Uncovering latent structure in valued graphs: a variational approach

Mahendra Mariadassou, Stephane S. Robin, Corinne C. Vacher

Uncovering Latent Structure in Valued Graphs

M. Mariadassou
Joint work with S. Robin and C. Vacher

Laboratoire MIG (UR INRA), Jouy-en-Josas, France.

Singapore, IMS, 10 May 2011

Outline

Yeast Protein Interaction Network (PIN)

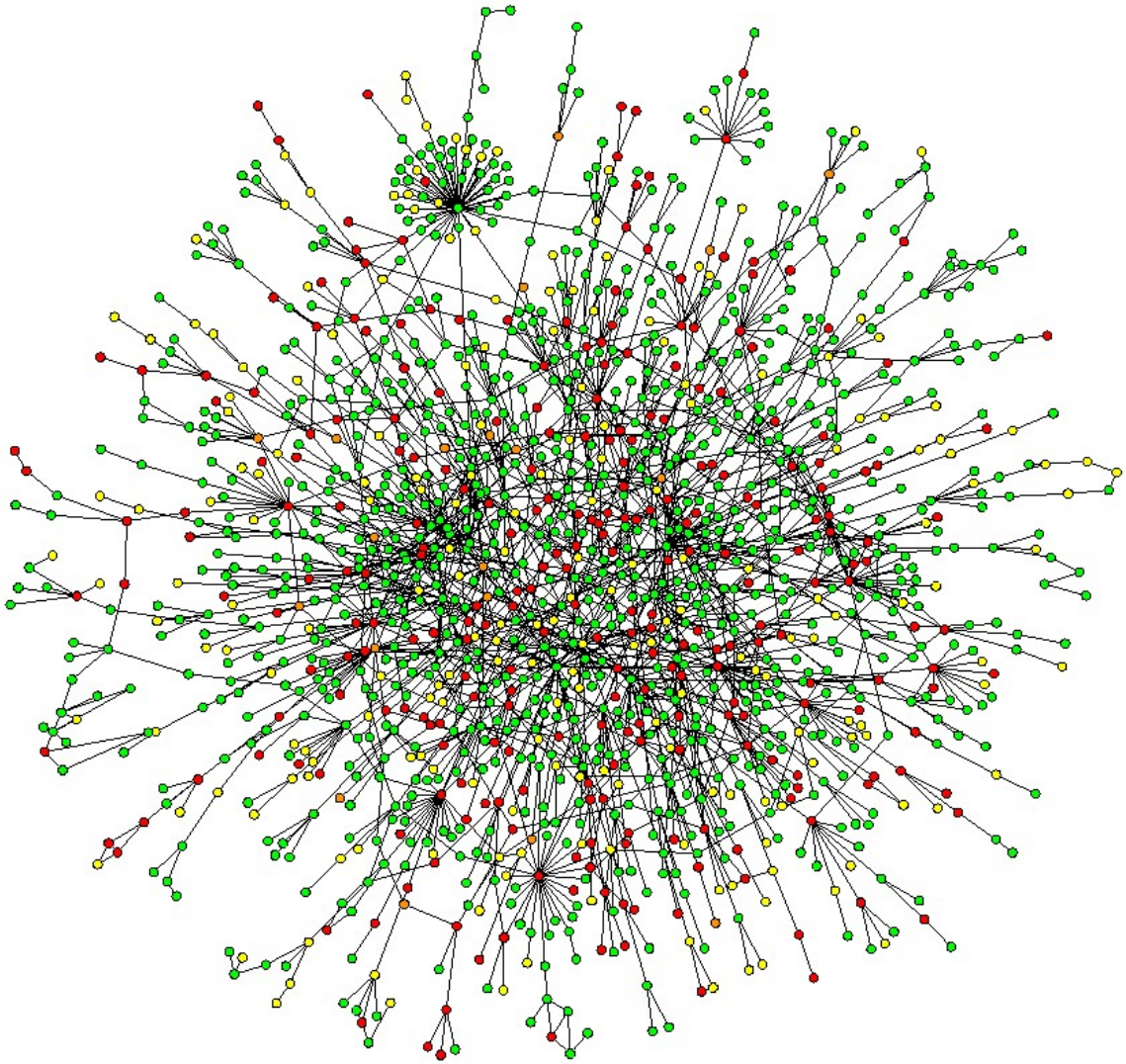

Figure: Yeast PIN. source: www.bordalierinstitute.com/images/yeastProteinInteractionNetwork.jpg

Goal: Simple Representation of the Graph

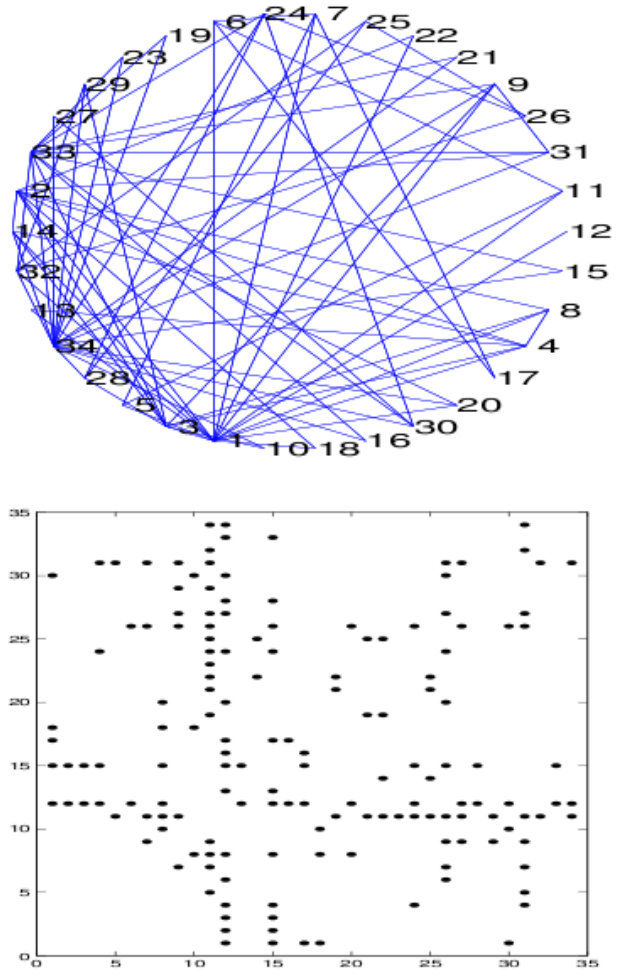

Figure: Zachary's karate club (Zachary 77)

