An introduction to network inference and mining

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Formation Biostatistique, Niveau 3

Outline

1. A brief introduction to networks/graphs
2. Network inference
3. Simple graph mining
   - Visualization
   - Global characteristics
   - Numerical characteristics calculation
   - Clustering

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1 A brief introduction to networks/graphs

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What is a network/graph? *réseau/graphe*

Mathematical object used to model **relational data between entities**.

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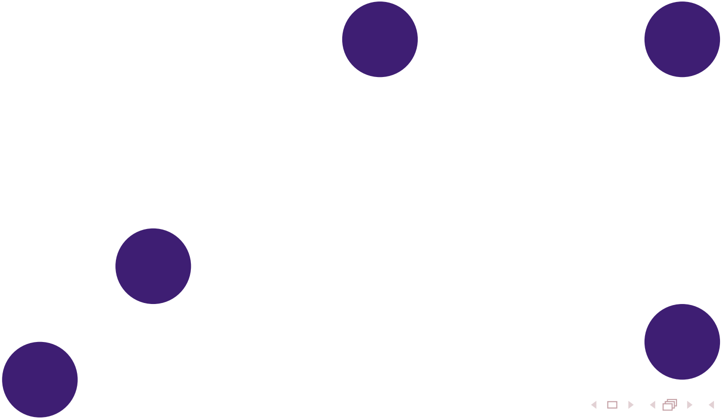
Mathematical object used to model **relational data between entities**.

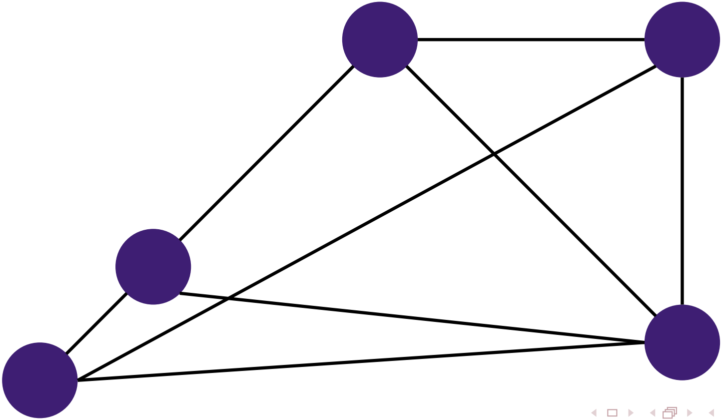
The entities are called the **nodes** or the **vertexes** (vertices in British) *nœuds/sommets*



What is a network/graph? *réseau/graphe*

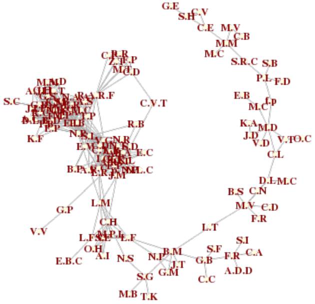
Mathematical object used to model **relational data between entities**.

A relation between two entities is modeled by an **edge** *arête*



(non biological) Examples

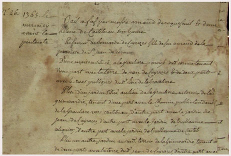
Social network: nodes: persons - edges: 2 persons are connected ("friends")



(Natty's facebook™[1] network)

(non biological) Examples

Modeling a large corpus of medieval documents



Notarial acts (mostly *baux à fief*, more precisely, land charters) established in a *seigneurie* named "Castelnau Montratier", written between 1250 and 1500, involving tenants and lords.[a]

