

Stochastic block models for networks

Applications in ecology

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On the R packages



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sbm

sbm

blockmodels

colSBM

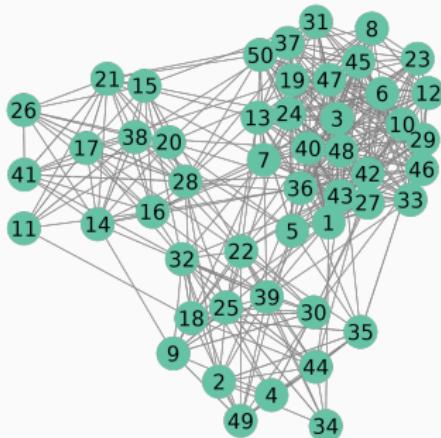
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1. Introduction
2. Probabilistic model
3. Inference

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

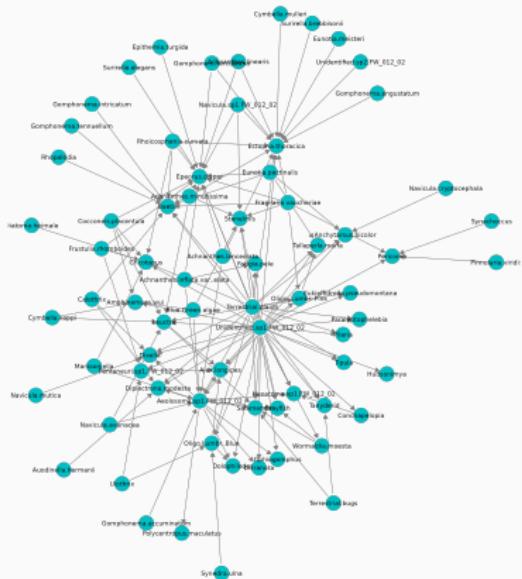


Pollination



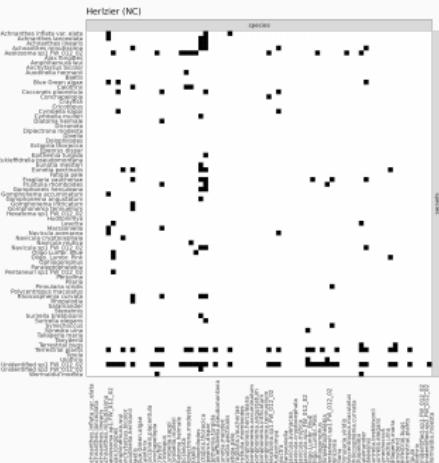
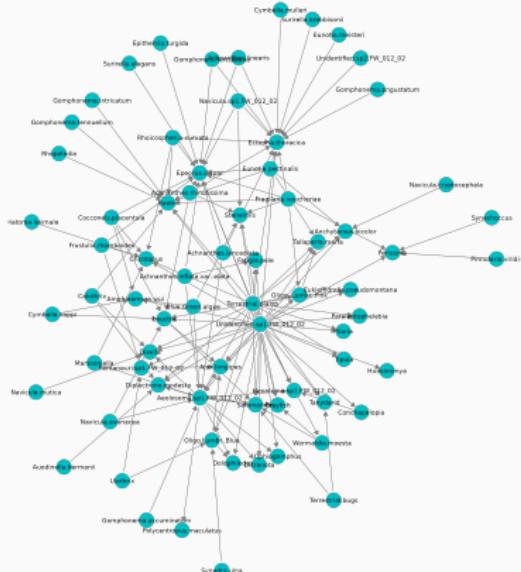
Predation networks: foodwebs

