Network science / Graph mining

Metrics for analyzing a connected world

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Outline

Outline

Graphs ?

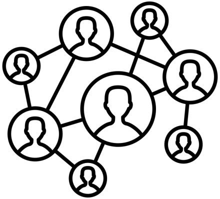


Figure: A graph: entities (nodes/vertices) and connections (edges)

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

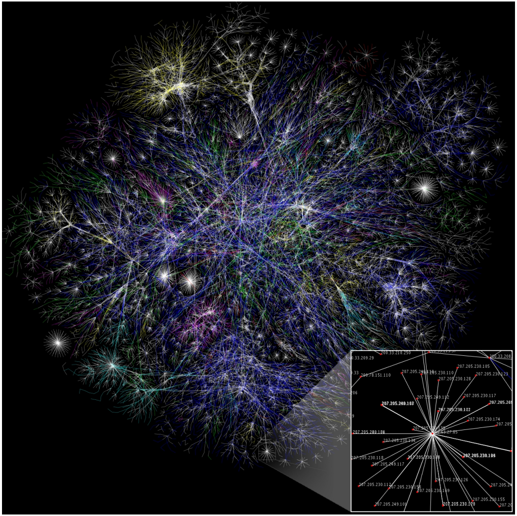


Figure: The Internet AS graph

The omnipresence of graphs in applications

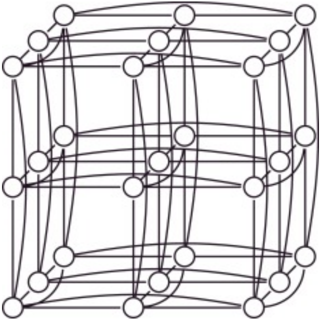


Figure: Interconnecting system-on-chips in a datacenter rack

The omnipresence of graphs in applications

- exemple use in social nets, epidemics...

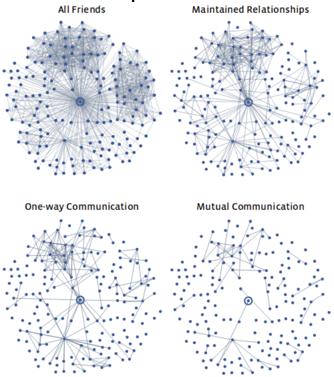


Figure 3.8: Four different views of a Facebook user's network neighborhood, showing the structure of links corresponding respectively to all declared friendships, maintained relationships, one-way communication, and reciprocal (i.e. mutual) communication. (Image from [286].)

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

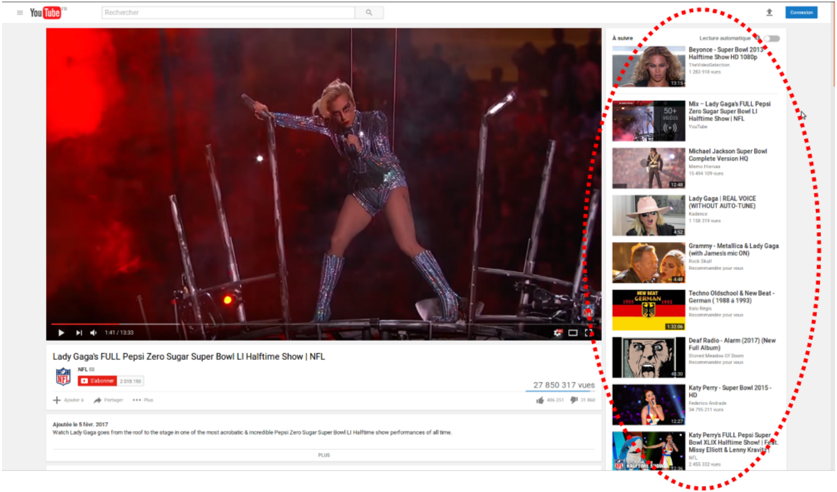
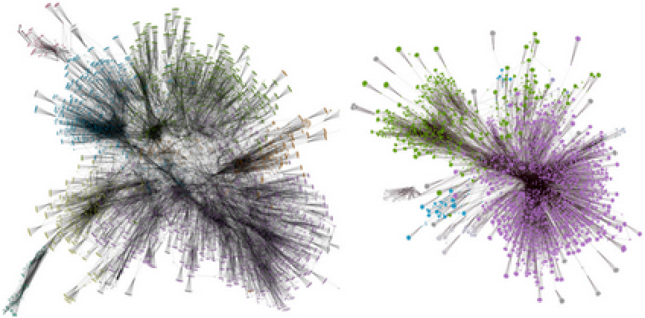


