Stochastic block models for networks

Applications in ecology

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April 2024

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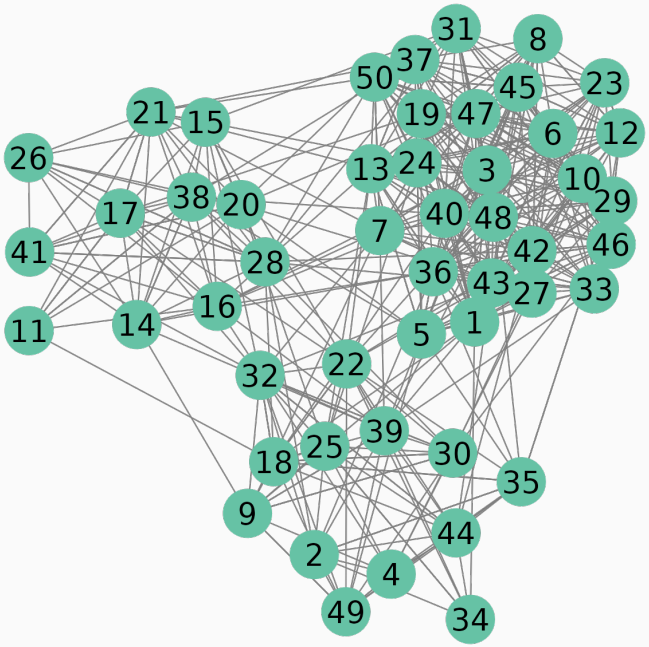
1. Introduction

2. Probabilistic model

3. Inference

Networks

Convenient tools to encode / represent interactions between entities



A network consists in:

- nodes/vertices which represent individuals / species / entities which may interact or not,
- links/edges/connections which stand for an interaction between a pair of nodes / dyads.

Social networks

- Friendship between individuals, 

- Linkedin 
- Twitter 
- Co-publication between researchers
- Advices between lawyers: oriented relation
- Enron email dataset
- Exchanges of seeds between farmers

Networks in ecology

- Ecosystems involve many species
- Interactions between species determine the functioning and evolution of ecosystems
- Several types of interactions

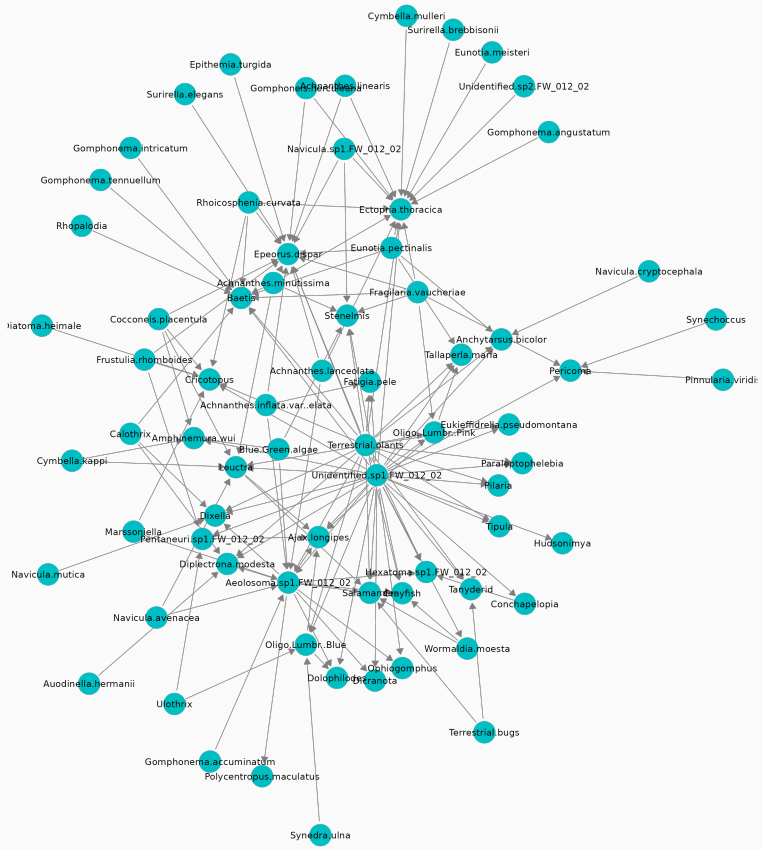
Predation

Parasitism

Pollination

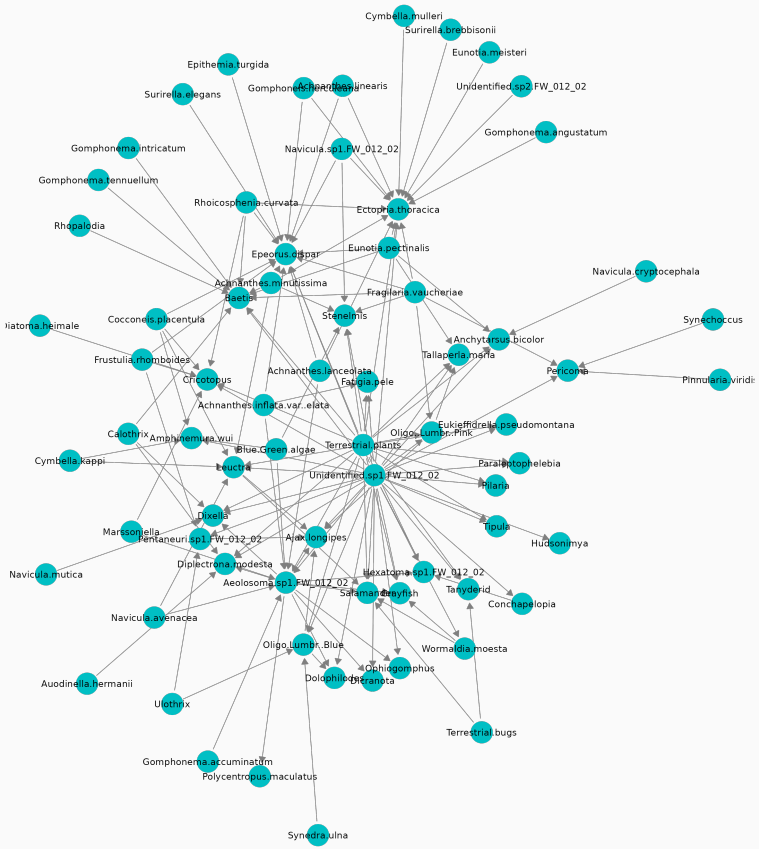
Predation networks: foodwebs

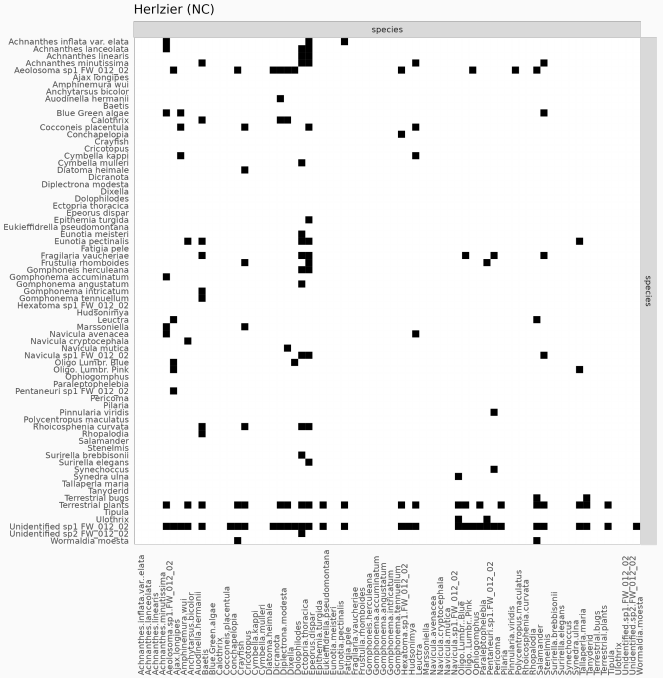
[Thompson and Townsend, 2003] Pine-forest stream foodweb issued from North-Caroline (71 species, 148 interactions)



Foodwebs: adjacency matrix

- $Y = (Y_{ij})_{1 \leq i,j, \leq n} = n \times n$ matrix
- $Y_{ij} = 1$ if i is eaten by j, 0 otherwise