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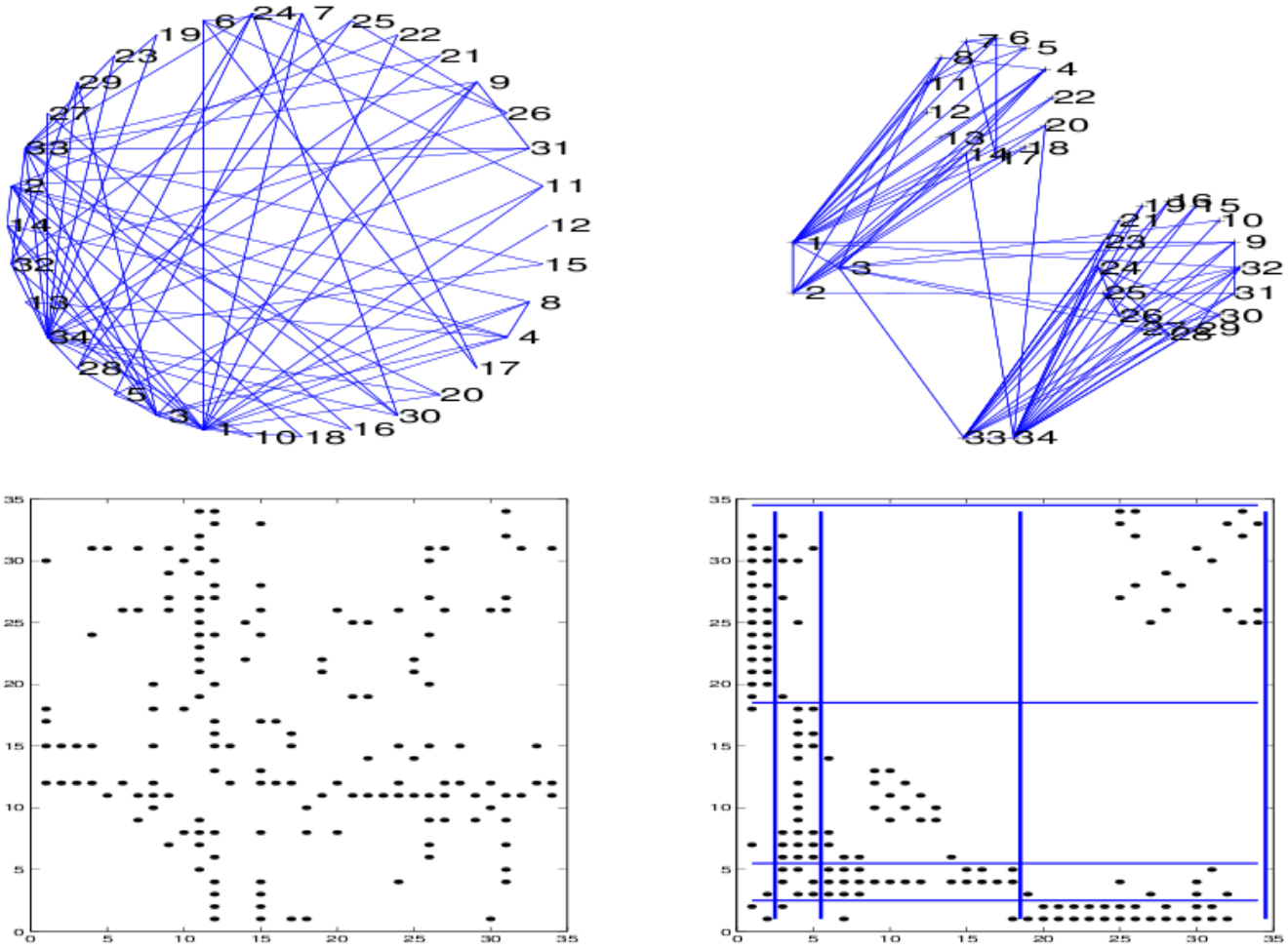

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Models for Networks

Classical Models

- Erdos-Renyi random graph (Erdos & Renyi 59);
- Degree distribution (Milo & al 04);
- Preferential Attachment (Barabasi & Albert 99);

Exponential Models

- ERGM (Holland & Leinhardt 81).

→ Local structure induced by relative frequencies of motifs.

Mixture Model

- Stochastic Block Model / MixNet (Holland & al 83, Fienberg & al 85, Snijders & Nowicki 97, Daudin & al 08)

→ Global structure induced by groups of similar nodes.

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MixNet Probabilistic Model (nodes)

Nodes heterogeneity

- The nodes are distributed among Q different classes (*e.g.* ●,▲,■);
- $\mathbf{Z} = (Z_i)_{i=1..n}$ i.i.d. vectors $Z_i = (Z_{i1}, \ldots, Z_{iQ}) \sim \mathcal{M}(1, \boldsymbol{\alpha})$ where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_Q)$ are the group proportions;
- Z_i is not observed.

