Masterclass in Machine Learning

Graph clustering and the Stochastic Bloc Model

Villiers-le-lac

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https://jchiquet.github.io/

AgroParisTech
Talents d'une planète soutenable

INRAE
la science pour la vie, l'humain, la terre

Setup and Reproducibility

```r
library(tidyverse) # data manipulation
library(igraph)    # graph manipulation
library(sbm)       # stochastic bloc model
library(missSBM)   # stochastic bloc model with missing data
library(aricode)   # clustering measures comparison
```

Outline

Outline

1. Motivations
2. Graph Partionning
3. The Stochastic Block Model (SBM)

Network data

Recommandation system: Epinion

Who-trust-whom online social network of a general consumer review site Epinions.com. Members of the site can decide whether to "trust" each other.

Social networks in ethnobiology

A seed exchange network in Kenya is collected on a limited space area, where all the 155 farmers are interviewed. Farmers provide information about other farmers with whom they have interacted.

Ecological networks: plant-pollinator network

Interaction network between predefined sets of plants and pollinators, by direct observation.

Companion data set: French political Blogosphere

Single day snapshot of almost 200 political blogs automatically extracted the 14 October 2006 and manually classified by the "Observatoire Présidentielle" project.

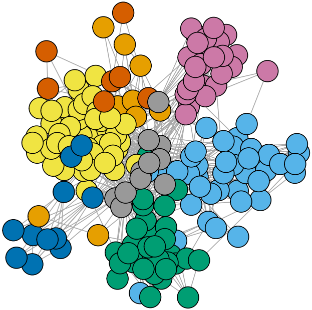
```
data("frenchblog2007", package = "missSBM")
blog <- frenchblog2007 %>%  delete_vertices(which(degree(frenchblog2007) <= 1))
summary(blog)

## IGRAPH 997d6c3 UN-- 192 1431 --
## + attr: name (v/c), party (v/c)

party <- V(blog)$party %>% as_factor()
party %>% table() %>% knitr::kable("latex")
```

.	Freq
green	9
right	40
center-rigth	32
left	57
center-left	11
far-left	7
liberal	25
analyst	11

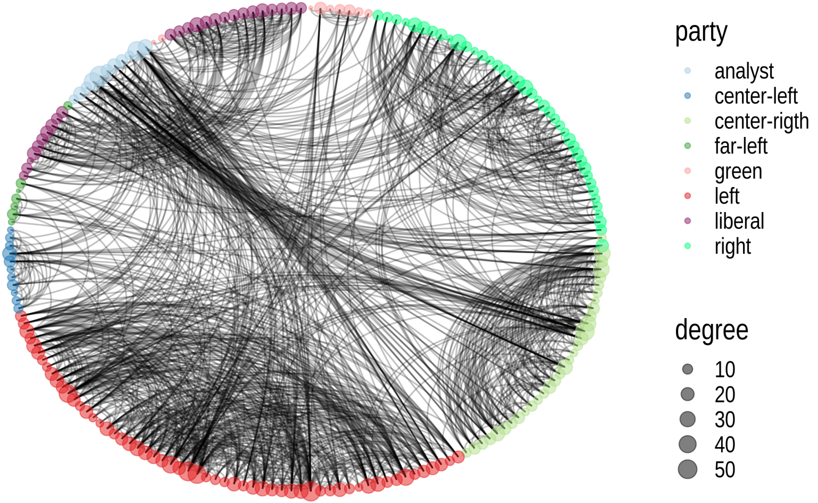
Visualization: graph view

A visual representation of the network data with nodes colored according to the political party each blog belongs to is achieved as follows:

```
plot.igraph(blog,
  vertex.color = party,
  vertex.label = NA
 )
```

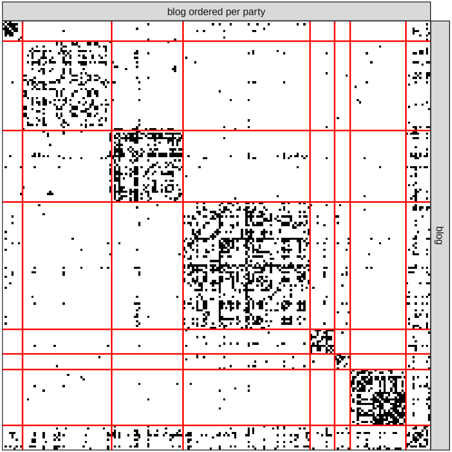


Visualization: graph view (advanced)



Visualization: matrix view

```
Y  <- as_adj(blog, sparse = FALSE)
sbm::plotMyMatrix(
  Y, dimLabels = list('blog', "blog ordered per party"),
  clustering = list(row = party))
```



Problematic

Remarks

- The pattern of connections between the nodes is highly related to the blog classification (political party)
- The data may support a natural grouping of the node which is not necessarily related to a predefined classification
- Same remark holds for any kind of clustering and unsupervised leaning problem

Objective: Graph clustering

Automatically find a partitioning of the nodes, i.e. a clustering, that groups together nodes with similar connectivity pattern.

Network data and binary graphs: minimal notation

A network is a collection of interacting entities. A graph is the mathematical representation of a network.