[a] http://graphcomp.univ-tlse2.fr

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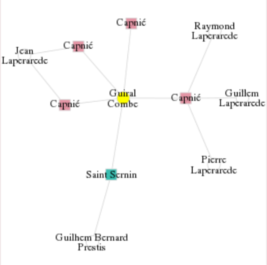
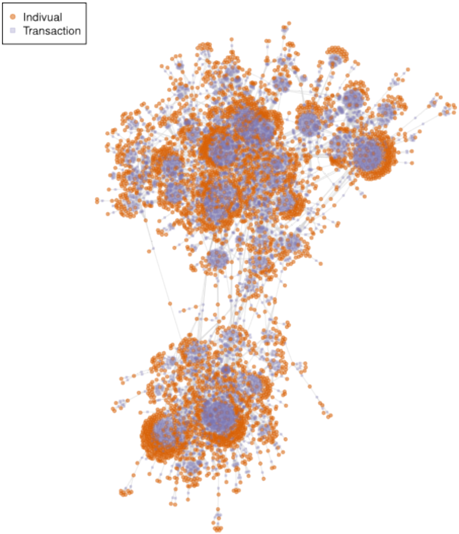


- nodes: transactions and individuals (3 918 nodes)
- edges: an individual is directly involved in a transaction (6 455 edges)

(non biological) Examples



Standard issues associated with networks

Inference

Giving data, how to build a graph whose edges represent the **direct** links between variables?

Example: co-expression networks built from microarray data (nodes = genes; edges = significant "direct links" between expressions of two genes)

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Graph mining (examples)

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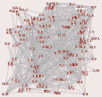

Random positions

Positions aiming at representing connected nodes closer

Standard issues associated with networks

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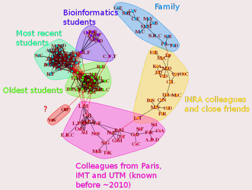
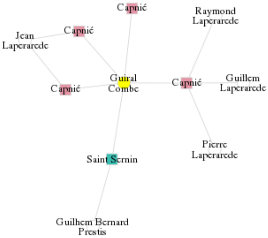
Graph mining (examples)

1. **Network visualization**: nodes **are not** a priori associated to a given position. How to represent the network in a meaningful way?
2. **Network clustering**: identify "communities" (groups of nodes that are densely connected and share a few links (comparatively) with the other groups)



More complex relational models

Nodes may be **labeled** by a factor



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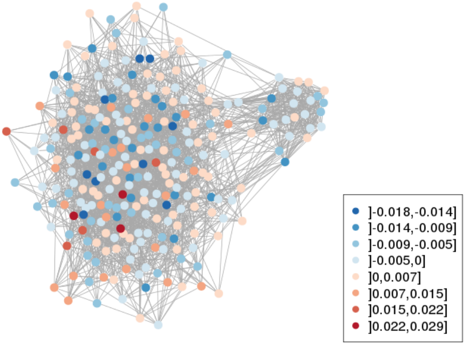

... or by a numerical information. [Laurent and Villa-Vialaneix, 2011]

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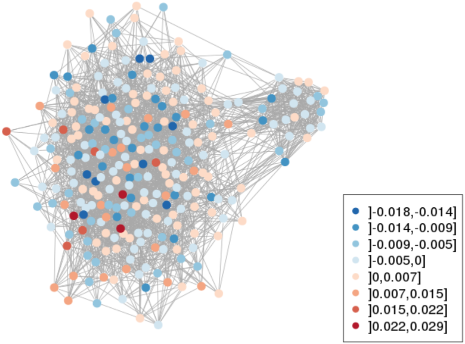

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Edges may also be labeled (type of the relation) or weighted (strength of the relation) or directed (direction of the relation).

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Framework

Data: large scale gene expression data

$$\begin{array}{c} \text{individuals} \\ n \simeq 30/50 \end{array} \left\{ \underbrace{X = \begin{pmatrix} . & . & . & . & . & . \\ . & . & X_i^j & . & . & . \\ . & . & . & . & . & . \end{pmatrix}}_{\text{variables (genes expression)},\ p \simeq 10^{3/4}} \right.$$

What we want to obtain: a network with

- nodes: genes;
- edges: significant and direct co-expression between two genes (track transcription regulations)

Advantages of inferring a network from large scale transcription data

1. **over raw data**: **focuses on the strongest direct relationships**: irrelevant or indirect relations are removed (more robust) and the data are easier to visualize and understand.
   Expression data are **analyzed all together** and not by pairs.

