Latent variable models in biology and ecology

Chapter 4: Stochastic Block Models and Latent Block Models

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Network data

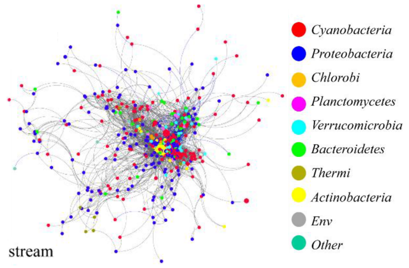
Networks can account for

- **Ecological networks** : Food web, Co-existence networks, Host-parasite interactions, Plant-pollinator interactions,
- **Social networks**
- **Inventory datasets**
- ...

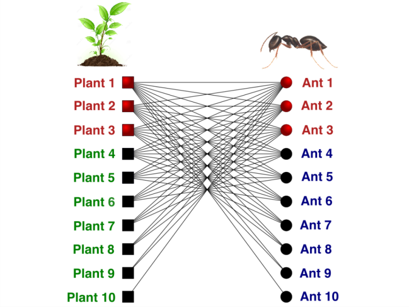
Bipartite / simple network

Networks may be or not bipartite: Interactions between nodes belonging to the same or to different functional group(s).

Simple network



Bipartite network



Terminology

A network consists in:

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

A network may be

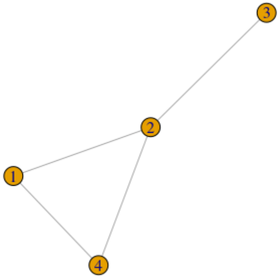
- directed / oriented (e.g. food web...),
- symmetric / undirected (e.g. coexistence network),
- with or without loops.

This distinction only makes sense for simple networks (not bipartite).

Network representation and adjacency matrix

For a non-directed network

$$Y = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

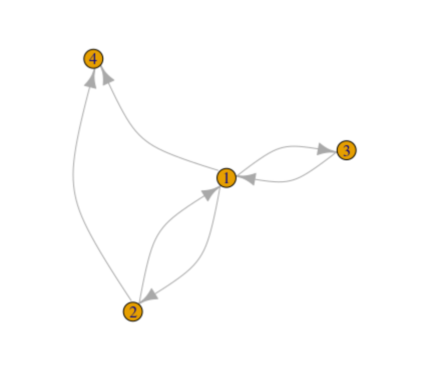


- n rows and n columns,
- symmetric matrix

Network representation and adjacency matrix

For a directed network

$$Y = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

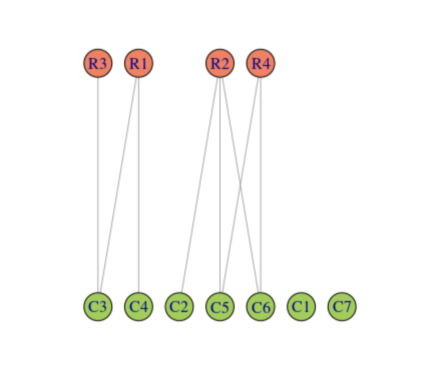


- n rows and n columns,
- non symmetric matrix

Bipartite network and incidence matrix

$$Y = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

- n rows and m columns, rectangular matrix.



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.

Goal

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

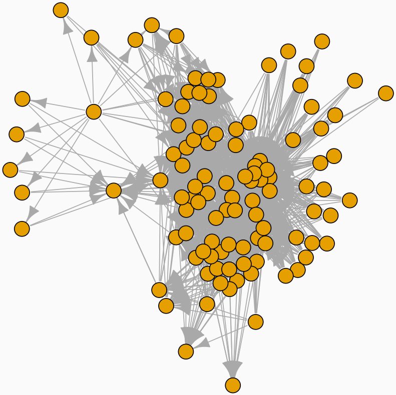
Network analysis

Aim : give a short description of the network, give a hint about its structure, look for heterogeneity in the connections

- Many metrics supplied for simple networks
- Have been extended to bipartite networks