Figure: Recommandations: contextual, personalized?

e.g.: recommendations on YouTube

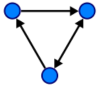


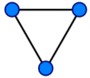
4-hops graphs from a YouTube video, new user (left) and returning user (ri

Figure: Blank profile vs. my recommandations

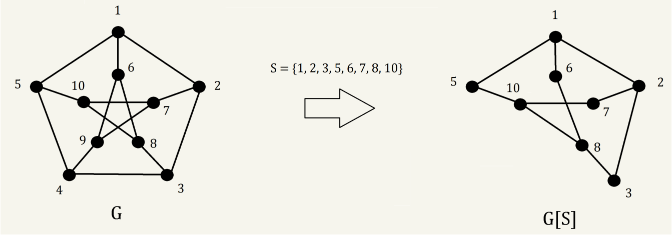
Core notions (1)

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

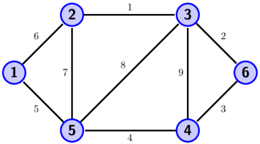




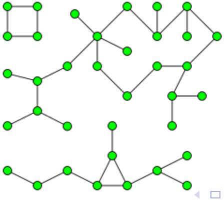
- A *subgraph* of G: formed by a subset of nodes/vertices and edges from G.



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

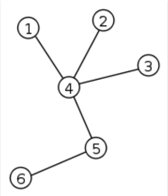


- Graph *connectivity:*
  - A graph is *connected* if there is a *path* btw any pair of vertices.
  - Otherwise, *connected components* are the subgraphs in which paths exist.

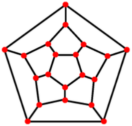


Core notions (3)

- 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 draw without any edges crossing each other.



Special *topologies*

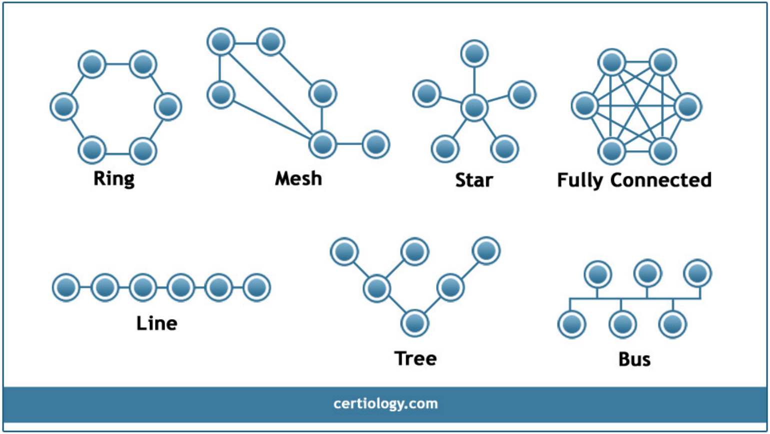
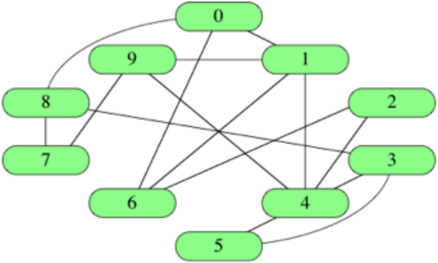


Figure: Graphs to remember, often used as illustrations

Adjacency list or edge list representations



Graph $G(V,E)$, with V: nodes and E: edges.
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 weigths for weighted graphs.

Example tool families for manipulating graphs

GraphX

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

X – Stream

Figure: Big graph processing on a single machine

neo4j

Figure: For a database-like handling of graphs

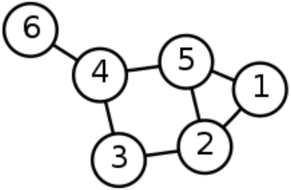
NetworkX

Figure: Prototyping in Python, lots of contributions

Stanford Large Network Dataset Collection

Outline

Basic notations



- $G(V,E)$: 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 $\Gamma(i)$.
  - $\Gamma(1) = \{2,5\}$

- 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:

