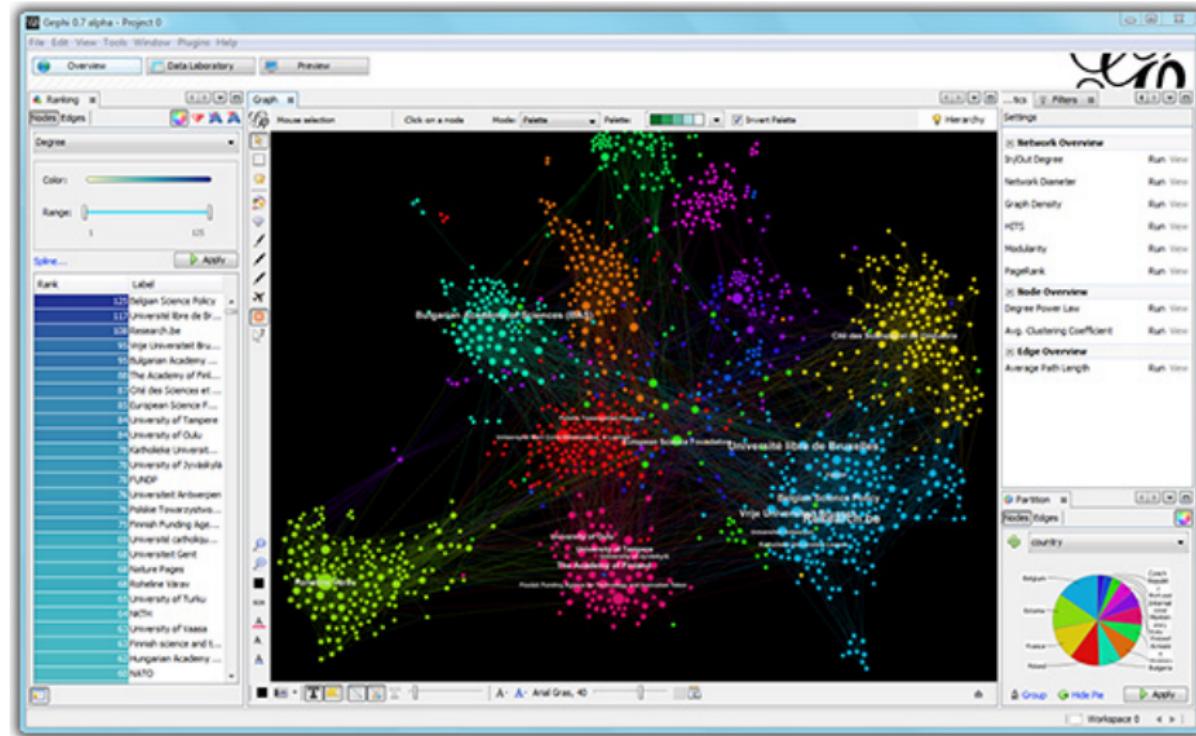
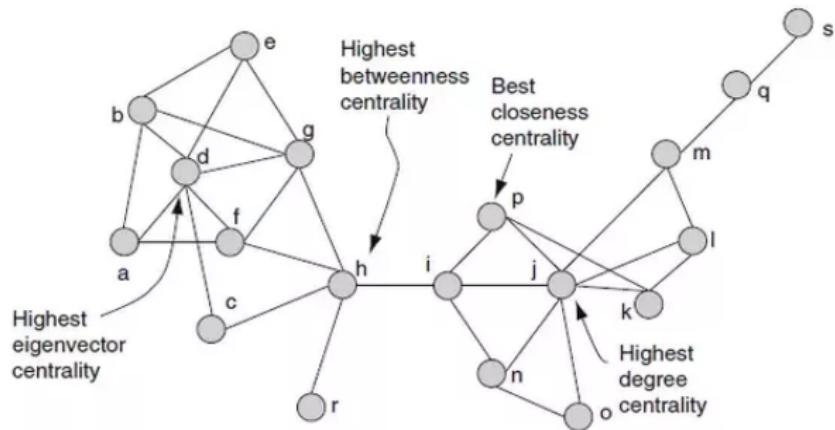


Figure: Gephi, <https://gephi.org/>

Eigenvector Centrality



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

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