Example : Chilean foodweb

[Kéfi et al., 2016]



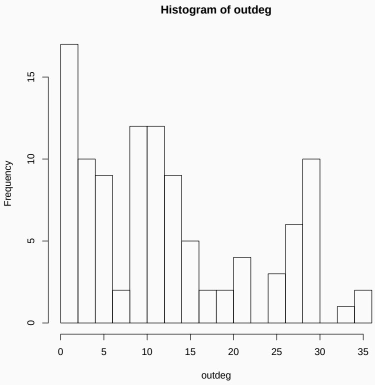
Degree

$$\begin{array}{rclrcl} \deg(u) & = & \sum_{v \in V}(u \leftrightarrow v), & \deg(v) & = & \sum_{u \in U}(u \leftrightarrow v) \\ \deg_i & = & \sum_{j=1}^{|V|} Y_{ij} & \deg_j & = & \sum_{i=1}^{|U|} Y_{ij} \end{array}$$

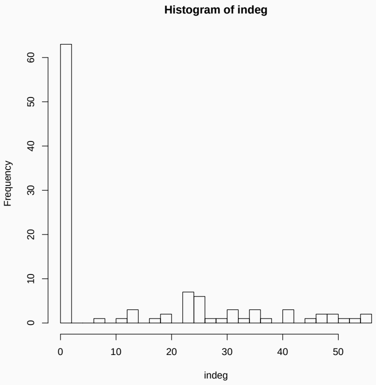
- Nodes with high degree are hubs
- Nodes with null degree are isolated
- If edges are oriented : in- and out- degrees can be computed.

Degrees on Chilean foodweb

Out degree distribution



In degree distribution



Closeness centrality

Property on a node

Definition

Determine whether a node can communicate with other nodes of the network directly or through the short paths.

$$C(u) = \frac{1}{\sum_{w \in U \cup V} d(u, w)}$$

where $d(u, w)$ is the length of the shortest path between u and w (through the network).

Note that, for bipartite networks

- A node $u \in U$ can have a minimum distance of 1 with $v \in V$.
- A node $u \in U$ can have a minimum distance of 2 with $u' \in U$.
- All paths between nodes of the same set are of even length.

Betweenness centrality

Property on a node

Definition

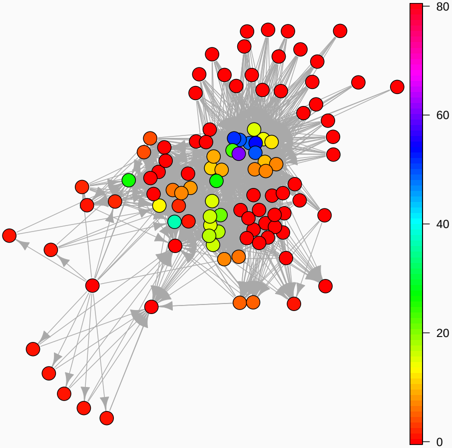
Betweenness centrality quantifies the number of times a node acts as a bridge along the shortest path between two other nodes.

The betweenness of a vertex v is computed as follows.

- For each pair of vertices (w, w'), compute the shortest paths between them. $\delta_{w,w'}$ is the number of shortest paths between (w, w')
- For each pair of vertices (w, w'), determine the fraction of shortest paths that pass through v : $\frac{\delta_{w,w'}(v)}{\delta_{w,w'}}$
- Sum this fraction over all pairs of vertices (w, w').

$$B(v) = \sum_{w \neq w' \neq v} \frac{\delta_{w,w'}(v)}{\delta_{w,w'}}$$

Betweenness centrality



Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
0.000	0.000	0.000	6.604	6.929	59.570

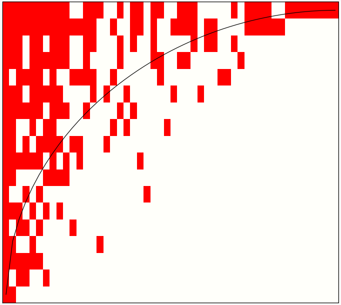
Nestedness

Property on the network

Definition

- Important property in ecology
- Defined as a pattern of interactions in which specialists (e.g. pollinators that visit few plant species) interact with plants that are visited by generalists.
- Mathematically, looking for a reordering of rows and columns such that Y is nested

Nestedness



- more generally used on incidence matrices,
- significance of the nestedness index computed by random permutations of the matrix,
- this food web is found to be nested.