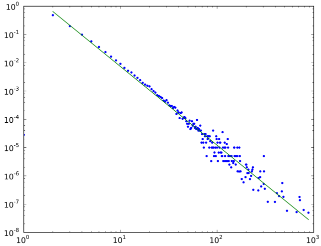


Figure: Degree distribution: x-axis is degree, y-axis is probability

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

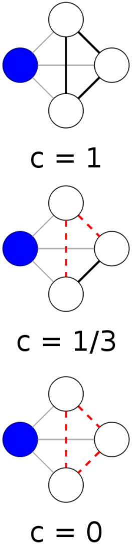
Clustering coefficient

- 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":*

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

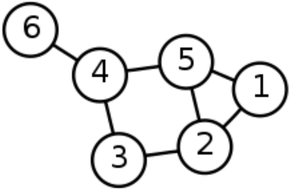
- Average clustering coefficient:

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

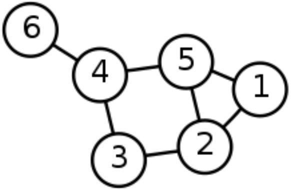


Path lengths

- *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 $\forall i \in V$.



Diameter



- *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.

Spectral analysis

The Laplacian matrix $L_G = D - A$:

- D *is the degree matrix a diagonal-matrix with* $D(i,i)$ *is the degree of the* i*th node in* G
- A *is the adjacency matrix, with* $A(i,j) = 1$ *if and only if* $(i,j) \in E$

$$L_G(i,j) = \begin{cases} deg(i) & \text{if } i = j \\ -1 & \text{if } (i,j) \in E \equiv 1 \\ 0 & \text{otherwise} \end{cases}$$

Labelled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2&0&0&0&0&0 \\ 0&3&0&0&0&0 \\ 0&0&2&0&0&0 \\ 0&0&0&3&0&0 \\ 0&0&0&0&3&0 \\ 0&0&0&0&0&1 \end{pmatrix}$	$\begin{pmatrix} 0&1&0&0&1&0 \\ 1&0&1&0&1&0 \\ 0&1&0&1&0&0 \\ 0&0&1&0&1&1 \\ 1&1&0&1&0&0 \\ 0&0&0&1&0&0 \end{pmatrix}$	$\begin{pmatrix} 2&-1&0&0&-1&0 \\ -1&3&-1&0&-1&0 \\ 0&-1&2&-1&0&0 \\ 0&0&-1&3&-1&-1 \\ -1&-1&0&-1&3&0 \\ 0&0&0&-1&0&1 \end{pmatrix}$

*For an (undirected) graph G and its **Laplacian matrix** $L = D - A$ with eigenvalues $\lambda_0 \leq \lambda_1 \leq ... \leq \lambda_{n-1}$:*

- $\lambda_0 = 0$, *as* $v_0 = (1, 1, ..., 1)$ *satisfies* $Lv_0 = 0$ *(row sum and column sum of* L *are* 0*)*
- *$\#$ of connected components in G is the algebraic multiplicity of the 0 eigenvalue (*$\implies \lambda_2 = 0$ *iff G is disconnected)*
- *the smallest non-zero eigenvalue of L is called the **spectral gap***
- *the second smallest eigenvalue of L (could be zero) is the **algebraic connectivity** of G*
- ...

Spectral analysis (3)

An example of a result: the diameter of a non complete graph G satisfies:

$$diam(G) \leq \lceil \frac{\log(vol(G)/\delta)}{\log \frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}} \rceil,$$

with δ the minimum degree of G and $vol(G)$ is the sum of the degrees of the vertices in G.

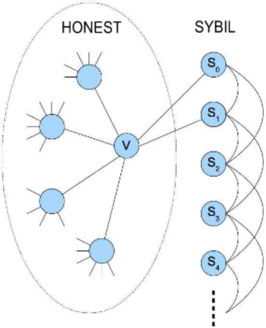
...and multiple results from graph theory, in general or for specific graphs

Conductance

- 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.

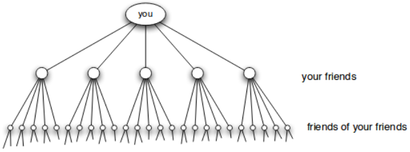


Expansion

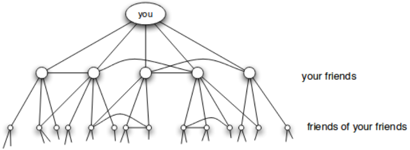
- *Expansion* of G: mean number of nodes that are reached in h hops from all nodes:

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

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



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



(b) *Triadic closure reduces the growth rate*

Resilience

- 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).

Outline

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.