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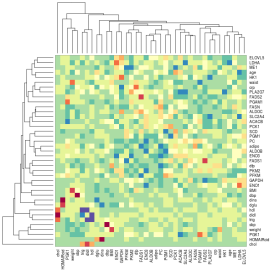
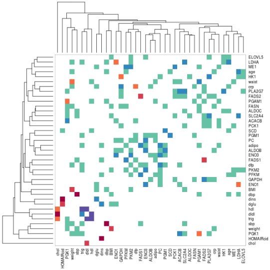
2. **over bibliographic network**: can handle **interactions with yet unknown** (not annotated) **genes** and deal with data collected in a particular condition.

Using *correlations*: relevance network [Butte and Kohane, 1999, Butte and Kohane, 2000]

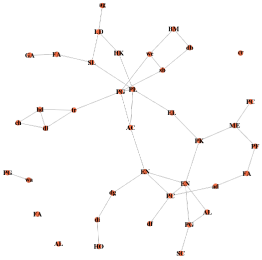
First (naive) approach: calculate correlations between expressions for all pairs of genes, threshold the smallest ones and build the network.



"Correlations"

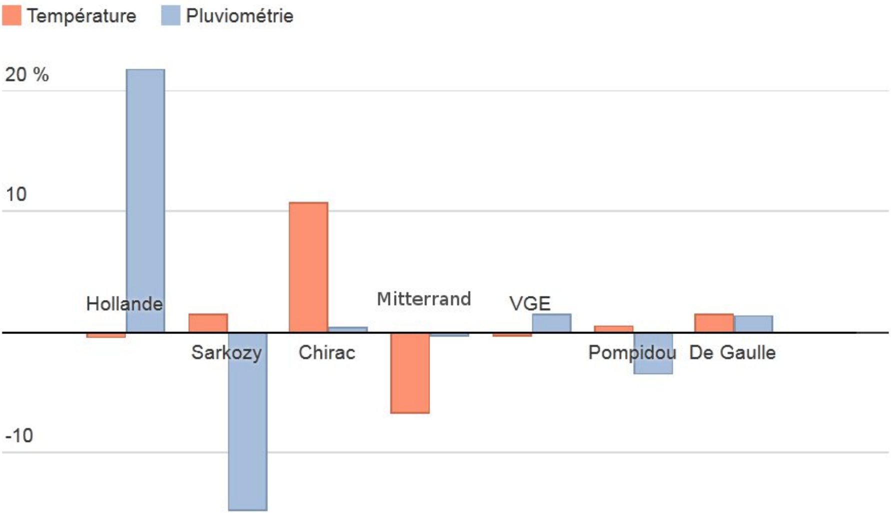


Thresholding



Graph

But correlation is not causality...