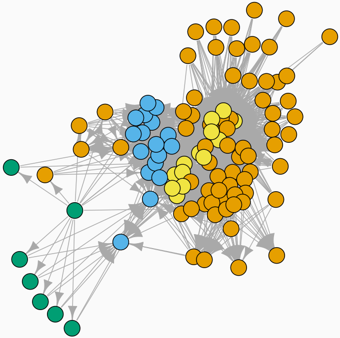
Modularity

Property on the network

Definition

Existence of clusters (blocks, module, communities) where nodes are much more connected than with other clusters

Modularity



1	2	3	4
69	17	7	13
- very low modularity.

Probabilistic approach

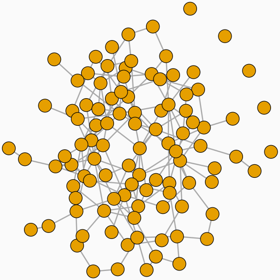
- Context: our matrix Y is the realization of a stochastic process.
- Aim: Propose a stochastic process is able to mimic heterogeneity in the connections.
- Advantage: benefit from the statistical tools (tests, model selection, etc...)

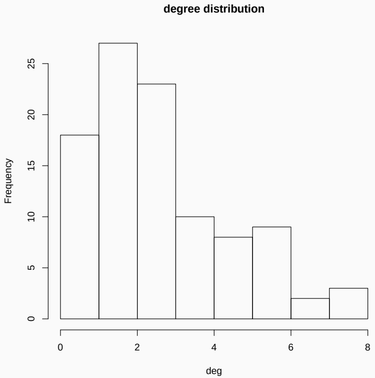
A first random graph model for network: null model