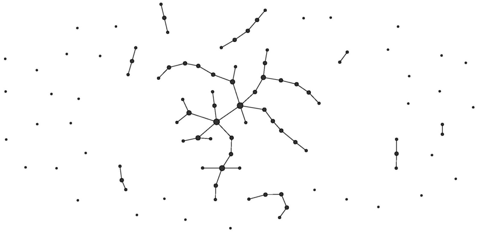
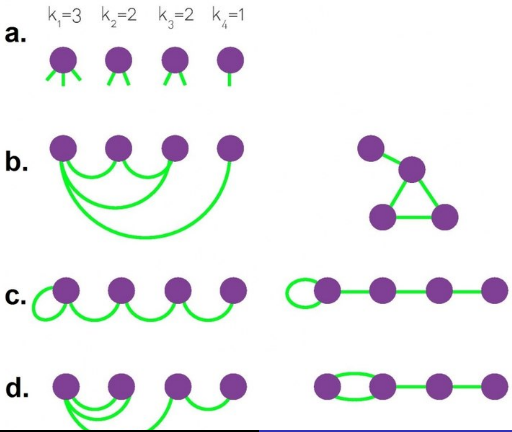


Figure: A random graph with $p = 0.01$.

- 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.
- For a large n, resulting degree distribution is Poisson.

The configuration model

- Arbitrary degree distribution: to choose
  - Create *n* nodes with each a given target degree, fitting the distribution
  - Loop: take one node with remaining "free" neighbor, and selected another node randomly to add an edge



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.

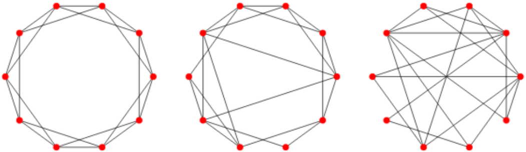


Figure 3.2: WS graphs with $n = 20$, $k = 4$, and $p = 0$ (left), $p = 0.2$ (middle), and $p = 1$ (right).

- 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: $p_i = \frac{d_i}{\Sigma_j d_j}$ (method called preferential attachment).

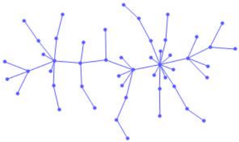


Figure: A Barabási-Albert graph with $n = 50$ and $m_0 = 1$.

- 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

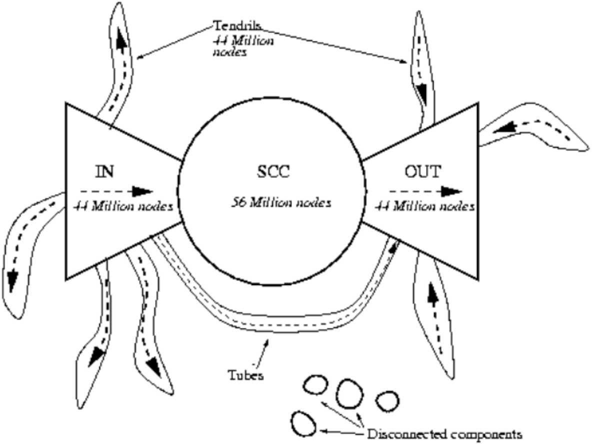
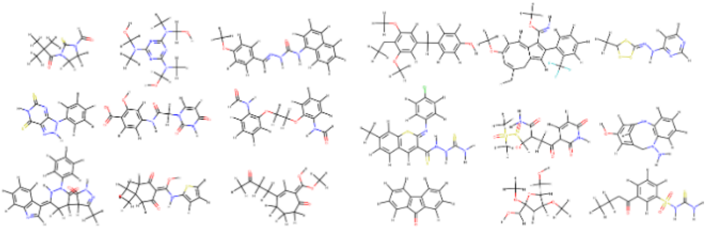


Figure: Bow-tie structure of the web

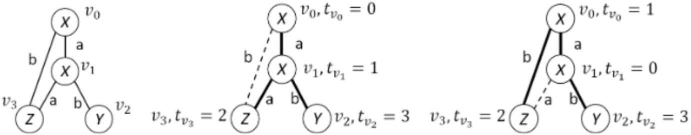
Generating graphs with neural nets: GraphGen (1)

- How to generate graphs from an unknown generative process?



(a) Real graphs (b) GraphGen

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



(a) Graph (b) DFS traversal on the graph (c) DFS traversal on the graph

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): $(0, 1, X, a, X), (1, 2, X, a, Z), (2, 0, Z, b, X), (1, 3, X, b, Y)$.

