Uncovering Latent Structure in Valued Graphs

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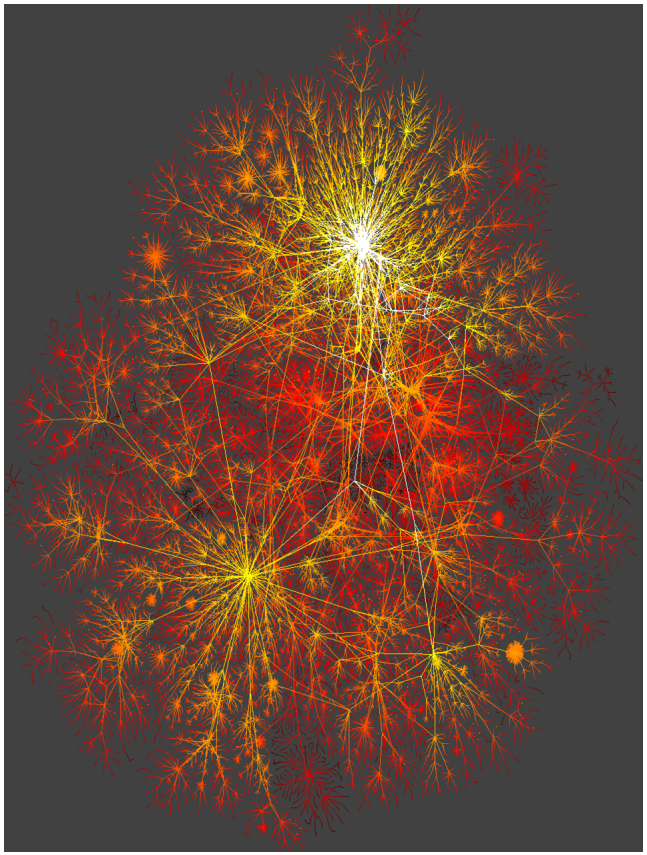
Motivations for the Study of Networks

Networks. . .

- Do exist:
  - → Electricity, transport,
  - → www networks,
- Represent or model interactions:
  - → Social relations,
  - → Metabolic pathways,
  - → Chemical reactions,
- Are hard to interpret as such:
  - → Many nodes/edges,
  - → Structure is hidden.



From Barabási website

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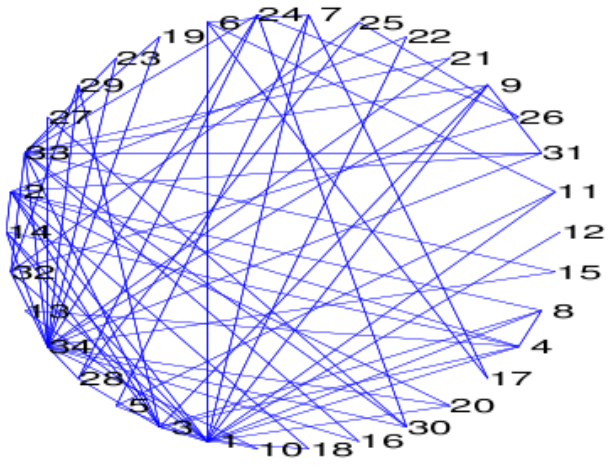
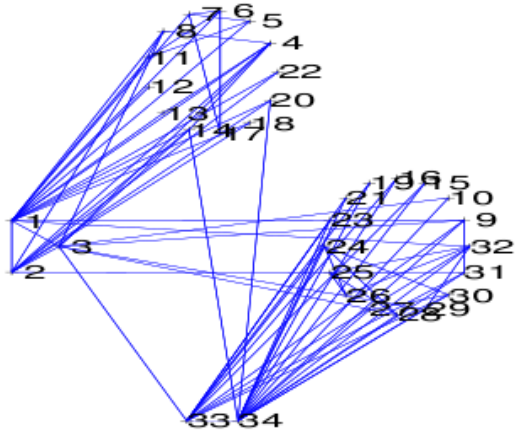
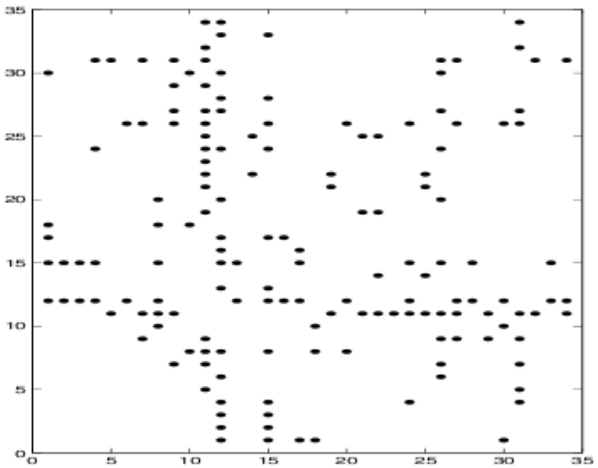
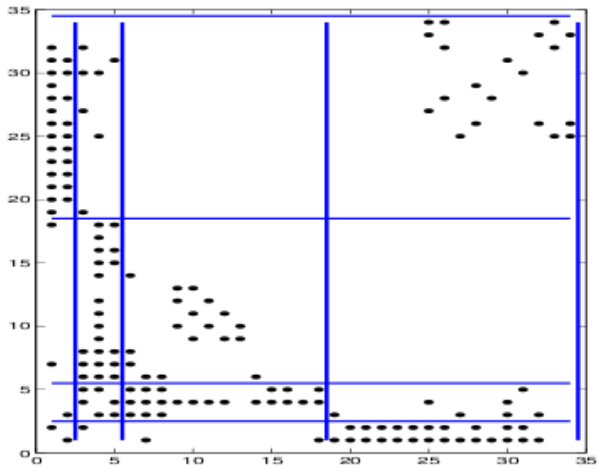
Goal: Simple Representation of the Graph