[Erdös and Rényi, 1959] Model for n nodes

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

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





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

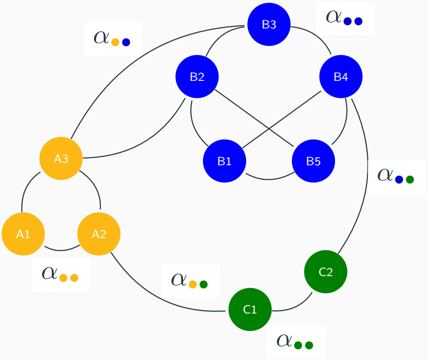
$$\mathbb{P}(Z_i = k) = \pi_k$$

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

(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



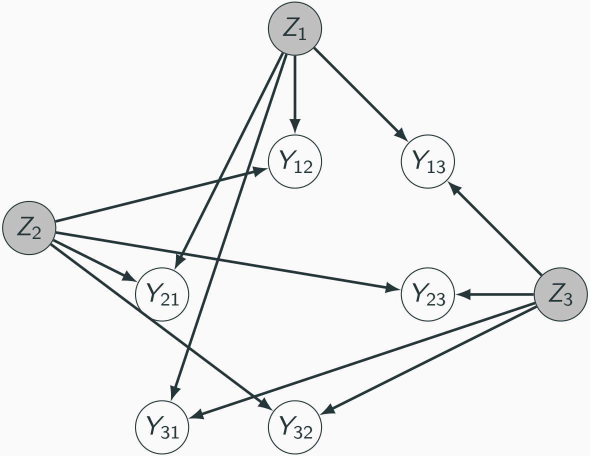
Parameters

Let n nodes divided into 3 clusters

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

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

DAG of the model

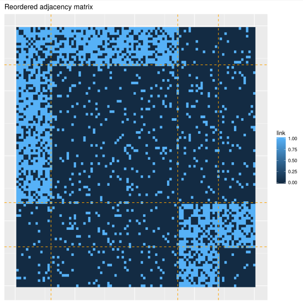


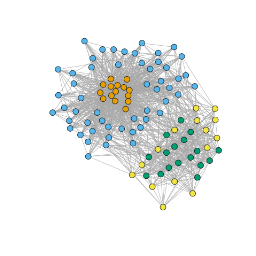
SBM : A great generative model

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

Networks with hubs generated by SBM

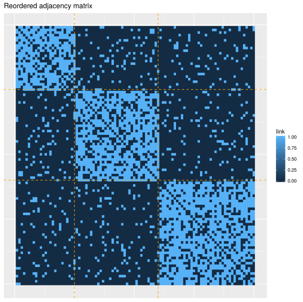
- $\pi = c(.15, .35, .15, .35)$
- $\alpha = \begin{pmatrix} 0.80 & 0.80 & 0.20 & 0.20 \\ 0.80 & 0.20 & 0.20 & 0.20 \\ 0.20 & 0.20 & 0.80 & 0.80 \\ 0.20 & 0.20 & 0.80 & 0.20 \end{pmatrix}$

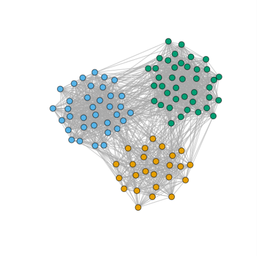




Community network generated by SBM

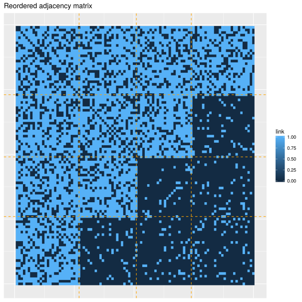
- $\pi = c(0.25, 0.35, 0.40)$
- $\alpha = \begin{pmatrix} 0.80 & 0.20 & 0.20 \\ 0.20 & 0.80 & 0.20 \\ 0.20 & 0.20 & 0.80 \end{pmatrix}$

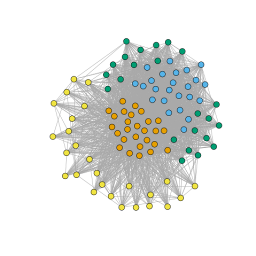




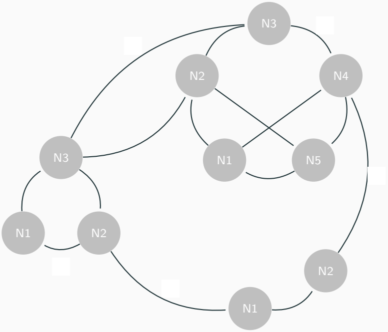
Nestedness generated by SBM

- $\pi = c(.15, .35, .15, .35)$
- $\alpha = \begin{pmatrix} 0.80 & 0.80 & 0.80 & 0.80 \\ 0.80 & 0.80 & 0.80 & 0.20 \\ 0.20 & 0.80 & 0.20 & 0.80 \\ 0.80 & 0.20 & 0.20 & 0.20 \end{pmatrix}$





Statistical inference



Stochastic Block Model

Let *n* nodes divided into

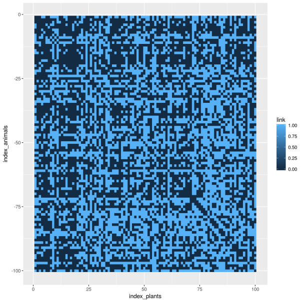
- $\mathcal{K} = \{\color{orange}{\bullet}, \color{blue}{\bullet}, \color{green}{\bullet}\}$, card($\mathcal{K}$) known
- $\pi_{\bullet} = ?$,
- $\alpha_{\color{orange}{\bullet}\color{blue}{\bullet}} = ?$

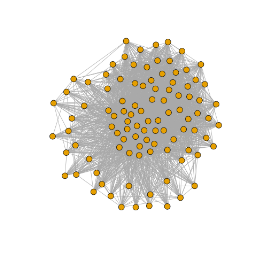
[Nowicki and Snijders, 2001], [Daudin et al., 2008]

R package: blockmodels, sbm

Statistical inference

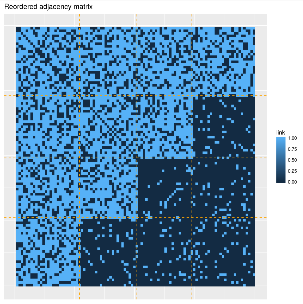
From....