Example: (9 nodes, 3 classes)

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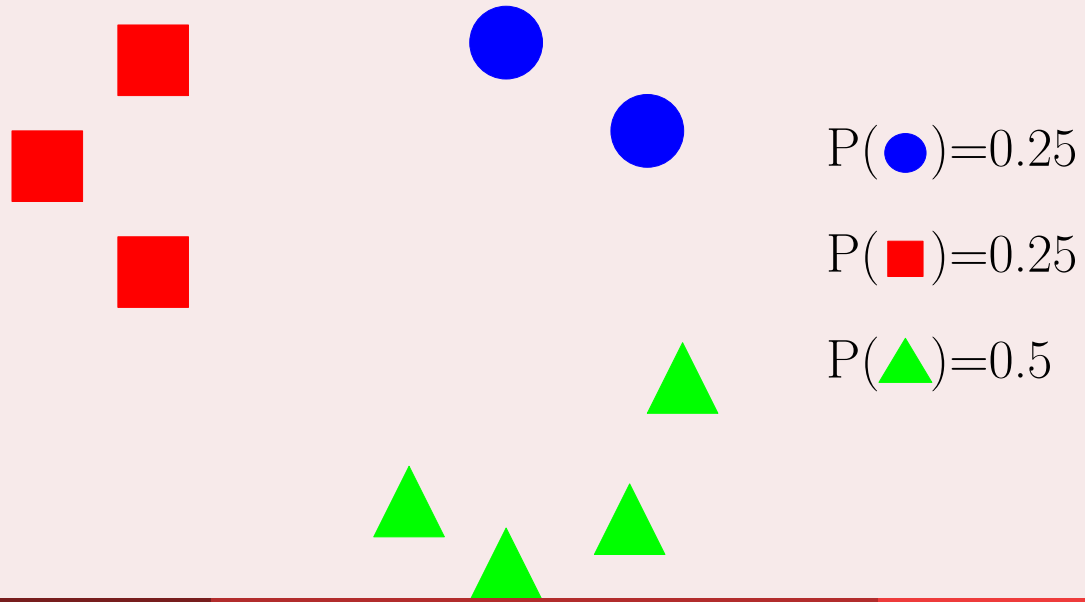

MixNet Probabilistic Model (edges)

Observations

- Edges values X_{ij} where $X_{ij} \in \mathbb{R}^s$;
- Conditional on $\mathbf{Z}$, the (X_{ij}) are independent with distribution

$$X_{ij}|\{Z_{iq} = 1, Z_{j\ell} = 1\} \sim f(., \theta_{q\ell})$$

- $\boldsymbol{\theta} = (\theta_{q\ell})_{q,\ell=1..Q}$ is the connectivity parameter.

Example: 3 classes with Poisson-valued edges

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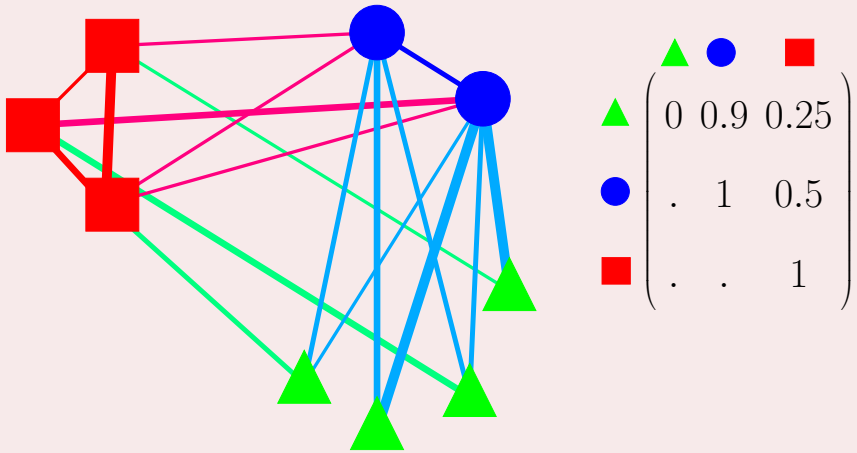

Flexibility of MixNet

Classical Distributions:

- f_θ can be any probability distribution;

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

$$X_{ij}|\{Z_{iq} = 1, Z_{j\ell} = 1\} \sim \mathcal{B}(\pi_{q\ell})$$

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

$$X_{ij}|\{Z_{iq} = 1, Z_{j\ell} = 1\} \sim \mathcal{P}(\lambda_{q\ell})$$

→ Poisson regression with homogeneous effects (PRMH) (counts with covariates): in ecological networks;

$$X_{ij}|\{Z_{iq} = 1, Z_{j\ell} = 1\} \sim \mathcal{P}(\lambda_{q\ell} \exp\{\beta^\intercal \mathbf{y}_{ij}\})$$

(Log)-Likelihood of the Model

- **Complete data likelihood**

$$\begin{aligned}\mathcal{L}(\mathbf{X},\mathbf{Z}) &= \ln \Pr(\mathbf{X},\mathbf{Z}) = \ln \Pr(\mathbf{Z}) P(\mathbf{X}|\mathbf{Z}) \\ &= \sum_i \sum_q Z_{iq} \ln \alpha_q + \sum_{i<j} \sum_{q,l} Z_{iq} Z_{jl} \ln f_{\theta_{ql}}(X_{ij})\end{aligned}$$

- **Observed data likelihood**

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

- Sum over $\mathcal{Q}^n$ is untractable, use EM algorithm instead.

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But...

- The random variables X_{ij} are not independent;
- The distribution $\Pr(.|\mathbf{X})$ of $\mathbf{Z}$ conditional on $\mathbf{X}$ is not a product distribution;

$\rightarrow$ Exact EM is not possible...

Variational Inference: Pseudo Likelihood

- If $\mathcal{R}_{\mathbf{X}}$ is a distribution over $\mathbf{Z}$, let

$$\mathcal{J}(\mathcal{R}_{\mathbf{X}}) = \mathcal{L}(\mathbf{X}) - KL(\mathcal{R}_{\mathbf{X}}, \Pr(.|\mathbf{X}))$$

- For $\mathcal{R}_{\mathbf{X}} = \Pr(.|\mathbf{X})$, $\mathcal{J}(\mathcal{R}_{\mathbf{X}}) = \mathcal{L}(\mathbf{X})$;
- **Variational approximation:** replace complicated distribution $\Pr(.|\mathbf{X})$ by a simple $\mathcal{R}_{\mathbf{X}}$ such that $KL(\mathcal{R}_{\mathbf{X}}, \Pr(.|\mathbf{X}))$ is minimal to obtain a tight lower bound of $\mathcal{L}(\mathbf{X})$.