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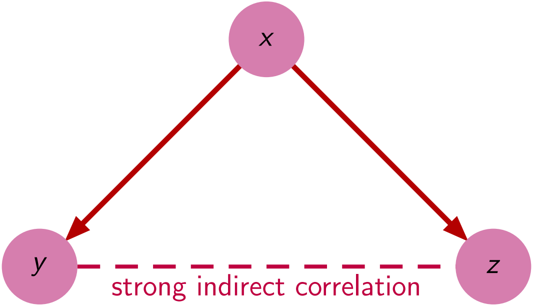


```
set.seed(2807); x <- runif(100)
y <- 2*x+1+rnorm(100,0,0.1); cor(x,y); [1] 0.9988261
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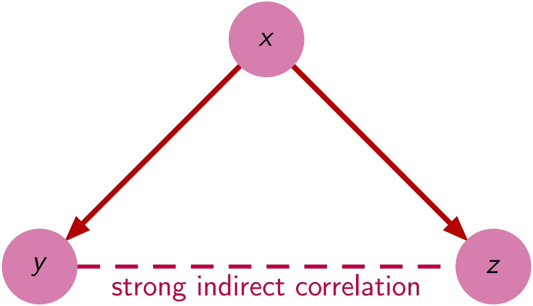


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♯ Partial correlation
cor(lm(y∼x)$residuals,lm(z∼x)$residuals) [1] -0.1933699
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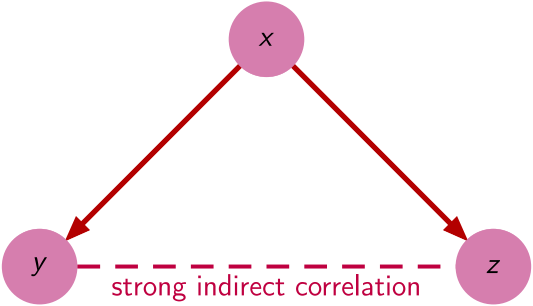

Networks are built using **partial correlations**, i.e., correlations between gene expressions **knowing the expression of all the other genes** (residual correlations).

Various approaches (and R packages) to infer gene expression networks

- **Graphical Gaussian Model** $(X_i)_{i=1,\ldots,n}$ are i.i.d. Gaussian random variables $\mathcal{N}(0,\Sigma)$ (gene expression); then

$$j \longleftrightarrow j' \text{(genes } j \text{ and } j' \text{ are linked)} \Leftrightarrow \mathbb{C}\mathrm{or}\left(X^j, X^{j'} | (X^k)_{k\neq j,j'}\right) > 0$$

$\mathbb{C}\mathbf{or}\left(X^j, X^{j'} | (X^k)_{k\neq j,j'}\right) \simeq \left(\Sigma^{-1}\right)_{j,j'} \Rightarrow$ find the partial correlations by means of $(\widehat{\Sigma}^n)^{-1}$.

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Problem: Σ is a p-dimensional matrix (with p large) and n is small compared to $p \Rightarrow (\widehat{\Sigma}^n)^{-1}$ is a poor estimate of Σ^{-1}!

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  - sparse approaches **[Friedman et al., 2008]**: packages glasso, huge, GGMselect **[Giraud et al., 2009]**, SIMoNe **[Chiquet et al., 2009]**, JGL **[Danaher et al., 2014]** or therese **[Villa-Vialaneix et al., 2014]**... (with unsupervised clustering or able to handle multiple populations data)

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- **Other methods**: Bayesian network learning **[Pearl, 1998, Pearl and Russel, 2002, Scutari, 2010]** bnlearn, mutual information **[Meyer et al., 2008]** minet...

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Settings

Notations

In the following, a **graph** $\mathcal{G} = (V, E, W)$ with:

- V: set of vertexes $\{x_1, \ldots, x_p\}$;
- E: set of edges;