Some Notations

Nodes

- n nodes labeled in $\{1, \ldots, n\}$;
- Q classes with different connectivity;
- $Z = Z_{iq}$ discrete latent variable, $Z_{iq} = 1$ if node i belongs to class q;
- $(Z_{i1}, \ldots, Z_{iQ}) \sim \mathcal{M}(1, \alpha_1, \ldots, \alpha_Q)$.

Edges

- X_{ij} = value of the edge from node i to node j: $i \overset{X_{ij}}{\rightarrow} j$
- Conditionally to Z, the X_{ij}s are independent with:

$$X_{ij} | i \in q, j \in l \sim f_{\theta_{ql}}$$

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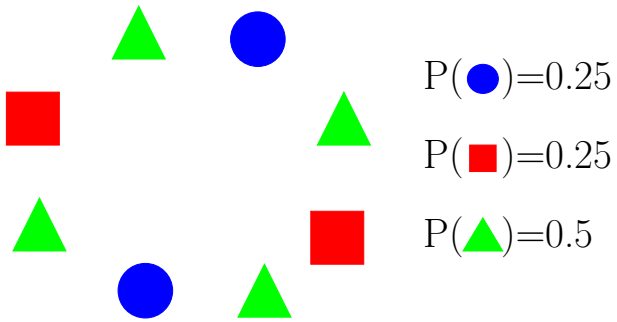
Example