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- Computing $\mathbb{E}_{\mathcal{R}_\mathbf{X}}[\mathcal{L}(\mathbf{X}, \mathbf{Z})]$ is easy, computing $\mathcal{H}(\mathcal{R}_\mathbf{X})$ is hard (in general).
- Restrict $\mathcal{R}_\mathbf{X}$ to a comfortable class of distributions:

$$\mathcal{R}_\mathbf{X}[\mathbf{Z}] = \prod_i h(Z_i; \boldsymbol{\tau}_i)$$

with $h(.; \boldsymbol{\tau}_i)$ the multinomial with paramater $\boldsymbol{\tau}_i = (\tau_{i1}, \ldots, \tau_{iQ})$.
Intuitively, $\tau_{iq} \simeq \Pr(Z_{iq} = 1|\mathbf{X})$.

- For such $\mathcal{R}_\mathbf{X}$,

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- Maximize pseudo-likelihood:

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- Step 1 **Optimize $\mathcal{J}$ w.r.t. (τ_i)**:
  - → Constraint: $\sum_q \tau_{iq} = 1$ for all i;
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$$\tilde{\tau}_{iq} \propto \alpha_q \prod_{j \neq i} \prod_{\ell=1}^{Q} f_{\theta_{q\ell}}(X_{ij})^{\tilde{\tau}_{jl}}$$

- Step 2 **Optimize $\mathcal{J}$ w.r.t. (α,θ)**:
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  - → Simple expression of $\tilde{\theta}_{ql}$ for classical distributions (weighted MLE).

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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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MixNet Properties

Identifiability

- Identifiablity of Parameters (Allman and al., 2009, 2011);
- Model Selection criteria (Daudin and al., 2008, Latouche and al., 2011)

Quality of Estimates

- VEM algorithm converge to a different optimum than ML in the general case (Gunawardana and Byrne (2005)), except for degenerated models;
- SBM are in a certain sense degenerated: $\Pr(.|\mathbf{X}) \to \delta_{\mathbf{Z}}$ (ongoing work of Celisse and Daudin, Mariadassou and Matias)

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Quality of the Estimates: Simulation Setup

- → Undirected graph with $Q = 3$ classes;
- → Poisson-valued edges;
- → $n = 100,\ 500$ vertices;
- → $\alpha_q \propto a^q$ for $a = 1,\ 0.5,\ 0.2$;
  - $a = 1$: balanced classes;
  - $a = 0.2$: unbalanced classes $(80.6\%,\ 16.1\%,\ 3.3\%)$
- → Connectivity matrix of the form $\begin{pmatrix} \lambda & \gamma\lambda & \gamma\lambda \\ \gamma\lambda & \lambda & \gamma\lambda \\ \gamma\lambda & \gamma\lambda & \lambda \end{pmatrix}$ for $\gamma = 0.1,\ 0.5,\ 0.9,\ 1.5$ and $\lambda = 2,\ 5$.
  - $\gamma = 1$: all classes equivalent (same connectivity pattern);
  - $\gamma \neq 1$: classes are different;
  - λ: mean value of an edge;
- → 100 repeats for each setup.

Quality of the Estimates: Results

- Root Mean Square Error (RMSE) = $\sqrt{Bias^2 + Variance}$

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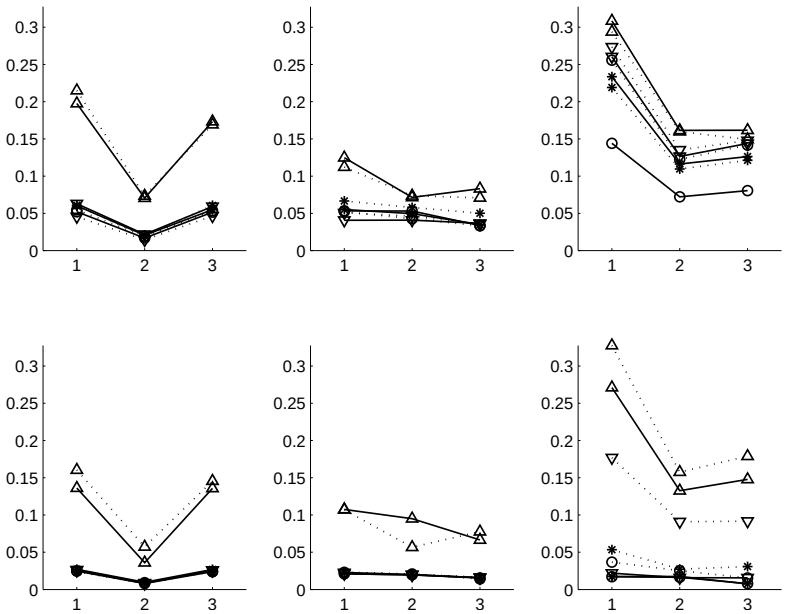
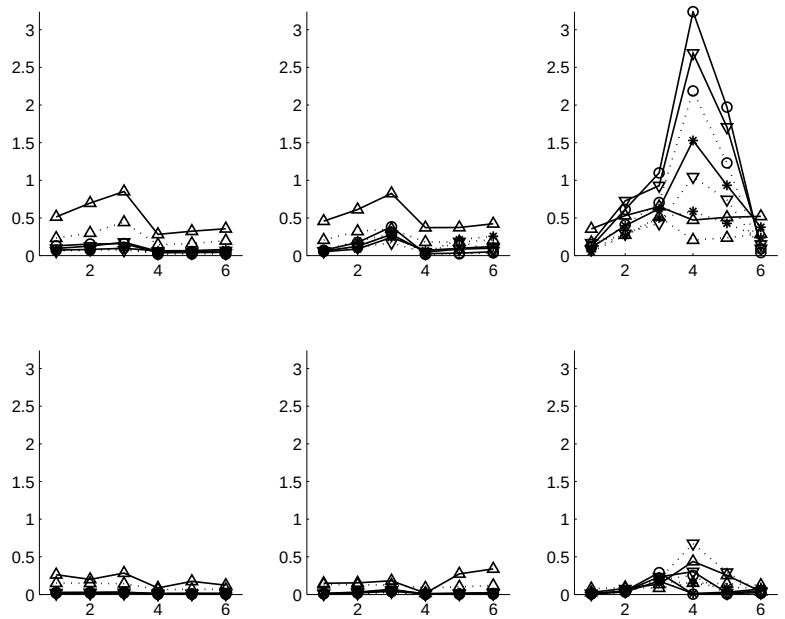
RMSE for the α_q



RMSE for the λ_{ql}



x-axis: $\alpha_1, \alpha_2, \alpha_3$

x-axis: $\lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{12}, \lambda_{13}, \lambda_{23}$

Top: $n = 100$, Bottom: $n = 500$

Left to right: $a = 1,\ 0.5,\ 0.2$

Solid line: $\lambda = 5$, dashed line: $\lambda = 2$

Symbols depend on γ: $\circ = 0.1$, $\nabla = 0.5$, $\Delta = 0.9$, $* = 1.5$

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.