Definition

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a mathematical structure consisting of

- a set $\mathcal{V} = \{1, \ldots, n\}$ of vertices or nodes
- a set $\mathcal{E} = \{e_1, \ldots, e_p : e_k = (i_k, j_k) \in (\mathcal{V} \times \mathcal{V})\}$ of edges or links
- The number of vertices $|\mathcal{V}|$ is called the order
- The number of edges $|\mathcal{E}|$ is called the size
- The neighbors of a vertex are the nodes directly connected to this vertex:
$$\mathcal{N}(i) = \{j \in \mathcal{V} : (i, j) \in \mathcal{E}\}.$$
- The degree d_i of a node i is given by its number of neighbors $|\mathcal{N}(i)|$.

Representation: adjacency matrix

The connectivity of a binary undirected (symmetric) graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is captured by the $|\mathcal{V}| \times |\mathcal{V}|$ matrix Y, called the adjacency matrix

$$(Y)_{ij} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

For a valued of weighted graph, a similar definition would be

$$(Y)_{ij} = \begin{cases} w_{ij} & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

where w_{ij} is the weight associated with edge $i \sim j$.

Remark

If the list of vertices is known, the only information which needs to be stored is the list of edges. In terms of storage, this is equivalent to a sparse matrix representation.

Outline

References

- Statistical Analysis of Network Data: Methods and Models,
  Eric Kolazcyk
  Chapter 4, Section 4
- Analyse statistique de graphes,
  Catherine Matias, Chapitre 3
- DS David Sontag's Lecture
  http://people.csail.mit.edu/dsontag/courses/ml13/slides/lecture16.pdf
- A Tutorial on Spectral Clustering,
  Ulrike von Luxburg

Outline

Principle

Form a partition of the nodes composed by "cohesive" sets, e.g.

1. vertices well connected among themselves
2. well separated from the remaining vertices

Agglomerative hierarchical clustering

1. Compute the dissimilarity between groups
2. Regroup the two most similar elements

Iterate until all element are in a single group

Output: n nested partitions from $\{\{1\},\ldots,\{n\}\}$ to $\{\{1,\ldots,n\}\}$

Ingredients

1. a dissimilarity measure between nodes
2. a distance measure between sets

Dissimilarity measures

Graph-specific

- Modularity: *fraction of edges that fall within a given groups minus expected fraction if edges were distributed at random*

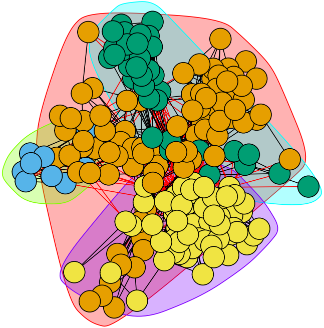
  For $\mathcal{C} = \{C_1, \ldots, C_K\}$ a candidate partition and $f_{ij}(\mathcal{C})$ the fraction of edges connecting vertices from C_i to C_j

$$\text{modularity}(\mathcal{C}) = \sum_{k=1}^{K} \left(f_{kk}(\mathcal{C}) - \mathbb{E}_{H_0}(f_{kk})\right)^2$$

- Betweeness: *number of shortest paths that go through a node in a graph or network*

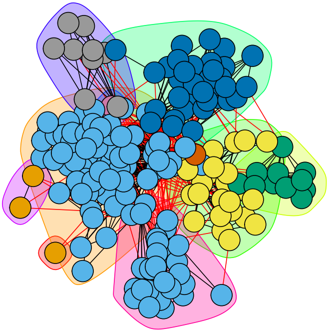
Examples of graph partionning I

```
hc <- cluster_fast_greedy(blog)
plot(hc, blog, vertex.label=NA)
```



Examples of graph partionning II

```
hc <- cluster_edge_betweenness(blog)
plot(hc, blog, vertex.label=NA)
```



Outline

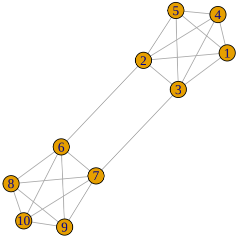
Motivation: graph-cut

Definition

The cut between two sets of nodes that form a partition in the graph is

$$\text{cut}(\mathcal{V}_A, \mathcal{V}_B) = \sum_{i \in \mathcal{V}_A, j \in \mathcal{V}_B} Y_{ij}, \qquad \mathcal{V}_A \cup \mathcal{V}_B = \mathcal{V}$$

Example: The graph cut between $\mathcal{V}_A = \{1, 2, 3, 4, 5\}$ and $\mathcal{V}_B = \{6, 7, 8, 9, 10\}$ is 2.



Min-cut

Idea: Find the 2-partition that minimizes the cut to form two homogeneous clusters.