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



Foodwebs: adjacency matrix

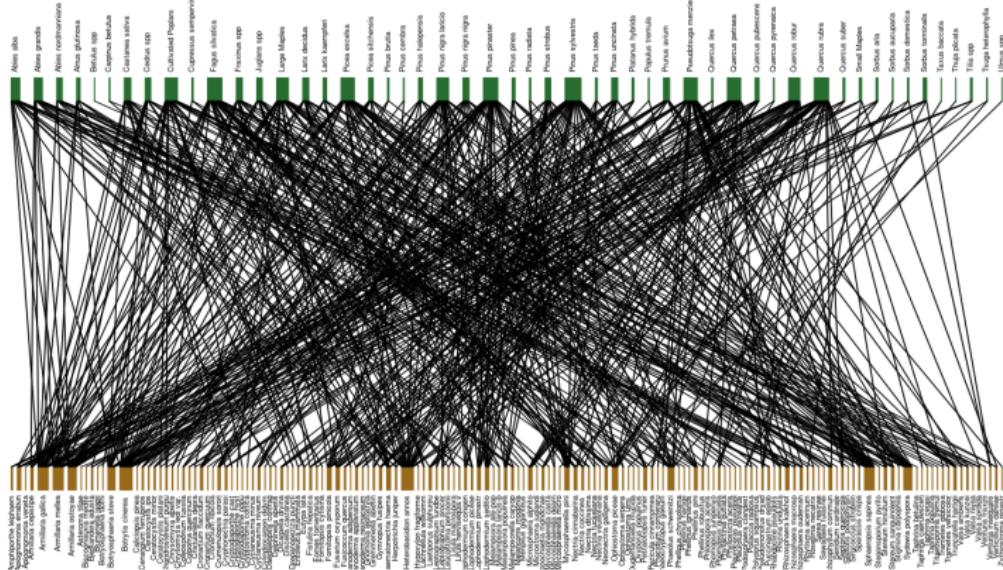
- $Y = (Y_{ij})_{1 \leq i,j, \leq n} = n \times n$ matrix
- $Y_{ij} = 1$ if i is eaten by j , 0 otherwise



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

Parasitism : tree-fungus network

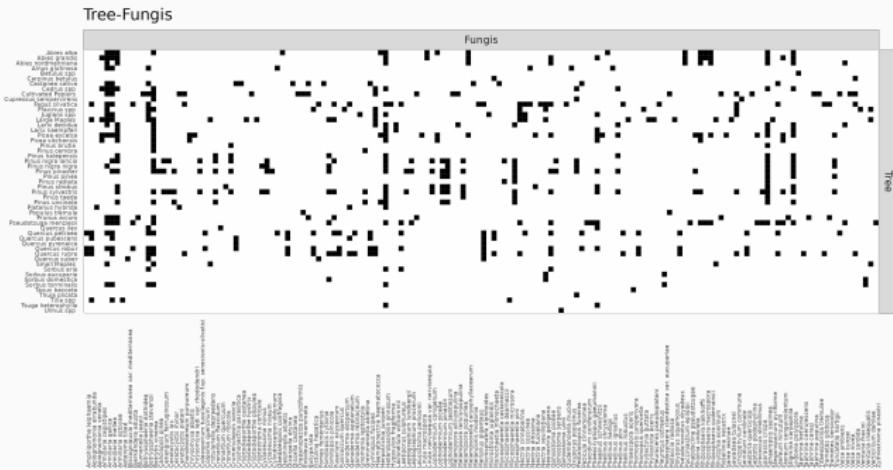
[Vacher et al., 2008] Parasitism relation between $n = 51$ tree species and $p = 154$ fungus species