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

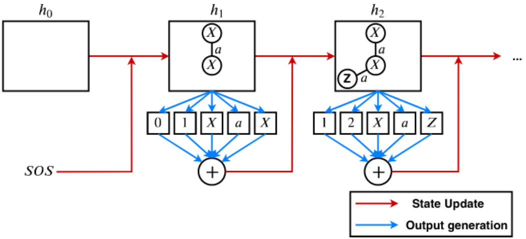
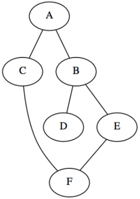


Figure 3: Architecture of GraphGen. Red arrows indicate data flow in the RNN whose hidden state h_i captures the state of the graph generated so far. Blue arrows show the information flow to generate the new edge tuple s_i.

Outline

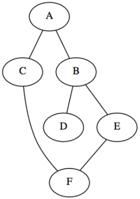
Depth first search



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

```python
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

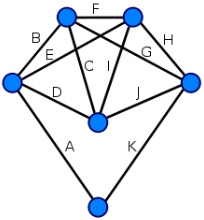


- *breadth* first:

```
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

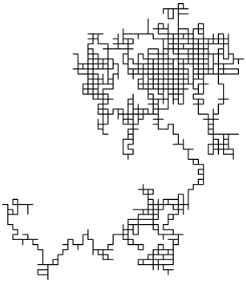
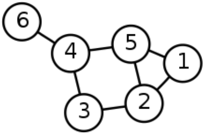


Figure: Random walk on a grid (i.e., 4 neighbors per node)



RDW(6,7hops)=(6,4,3,4,5,4,3,2)

Random walks - app1: sampling (biased)

- 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: $P_j = \frac{d_j}{\Sigma_{i=0}^{n} d_i}$

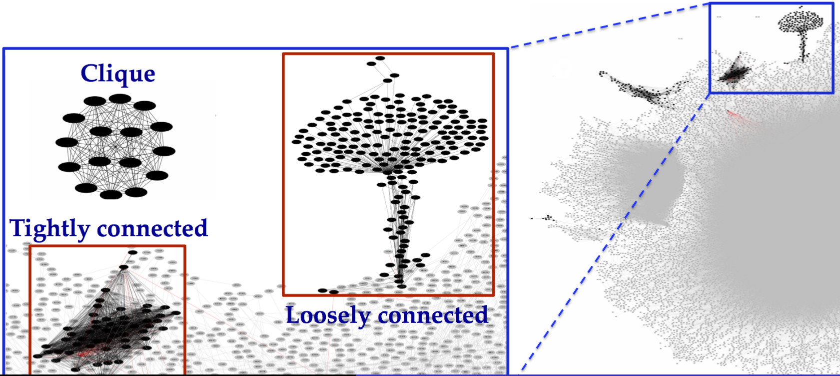
Random walks - app1: sampling (uniform)

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

- 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.

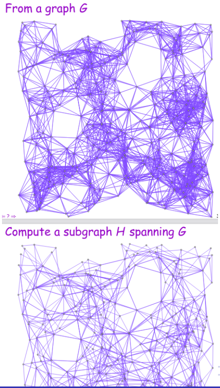


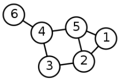
Spanner

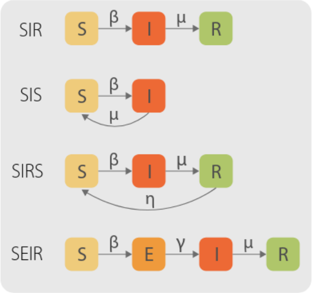
- A spanner H of a graph G: subgraph of G with *few* edges and *short* distances.[2] Tradeoff between number of edges and distance stretch.
- (α,β)-spanner of $G \iff \forall(u,v)$: $dist_H((u,v)) \leq \alpha \times dist_G((u,v)) + \beta$, with α: multiplicative stretch, β: additive stretch.