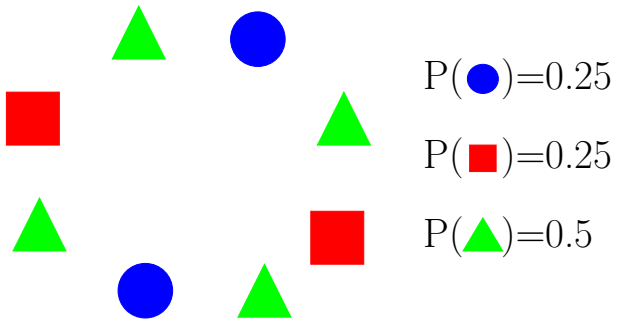
- **Nodes:**



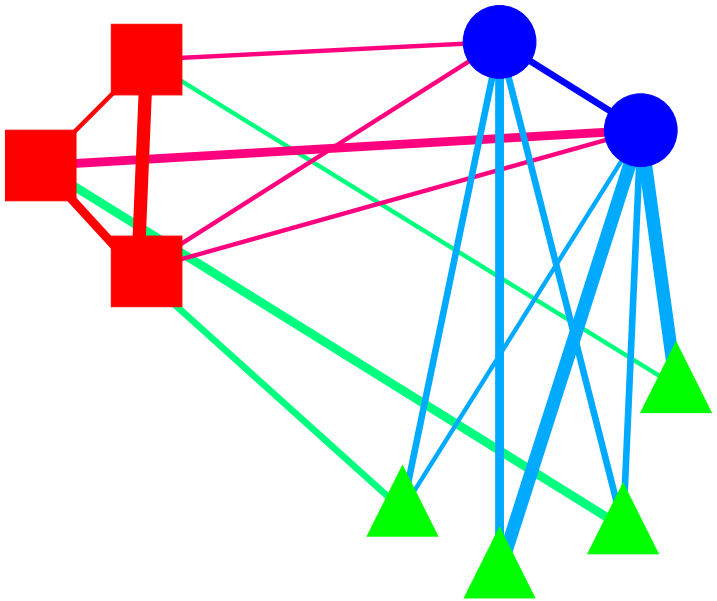
- **Edge (Poisson)**

Example

- **Nodes:**



- **Edge (Poisson)**



$$\begin{array}{c} \\ \blacktriangle \\ \bullet \\ \blacksquare \end{array} \begin{array}{c} \begin{array}{ccc} \blacktriangle & \bullet & \blacksquare \end{array} \\ \begin{pmatrix} 0 & 0.9 & 0.25 \\ . & 1 & 0.5 \\ . & . & 1 \end{pmatrix} \end{array}$$

Flexibility of MixNet

- **Classical Distributions:**

→ f_θ can be any probability distribution;

→ Bernoulli (interaction graph): presence/absence of an edge;

→ Multinomial (labelled graph): nature of the connection (friend, lover, colleague);

→ Poisson (count): in coauthorship networks, number of copublished papers;

→ Gaussian (intensity): intensity of the connection (airport network);

MixNet easily generates graphs.

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Pseudo-Likelihood

Maximum Likelihood Approach

- Observed data likelihood:

$$\mathcal{L}(\mathbf{X}) = \ln \sum_{\mathbf{Z}} \exp \mathcal{L}(\mathbf{X}, \mathbf{Z})$$

- The observed data likelihood requires a sum over Q^n terms, and is thus untractable;
- EM-like strategies require the knowledge of $\Pr(\mathbf{Z}|\mathbf{X})$, also untractable (no conditional independence) and also fail.

Variational Inference: Pseudo Likelihood

- Optimize in $\mathcal{R}_{\mathbf{X}}$ the function $\mathcal{J}(\mathcal{R}_{\mathbf{X}})$ given by :

$$\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}]) = \mathcal{L}(\mathbf{X}) - KL(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}], \Pr(\mathbf{Z}|\mathbf{X})) = \mathcal{H}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}]) - \sum_{\mathbf{Z}} \mathcal{R}_{\mathbf{X}}[\mathbf{Z}] \mathcal{L}(\mathbf{X}, \mathbf{Z})$$

- For simple $\mathcal{R}_{\mathbf{X}}$, $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ is tractable.

2 Steps Iterative Algorithm

- Step 1 **Optimize** $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ **w.r.t.** $\mathcal{R}_{\mathbf{X}}[\mathbf{Z}]$:
  - → Restriction to a "comfortable" class of functions;
  - → $\mathcal{R}_{\mathbf{X}}[\mathbf{Z}] = \prod_i h(\mathbf{Z}_i; \boldsymbol{\tau}_i)$, with $h(.; \boldsymbol{\tau}_i)$ the multinomial distribution;
  - → τ_{iq} is a variational parameter to be optimized using a fixed point algorithm:

$$\tilde{\tau}_{iq} \propto \alpha_q \prod_{j \neq i} \prod_{l=1}^{Q} f_{\theta_{ql}}(X_{ij})^{\tilde{\tau}_{jl}}$$

- Step 2 **Optimize** $\mathcal{J}(\mathcal{R}_{\mathbf{X}}[\mathbf{Z}])$ **w.r.t.** (α, θ):
  - → Constraint: $\sum_q \alpha_q = 1$

$$\begin{aligned} \tilde{\alpha}_q &= \sum_i \tilde{\tau}_{iq}/n \\ \tilde{\theta}_{ql} &= arg\max_{\theta} \sum_{ij} \tilde{\tau}_{iq}\tilde{\tau}_{jl} \log f_{\theta}(X_{ij}) \end{aligned}$$

  - → Simple expression of $\tilde{\theta}_{ql}$ for classical distributions.