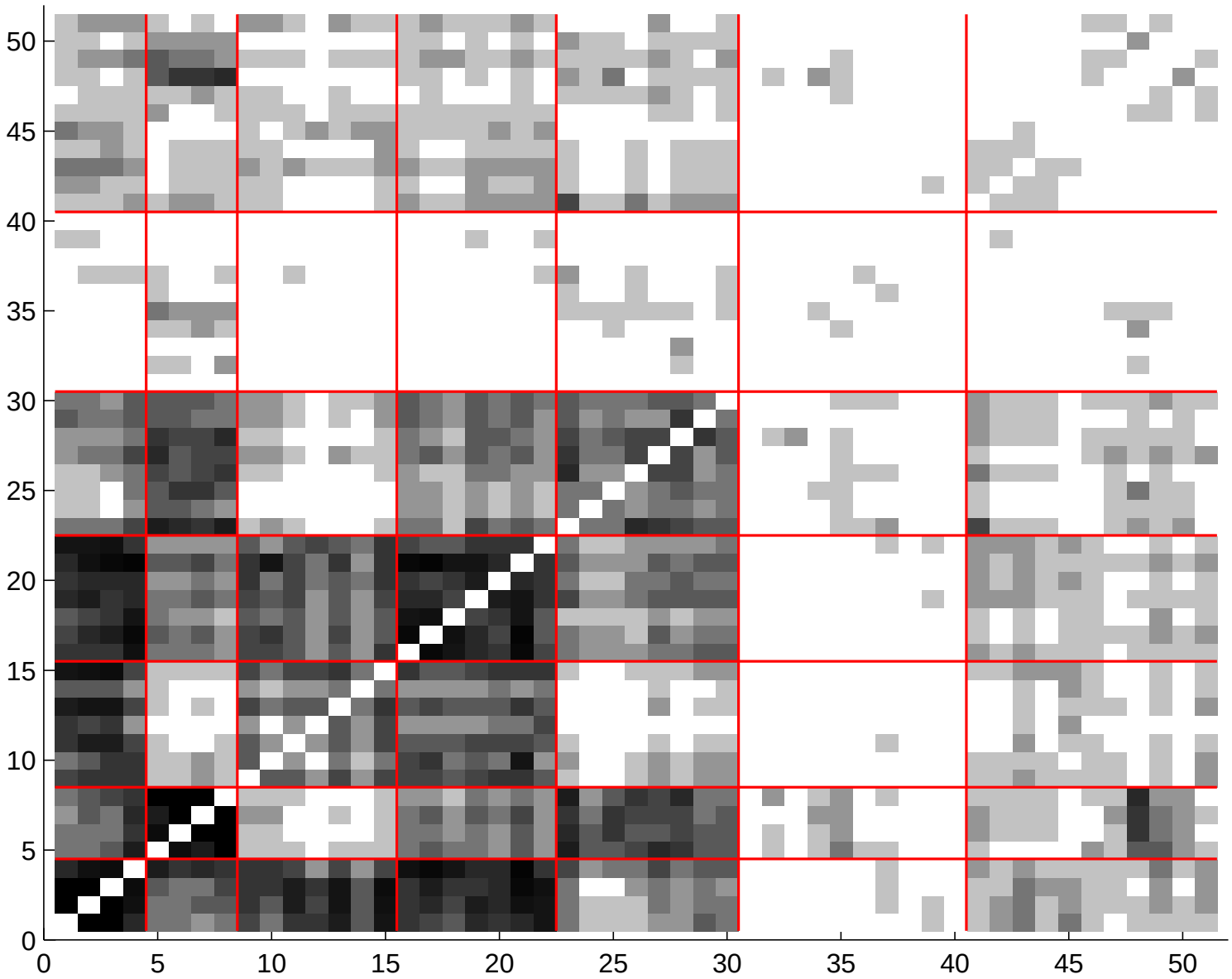
Fungi Trees Interactions

- **Dataset** Parisitic behavior of 154 fungi on 51 trees;
- **Network** Valued Network on trees: $X_{tt'}$ = number of fungis infecting both t and t'.
- **Goal** Identify groups of trees sharing similar interactions: is similarity driven by evolution or geography ?
- **Poisson Model** We assume