Min-cut problem

Based on this principle, the normalized cut consider the connectivity between groups relative to the volume of each groups

$$\arg\min_{\{\mathcal{V}_A,\mathcal{V}_B\}} \mathrm{cut}^N(\mathcal{V}_A,\mathcal{V}_B),$$

where $\mathrm{Vol}(\mathcal{V}_S)) = \sum_{i\in\mathcal{S}} d_i$ and

$$\begin{aligned}\mathrm{cut}^N(\mathcal{V}_A,\mathcal{V}_B) &= \frac{\mathrm{cut}(\mathcal{V}_A,\mathcal{V}_B)}{\mathrm{Vol}(\mathcal{V}_A)} + \frac{\mathrm{cut}(\mathcal{V}_A,\mathcal{V}_B)}{\mathrm{Vol}(\mathcal{V}_B)} \\ &= \mathrm{cut}(\mathcal{V}_A,\mathcal{V}_B)\frac{\mathrm{Vol}(\mathcal{V}_A)+\mathrm{Vol}(\mathcal{V}_B)}{\mathrm{Vol}(\mathcal{V}_A)\mathrm{Vol}(\mathcal{V}_B)}\end{aligned}$$

$\rightsquigarrow$ The term in $(\mathrm{Vol}(\mathcal{V}_A),\mathrm{Vol}(\mathcal{V}_B))$ encourages balance groups/cuts

Solving min-cut for 2 clusters

Let

$$x = (x_i)_{i=1,\dots,n} = \begin{cases} -1 & \text{if} \quad i \in \mathcal{V}_A, \\ 1 & \text{if} \quad i \in \mathcal{V}_B. \end{cases}$$

Then, letting D the diagonal matrix of degrees,

$$x^\top (D - Y)x = x^\top Dx - (x^\top Dx - 2\text{cut}(\mathcal{V}_A, \mathcal{V}_B)),$$

so that

$$\text{cut}(\mathcal{V}_A, \mathcal{V}_B) = \frac{1}{2} x^\top (D - Y)x.$$

Solving Min-cut for 2 clusters

Normalized graph-cut $\Leftrightarrow$ integer programming problem

$$\arg\min_{\{\mathcal{V}_A,\mathcal{V}_B\}} \mathrm{cut}^N(\mathcal{V}_A,\mathcal{V}_B)$$

$$\Leftrightarrow \quad \arg\min_{x\in\{-1,1\}^n} \frac{x^\top(D-Y)x}{x^\top Dx}, \quad \text{s.c.} \quad x^\top D\mathbf{1}_n = 0,$$

where the constraint imposes only discrete values in x.

Relax version

If we relax to $x \in [-1,1]^n$, it turns to a simple eigenvalue problem

$$\arg\min_{x\in[-1,1]^n} x^\top(D-Y)x, \quad \text{s.c.} \quad x^\top Dx = 1 \Leftrightarrow (D-Y)x = \lambda Dx.$$

where $\mathbf{L} = D - Y$ is called the Laplacian matrix of the graph $\mathcal{G}$.

Solving Min-cut for 2 clusters

Normalized graph-cut $\Leftrightarrow$ integer programming problem

$$\arg\min_{\{\mathcal{V}_A,\mathcal{V}_B\}} \mathrm{cut}^N(\mathcal{V}_A,\mathcal{V}_B)$$

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Graph Laplacian: spectrum

Proposition (Spectrum of $\mathbf{L}$)

The $n \times n$ matrix $\mathbf{L}$ has the following properties:

$$\mathbf{x}^\top \mathbf{L} \mathbf{x} = \frac{1}{2} \sum_{i,j} Y_{ij} (x_i - x_j)^2, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

- $\mathbf{L}$ *is a symmetric, positive semi-definite matrix,*
- $\mathbf{1}_n$ *is in the kernel of L since $L\mathbf{1}_n = 0$,*
- *The first normalized eigen vector with eigen value $\lambda > 0$ is solution to the relaxed graph cut problem*

The Laplacian is easily (and fastly) computed in R thanks to the **igraph** package:

```
L <- laplacian_matrix(blog)
```

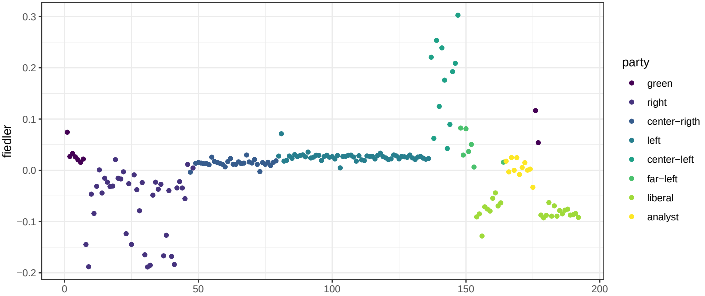
Bi-partionning and the Fiedler vector

Fiedler vector is the named sometimes given to the normalized eigen vector associated with the smallest positive eigen-value of $\mathbf{L}$.