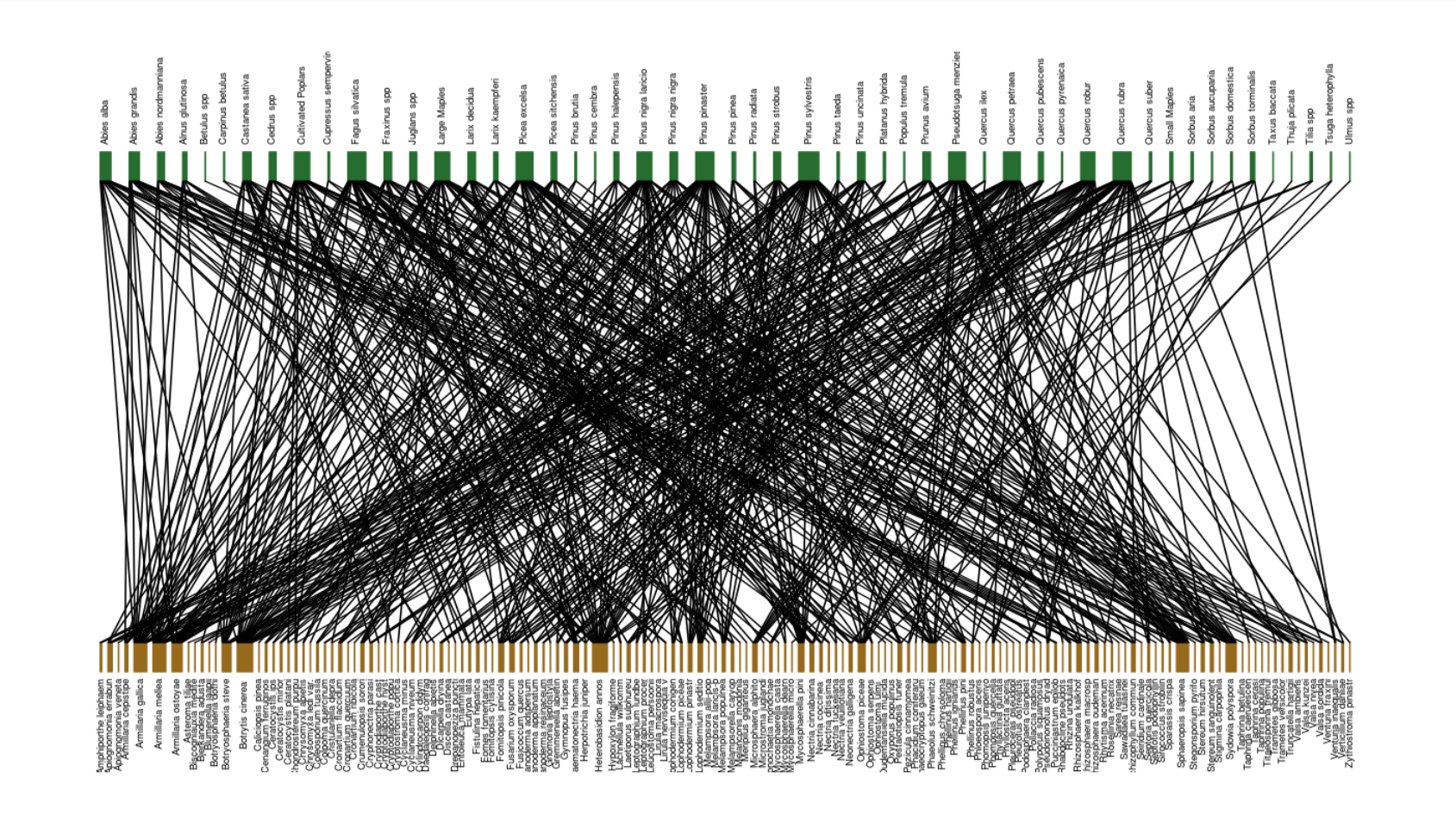




Directed binary relation : Y non symetric and 0/1.

Parasitism : tree-fungus network

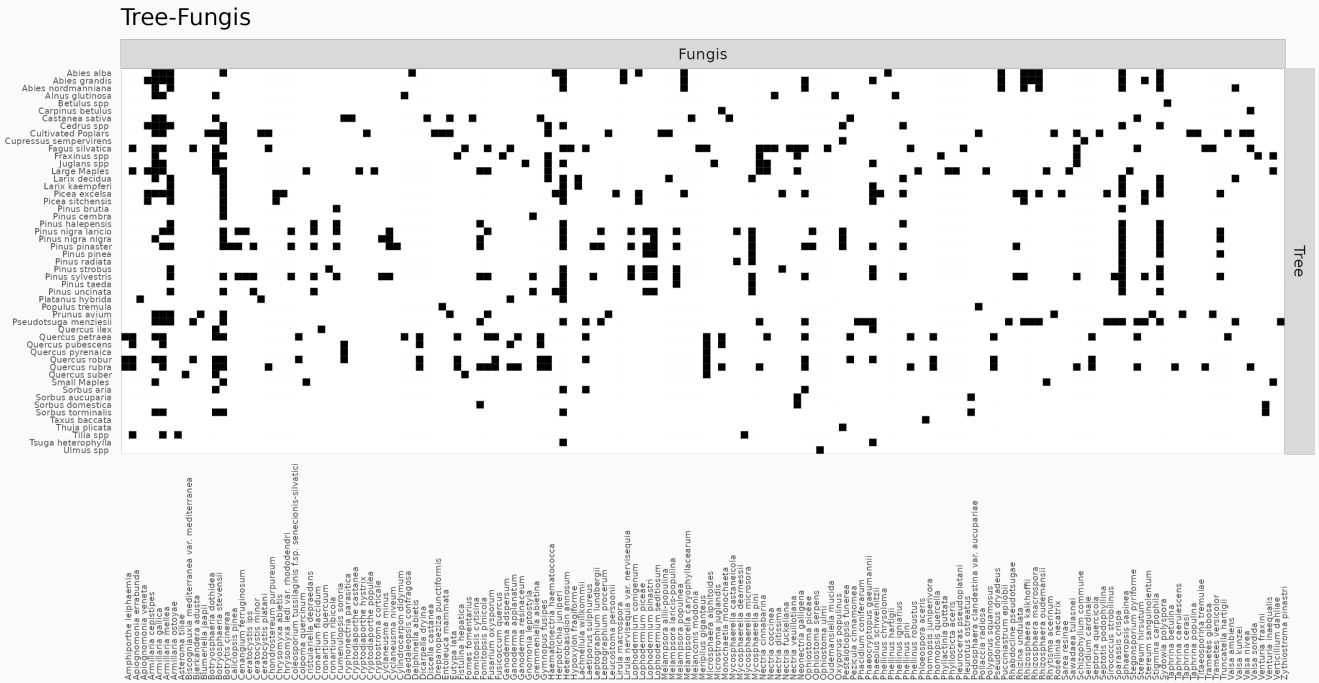
[Vacher et al., 2008] Parasitism relation between $n = 51$ tree species and $p = 154$ fungus species



Nodes of two types: bipartite network

Parasitism : tree-fungus incidence matrix

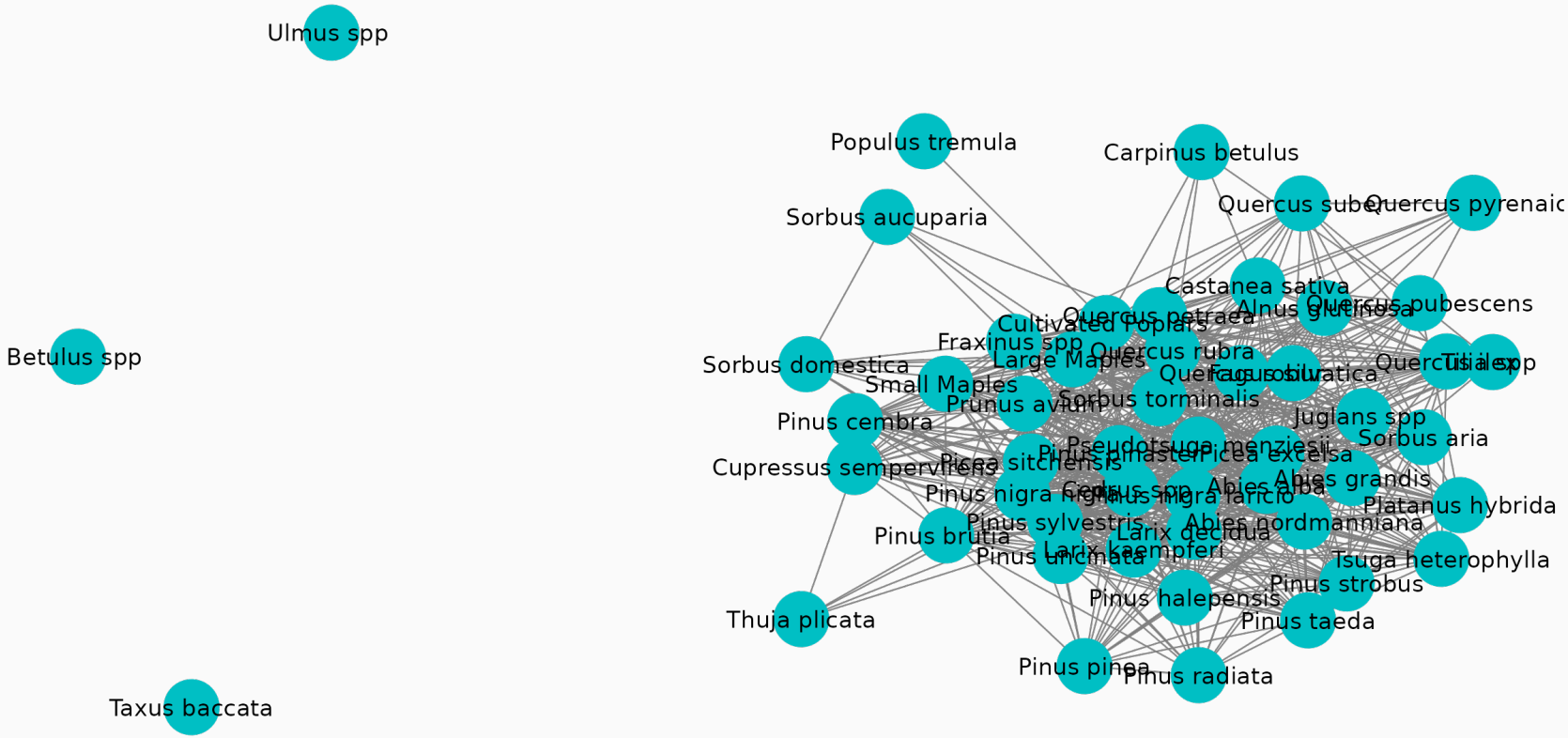
- $Y = (Y_{ij})_{1 \leq i,j, \leq n} = n \times p$ matrix
- $Y_{ij} = 1$ if tree i is parasited by fungus j, 0 otherwise



Binary bipartite network: Y non square and 0/1.