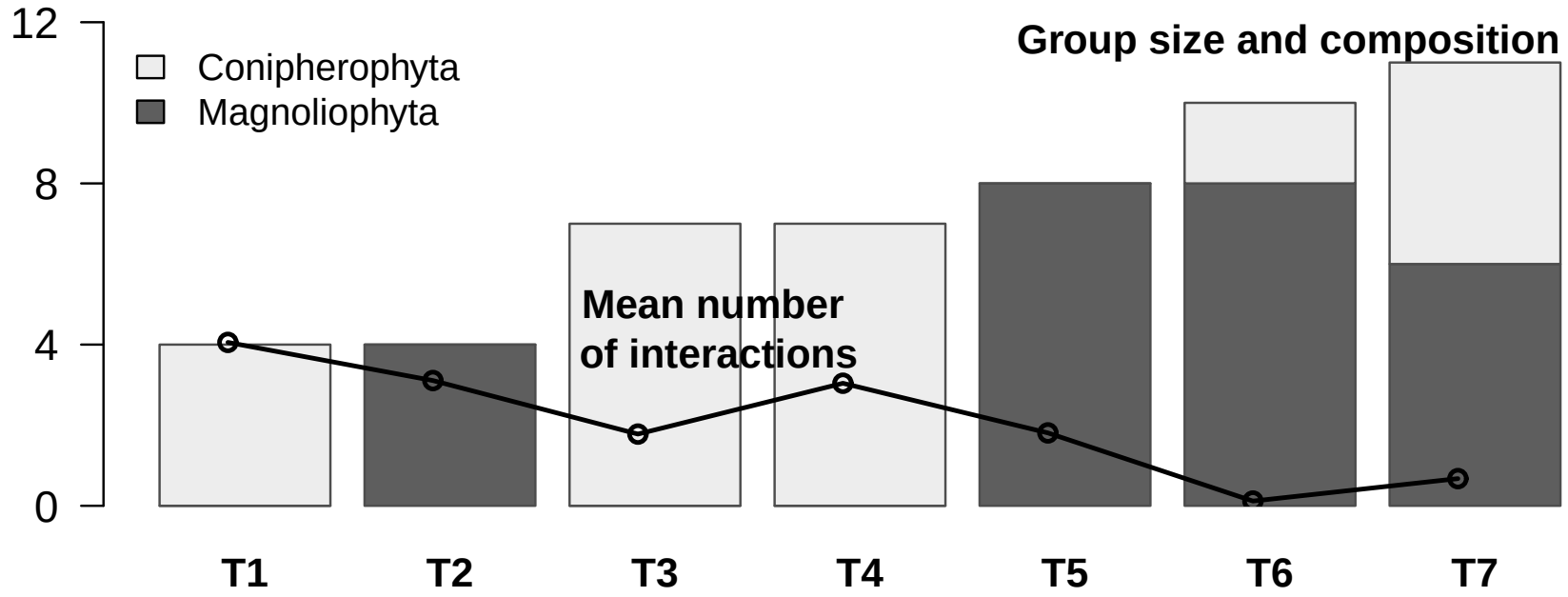
$$X_{ij}|\{Z_{iq} = 1, Z_{j\ell} = 1\} \sim \mathcal{P}(\lambda_{q\ell})$$

- **Covariate**
  - Phylogenetic relatedness measured by genetic\taxonomic distance;
  - Geographical relatedness measured by Jaccard distance;

With no covariate (7 classes)



Groups of Trees: No Covariate



- Taxonomic rank: species ¡ genus ¡ family ¡ order ¡ class ¡ phylum;
- Strong effect of taxonomic rank on the group composition;
- Groups T1, T2, T3, T4 are even monofamily;
- Need to account for taxonomic distance.

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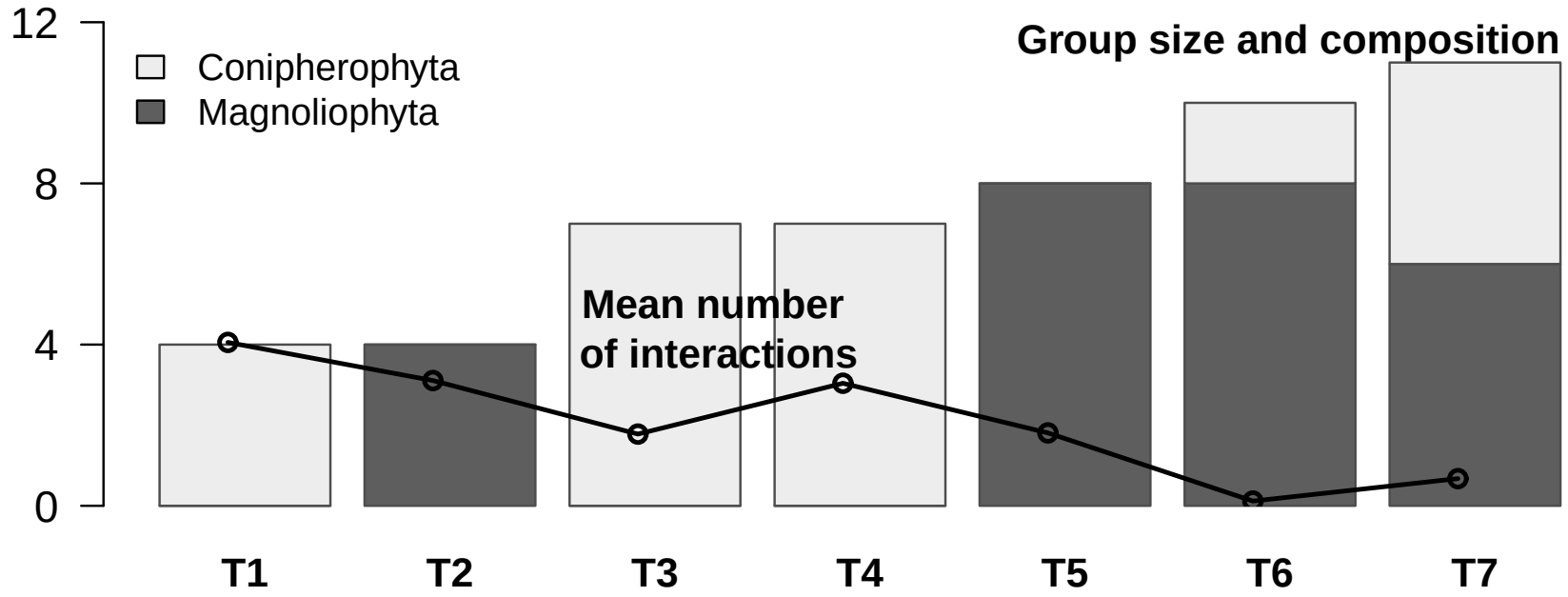

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Groups of Trees: No Covariate (II)

$\widehat{\lambda}_{q\ell}$	T1	T2	T3	T4	T5	T6	T7
T1	14.46	4.19	5.99	7.67	2.44	0.13	1.43
T2	4.19	14.13	0.68	2.79	4.84	0.53	1.54
T3	5.99	0.68	3.19	4.10	0.66	0.02	0.69
T4	7.67	2.79	4.10	7.42	2.57	0.04	1.05
T5	2.44	4.84	0.66	2.57	3.64	0.23	0.83
T6	0.13	0.53	0.02	0.04	0.23	0.04	0.06
T7	1.43	1.54	0.69	1.05	0.83	0.06	0.27
$\widehat{\alpha}_q$	7.8	7.8	13.7	13.7	15.7	19.6	21.6

- T1, T2, T3, T4, T5: trees sharing lots of parasites;
- T6, T7: Trees with sharing few parasites with any other.