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Model Selection Criterion

- BIC-like criterion to select the number of classes;
- The likelihood can be split: $\mathcal{L}(\mathbf{X}, \mathbf{Z}|Q) = \mathcal{L}(\mathbf{X}|\mathbf{Z}, Q) + \mathcal{L}(\mathbf{Z}|Q)$;
- These terms can be penalized separately:

$$\begin{aligned} \mathcal{L}(\mathbf{X}|\mathbf{Z}, Q) &\rightarrow \text{pen}_{\mathbf{X}|\mathbf{Z}} = P_Q \log n(n-1) \\ \mathcal{L}(\mathbf{Z}|Q) &\rightarrow \text{pen}_{\mathbf{Z}} = (Q-1)\log(n) \end{aligned}$$

$$ICL(Q) = \max_{\theta} \mathcal{L}(\mathbf{X}, \tilde{\mathbf{Z}}|\theta, m_Q) - \frac{1}{2}\left(P_Q \log n(n-1) - (Q-1)\log(n)\right)$$

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Number of Classes

→ Undirected graph with $Q^\star = 3$ classes and Poisson edges;

→ $n = 50,\ 100,\ 500,\ 1000$ vertices;

→ $\alpha_q = (57.1\%, 28, 6\%, 14, 3\%)$;

→ Connectivity matrix of the form $\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$

	Q		
n	2	3	4
50	82	**17**	1
100	7	**90**	3
500	0	**100**	0
1000	0	**100**	0

Table: Frequency of selected Q for various n.

Fungi Trees Interactions

- **Dataset** Interactions between 154 fungi and 51 trees European species. Fungus f is connected to tree t if it has been collected on it.
- **Projected Graphs** For each species, we define the projected graph:
  for trees $X_{tt'}$ = Number of common fungi,
  for fungi $X_{ff'}$ = Number of common trees,
- **Poisson Model** For both species, we assume that the intensities have Poisson distributions: $X \simeq \mathcal{P}(\lambda_{ql})$.
- **Number of classes**. The ICL criterion selects:
  - 7 classes for trees;
  - 9 classes for fungi.

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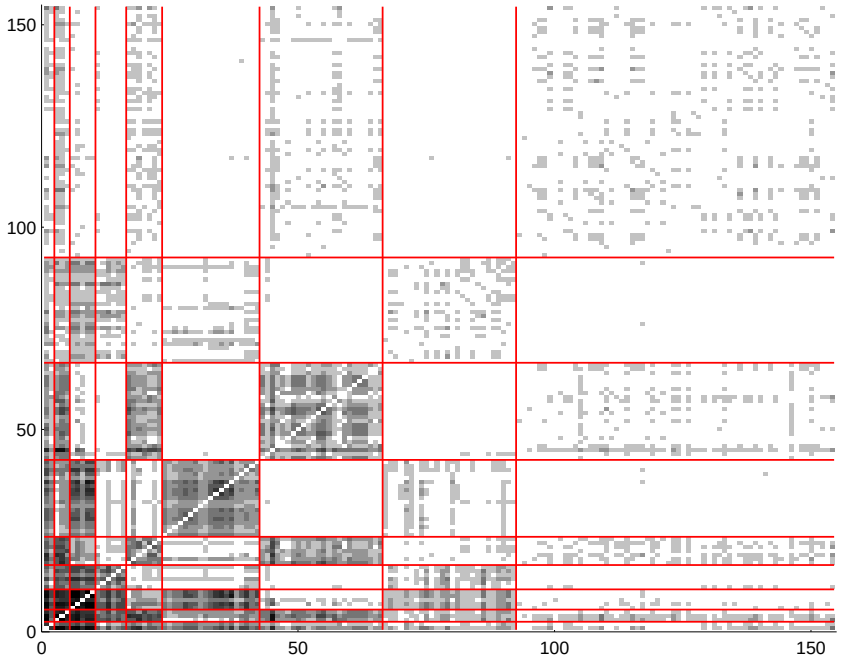
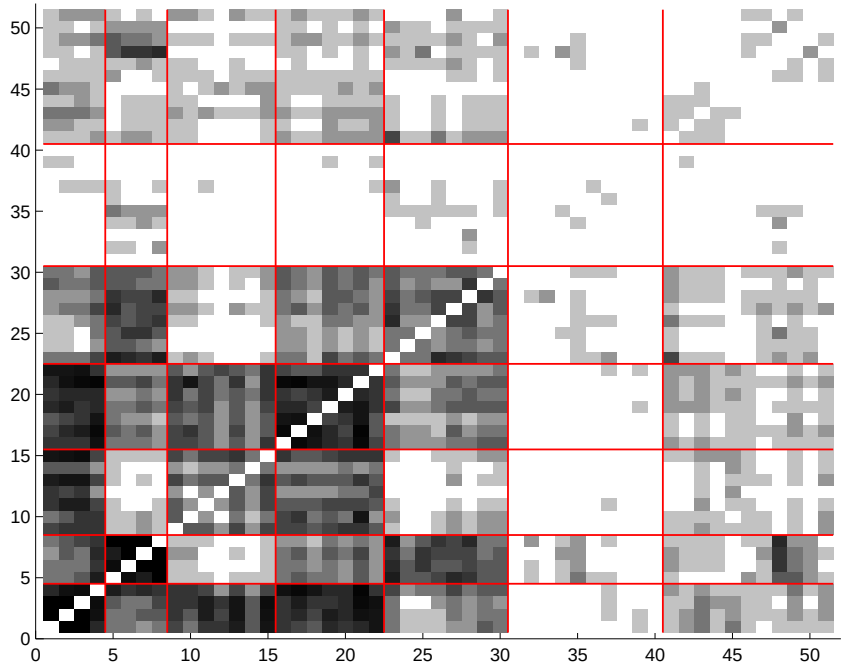
Results of Clustering