Nodes of two types: bipartite network

Parasitism : tree-fungus incidence matrix

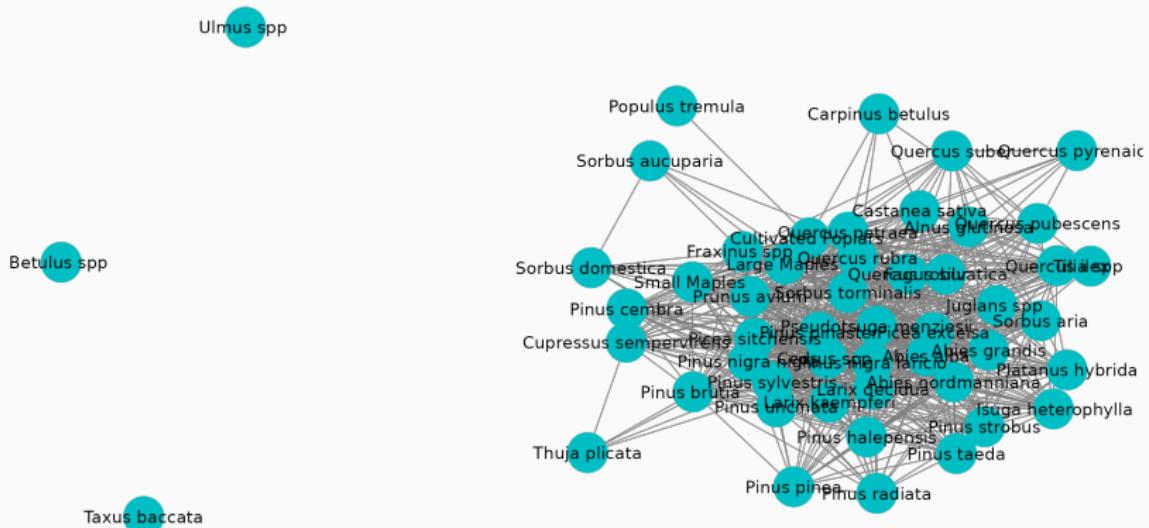
- $Y = (Y_{ij})_{1 \leq i,j \leq n} = n \times p$ matrix
- $Y_{ij} = 1$ if tree i is parasited by fungus j , 0 otherwise



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



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: characterize / 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

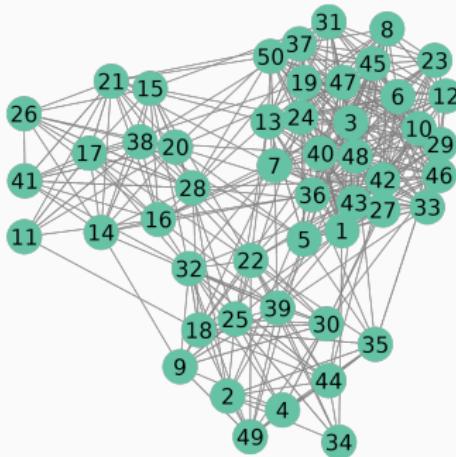
- Can we find groups of trees and fungi that are preferentially associated?

Ecological questions ii

Parasite networks between trees

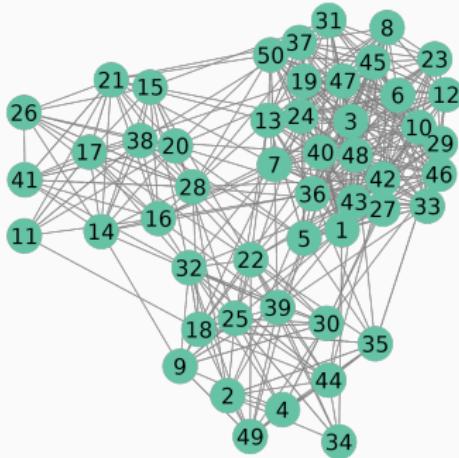
- Do any of the three distances (genetic, geographic or taxonomic) contributes to shape the number of shared parasites?
- Are the covariates sufficient to explain the interactions?

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 !

1. Introduction
2. Probabilistic model
 - 2.1 Stochastic Block Model
 - 2.2 Bipartite stochastic block models
 - 2.3 Some possible extensions
3. Inference

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

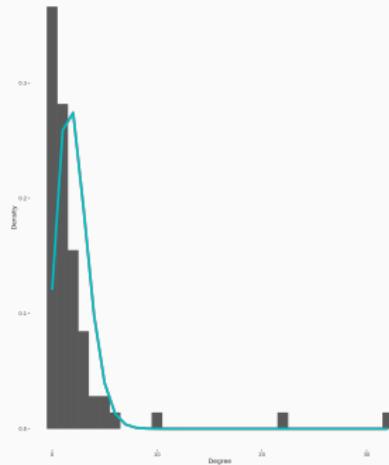
$$\forall 1 \leq i, j \leq n, \quad Y_{ij} \stackrel{i.i.d.}{\sim} \text{Bern}(p),$$