Groups of Trees: With Covariate

Model: $X_{ij} \sim \mathcal{P}(\lambda_{ql} e^{\beta y_{ij}})$ with y_{ij} taxonomic distance

- $\hat{Q} = 4$ classes;
- $\hat{\beta} = -0.317$;

	T'1	T'2	T'3	T'4
T1	0	0	0	4
T2	0	0	0	4
T3	2	5	0	0
T4	0	2	0	5
T5	0	2	0	6
T6	0	0	10	0
T7	7	2	2	0

$\widehat{\lambda}_{q\ell}$	T'1	T'2	T'3	T'4
T'1	0.75	2.46	0.40	3.77
T'2	2.46	4.30	0.52	8.77
T'3	0.40	0.52	0.080	1.05
T'4	3.77	8.77	1.05	14.22
$\widehat{\alpha}_q$	17.7	21.5	23.5	37.3

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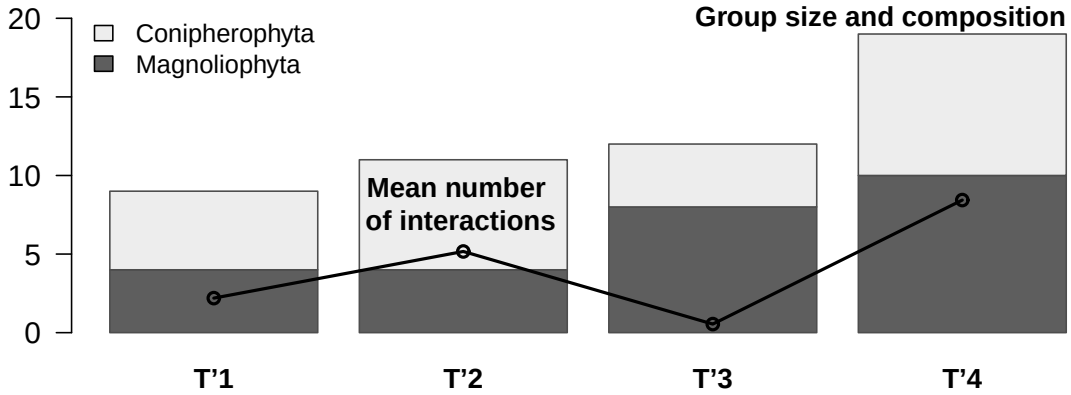

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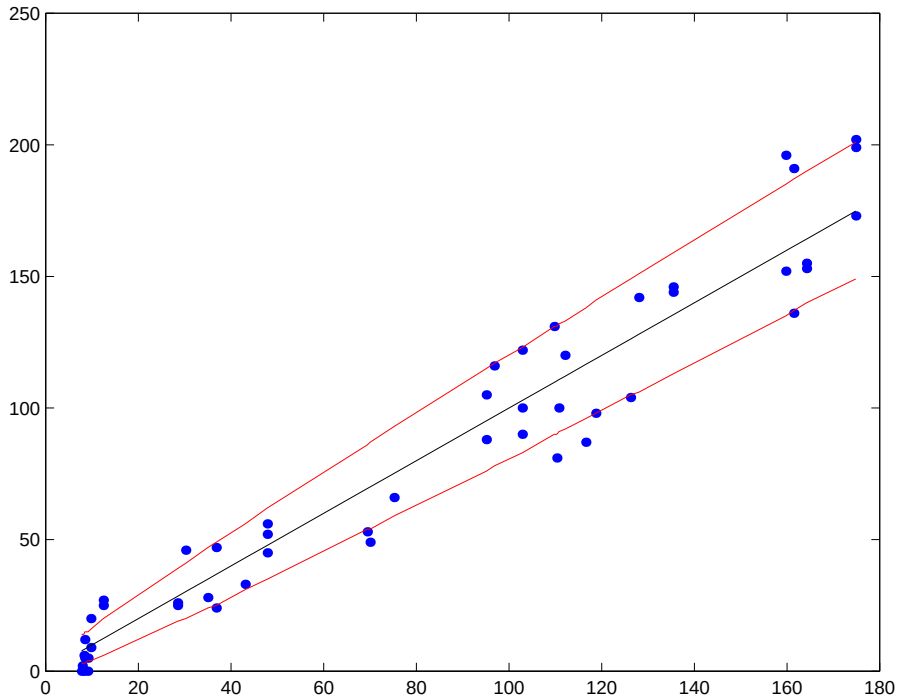
Goodness of fit