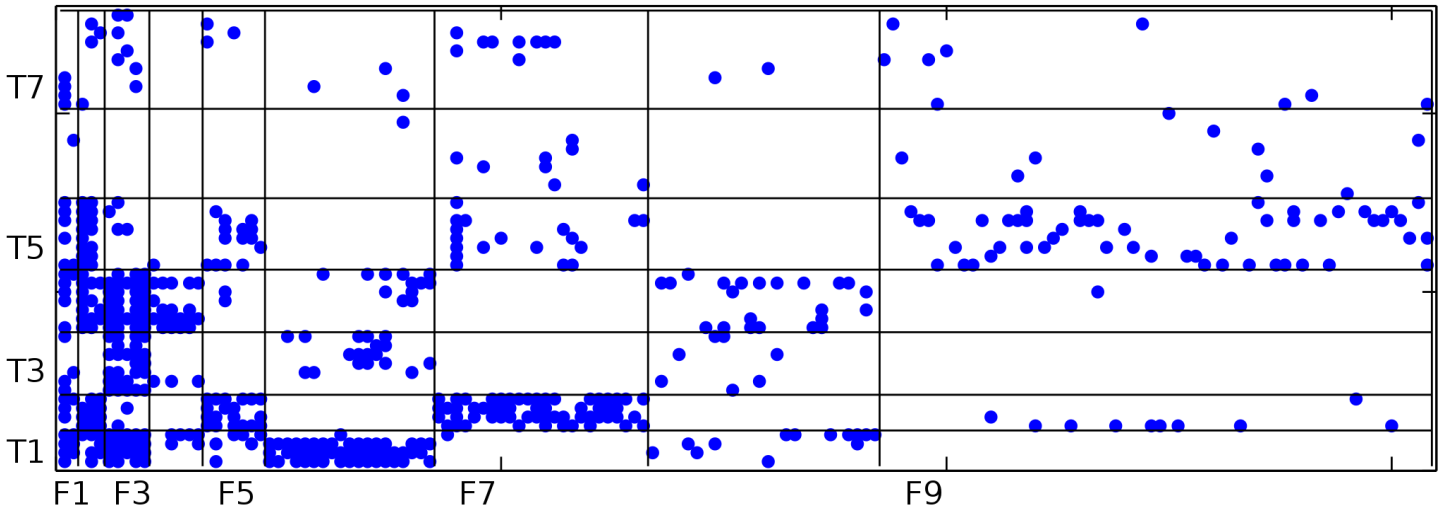
Fungi Network



Trees Network



Clustered Interaction Network



- Tree classes are associated with phylogenetic history;
- Fungus classes are associated with nutritional strategy;
- Consistent with (known) tree speciation prior to fungus speciation;
- Identify generalist and specialist fungi classes.

Summary

- Flexible probabilistic model to detect structure in complex valued graphs;
- Pseudo-likelihood estimators computed obtained through variational EM;
- A statistical criterion to choose the number of classes;
- Package available at `http://pbil.univ-lyon1.fr/software/MixNet`.

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E. Coli Reaction Network

- **Reaction Network of E.Coli**:
  - → data from `http://www.biocyc.org/`,
  - → $n = 605$ vertices (reactions) and $1\,782$ edges.
  - → 2 reactions i and j are connected if the product of i is the substrate of j (cofactors excluded),
  - → V. Lacroix and M.-F. Sagot (INRIA - Hélix).