$\rightarrow$ solves the relaxed min-cut problem

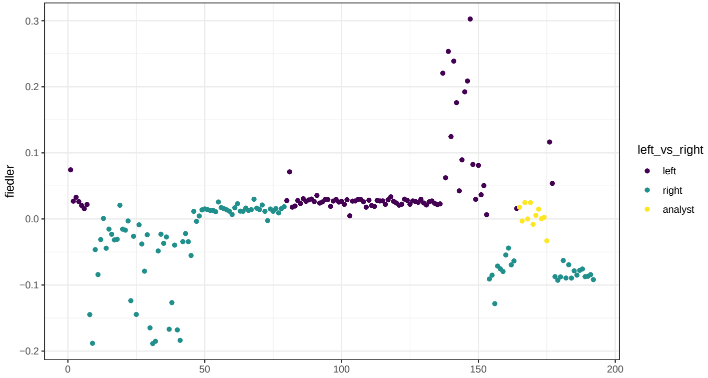
$\rightarrow$ can be used to compute a bi-partition of a graph.

```
spec_L <- eigen(L); practical_zero <- 1e-12
lambda  <- min(spec_L$values[spec_L$values>practical_zero])
fiedler <- spec_L$vectors[, which(spec_L$values == lambda)]
qplot(y = fiedler, colour = party) + viridis::scale_color_viridis(discrete = TRUE)
```



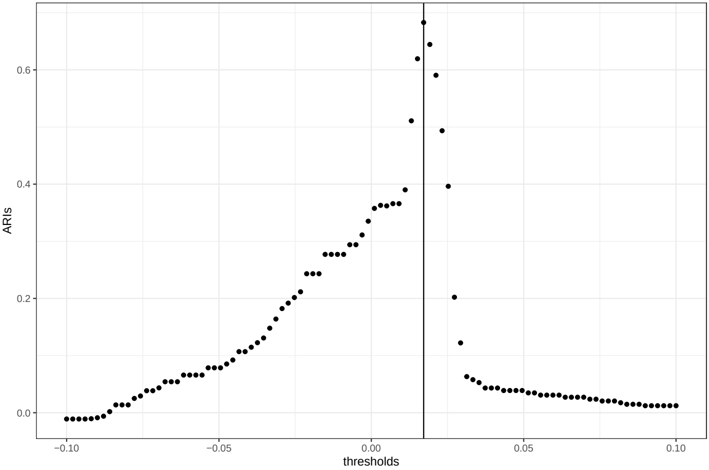
Example on a simplied left/right view

```
left_vs_right <-
  forcats::fct_collapse(party,
    left = c("green", "left", "far-left", "center-left"),
    right = c("right", "liberal", "center-rigth"),
    analyst = "analyst"
  )
qplot(y = fiedler, colour = left_vs_right) +  viridis::scale_color_viridis(discrete
```



"Validation"

```
thresholds <- seq(-.1, .1, len = 100)
ARIs <- map_dbl(thresholds, ~ARI(left_vs_right, fiedler > .))
qplot(thresholds, ARIs) + geom_vline(xintercept = thresholds[which.max(ARIs)]) + th
```



Spectral clustering

From the definition of the Laplacian matrix,

- The multiplicity of the first eigen value (0) of $\mathbf{L}$ determines the number of connected components in the graph.
- The larger the second non trivial (positive) eigenvalue, the higher the connectivity of $\mathcal{G}$.

General Heuristic

1. Compute spectral decompostion of $\mathbf{L}$ to perform clustering in the eigen space
2. For a graph with K connected components, the first K eigen-vectors are $\mathbf{1}$ spanning the eigenspace associated with eigenvalue 0
3. Applying a simple clustering algorithm to the rows of the K first eigenvectors separate the components

$\rightsquigarrow$ Generalizes to graphs with a single component (tends to separates groups of nodes which are highly connected together)

Some variants

Definition ((Normalized) Laplacian)

The normalized Laplacian matrix $\mathbf{L}$ is defined by

$$\mathbf{L}_N = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}.$$

Definition ((Absolute) Graph Laplacian)

The absolute Laplacian matrix $\mathbf{L}_{abs}$ is defined by

$$\mathbf{L}_{abs} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{L}_N,$$

with eigenvalues $1 - \lambda_n \leq \cdots \leq 1 - \lambda_2 \leq 1 - \lambda_1 = 1$, where $0 = \lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of $\mathbf{L}_N$.

Normalized Spectral Clustering

by Ng, Jordan and Weiss (2002)

Input: Adjacency matrix and number of classes Q

Compute the normalized graph Laplacian $\mathbf{L}$
Compute the eigen vectors of $\mathbf{L}$ associated with the Q smallest eigenvalues
Define $\mathbf{U}$, the $n \times Q$ matrix that encompasses these Q vectors
Define $\tilde{\mathbf{U}}$, the row-wise normalized version of $\mathbf{U}$: $\tilde{u}_{ij} = \frac{u_{ij}}{\|\mathbf{U}_i\|_2}$
Apply k-means to $(\tilde{\mathbf{U}}_i)_{i=1,\dots,n}$

Output: vector of classes $\mathbf{C} \in \mathcal{Q}^n$, such as $C_i = q$ if $i \in q$