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The **connected components**/*composantes connexes* of a graph are all its connected subgraphs.

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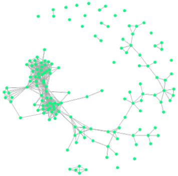
Example 1: Natty's FB network has 21 connected components with 122 vertexes (professional contacts, family and closest friends) or from 1 to 5 vertexes (isolated nodes)



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Example 2: Medieval network: 10 542 nodes and the largest connected component contains 10 025 nodes ("giant component" / *composante géante*).

Visualization tools help understand the graph macro-structure

Purpose: How to display the nodes in a **meaningful** and **aesthetic** way?

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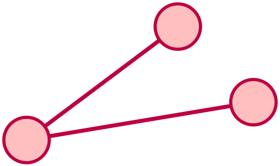
Standard approach: **force directed placement** algorithms (FDP)

algorithmes de forces (e.g., [Fruchterman and Reingold, 1991])



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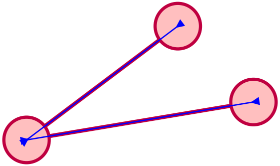

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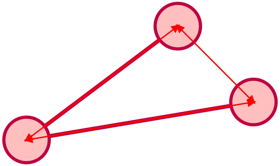

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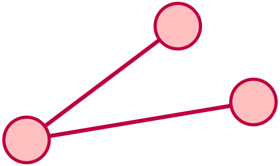

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iterative algorithm until stabilization of the vertex positions.

Visualization software

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- free software **Gephi**[2] (interactive software, supports zooming and panning)

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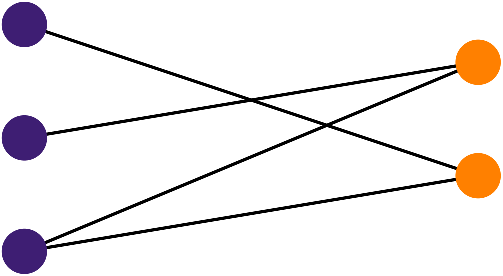
Peculiar graphs

Medieval network (largest connected component):

- 10 025 vertexes: transactions or persons;
- edges model the active involvement of a person in a transaction.

⇒ **Bipartite graph** / *graphe biparti*



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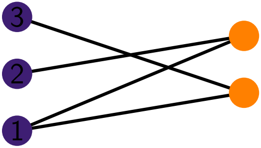
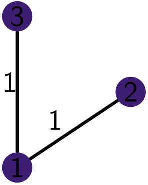
Projected graphs:

- individuals: nodes are the 3 755 individuals and edges weighted by the number of common transactions;
- transactions (not used): nodes are the 6 270 transactions and edges are weighted by the number of common actively involved persons.





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Density: Number of edges divided by the number of pairs of vertexes. *Is the network densely connected?*