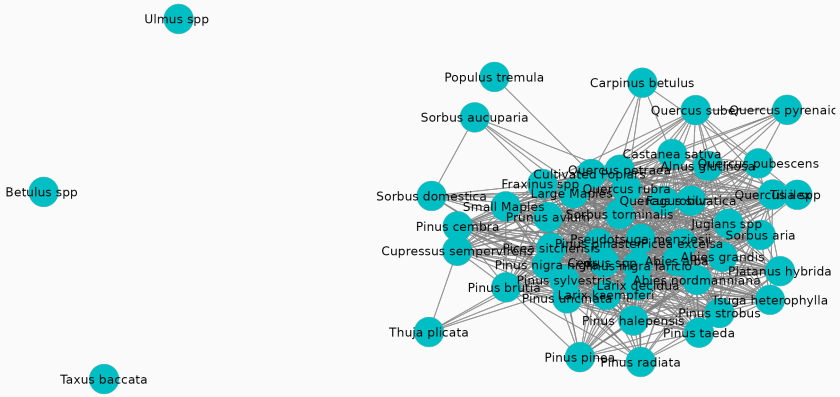
Parasitism : tree-tree network

[Vacher et al., 2008] Number of shared fungus between any pair of the $n = 51$ tree species



Parasitism : weighted adjacency matrix

Y_{ij}: number of shared fungal parasites (fungus hosted by both species)



Weighted non-oriented network: Y symetric and $\in \mathbb{N}$.

Additional information: covariates on pair of trees

For each pair of tree species, 3 distances were also measured:

- taxonomic distance (x^1)
- geographic distance (x^2)
- genetic distance (x^3)

Ecological questions i

→ Ecological aim: caracterize / understand / compare ecosystem organizations.

Foodwebs

- How is organized the network? Can I gather species with similar behavior (trophic levels)?
- Do two given species play the same role in the network?

Fungus-tree networks

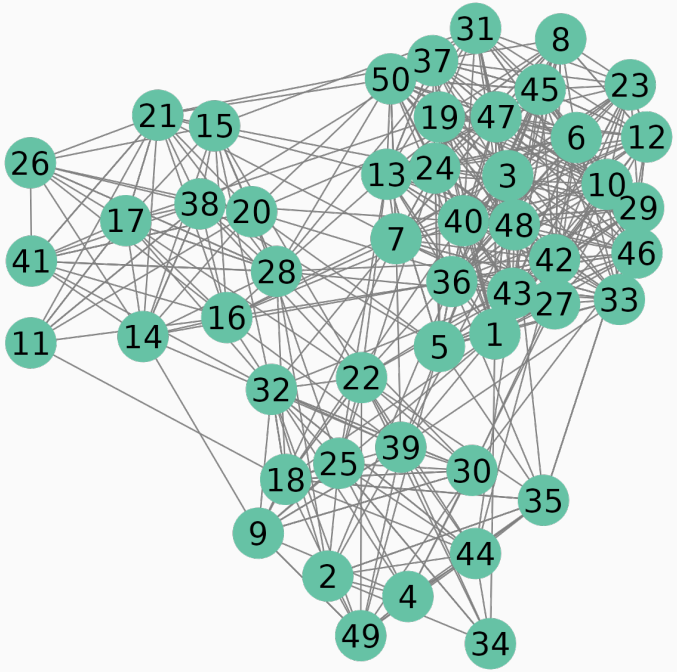
- Can we find groups of trees and fungi that are preferentially associated?

Ecological questions ii

Parasite networks between trees

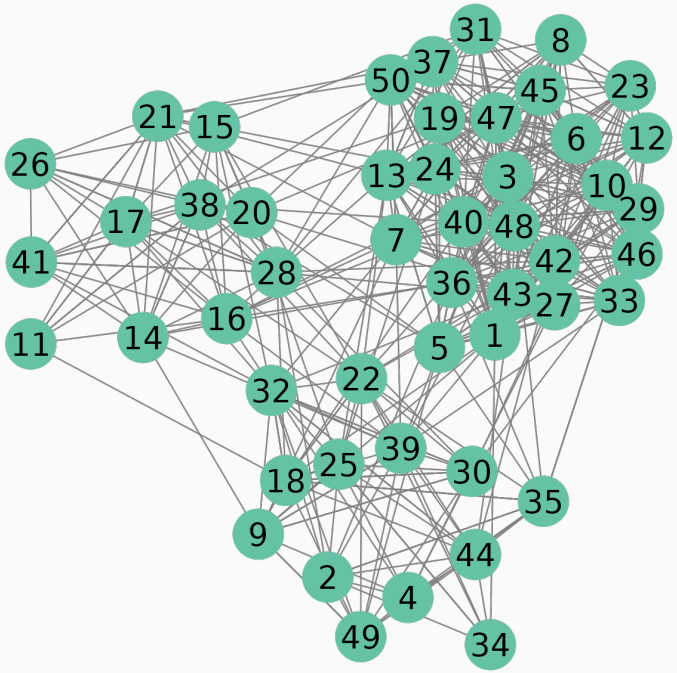
- Do any of the three distances (genetic, geographic or taxonomic) contributes to shape the number of shared parasites?
- Are the covariates sufficient to explain the interactions?

Statistical inference: available data



- the network provided as:
  - an adjacency matrix (for simple network) or an incidence matrix (for bipartite network),
  - a list of pair of nodes / dyads which are linked.
- some additional covariates on nodes, dyads which can account for sampling effort.

Statistical inference: goal



- Unraveling / describing / modeling the network topology.
- Discovering particular structure of interactions between some subsets of nodes.
- Understanding node heterogeneity.
- Not inferring the network !

Probabilistic approach

- Context: our matrix Y is the realization of a stochastic process.
- Aim: Propose a stochastic process is able to mimic heterogeneity in the connections.
- Advantage: benefit from the statistical tools (tests, model selection, etc...)

A first random graph model for network

Erdős-Rényi (1959) Model for n nodes

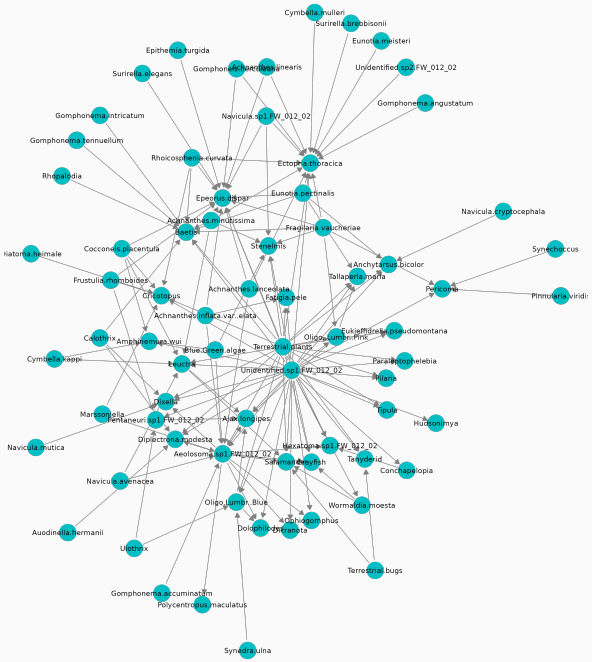
$$\forall 1 \leq i, j \leq n, \quad Y_{ij} \overset{i.i.d.}{\sim} \mathcal{B}\text{ern}(p),$$

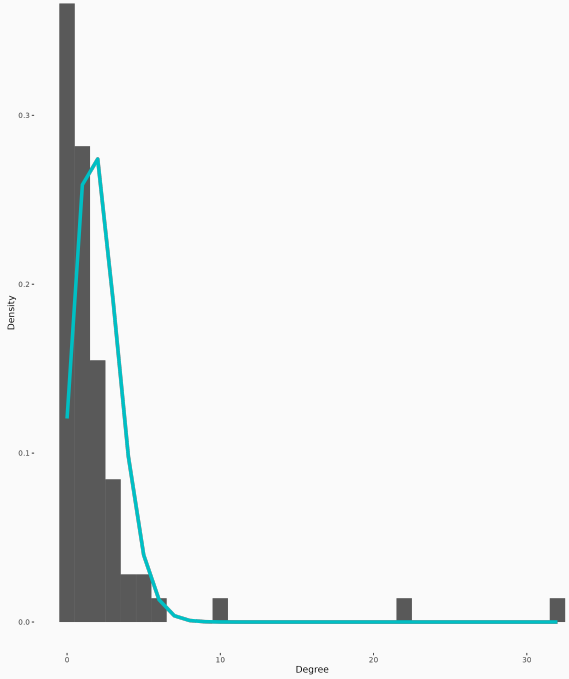
where $p \in [0, 1]$ is the probability for a link to exist.