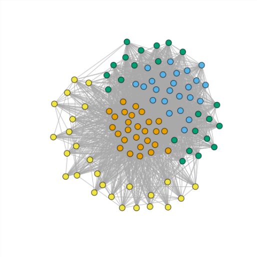




Statistical inference

... to





Tasks

- Find the clusters
- Find the number of clusters
- Practical implementation
- Theoretical results

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 $i = 1, \ldots, n_1$ partitionned into K_1 clusters, nodes $j = 1, \ldots, n_2$ partitionned into K_2 clusters
- $$\begin{array}{ll} Z_i^1 = k & \text{if node } i \text{ belongs to cluster (block) } k \\ Z_j^2 = \ell & \text{if node } j \text{ belongs to cluster (block) } \ell \end{array}$$
- Z_i^1, Z_j^2 independent variables

$$\mathbb{P}(Z_i^1 = k) = \pi_k^1, \quad \mathbb{P}(Z_j^2 = \ell) = \pi_\ell^2$$

Probabilistic model for binary bipartite networks

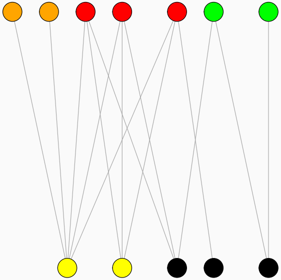
Conditionally to $(Z_i^1)_{i=1,\dots,n_1}, (Z_j^2)_{j=1,\dots,n_2}$**...**

(Y_{ij}) independent and

$$Y_{ij}|Z_i^1, Z_j^2 \sim \mathcal{B}ern(\alpha_{Z_i^1,Z_j^2}) \quad \Leftrightarrow \quad \mathbb{P}(Y_{ij} = 1|Z_i^1 = k, Z_j^2 = \ell) = \alpha_{k\ell}$$

[Govaert and Nadif, 2008]

Latent Block Model : illustration



Latent Block Model

- n_1 row nodes $\mathcal{K}_1 = \{\textcolor{red}{\bullet}, \textcolor{orange}{\bullet}, \textcolor{green}{\bullet}\}$ classes
- $\pi^1_\bullet = \mathbb{P}(i \in \bullet)$, $\bullet \in \mathcal{K}_1, i = 1, \dots, n$
- n_2 column nodes $\mathcal{K}_2 = \{\textcolor{yellow}{\bullet}, \bullet\}$ classes
- $\pi^2_\bullet = \mathbb{P}(j \in \bullet)$, $\bullet \in \mathcal{K}_2, j = 1, \dots, m$
- $\alpha_{\textcolor{red}{\bullet}\textcolor{yellow}{\bullet}} = \mathbb{P}(i \leftrightarrow j | i \in \textcolor{red}{\bullet}, j \in \textcolor{yellow}{\bullet})$

$$
\begin{aligned}
Z^1_i = \mathbf{1}_{\{i \in \bullet\}} &\sim^{\text{iid}} \mathcal{M}(1, \boldsymbol{\pi}^1), \quad \forall \bullet \in \mathcal{Q}_1, \\
Z^2_j = \mathbf{1}_{\{j \in \bullet\}} &\sim^{\text{iid}} \mathcal{M}(1, \boldsymbol{\pi}^2), \quad \forall \bullet \in \mathcal{Q}_2, \\
Y_{ij} \mid \{i \in \textcolor{red}{\bullet}, j \in \textcolor{yellow}{\bullet}\} &\sim^{\text{ind}} \mathcal{B}ern(\alpha_{\textcolor{red}{\bullet}\textcolor{yellow}{\bullet}})
\end{aligned}
$$

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

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

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: blockmodels, 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 $i = 1, \dots, n$ are partitioned into K clusters
- Z_i independent variables

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

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

(Y_{ij}) independent and

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

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

Statistical Inference

- Selection of the number of clusters K for SBM or K_1, K_2 for LBM
- Estimation of the parameters $\pi, \boldsymbol{\theta}$ for a given number of clusters
- Clustering $\hat{\mathbf{Z}}$

Likelihood for SBM

For directed network .