- **Question**:
  - → Interpretation of the connectivity structure of classes?

- **MixNet results**:
  - → ICL gives $\hat{Q} = 21$ classes,
  - → Most classes correspond to pseudo-cliques,

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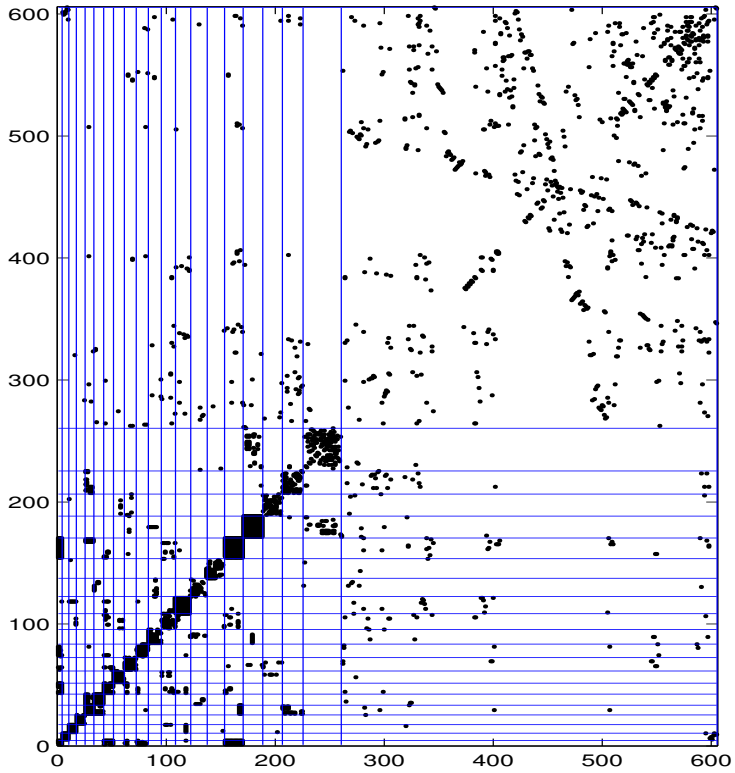
Biological interpretation of the groups I

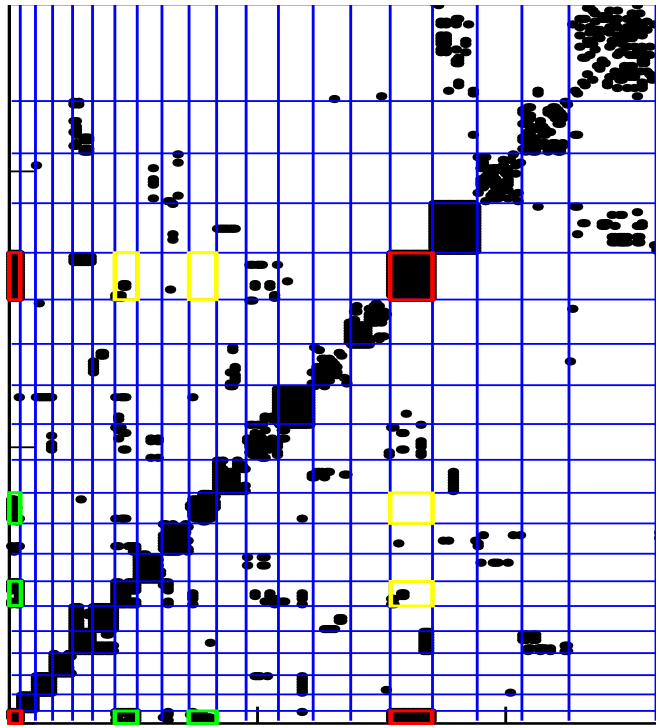
- Dot-plot representation
  - → adjacency matrix (sorted)
- Biological interpretation:
  - → Groups 1 to 20 gather reactions involving all the same compound either as a substrate or as a product,
  - → A compound (chorismate, pyruvate, ATP,*etc*) can be associated to each group.
- The structure of the metabolic network is governed by the compounds.



Biological interpretation of the groups II

- → Classes 1 and 16 constitute s single clique corresponding to a single compound (pyruvate),
- → They are split into two classes because they interact differently with classes 7 (CO2) and 10 (AcetylCoA)
- → Connectivity matrix (sample):

q, l	1	7	10	16
1	1.0			
7	.11	.65		
10	.43		.67	
16	1.0	.01	ϵ	1.0



Adjacency matrix (sample)