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

Consequence

$$\deg(i) \sim_{i.i.d} \text{Bin}(n, p)$$

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

1. Introduction

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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

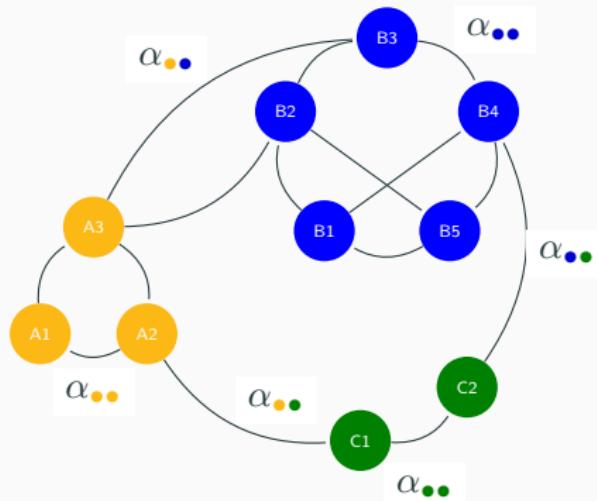
$$\mathbb{P}(Z_i = k) = \pi_k$$

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

(Y_{ij}) independant and

$$Y_{ij}|Z_i, Z_j \sim \text{Bern}(\alpha_{Z_i, Z_j}) \Leftrightarrow P(Y_{ij} = 1|Z_i = k, Z_j = \ell) = \alpha_{k\ell}$$

Stochastic Block Model : illustration



Parameters

Let n nodes divided into 3 clusters

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

$$Z_i = \mathbf{1}_{\{i \in \bullet\}} \sim^{\text{iid}} \mathcal{M}(1, \pi), \quad \forall \bullet \in \mathcal{K},$$

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

SBM : A great generative model

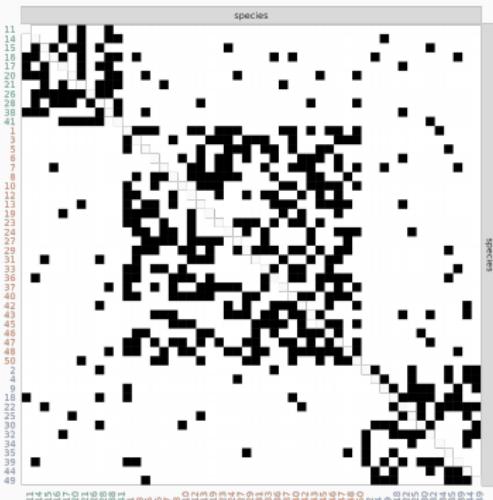
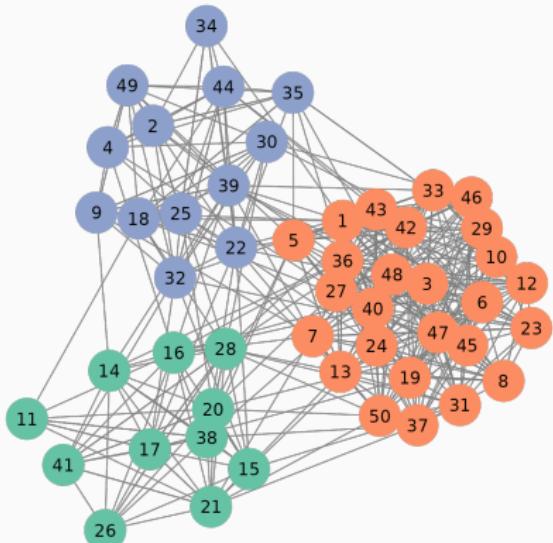
- Generative model : easy to simulate
- No a priori on the type of structure
- Combination of modularity, nestedness, etc...