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

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

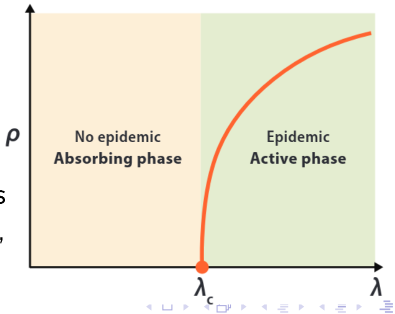






Epidemic on graph nodes: models with states Susceptible, Infected, Recovered, Exposed.[9]

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



Epidemics on graphs (2)

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

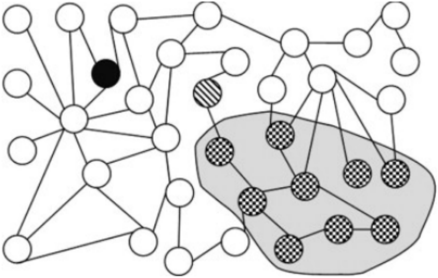


Fig. 1. Example of a social network. Black node denotes the globally central node; chequered nodes denote the potential market; hatched node denotes the node central w.r.t. the potential market.

Figure: cf "A targeted approach to viral marketing"

Outline

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.

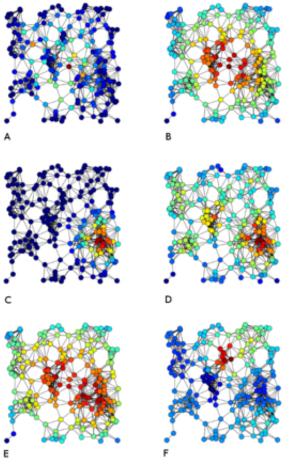
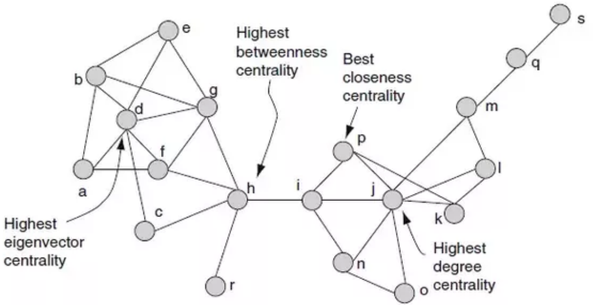


Figure: Various importance results

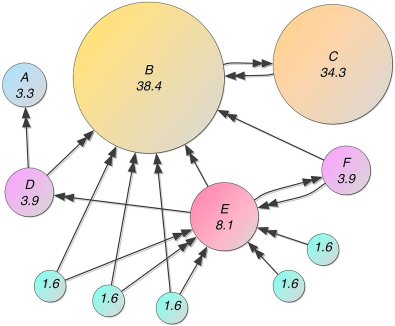
Degree centrality



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

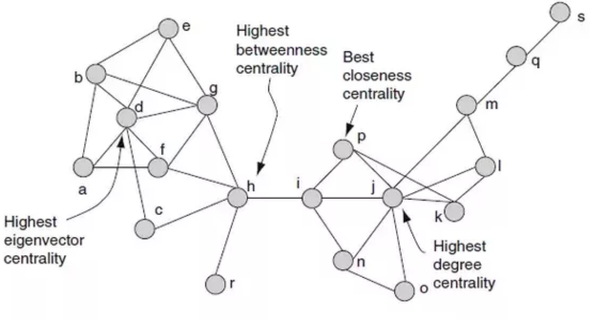
$$C_d(i) = \frac{d(i)}{n-1}$$

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.

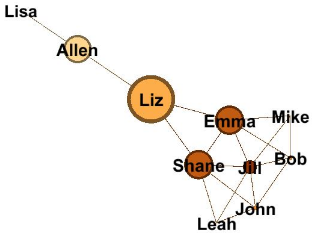
$$PR(i) = \sum_{j \in \Gamma(i)} \frac{PR(j)}{|\Gamma_{out}(j)|}$$



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

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

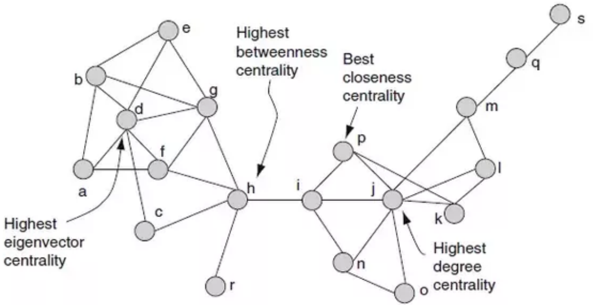
Eccentricity



An important node is not *eccentered*

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

Betweeness centrality

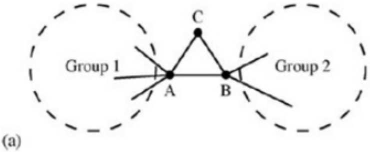


An important node is a node that lies on many *shortest paths*

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

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

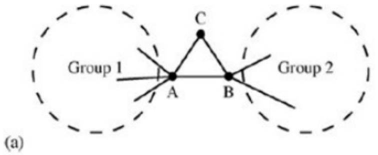
Random walk betweeness centrality



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.