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Examples

Example 1: Natty's FB network

- 152 vertexes, 551 edges $\Rightarrow$ density $= \frac{551}{152 \times 151/2} \simeq 4.8\%$;
- largest connected component: 122 vertexes, 535 edges $\Rightarrow$ density $\simeq 7.2\%$.

Example 2: Medieval network (largest connected component): 10 025 vertexes, 17 612 edges $\Rightarrow$ density $\simeq 0.035\%$.
Projected network (individuals): 3 755 vertexes, 8 315 edges $\Rightarrow$ density $\simeq 0.12\%$.

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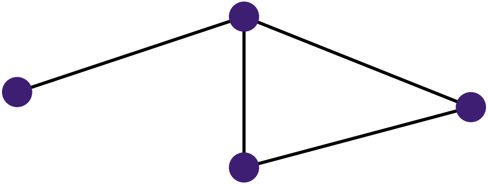
Density: Number of edges divided by the number of pairs of vertexes. *Is the network densely connected?*

Transitivity: Number of triangles divided by the number of triplets connected by at least two edges. *What is the probability that two friends of mine are also friends?*



Density is equal to $\frac{4}{4\times 3/2} = 2/3$; Transitivity is equal to $1/3$.

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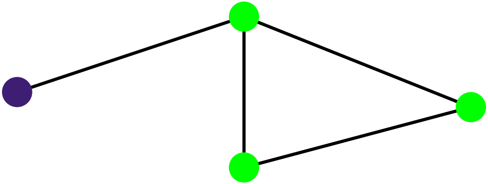

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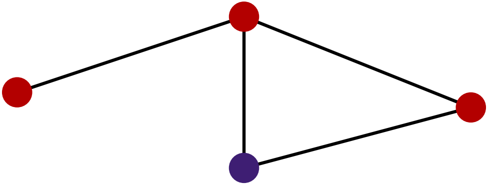

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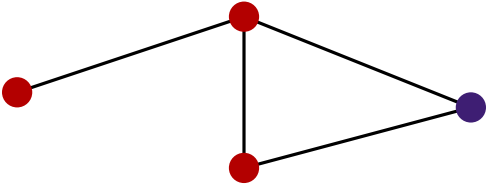

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Examples

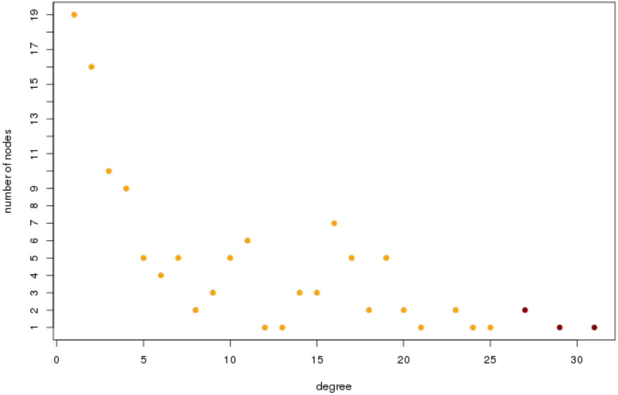
Example 1: Natty's FB network

- density $\simeq$ 4.8%, transitivity $\simeq$ 56.2%;
- largest connected component: density $\simeq$ 7.2%, transitivity $\simeq$ 56.0%.

Example 2: Medieval network (projected network, individuals): density $\simeq$ 0.12%, transitivity $\simeq$ 6.1%.

Extracting important nodes

1. **vertex degree** *degré*: number of edges adjacent to a given vertex or $d_i = \sum_j W_{ij}$. Vertexes with a high degree are called **hubs**: measure of the vertex popularity.



Number of nodes (y-axis) with a given degree (x-axis)

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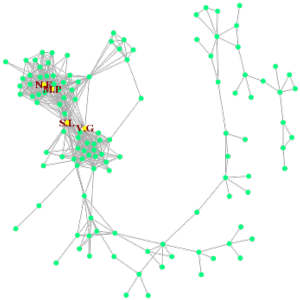

Two hubs are students who have been hold back at school and the other two are from my most recent class.

Extracting important nodes

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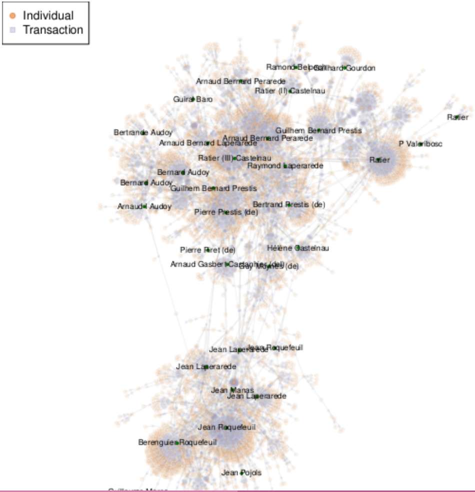