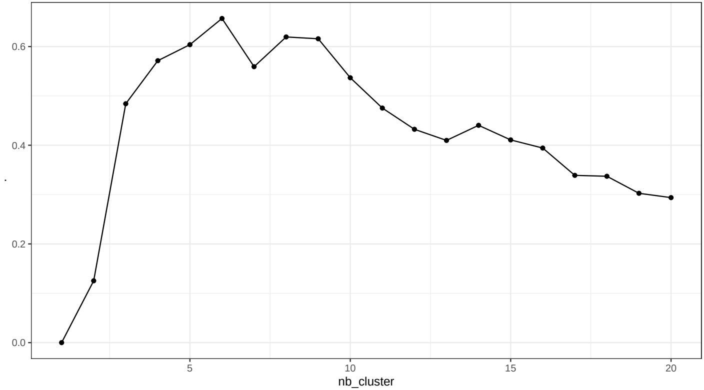
Implementation of normalized spectral clustering

```
spectral_clustering <- function(graph, nb_cluster, normalized = TRUE) {

  ## Compute Laplacian matrix
  L <- laplacian_matrix(graph, normalized = normalized)
  ## Generates indices of last (smallest) K vectors
  selected <- rev(1:ncol(L))[1:nb_cluster]
  ## Extract an normalized eigen-vectors
  U <- eigen(L)$vectors[, selected, drop = FALSE]  # spectral decomposition
  U <- sweep(U, 1, sqrt(rowSums(U^2)), '/')
  ## Perform k-means
  res <- kmeans(U, nb_cluster, nstart = 40)$cl

  res
}
```

Application to the French blogosphere (1)

Perform spectral clustering on the blogosphere for various numbers of group:

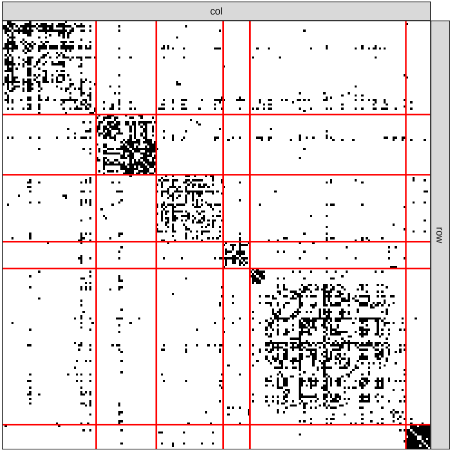
```
nb_cluster <- 1:20
map(nb_cluster, ~spectral_clustering(blog, .)) %>%
  map_dbl(ARI, party) %>% qplot(nb_cluster, y = .) + geom_line() + theme_bw()
```



Application to the French blogosphere (2)

Once reorder according to the best clustering (obtained $k = 6$) groups, the orginal data matrix looks as follows

```r
plotMyMatrix(as_adj(blog, sparse = FALSE),
  clustering = list(row = spectral_clustering(blog, 6)))
```



Outline

References

- Statistical Analysis of Network Data: Methods and Models
  Eric Kolazcyk
  Chapters 5 and 6

- Mixture model for random graphs, Statistics and Computing
  Daudin, Robin, Picard
  pbil.univ-lyon1.fr/members/fpicard/franckpicard_fichiers/pdf/DPR08.pdf

- Analyse statistique de graphes,
  Catherine Matias
  Chapitre 4, Section 4

Motivations

Last section: find an underlying organization in a observed network

Spectral or hierachical clustering for network data

$\rightsquigarrow$ Not model-based, thus no statistical inference possible

Now: clustering of network based on a probabilistic model of the graph

Become familiar with

- the stochastic block model, a random graph model tailored for clustering vertices,
- the variational EM algorithm used to infer SBM from network data.

$$\text{hierarchical/kmeans clustering} \leftrightarrow \text{Gaussian mixture models}$$
$$\Updownarrow$$
$$\text{hierarchical/spectral clustering for network} \leftrightarrow \text{Stochastic block model}$$

Outline

A mathematical model: Erdös-Rényi graph

Definition

Let $\mathcal{V} = 1, \ldots, n$ be a set of fixed vertices. The (simple) Erdös-Rényi model $\mathcal{G}(n, \pi)$ assumes random edges between pairs of nodes with probability π. In orther word, the (random) adjacency matrix $\mathbf{X}$ is such that

$$Y_{ij} \sim \mathcal{B}(\pi)$$

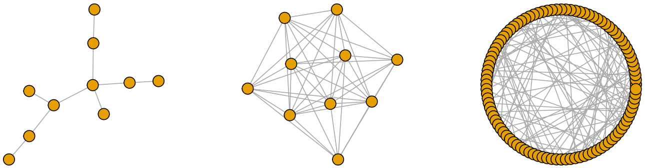
Proposition (degree distribution)

The (random) degree D_i of vertex i follows a binomial distribution:

$$D_i \sim b(n-1, \pi).$$

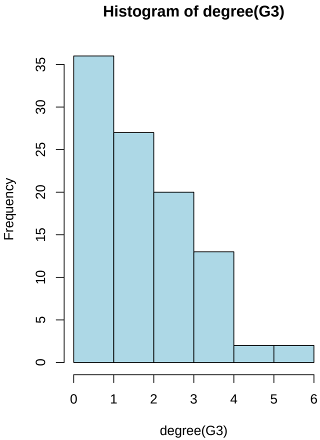
Erdös-Rényi - example

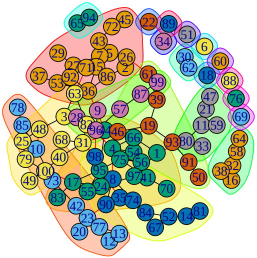
```
G1 <- igraph::sample_gnp(10, 0.1)
G2 <- igraph::sample_gnp(10, 0.9)
G3 <- igraph::sample_gnp(100, .02)
par(mfrow=c(1,3))
plot(G1, vertex.label=NA) ; plot(G2, vertex.label=NA)
plot(G3, vertex.label=NA, layout=layout.circle)
```