References

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

Modelling communities

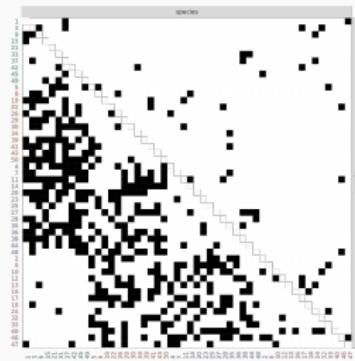
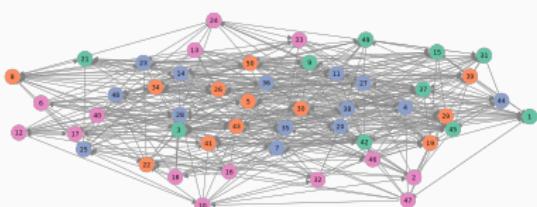
$$p = \begin{pmatrix} \underline{0.45} & 0.05 & 0.05 \\ 0.05 & \underline{0.45} & 0.05 \\ 0.05 & 0.05 & \underline{0.45} \end{pmatrix} \quad \nu = (0.25, 0.5, 0.25)$$



Modelling foodwebs

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

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



1. Introduction

2. Probabilistic model

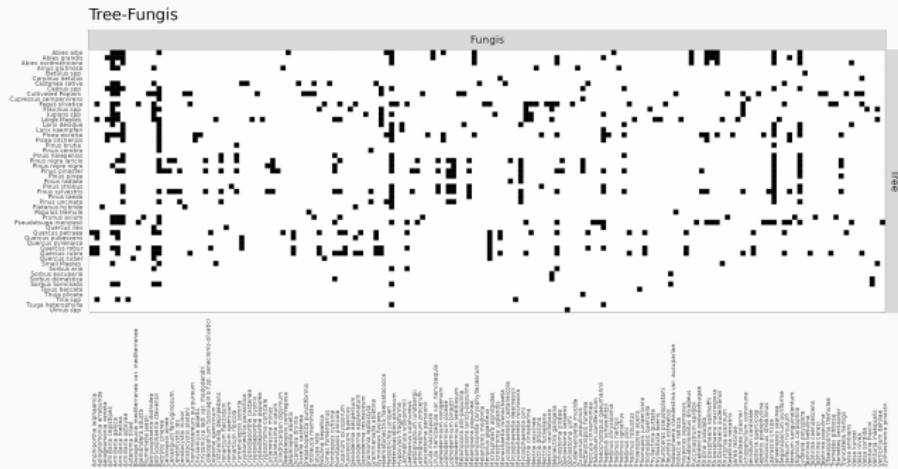
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2.3 Some possible extensions

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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 $i = 1, \dots, n$ partitionned into K clusters, nodes $j = 1, \dots, p$ partitionned into L clusters
- $Z_i = k$ if node i belongs to cluster (block) k
 $W_j = \ell$ if node j belongs to cluster (block) ℓ
- $(Z_i)_{i=1,\dots,n}, (W_j)_{j=1,\dots,p}$ 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 $(W_i)_{i=1,\dots,n}, (W_j)_{j=1,\dots,p} \dots$

(Y_{ij}) independent and

$$Y_{ij}|Z_i, W_j \sim \text{Bern}(\alpha_{Z_i, W_j}) \Leftrightarrow \mathbb{P}(Y_{ij} = 1|Z_i = k, W_j = \ell) = \alpha_{k\ell}$$

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

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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 $i = 1, \dots, n$ 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

$$Y_{ij}|Z_i, Z_j \sim \text{Bern}(\text{logit}(\alpha_{Z_i, Z_j} + \theta \cdot x_{ij})) \quad \text{if binary data}$$

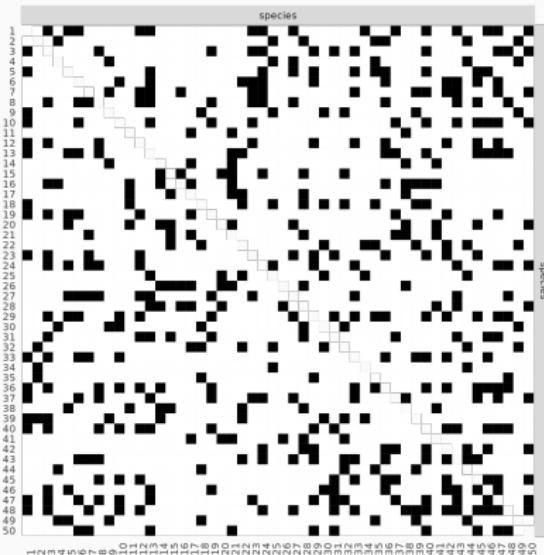
$$Y_{ij}|Z_i, Z_j \sim \mathcal{P}(\exp(\alpha_{Z_i, Z_j} + \theta \cdot x_{ij})) \quad \text{if counting data}$$