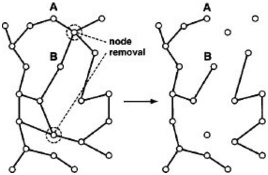
An important node see *regularly* random data flows

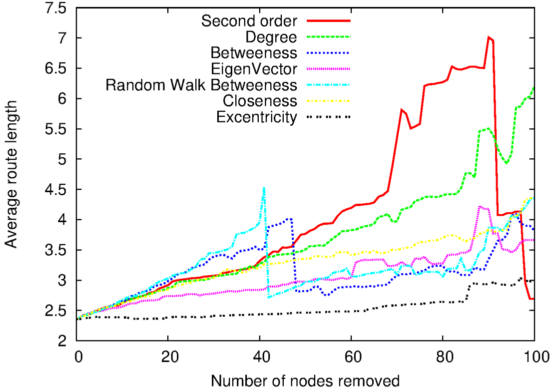
- Let an unbiased random walk running on the graph
- Each node records *return time* of the walk in Ξ_i
- After N visits on a node i, its standart deviation is:

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

Important nodes have a low standart deviation of those return times

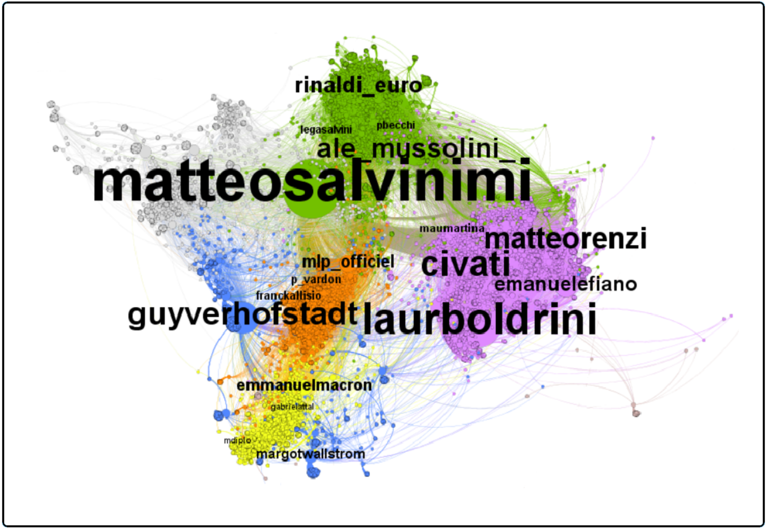
Removal impact on path lengths





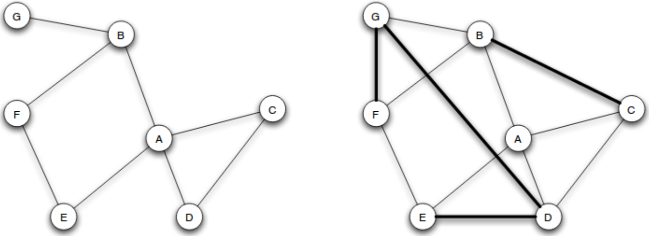
Outline

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".*



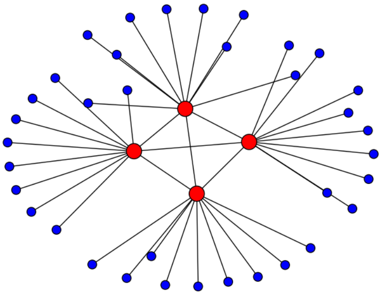
(a) *Before new edges form.* (b) *After new edges form.*

- $\{G, B, F\}$ 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":



Node removal

- Removing nodes or edges sequentially, to obtain a *dendogram*[3]