Erdös-Rény - limitations: very homegeneous

```
average.path.length(G3); diameter(G3)

## [1] 5.233395
## [1] 12
```





Mechanism-based model: preferential attachment

The graph is defined dynamically as follows

Definition

Start from a initial graph $\mathcal{G}_0 = (\mathcal{V}_0, \mathcal{E}_0)$, then for each time step,

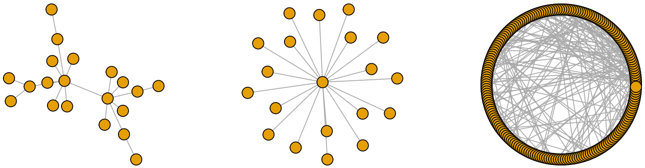
1. At t a new node V_t is added
2. V_t is connected to $i \in V_{t-1}$ with probability

$$D_i^\alpha + \mathrm{cst.}$$

$\rightsquigarrow$ Nodes with high degree get more connections thus richers get richers

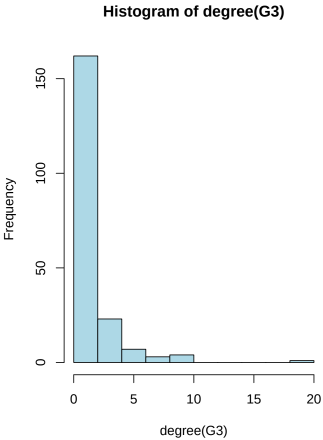
Preferential attachment - example

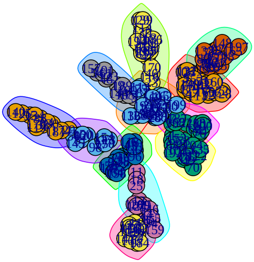
```
G1 <- igraph::sample_pa(20, 1, directed=FALSE)
G2 <- igraph::sample_pa(20, 5, directed=FALSE)
G3 <- igraph::sample_pa(200, directed=FALSE)
par(mfrow=c(1,3))
plot(G1, vertex.label=NA) ; plot(G2, vertex.label=NA)
plot(G3, vertex.label=NA, layout=layout.circle)
```



Preferential attachment - limitations

```
average.path.length(G3); diameter(G3)

## [1] 6.019397
## [1] 15
```





Limitations

- Erdös-Rényi
  The ER model does not fit well real world network
  - As can been seen from its degree distribution
  - ER is generally too homogeneous
- Preferential attachment
  - Is defined through an algorithm so performing statistics is complicated
  - Is stucked to the power-law distribution of degrees

The Stochastic Block Model

The SBM[1] generalizes ER in a mixture framework. It provides

- a statistical framework to adjust and interpret the parameters
- a flexible yet simple specification that fits many existing network data

[1] Other models exist (e.g. exponential model for random graphs) but less popular.

Outline

Stochastic Block Model: definition

Mixture model point of view: mixture of Erdös-Rényi

Latent structure

Let $\mathcal{V} = \{1, .., n\}$ be a fixed set of vertices. We give each $i \in \mathcal{V}$ a latent label among a set $\mathcal{Q} = \{1, \dots, Q\}$ such that

- $\alpha_q = \mathbb{P}(i \in q), \quad \sum_q \alpha_q = 1;$
- $Z_{iq} = \mathbf{1}_{\{i \in q\}}$ are independent hidden variables.

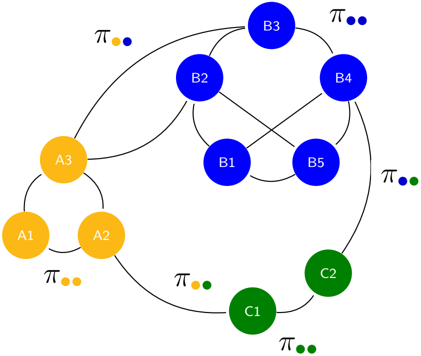
The conditional distribution of the edges

Connexion probabilities depend on the node class belonging:

$$Y_{ij} | \{i \in q, j \in \ell\} \sim \mathcal{B}(\pi_{q\ell}) \qquad \left(\Leftrightarrow Y_{ij} | \{Z_{iq} Z_{j\ell} = 1\} \sim \mathcal{B}(\pi_{q\ell}). \right)$$

The $Q \times Q$ matrix $\boldsymbol{\pi}$ gives for all couple of labels $\pi_{q\ell} = \mathbb{P}(Y_{ij} = 1 | i \in q, j \in \ell)$.