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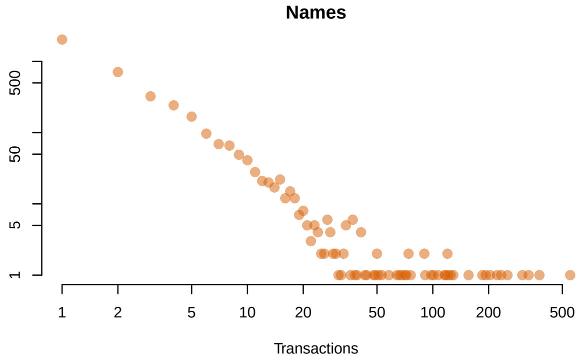

This distribution indicates **preferential attachement** *attachement préférentiel*.

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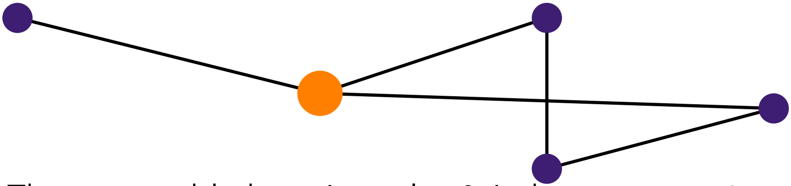

The orange node's degree is equal to 2, its betweenness to 4.

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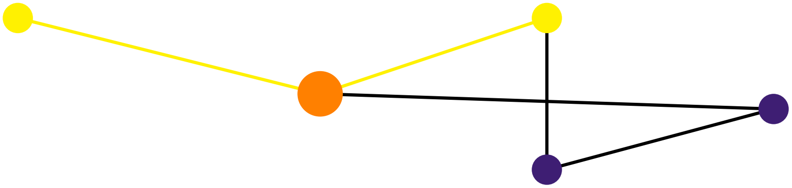

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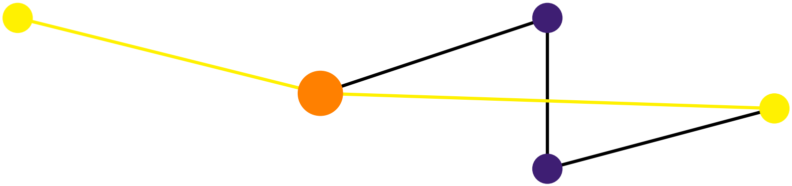

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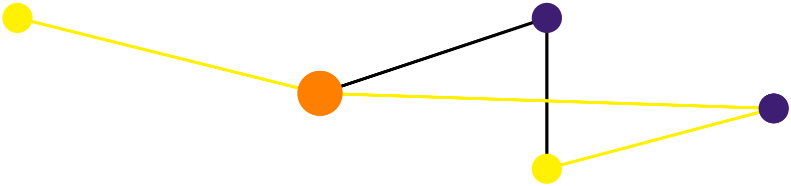

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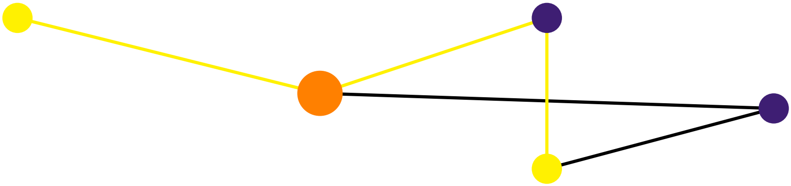

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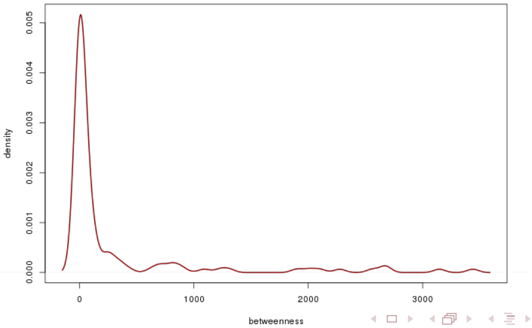

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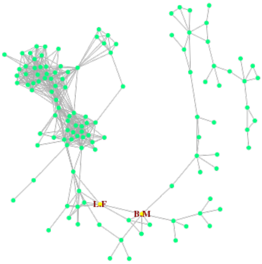

Vertexes with a high betweenness ($> 3\ 000$) are 2 political figures.

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   Example 2: In the medieval network: moral persons such as the "Chapter of Cahors" or the "Church of Flaugnac" have a high betweenness despite a low degree.

Vertex clustering *classification*

Cluster vertexes into groups that are **densely connected** and share **a few links** (comparatively) **with the other groups**. Clusters are often called **communities** *communautés* (social sciences) or **modules** *modules* (biology).

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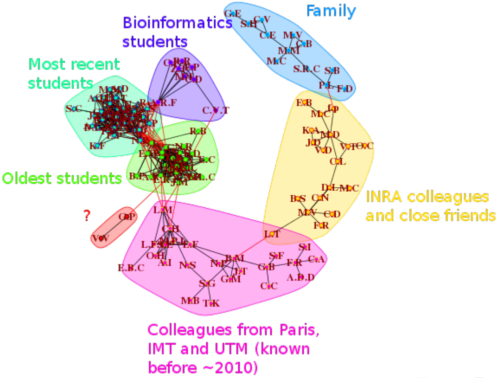
Example 1: Natty's facebook network



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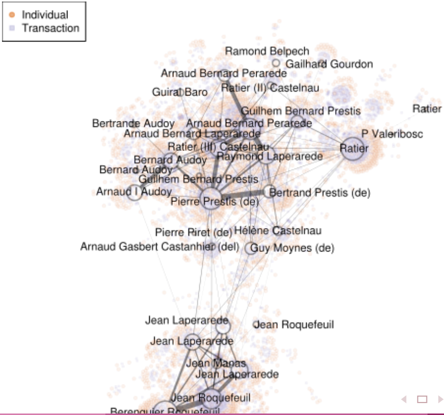

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Several clustering methods:

- min cut minimization minimizes the number of edges between clusters;
- spectral clustering [von Luxburg, 2007] and kernel clustering uses eigen-decomposition of the **Laplacian**/*Laplacien*

$$L_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j \\ d_i & \text{otherwise} \end{cases}$$

  (matrix strongly related to the graph structure);
- Generative (Bayesian) models [Zanghi et al., 2008];
- Markov clustering simulate a flow on the graph;
- **modularity maximization**