Complete likelihood $(\mathbf{Y})$ et $(\mathbf{Z})$

$$
\begin{aligned}
\ell_c(\mathbf{Y},\mathbf{Z};\theta) &= p(\mathbf{Y}|\mathbf{Z};\boldsymbol{\alpha})p(\mathbf{Z};\boldsymbol{\pi}) \\
&= \prod_{(i\neq j)=1}^{n} f_{\alpha_{Z_i,Z_j}}(Y_{ij}) \times \prod_{i=1}^{n} \pi_{Z_i} \\
&= \prod_{(i\neq j)=1}^{n} \prod_{k=1}^{K} \prod_{\ell=1}^{K} \left(f_{\alpha_{k,\ell}}(Y_{ij})\right)^{\mathbf{1}_{Z_i=k}\mathbf{1}_{Z_j=\ell}} \times \prod_{i=1}^{n} \prod_{k=1}^{K} (\pi_k)^{\mathbf{1}_{Z_i=k}}
\end{aligned}
$$

Marginal likelihood $(\mathbf{Y})$

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

Marginal likelihood : remark

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

Remark

$\mathcal{Z} = \{1,\dots,K\}^n \Rightarrow$ 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) :

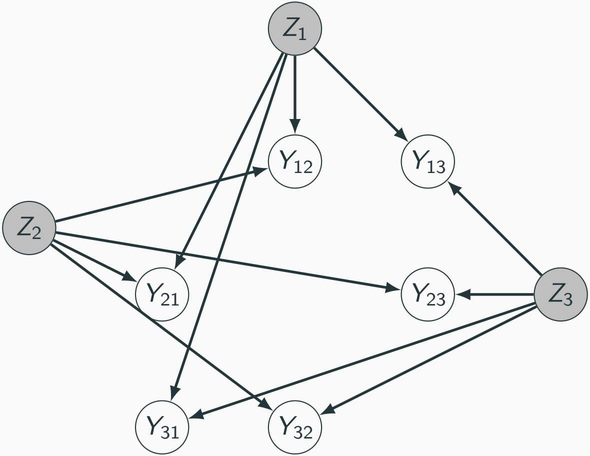
- **Step E**: compute

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

- **Step M**:

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

Limitations of standard EM



- Step E requires the computation of $\mathbb{E}_{\mathbf{Z}|\mathbf{Y},\theta^{(t-1)}}\left[\log \ell_c(\mathbf{Y},\mathbf{Z};\theta)\right]$
- However, once conditioned by par $\mathbf{Y}$, the $\mathbf{Z}$ are not independent anymore: complex distribution if K and n big.

Variational EM : maximization of a lower bound

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

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

Central identity

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

Note that:

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

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

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

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 VE** Maximization w.r.t. τ

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

Variational EM

Algorithm

- **Step M** Maximization w.r.t. θ

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

VE-step for 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)

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

VE-step for SBM ii

with

$$\begin{aligned}
\log \ell_c(\mathbf{Y}, \mathbf{Z}; \theta) &= \log p(\mathbf{Y}|\mathbf{Z}; \theta) + \log p(\mathbf{Z}; \theta)\,, \\
&= \sum_{i,j=1, i\neq j}^{n} \log p(Y_{ij}|Z_i, Z_j; \theta) + \sum_{i=1}^{n} \log \pi_{Z_i}\,. \\
&= \sum_{i,j=1, i\neq j}^{n} \sum_{k,\ell=1}^{K} Z_{ik} Z_{j\ell} \log p(Y_{ij}|\alpha_{k\ell}) + \sum_{i=1}^{n} \sum_{k=1}^{K} Z_{ik} \log \pi_k
\end{aligned}$$

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

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

VE-step for SBM iii

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

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

VE-step for SBM iv

- 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.