Consequence

$$\deg(i) \sim_{i.i.d} \mathcal{B}\text{in}(n, p)$$

Confrontation to a real network





Not enough variability in the degree

Limitations of an ER graph to describe real networks

- Homogeneity of the connections
- Degree distribution too concentrated, no high degree nodes,
- All nodes are equivalent (no nestedness...),
- No modularity, no hubs

Stochastic Block Model

[Nowicki and Snijders, 2001] Let (Y_{ij}) be an adjacency matrix

Latent variables

- The nodes $i = 1, \ldots, n$ are partitionned into K clusters
- $Z_i = k$ if node i belongs to cluster (block) k
- Z_i independant variables

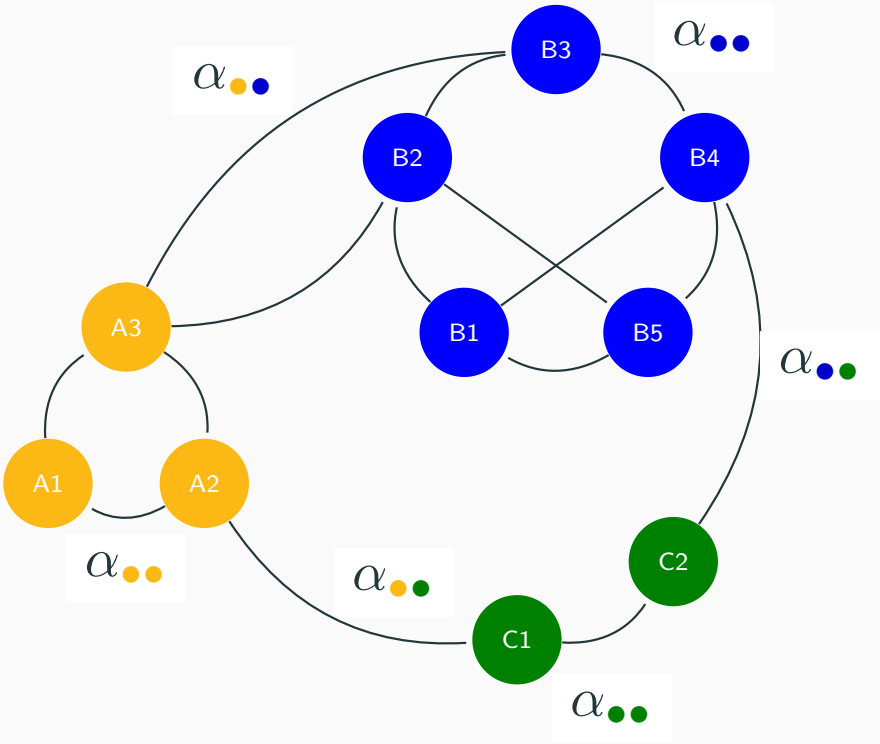
$$\mathbb{P}(Z_i = k) = \pi_k$$

Conditionally to $(Z_i)_{i=1,\ldots,n}$...

(Y_{ij}) independant and

$$Y_{ij}|Z_i, Z_j \sim \mathcal{B}ern(\alpha_{Z_i,Z_j}) \quad \Leftrightarrow \quad P(Y_{ij} = 1|Z_i = k, Z_j = \ell) = \alpha_{k\ell}$$

Stochastic Block Model : illustration



Parameters

Let n nodes divided into 3 clusters

- $\mathcal{K} = \{\bullet, \bullet, \bullet\}$ clusters
- $\pi_\bullet = \mathbb{P}(i \in \bullet),\ \bullet \in \mathcal{K}, i = 1, \ldots, n$
- $\alpha_{\bullet\bullet} = \mathbb{P}(i \leftrightarrow j | i \in \bullet, j \in \bullet)$

$$Z_i = \mathbf{1}_{\{i \in \bullet\}} \sim^{\text{iid}} \mathcal{M}(1, \pi), \quad \forall \bullet \in \mathcal{K},$$
$$Y_{ij} \mid \{i \in \bullet, j \in \bullet\} \sim^{\text{ind}} \mathcal{B}(\alpha_{\bullet\bullet})$$

SBM : A great generative model

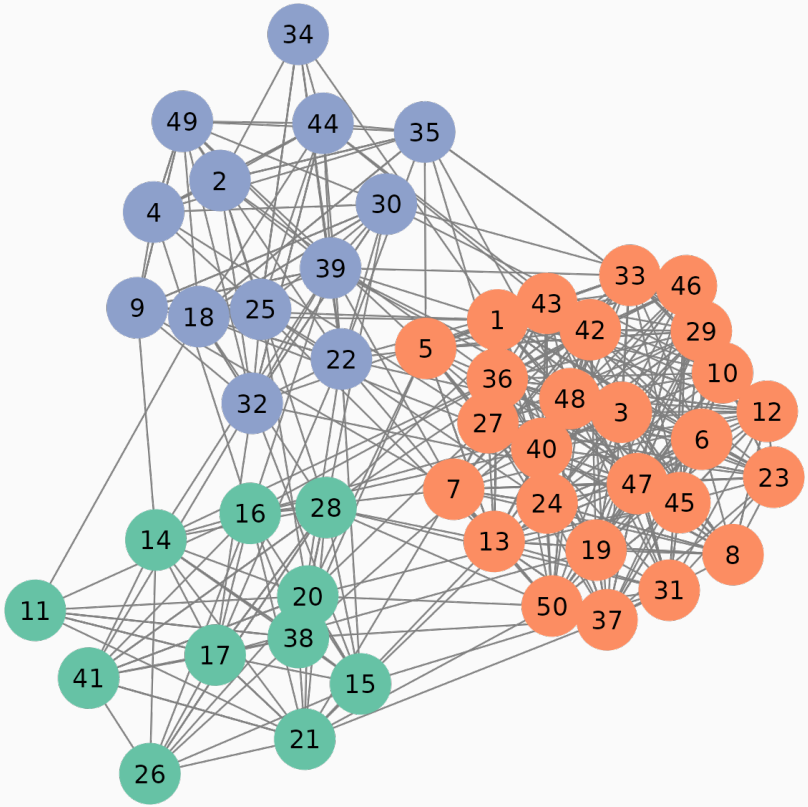
- Generative model : easy to simulate
- No a priori on the type of structure
- Combination of modularity, nestedness, etc...

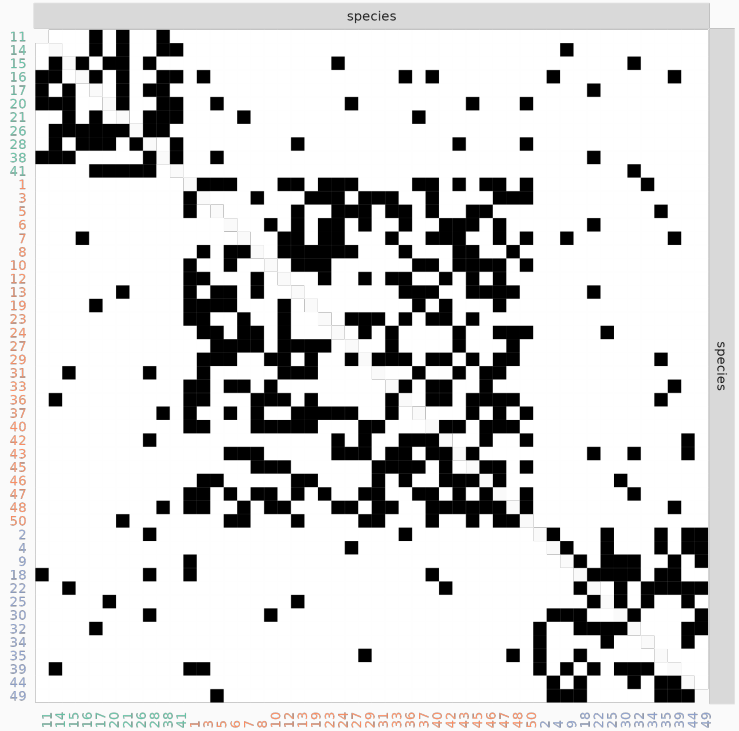
References

- Other ways to model heterogeneity in networks [Matias, Catherine and Robin, Stéphane, 2014]
- Review paper on SBM [Lee and Wilkinson, 2019]

Modelling communities

$$\boldsymbol{\alpha} = \begin{pmatrix} \underline{0.45} & 0.05 & 0.05 \\ 0.05 & \underline{0.45} & 0.05 \\ 0.05 & 0.05 & \underline{0.45} \end{pmatrix} \qquad \pi = (0.25, 0.5, 0.25)$$