- ... (clustering jungle... see e.g., [Fortunato and Barthélémy, 2007, Schaeffer, 2007, Brohée and van Helden, 2006])

Find clusters by modularity optimization *modularité*

The **modularity** [Newman and Girvan, 2004] of the partition $(\mathcal{C}_1, \ldots, \mathcal{C}_K)$ is equal to:

$$\mathcal{Q}(\mathcal{C}_1, \ldots, \mathcal{C}_K) = \frac{1}{2m} \sum_{k=1}^{K} \sum_{x_i, x_j \in \mathcal{C}_k} (W_{ij} - P_{ij})$$

with P_{ij}: weight of a "null model" (graph with the same degree distribution but no preferential attachment):

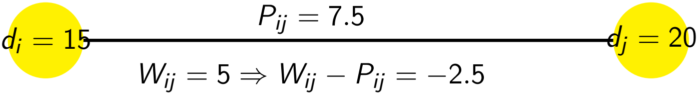
$$P_{ij} = \frac{d_i d_j}{2m}$$

with $d_i = \frac{1}{2} \sum_{j \neq i} W_{ij}$.

Interpretation

A good clustering should **maximize the modularity**:

- $\mathcal{Q} \nearrow$ when (x_i, x_j) are in the **same cluster** and $W_{ij} \gg P_{ij}$
- $\mathcal{Q} \searrow$ when (x_i, x_j) are in **two different clusters** and $W_{ij} \gg P_{ij}$ $(m = 20)$



i and j in the same cluster decreases the modularity

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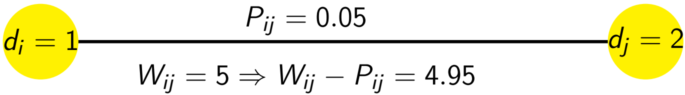

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- Modularity
    - **helps separate hubs** ($\neq$ spectral clustering or min cut criterion);
    - is not an increasing function of the number of clusters: useful to **choose the relevant number of clusters** (with a grid search: several values are tested, the clustering with the highest modularity is kept) but modularity has a **small resolution default** (see **[Fortunato and Barthélémy, 2007]**)

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Main issue: Optimization = **NP-complete problem** (exhaustive search is not not usable)

Different solutions are provided in [Newman and Girvan, 2004, Blondel et al., 2008, Noack and Rotta, 2009, Rossi and Villa-Vialaneix, 2011] (among others) and some of them are implemented in the R package igraph.

Open issues with clustering (not addressed)

- overlapping communities *communautés recouvrantes*;
- hierarchical clustering **[Rossi and Villa-Vialaneix, 2011]** provides an approach;
- "organized" clustering (projection on a small dimensional grid) and clustering for visualization **[Boulet et al., 2008, Rossi and Villa-Vialaneix, 2010, Rossi and Villa-Vialaneix, 2011]**;
- ...

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