M-step for SBM i

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

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

Maximization with respect to $\boldsymbol{\pi}$ is quite direct:

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

For the Bernoulli SBM:

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

M-step for SBM ii

If the edge probabilities depend on covariates:

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

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

- Really fast
- Strongly depend on the initial values

Penalized likelihood criterion

- Selection of the number of clusters K (or K_1, K_2 in the LBM)
- Integrated Classification Likelihood (ICL) [Biernacki et al., 2000]

$$ICL(\mathcal{M}_{\mathbf{K}}) = \log \ell_c(\mathbf{Y}, \hat{\mathbf{Z}}; \hat{\theta}_{\mathbf{K}}) - \mathrm{pen}(\mathcal{M}_{\mathbf{K}}) \tag{2}$$

where

$$\hat{Z}_i = \underset{k \in \{1,\ldots,K\}}{\arg\max}\ \hat{\tau}_{ik}. \tag{3}$$

- Integrated Complete Likelihood (ICL)

$$ICL(\mathcal{M}_{\mathbf{K}}) = \mathbb{E}_{p(\cdot|\mathbf{Y},\hat{\theta}_{\mathbf{K}})}[\log \ell_c(\mathbf{Y}, \hat{\mathbf{Z}}; \hat{\theta}_{\mathbf{K}}) - \mathrm{pen}(\mathcal{M}_{\mathbf{K}}) \tag{4}$$

Expression of the penalization

For SBM

$$pen_{\mathcal{M}} = \begin{cases} -\frac{1}{2}\left\{(K-1)\log(n) + K^2\log\left(n^2-n\right)\right\} & \text{for directed network} \\ -\frac{1}{2}\left\{\underbrace{(K-1)\log(n)}_{\text{Clust.}} + \frac{K(K+1)}{2}\log\left(\frac{n^2-n}{2}\right)\right\} & \text{for undirected network} \end{cases}$$

For LBM

$$pen_{\mathcal{M}} = -\frac{1}{2}\left\{\underbrace{(K_1-1)\log(n_1) + (K_2-1)\log(n_2)}_{\text{Bi-Clust.}} + \underbrace{(K_1K_2)\log(n_1n_2)}_{\text{Connection}}\right\}$$

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.

Comments on the ICL versus BIC

Conjecture

$$BIC(\mathcal{M}) \quad = \quad \log \ell(\mathbf{Y}; \hat{\theta}, \mathcal{M}) - \mathrm{pen}(\mathcal{M})$$

with the same penalty

- Under this conjecture

$$\begin{aligned} ICL(\mathcal{M}) \quad &= \quad BIC(\mathcal{M}) + \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{Y}; \hat{\theta}_{\mathbf{K}}) \log p(\mathbf{Z}|\mathbf{Y}; \hat{\theta}_{\mathbf{K}}) \\ &= \quad BIC(\mathcal{M}) - \mathcal{H}(p(\cdot|\mathbf{Y}; \theta)) \end{aligned}$$

- As a consequence, because of the entropy, ICL will encourage clustering with well-separated groups
-

$$\widehat{ICL}(\mathcal{M}) = BIC(\mathcal{M}) + \sum_{\mathbf{Z}} \mathcal{R}_{\mathbf{Y}}(\mathbf{Z}, \widehat{\tau}) \log \mathcal{R}_{\mathbf{Y}, \widehat{\tau}}(\mathbf{Z}) - \mathbf{KL}[\mathcal{R}_{\mathbf{Y}, \widehat{\tau}}, p(\cdot|\mathbf{Y}; \widehat{\theta})] \,.$$

Algorithm in practice

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

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]

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,

Probabilistic model for networks in a nutshell

SBM/LBM

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

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