Stochastic Block Model: the big picture



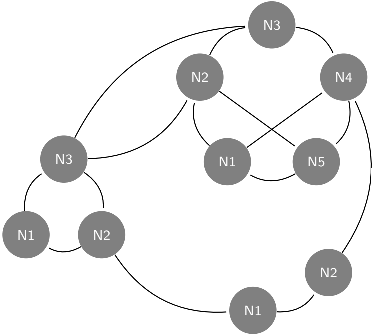
Stochastic Block Model

Let n nodes divided into

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

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

Stochastic Block Model: unknown parameters



Stochastic Block Model

Let n nodes divided into

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

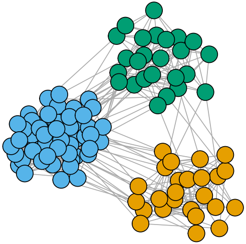
$$Z_i = \mathbf{1}_{\{i \in \bullet\}} \ \sim^{\text{iid}} \mathcal{M}(1, \alpha), \quad \forall \bullet \in \mathcal{Q},$$

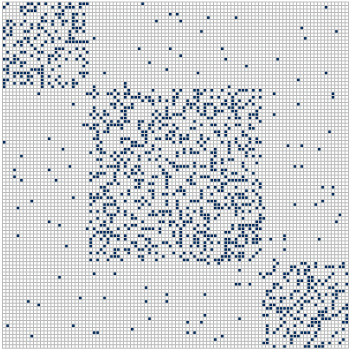
$$Y_{ij} \mid \{i \in {\color{orange}\bullet}, j \in {\color{blue}\bullet}\} \sim^{\text{ind}} \mathcal{B}(\pi_{{\color{orange}\bullet}{\color{blue}\bullet}})$$

Stochastic block models – examples of topology

Community network

```
pi <- matrix(c(0.3,0.02,0.02,0.02,0.3,0.02,0.02,0.02,0.3),3,3)
communities <- igraph::sample_sbm(100, pi, c(25, 50, 25))
par(mfrow = c(1,2))
plot(communities, vertex.label=NA, vertex.color = rep(1:3,c(25, 50, 25)))
corrplot(as_adj(communities, sparse =FALSE), tl.pos = "n", cl.pos = 'n')
```

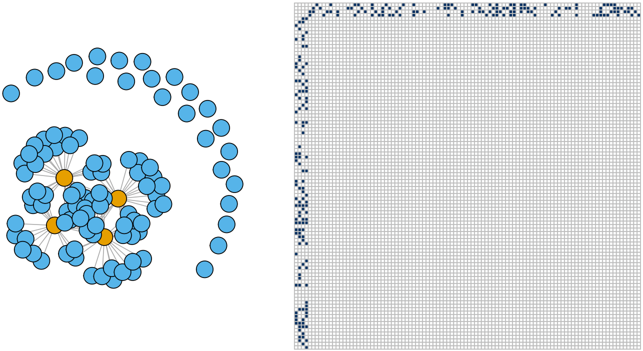




Stochastic block models – examples of topology

Star network

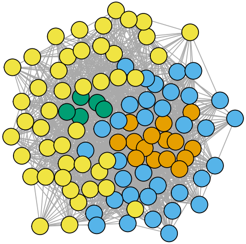
```r
pi <- matrix(c(0.05,0.3,0.3,0),2,2)
star <- igraph::sample_sbm(100, pi, c(4, 96))
par(mfrow = c(1,2))
plot(star, vertex.label=NA, vertex.color = rep(1:2,c(4,96)))
corrplot(as_adj(star, sparse =FALSE), tl.pos = "n", cl.pos = 'n')
```

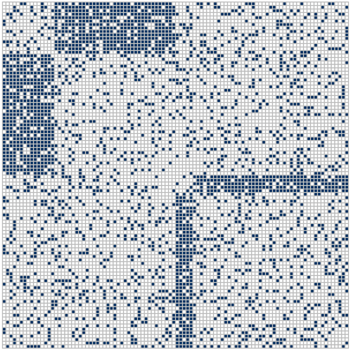


Stochastic block models – examples of topology

Bipartite network

```
pi <- matrix(c(.2,1-.2,.2,.2,1-.2,.2,.2,.2,.2,.2, .2,1-.2,.2,.2,1-.2,.2),4,4)
bipar <- igraph::sample_sbm(100, pi, c(15, 35, 5, 45))
par(mfrow = c(1,2))
plot(bipar, vertex.label=NA, vertex.color = rep(1:4,c(15, 35, 5, 45)))
corrplot(as_adj(bipar, sparse =FALSE), tl.pos = "n", cl.pos = 'n')
```





Degree distributions

Conditional degree distribution

The conditional degree distribution of a node $i \in q$ is

$$D_i | i \in q \sim \mathrm{b}(n-1, \bar{\pi}_q) \approx \mathcal{P}(\lambda_q), \qquad \bar{\pi}_q = \sum_{\ell=1}^{Q} \alpha_\ell \pi_{q\ell}, \quad \lambda_q = (n-1)\bar{\pi}_q$$

Conditional degree distribution

The degree distribution of a node i can be approximated by a mixture of Poisson distributions:

$$\mathbb{P}(D_i = k) = \sum_{q=1}^{Q} \alpha_q \exp\{-\lambda_q\} \frac{\lambda_q^k}{k!}$$

Outline

Likelihoods

Complete data likelihood

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

Marginal likelihood $(\mathbf{Y})$

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

$\boldsymbol{\mathcal{Z}} = \{1, \dots, K\}^n$: impossible to compute when K and n increase.