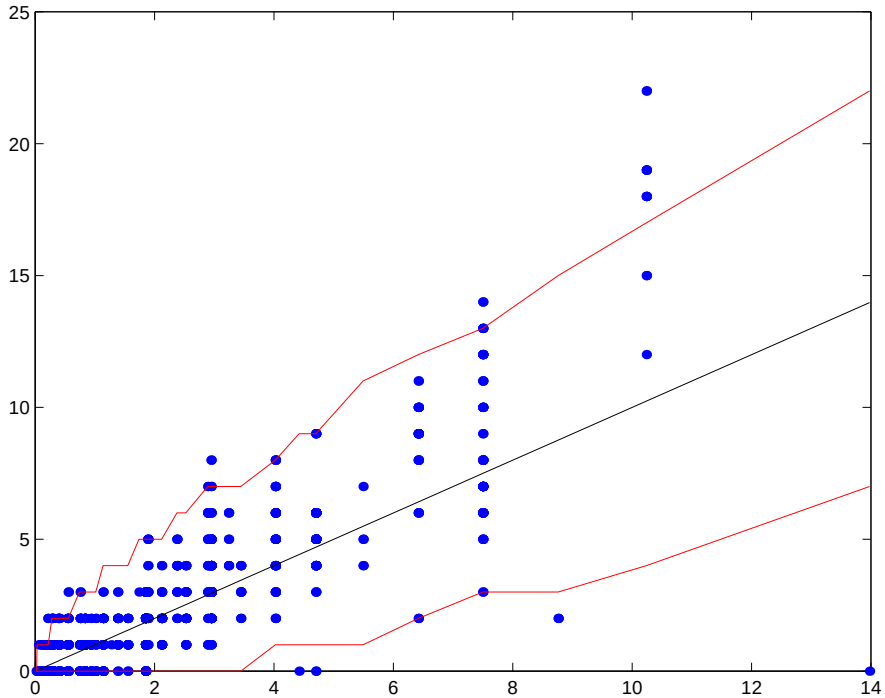
Check predictive power of the model for

Weighted degree



$$K_i = \sum_{j \neq i} X_{ij}$$

Single Edge Value



$$X_{ij}$$

Other covariates

- Genetic distance: same effect than taxonomic distance;
- Jaccard distance: no effect;

→ Main sources of similarity in trees parasitic assemblages are evolutionary processes and not ecological processes.

Tree interaction network				
Factor	Covariate	Q (PM)	Q (PRMH)	Δ ICL
Phylogenetic relatedness	Taxonomic Distance	7	4	116.0
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Geographical overlap	Jaccard distance	7	7	-8.6

Table: Effect of covariates. Δ ICL = gain of switching from PM to PRMH.

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MixNet

- Flexible probabilistic model to detect structure in complex valued graphs;
- Pseudo-likelihood estimators computed through variational EM (consistency ?);
- A statistical model selection criteria for the number of classes;
- Package available at `http://pbil.univ-lyon1.fr/software/MixNet`.

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- Similarity in parasitic assemblages of two trees explained by phylogenetic relatedness, not geographical overlap.

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E. Coli Reaction Network

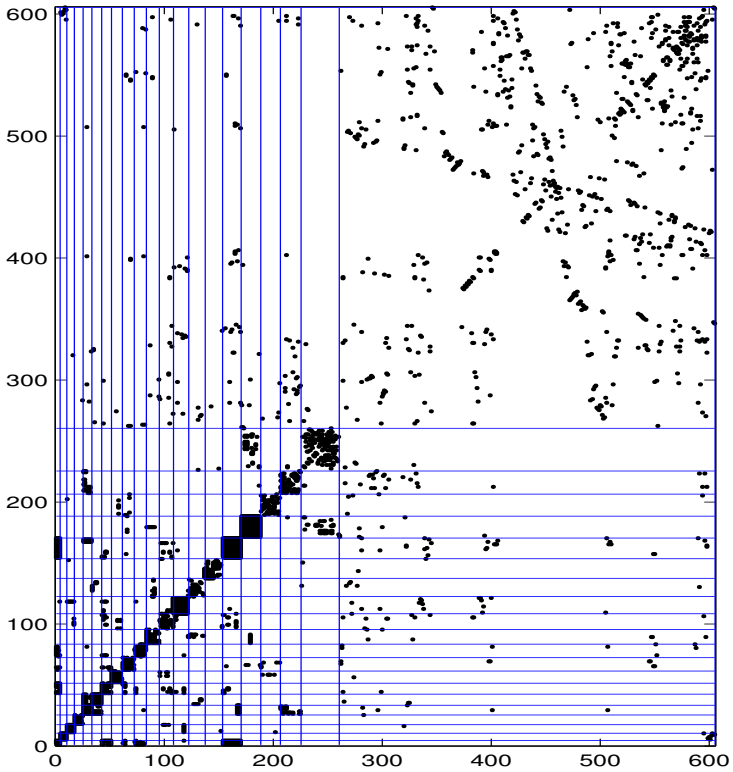
- **Reaction Network of E.Coli**:
  - → data from `http://www.biocyc.org/`,
  - → $n = 605$ vertices (reactions) and $1\,782$ edges.
  - → 2 reactions i and j are connected if the product of i is the substrate of j (cofactors excluded),
  - → V. Lacroix and M.-F. Sagot (INRIA - Hélix).

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

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

Biological interpretation of the groups I

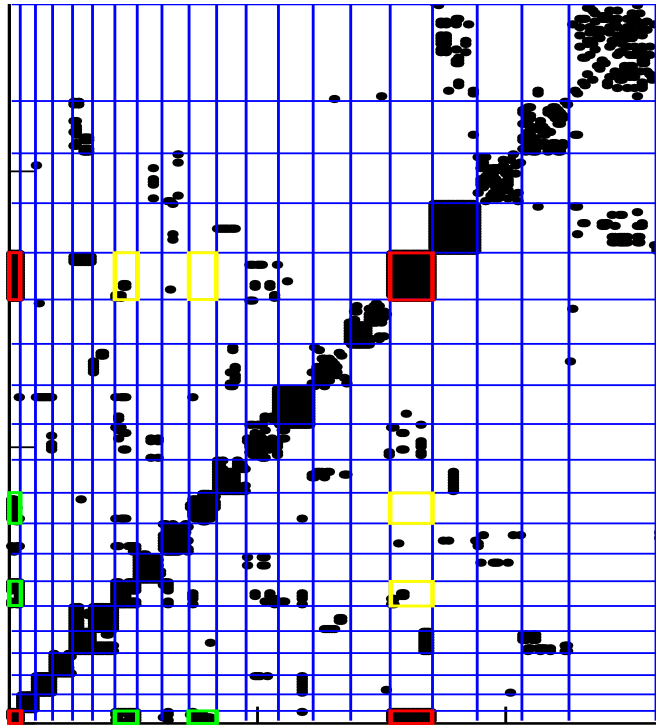
- Dot-plot representation
  - → adjacency matrix (sorted)
- Biological interpretation:
  - → Groups 1 to 20 gather reactions involving all the same compound either as a substrate or as a product,
  - → A compound (chorismate, pyruvate, ATP,*etc*) can be associated to each group.
- The structure of the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