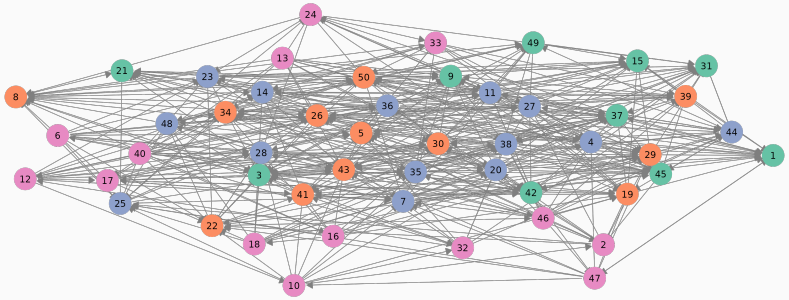


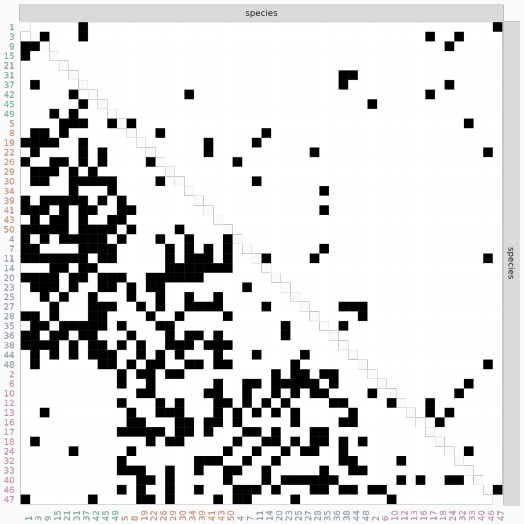


Modelling foodwebs

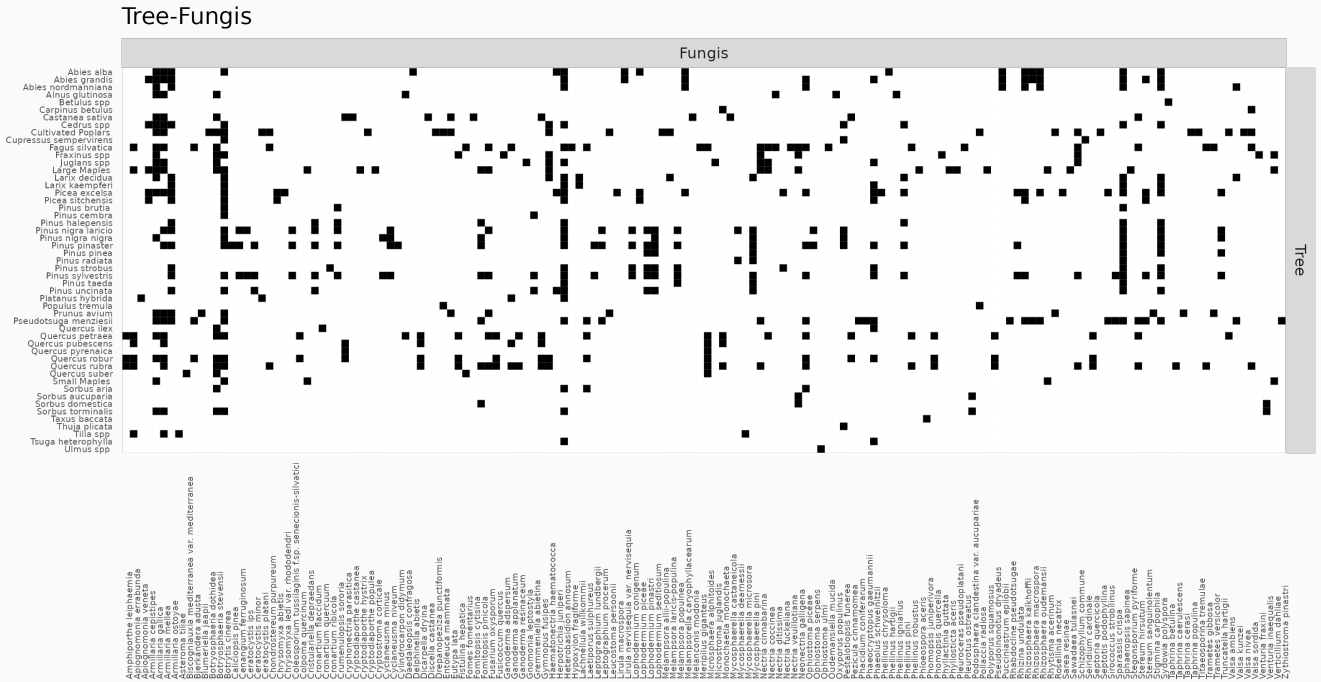
$$\boldsymbol{\alpha} = \begin{pmatrix} 0.10 & 0.02 & 0.02 & 0.02 \\ \underline{0.50} & 0.10 & 0.02 & 0.02 \\ \underline{0.50} & \underline{0.40} & 0.10 & 0.02 \\ 0.02 & \underline{0.40} & \underline{0.40} & 0.10 \end{pmatrix}$$

$$\pi = (0.2, .25, 0.30, 0.25)$$





Probabilistic model for binary bipartite networks



Requires adaptation to bipartite networks: blocks for rows and cols

Probabilistic model for binary bipartite networks

Let Y_{ij} be a bi-partite network. Individuals in row and cols are not the same.

Latent variables : bi-clustering

- Nodes $i = 1, \ldots, n$ partitionned into K clusters, nodes $j = 1, \ldots, p$ partitionned into L clusters
- $$Z_i = k \quad \text{if node } i \text{ belongs to cluster (block) } k$$
  $$W_j = \ell \quad \text{if node } j \text{ belongs to cluster (block) } \ell$$
- $(Z_i)_{i=1,\ldots,n}, (W_j)_{j=1,\ldots,p}$ independent variables

$$\mathbb{P}(Z_i = k) = \pi_k, \quad \mathbb{P}(W_j = \ell) = \rho_\ell$$

Probabilistic model for binary bipartite networks

Conditionally to $(W_i)_{i=1,\dots,n}, (W_j)_{j=1,\dots,p}$...

(Y_{ij}) independent and

$$Y_{ij}|Z_i, W_j \sim \mathcal{B}ern(\alpha_{Z_i,W_j}) \quad \Leftrightarrow \quad \mathbb{P}(Y_{ij} = 1|Z_i = k, W_j = \ell) = \alpha_{k\ell}$$

Also called Latent Block Models [Govaert and Nadif, 2008]

Exercice

Go to the tutorial and simulate networks with your own structures.

Valued-edge networks

Values-edges networks

Information on edges can be something different from presence/absence.
It can be:

1. a count of the number of observed interactions,
2. a quantity interpreted as the interaction strength,

Natural extensions of SBM and LBM

1. Poisson distribution: $Y_{ij} \mid \{i \in \bullet, j \in \bullet\} \sim^{\text{ind}} \mathcal{P}(\lambda_{\bullet\bullet})$,
2. Gaussian distribution: $Y_{ij} \mid \{i \in \bullet, j \in \bullet\} \sim^{\text{ind}} \mathcal{N}(\mu_{\bullet\bullet}, \sigma^2)$, [Mariadassou et al., 2010]
3. More generally,

$$Y_{ij} \mid \{i \in \bullet, j \in \bullet\} \sim^{\text{ind}} \mathcal{F}(\theta_{\bullet\bullet})$$

Multiplex networks

Several kind of interactions between nodes For instance :

- Love and friendship
- Working relations and friendship
- In ecology : mutualistic and competition

Block model for multiplex networks

$Y_{ij} \in \{0,1\}^Q = (Y_{ij}^a, Y_{ij}^b), \forall w \in \{0,1\}^2$

$$\mathbb{P}((Y_{ij}^a, Y_{ij}^b) = w | Z_i = k, Z_j = \ell) = \alpha_{k\ell}^w$$

[Kéfi et al., 2016], [Barbillon et al., 2017]

In R package: sbm when two relations are at stake.

Remark: a particular case of multiplex network is dynamic network, [Matias and Miele, 2017].

Taking into account covariates

Sometimes covariates are available. They may be on:

- nodes,
- edges,
- both.

1. They can be used a posteriori to explain blocks inferred by SBM.
2. Extension of the SBM which takes into account covariates. Blocks are structure of interaction which is not explained by covariates !

If covariates are sampling conditions, case 2 be may more interesting.

SBM with covariates

- As before : (Y_{ij}) be an adjacency matrix
- Let $x^{ij} \in \mathbb{R}^p$ denote covariates describing the pair (i, j)

Latent variables : as before

- The nodes $i = 1, \ldots, n$ are partitioned into K clusters
- Z_i independent variables

$$\mathbb{P}(Z_i = k) = \pi_k$$

Conditionally to $(Z_i)_{i=1,\ldots,n}$...

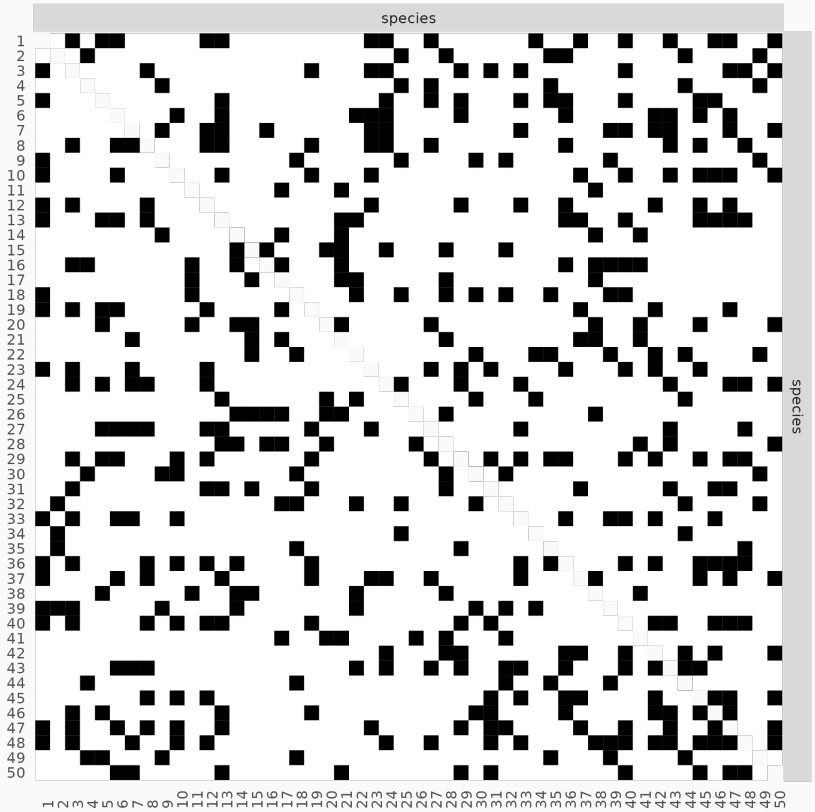
(Y_{ij}) independent and

$$\begin{aligned} Y_{ij}|Z_i, Z_j &\sim \mathcal{B}ern(\text{logit}(\alpha_{Z_i,Z_j} + \theta \cdot x_{ij})) \quad \text{if binary data} \\ Y_{ij}|Z_i, Z_j &\sim \mathcal{P}(\exp(\alpha_{Z_i,Z_j} + \theta \cdot x_{ij})) \quad \text{if counting data} \end{aligned}$$

If $K = 1$: all the connection heterogeneity is explained by the covariates.