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

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 - 3.2 Model selection

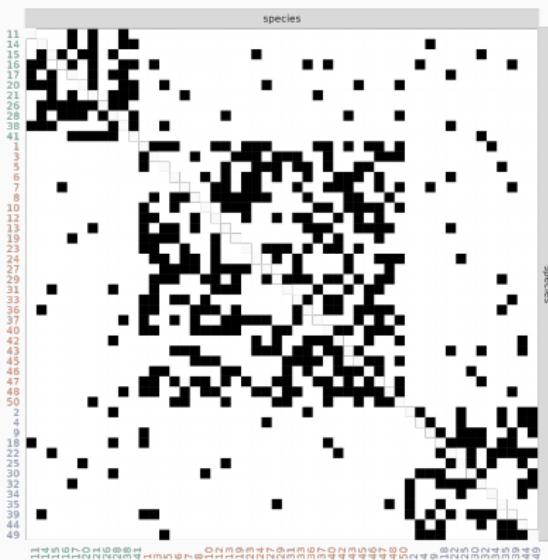
Aim

Going from...



Aim

... to



Statistical inference

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

Presented in details for binary SBM.

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Likelihood for Bernoulli SBM

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

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

Marginal likelihood (\mathbf{Y})

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

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

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

- **Step M:**

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

Limitations of standard EM i

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

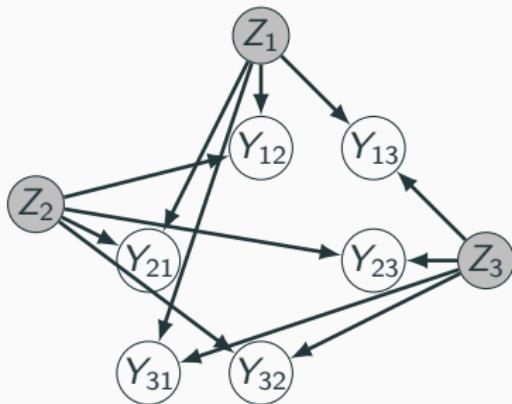
■

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

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

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

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

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

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

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

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

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

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)

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

with

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

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

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

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

Maximization with respect to π is quite direct:

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

For the Bernoulli SBM:

$$\hat{\alpha}_{kl} = \frac{\sum_{i,j=1, i \neq j}^n \hat{\tau}_{ik} \hat{\tau}_{jl} Y_{ij}}{\sum_{i,j=1, i \neq j}^n \hat{\tau}_{ik} \hat{\tau}_{jl}}$$

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

- Really fast
- Strongly depend on the initial values

1. Introduction
2. Probabilistic model
3. Inference
 - 3.1 Parameters estimation
 - 3.2 Model selection

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]

$$ICL(\mathcal{M}_K) = \log \ell_c(\mathbf{Y}, \hat{\mathbf{Z}}; \hat{\theta}_K) - \text{pen}(\mathcal{M}_K) \quad (2)$$

where

$$\hat{\mathbf{Z}}_i = \arg \max_{k \in \{1, \dots, K\}} \hat{\tau}_{ik}. \quad (3)$$

- Integrated Complete Likelihood (ICL)

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

Expression of the penalization for SBM

- For directed network

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

- 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

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

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

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

with the same penalty

- Under this conjecture

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

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

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

Algorithm in practice

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

Stepwise procedure

Starting from K

- **Split** : if $K < K_{\max}$
 - 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 $K > K_{\min}$
 - 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 [\[Tabouy et al., 2019\]](#)

Probabilistic model for networks in a nutshell

SBM/LBM

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

Now it's time
to practice!



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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