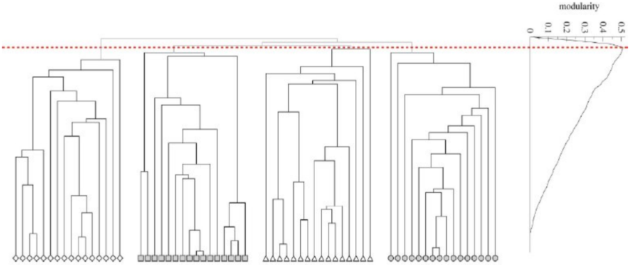
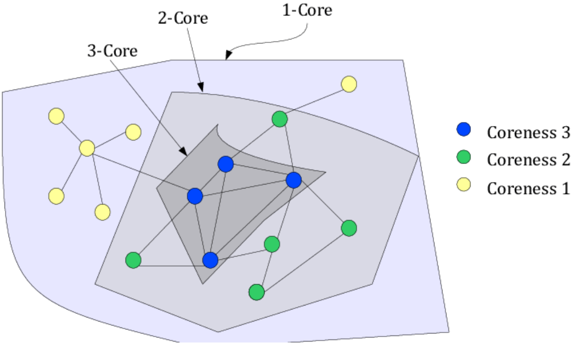


Fig.: A network dendrogram (aka hierarchical tree)

[3] *http://perso.crans.org/aynaud/communities/api.html*

k-core



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

- *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 $c_i \neq c_j$)

Iterate: 1) assign community to each node that maximizes modularity, 2) build the resulting graph

Outline

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

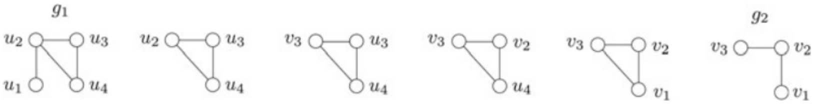
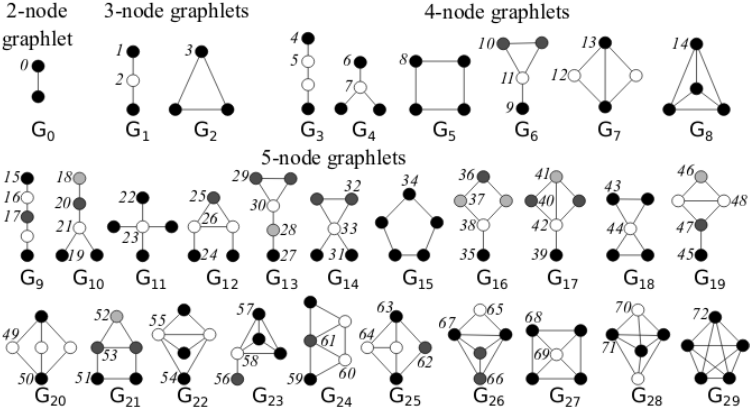


Figure: An edit path λ between to graphs G_1 and G_2

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

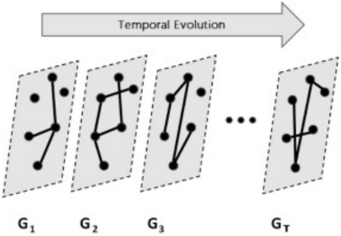


Outline

1. Graphs and representations
2. Classical metrics
3. Modeling and generating graphs
4. Exploring graphs
5. Importance metrics
6. Community metrics
7. Comparing graphs
8. TVGs: time varying graphs

The time dimension

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



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

The time dimension for community analysis

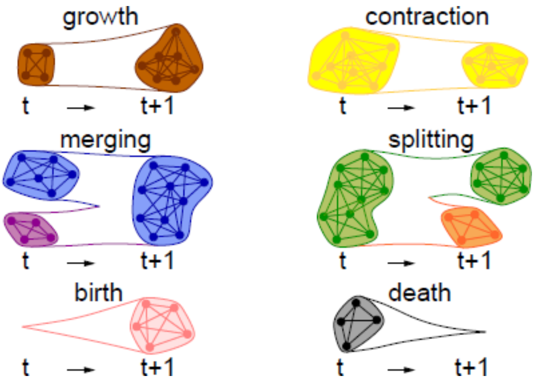


Figure: The fate of communities, observation possible through the time dimension

A model for time-varying graphs

- 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

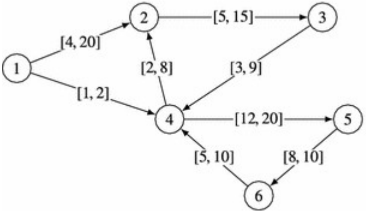


Figure: A directed TVG, with fix nodes, but dynamic edges

- A *journey*: temporal extension of the notion of path.
- A sequence of tuples $\mathcal{J} = \{(e_1, t_1), (e_2, t_2) ..., (e_k, t_k)\}$, 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.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

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

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