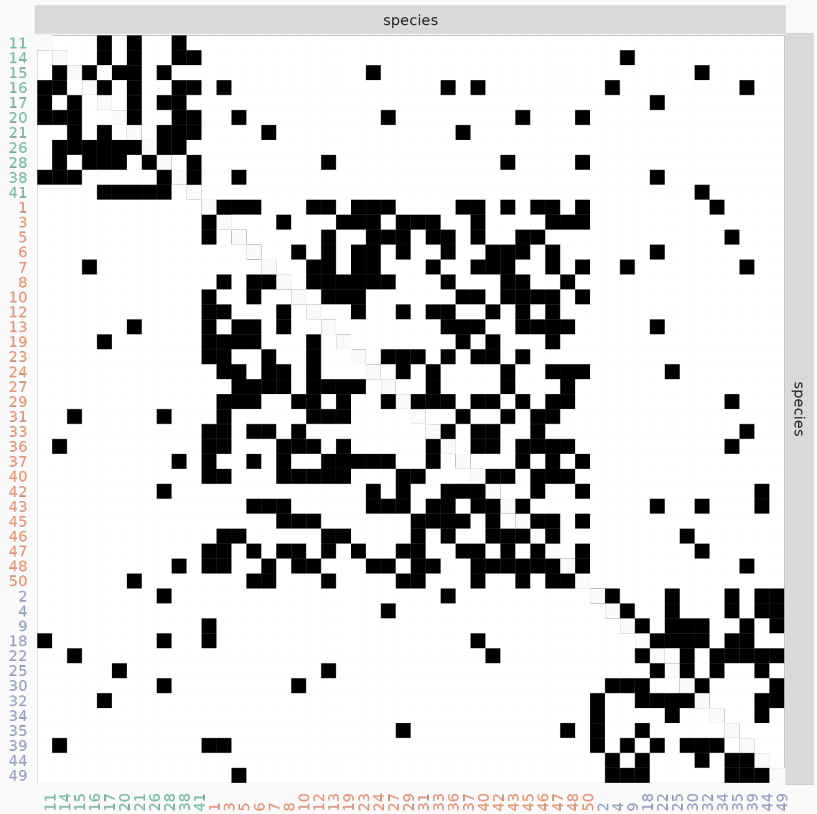
Aim

Going from...



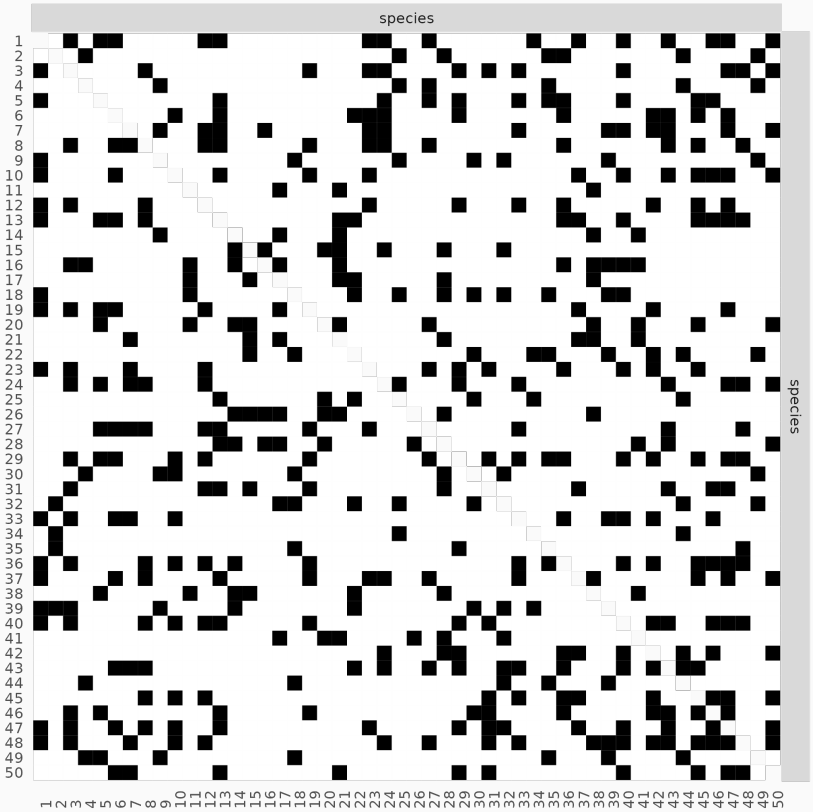
Aim

... to


species
species
11 14 15 16 17 20 21 26 28 38 41 1 3 5 6 7 8 10 12 13 19 23 24 27 29 31 33 36 37 40 42 43 45 46 47 48 50 2 4 9 18 22 25 30 32 34 35 39 44 49

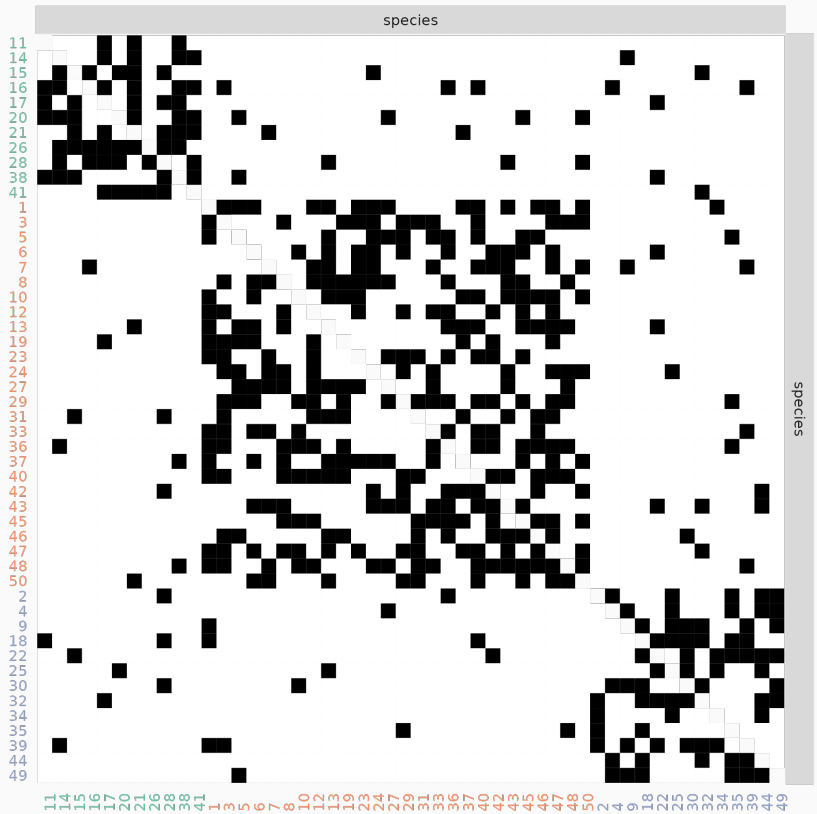
Aim

Going from...



Aim

... to


species
species
11 14 15 16 17 20 21 26 28 38 41 1 3 5 6 7 8 10 12 13 19 23 24 27 29 31 33 36 37 40 42 43 45 46 47 48 50 2 4 9 18 22 25 30 32 34 35 39 44 49

Statistical challlenges

- Selection of the number of clusters
  - K for SBM , K and L for bipartite SBM
- Estimation of the parameters $(\pi, \boldsymbol{\theta})$ for a given number of clusters
- Clustering $\hat{\mathbf{Z}}$

Presented in details for binary SBM.

Likelihood for Bernoulli SBM

Complete likelihood (Y) et (Z)

$$\begin{aligned}
\ell_c(\mathbf{Y}, \mathbf{Z}; \theta) &= p(\mathbf{Y}|\mathbf{Z}; \boldsymbol{\alpha}) p(\mathbf{Z}; \pi) \\
&= \prod_{i \neq j} f_{\alpha_{Z_i, Z_j}}(Y_{ij}) \times \prod_i \pi_{Z_i} \\
&= \prod_{i,j} \alpha_{Z_i, Z_j}^{Y_{ij}} (1 - \alpha_{Z_i, Z_j})^{1 - Y_{ij}} \prod_i \pi_{Z_i}
\end{aligned}$$

Marginal likelihood (Y)

$$\ell(\mathbf{Y}; \theta) = \sum_{\mathbf{Z} \in \mathcal{Z}} \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) \,. \tag{1}$$

$$\log \ell(\mathbf{Y}; \theta) = \log \sum_{\mathbf{Z} \in \mathcal{Z}} \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) \,. \tag{2}$$

Marginal likelihood : remark

$$\log \ell(\mathbf{Y}; \theta) = \log \sum_{\mathbf{Z} \in \mathcal{Z}} \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)\,.$$

Remark

$\mathcal{Z} = \{1, \ldots, K\}^n \Rightarrow$ when K and n increase, impossible to compute.

Standard tool to maximize the likelihood when latent variables involved : EM algorithm.

From EM to variational EM

Standard EM

At iteration (t) :

- **Step E**: compute

$$Q(\theta|\theta^{(t-1)}) = \mathbb{E}_{\mathbf{Z}|\mathbf{Y},\theta^{(t-1)}}\left[\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)\right]$$

- **Step M**:

$$\theta^{(t)} = \arg\max_{\theta} Q(\theta|\theta^{(t-1)})$$

Limitations of standard EM i

Step E requires the computation of $\mathbb{E}_{\mathbf{Z}|\mathbf{Y},\theta^{(t-1)}}[\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)]$

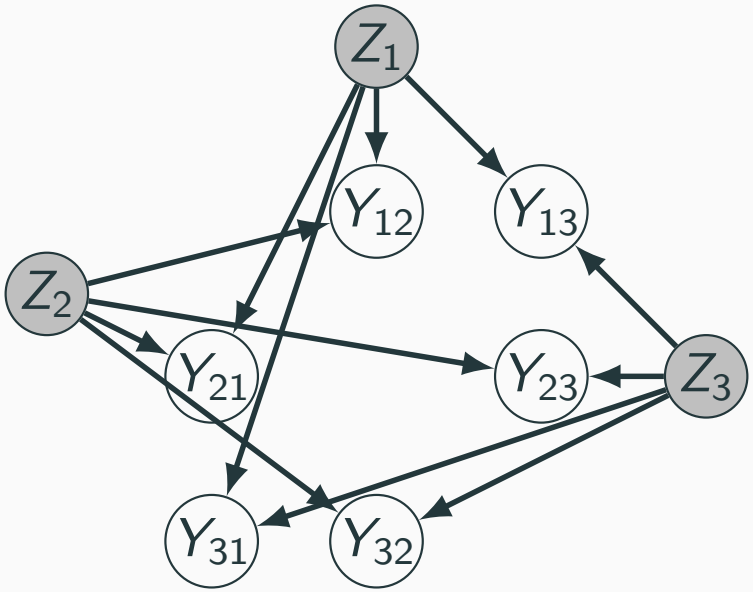
-

$$\begin{aligned}
\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) &= \log\left[\prod_{i \neq j} \alpha_{Z_i, Z_j}^{Y_{ij}} (1 - \alpha_{Z_i, Z_j})^{1 - Y_{ij}}\right] + \log\left[\prod_i \pi_{Z_i}\right] \\
&= \sum_{i \neq j} \sum_{k,\ell=1}^{K} Z_{ik} Z_{j\ell} \left[Y_{ij} \log \alpha_{k\ell} + (1 - Y_{ij}) \log(1 - \alpha_{k\ell})\right] \\
&\quad + \sum_{i,k=1}^{n,K} Z_{ik} \log \pi_k
\end{aligned}$$

with $Z_{ik} = \mathbf{1}_{Z_i = k}$

Limitations of standard EM ii

- However, once conditioned by par $\mathbf{Y}$, the $\mathbf{Z}$ are not independent anymore



$$p(\mathbf{Z}|\mathbf{Y}, \theta^{(t-1)}) \neq \prod_{i=1}^{n} p(Z_i|\mathbf{Y}, \theta^{(t-1)})$$

Variational EM : maximization of a lower bound

Idea : replace the complicated distribution $p(\mathbf{Z}|\mathbf{Y};\theta)$ by a simpler one.

Let $\mathcal{R}_{\mathbf{Y},\tau}$ be any distribution on $\mathbf{Z}$

Central identity

$$\begin{aligned}
\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) &= \log \ell(\mathbf{Y};\theta) - \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, p(\cdot|\mathbf{Y};\theta)] \quad \leq \log \ell(\mathbf{Y};\theta) \\
&= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}\left[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta)\right] - \sum_{\mathbf{Z}} \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}) \log \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}) \\
&= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}\left[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta)\right] + \mathcal{H}\left(\mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z})\right)
\end{aligned}$$

Note that:

$$\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) = \log \ell(\mathbf{Y};\theta) \Leftrightarrow \mathcal{R}_{\mathbf{Y},\tau} = p(\cdot|\mathbf{Y};\theta)$$

⏩ skip mathematicals details on VEM

Proof i

By Bayes

$$\begin{aligned} \log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) &= \log p(\mathbf{Z}|\mathbf{Y}; \theta) + \log \ell(\mathbf{Y}; \theta) \\ \log \ell(\mathbf{Y}; \theta) &= \log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) - \log p(\mathbf{Z}|\mathbf{Y}; \theta) \end{aligned}$$

By integration against $\mathcal{R}_{\mathbf{Y},\tau}$:

$$\begin{aligned} \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \ell(\mathbf{Y}; \theta)] &= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log p(\mathbf{Z}|\mathbf{Y}; \theta)] \\ \log \ell(\mathbf{Y}; \theta) &= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log p(\mathbf{Z}|\mathbf{Y}; \theta)] \end{aligned}$$

Proof ii

As a consequence:

$$
\begin{aligned}
\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) &= \log \ell(\mathbf{Y};\theta) - \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, p(\cdot|\mathbf{Y};\theta)] \\
&= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log p(\mathbf{Z}|\mathbf{Y};\theta)] \\
&\quad -\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}\left[\log \frac{\mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z})}{p(\mathbf{Z}|\mathbf{Y};\theta)}\right] \\
&= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log p(\mathbf{Z}|\mathbf{Y};\theta)] \\
&\quad \underbrace{-\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z})]}_{\mathcal{H}(\mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}))} + \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log p(\mathbf{Z}|\mathbf{Y};\theta)]
\end{aligned}
$$

Variational EM

- Maximization of $\log \ell(\mathbf{Y}; \theta)$ w.r.t. θ replaced by maximization of the lower bound $\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau})$ w.r.t. τ and θ.
- **Benefit** : we choose $\mathcal{R}_{\mathbf{Y},\tau}$ such that the maximization calculus can be done explicitly
  - In our case: mean field approximation : neglect dependencies between the (Z_i)

$$P_{\mathcal{R}_{\mathbf{Y},\tau}}(Z_i = k) = \tau_{ik}$$

Variational EM

Algorithm

At iteration (t), given the current value $(\theta^{(t-1)}, \mathcal{R}_{\mathbf{Y},\tau^{(t-1)}})$,

- **Step 1 (VE)** Maximization w.r.t. τ

$$\begin{aligned}\tau^{(t)} &= \arg\max_{\tau\in\mathcal{T}} \mathcal{I}_{\theta^{(t-1)}}(\mathcal{R}_{\mathbf{Y},\tau}) \\ &= \arg\max_{\tau\in\mathcal{T}} \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}\left[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta^{(t-1)})\right] + \mathcal{H}\left(\mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z})\right)\end{aligned}$$

Note that

$$\begin{aligned}\tau^{(t)} &= \arg\max_{\tau\in\mathcal{T}} \log \ell(\mathbf{Y};\theta^{(t-1)}) - \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, p(\cdot|\mathbf{Y};\theta^{(t-1)})] \\ &= \arg\min_{\tau\in\mathcal{T}} \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, p(\cdot|\mathbf{Y};\theta^{(t-1)})]\end{aligned}$$

Variational EM

Algorithm

- **Step 2 (M)** Maximization w.r.t. θ

$$\begin{aligned}
\theta^{(t)} &= \arg\max_{\theta} \mathcal{I}_{\theta}(\mathcal{R}_{\mathbf{Y},\tau^{(t)}}) \\
&= \arg\max_{\theta} \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau^{(t)}}} [\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)] + \mathcal{H}\left(\mathcal{R}_{\mathbf{Y},\tau^{(t)}}(\mathbf{Z})\right) \\
&= \arg\max_{\theta} \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau^{(t)}}} [\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta)]
\end{aligned}$$

Details of the VE-step for binary SBM i

$$\tau^{(t)} = \arg\min_{\tau} \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, p(\cdot|\mathbf{Y}; \theta^{(t-1)})] = \arg\max_{\tau} \mathcal{I}_{\theta^{(t-1)}}(\mathcal{R}_{\mathbf{Y},\tau}) \,.$$

(we drop out the index $^{(t-1)}$ on θ)

$$\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) \quad = \quad \sum_{\mathbf{Z}} \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}) \log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) - \sum_{\mathbf{Z}} \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}) \log \mathcal{R}_{\mathbf{Y},\tau}(\mathbf{Z}) \,,$$

with

$$\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) \quad = \quad \sum_{i,j=1, i\neq j}^{n} \sum_{k,\ell=1}^{K} Z_{ik} Z_{j\ell} \log p(Y_{ij}|\alpha_{k\ell}) + \sum_{i=1}^{n} \sum_{k=1}^{K} Z_{ik} \log \pi_k$$

Details of the VE-step for binary SBM ii

Integration of the $\mathbf{Z}$ where $\mathbf{Z} \sim \mathcal{R}_{\mathbf{Y},\tau}$

$$\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) = \sum_{i,j=1,i\neq j}^{n} \sum_{k,\ell=1}^{K} \tau_{iq}\tau_{j\ell} \log p(Y_{ij}|\alpha_{k\ell}) + \sum_{i=1}^{n}\sum_{k=1}^{K} \tau_{ik} \log \pi_k$$

Maximization under the constraint: $\forall i = 1 \dots n$, $\sum_{k=1}^{K} \tau_{ik} = 1$.

- Derivatives of

$$\mathcal{I}_\theta(\mathcal{R}_{\mathbf{Y},\tau}) + \sum_{i=1}^{n} \lambda_i \left[\sum_{k=1}^{K} \tau_{ik} - 1 \right]$$

with respect to $(\lambda_i)_{i=1\dots n}$ and $(\tau_{ik})_{i=1\dots n, k=1\dots K}$ where λ_i are the Lagrange multipliers,

Details of the VE-step for binary SBM iii

- Leads to collection of equations: for $i = 1 \dots n$ and $k = 1 \dots K$,

$$\sum_{\ell=1}^{K} \sum_{j=1, j \neq i}^{n} \log p(Y_{ij} | \alpha_{k\ell}) \tau_{j\ell} + \log \pi_k - \log \tau_{ik} + 1 + \lambda_i = 0 \,,$$

- Leads to the following fixed point problem:

$$\widehat{\tau}_{ik} = e^{1+\lambda_i} \alpha_k \prod_{j=1, j \neq i}^{n} \prod_{\ell=1}^{K} p(Y_{ij} | \alpha_{k\ell})^{\widehat{\tau}_{j\ell}}, \quad \forall i = 1 \dots n, \forall k = 1 \dots K \,,$$

which has to be solved under the constraints $\forall i = 1 \dots n$, $\sum_{k=1}^{K} \tau_{ik} = 1$. This optimization problem is solved using a standard fixed point algorithm.

Details of the M-step for binary SBM i

$$\theta^{(t)} = \arg\max_{\theta} \mathcal{I}_{\theta^{(t)}}\left(\mathcal{R}_{\mathbf{Y},\tau^{(t)}}\right)$$

under the constraints: $\sum_{k=1}^{k} \pi_k = 1$.

Maximization with respect to π is quite direct:

$$\widehat{\pi}_q = \frac{1}{n}\sum_{i=1}^{n} \widehat{\tau}_{ik}$$

For the Bernoulli SBM:

$$\widehat{\alpha}_{k\ell} = \frac{\sum_{i,j=1,i\neq j}^{n} \widehat{\tau}_{ik}\widehat{\tau}_{j\ell}\, Y_{ij}}{\sum_{i,j=1,i\neq j}^{n} \widehat{\tau}_{ik}\widehat{\tau}_{j\ell}}$$

Details of the M-step for binary SBM ii

If the edge probabilities depend on covariates:

$$\text{logit}(p_{k\ell}) = \alpha_{k\ell} + \beta \cdot x_{ij} \,,$$

then the optimization of $(\alpha_{k\ell})$ and (β) at step M of the VEM is not explicit anymore and one should resort to optimization algorithms such as Newton-Raphson algorithm.

In practice

- Non stochastic algorithm
- Really fast
- Strongly depends on the initial values
- Asymptotic theoretical properties of the variational estimators

Output

For a given number of blocks K:

- $\widehat{\theta}_K$
- $\widehat{\tau}_{ik} \approx P(Z_i = k|\mathbf{Y}, \widehat{\theta}_K)$
- $$\hat{Z}_i = \underset{k \in \{1,\dots,K\}}{\arg\max}\ \hat{\tau}_{ik}$$
- Hopefully : you can reorder the matrix according to the block affectations and see a structure appearing.

Selecting the number of blocks

- The number of parameters increases with K

$$nb(K) = \underbrace{K-1}_{\text{block. prop}} + \underbrace{\frac{K(K+1)}{2}}_{\alpha_{k\ell}}$$

  (for undirected network)
- The fit of the model to the data is better with large K

$$\log \ell(\mathbf{Y}; \widehat{\theta}_K)$$

- Balance between complexity and fit: penalized likelihood criterion

$$\text{Crit}(K) = \log \ell(\mathbf{Y}; \widehat{\theta}_K) - \text{pen}(\mathcal{M}_K)$$

  - Cf : AIC, BIC, ...
  - Penalty is such that we have asymptotic guaranties to select the "true" model

In our model

- Unable to compute the marginal likelihood but able to compute the complete likelihood
- BIC on the complete likelihood

$$\log \ell_c(\mathbf{Y}, \mathbf{Z}; \hat{\theta}_{\mathbf{K}}) - \mathrm{pen}(\mathcal{M}_{\mathbf{K}})$$

- See after for the expression of the penalty term
- But : Z unknown

ICL criterion

- Integrated Classification Likelihood (ICL) [Biernacki et al., 2000]

$$ICL(\mathcal{M}_{\mathbf{K}}) = \log \ell_c(\mathbf{Y}, \hat{\mathbf{Z}}; \hat{\theta}_{\mathbf{K}}) - \mathrm{pen}(\mathcal{M}_{\mathbf{K}})$$

where

$$\hat{Z}_i = \underset{k \in \{1,\dots,K\}}{\arg\max}\ \hat{\tau}_{ik}.$$

- Integrated Complete Likelihood (ICL)

$$ICL(\mathcal{M}_{\mathbf{K}}) = \mathbb{E}_{p(\cdot|\mathbf{Y},\hat{\theta}_{\mathbf{K}})}[\log \ell_c(\mathbf{Y}, \mathbf{Z}; \hat{\theta}_{\mathbf{K}})] - \mathrm{pen}(\mathcal{M}_{\mathbf{K}})$$

Expression of the penalization for SBM

- For directed network

$$pen_{\mathcal{M}} = \frac{1}{2}\left\{(K-1)\log(n) + K^2 \log\left(n^2 - n\right)\right\}$$

- For undirected network

$$pen_{\mathcal{M}} = \frac{1}{2}\left\{\underbrace{(K-1)\log(n)}_{\text{Clust.}} + \frac{K(K+1)}{2}\log\left(\frac{n^2-n}{2}\right)\right\}$$

Expression of the penalization for bipartite SBM

$$pen_{\mathcal{M}} = -\frac{1}{2}\left\{ \underbrace{(K-1)\log(n) + (L-1)\log(p)}_{\text{Bi-Clust.}} + \underbrace{(KL)\log(np)}_{\text{Connection}} \right\}$$

Advantages of ICL

- its capacity to outline the clustering structure in networks
- Involves a trade-off between goodness of fit and model complexity
- ICL values : goodness of fit AND clustering sharpness.

Algorithm in practice

- Going trough the models and initiate VEM at the same time
- Bounds on K : $\{K_{\text{min}}, \ldots, K_{\text{max}}\}$

Stepwise procedure

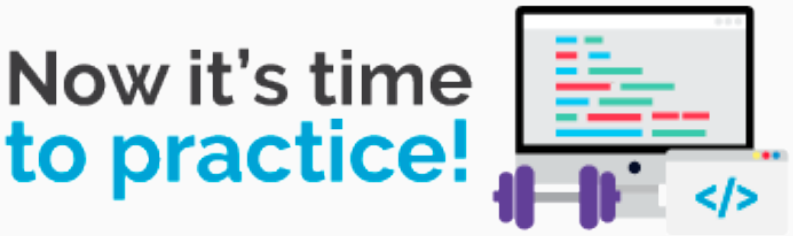
Starting from K

- **Split** : if $K < K_{\text{max}}$
  - Maximize the likelihood (lower bound) of $\mathcal{M}_{K+1}$
  - K initializations of the VEM are proposed : split each cluster into 2 clusters
- **Merge** : If $K > K_{\text{min}}$
  - Maximize the likelihood (lower bound) of model $\mathcal{M}_{K-1}$
  - $\frac{K(K-1)}{2}$ initializations of the VEM are proposed : merging all the possible pairs of clusters

Theoretical properties for SBM

- Identifiability and a first consistency result by [Celisse et al., 2012]
- Consistency of the posterior distribution of the latent variables [Mariadassou and Matias, 2015]
- Consistency and properties of the variational estimators [Bickel et al., 2013]

Exercice



- Go back to the tutorial and estimate the parameters of your simulated networks.
- Do you obtain the same clusters?
- Decrease the number of nodes. What do you expect?

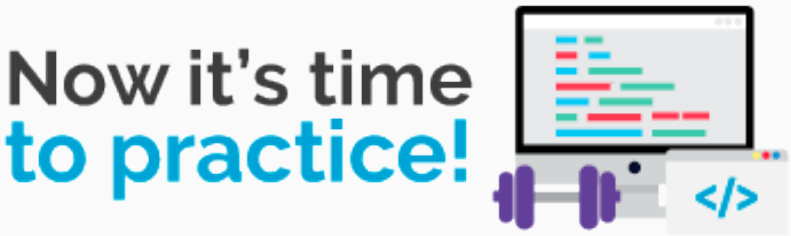
Other extensions

- Time evolving networks Matias
- Multipartite, Multiplexe networks (R-package sbm, Bar-Hen, Barbillon, Donnet)
- Multilevel networks (individuals and organizations) (Chabbert-Liddell)
- Missing data in the network [Tabouy et al., 2019]

Probabilistic model for networks in a nutshell

SBM/LBM

- generative models,
- flexible,
- comprehensive models which can be linked to a lot of classical descriptors.



Comprehensive R package available on CRAN and Github gathering several block models and there in references with vignettes.

https://grosssbm.github.io/sbm/

Illustration from there

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