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**:

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

With SBM,

$$\mathbb{E}_{\mathbf{Z}|\mathbf{Y}}\big[\log L(\boldsymbol{\theta};\mathbf{Y},\mathbf{Z})\big] = \sum_{i,q}\tau_{iq}\log\alpha_q + \sum_{i<j,q,\ell}\eta_{ijq\ell}\log\pi_{q\ell}^{Y_{ij}}(1-\pi_{q\ell})^{1-Y_{ij}}$$

where $\tau_{iq}, \eta_{ijq\ell}$ are the posterior probabilities:

- $\tau_{iq} = \mathbb{P}(Z_{iq}=1|\mathbf{Y}) = \mathbb{E}\left[Z_{iq}|\mathbf{Y}\right].$
- $\eta_{ijq\ell} = \mathbb{P}(Z_{iq}Z_{j\ell}=1|\mathbf{Y}) = \mathbb{E}\left[Z_{iq}Z_{j\ell}|\mathbf{Y}\right].$

The EM strategy does not apply directly for SBM

Ouch: another intractability problem

- the Z_{iq} are not independent conditional on $(X_{ij}, i < j)$ ...
- we cannot compute $\eta_{ijq\ell} = \mathbb{P}(Z_{iq}Z_{j\ell} = 1|\mathbf{Y}) = \mathbb{E}\left[Z_{iq}Z_{j\ell}|\mathbf{Y}\right]$,
- the conditional expectation $Q(\boldsymbol{\theta})$, i.e. the main EM ingredient, is intractable.

Solution: mean field approximation

Approximate $\eta_{ijq\ell}$ by $\tau_{iq}\tau_{j\ell}$, i.e., assume conditional independence between Z_{iq}
$\rightsquigarrow$ This can be formalized in the variational framework

Revisting the EM algorithm I

Proposition

Consider a distribution $\mathbb{Q}$ *for the* $\{Z_{iq}\}$. *We have*

$$\log L(\boldsymbol{\theta}; \mathbf{Y}) = \mathbb{E}_{\mathbb{Q}}[\log L(\boldsymbol{\theta}, \mathbf{Y}, \mathbf{Z})] + \mathcal{H}(\mathbb{Q}) + \mathrm{KL}(\mathbb{Q} \mid \mathbb{P}(\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta})),$$

where $\mathcal{H}$ *is the entropy and* $\mathrm{KL}(\cdot|\cdot)$ *is the Kullback-Leibler divergence:*

$$\mathcal{H}(\mathbb{Q}) = -\sum_z \mathbb{Q}(z) \log \mathbb{Q}(z) = -\mathbb{E}_{\mathbb{Q}}[\log \mathbb{Q}(Z)]$$

$$\mathrm{KL}(\mathbb{Q} \mid \mathbb{P}(\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta})) = \sum_z \mathbb{Q}(z) \log \frac{\mathbb{Q}(z)}{\mathbb{P}(\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta})} = \mathbb{E}_{\mathbb{Q}}\left[\log \frac{\mathbb{Q}(z)}{\mathbb{P}(\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta})}\right]$$

Revisting the EM algorithm II

Let

$$J(\mathbb{Q}, \boldsymbol{\theta}) \triangleq \mathbb{E}_{\mathbb{Q}} \left(\log L(\boldsymbol{\theta}; \mathbf{Y}, \mathbf{Z}) \right) + \mathcal{H}(\mathbb{Q})$$

The steps in the EM algorithm may be viewed as:

Expectation step : choose $\mathbb{Q}$ to maximize $J(\mathbb{Q}; \boldsymbol{\theta}^{(t)})$

The solution is $\mathbb{P}(\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta}^{(t)})$

Maximization step : choose $\boldsymbol{\theta}$ to maximize $J(\mathbb{Q}^{(t)}; \boldsymbol{\theta})$

The solution maximizes $\mathbb{E}_{\mathbf{Z}|\mathbf{Y}; \boldsymbol{\theta}^{(t)}} \left(\log L(\boldsymbol{\theta}; \mathbf{Y}, \mathbf{Z}) \right)$

Variational approximation for SBM

Problem for SBM

$\mathbb{P}(\mathbf{Z}|\mathbf{Y};\boldsymbol{\theta}^{(t)})$ cannot be computed thus the E-step cannot be solved.

Idea

Choose $\mathbb{Q}$ in a class of function so that the E-step can be solved.

Family of distribution that factorizes

We chose $\mathbb{Q}$ the multinomial distribution so that

$$\mathbb{Q}(\mathbf{Z}) = \prod_{i=1}^{n} \mathbb{Q}_i(Z_i) = \prod_{i=1}^{n} \prod_{q=1}^{Q} \tau_{iq}^{Z_{iq}},$$

where $\tau_{iq} = \mathbb{Q}_i(Z_i = q) = \mathbb{E}_{\mathbb{Q}}(Z_{iq})$, with $\sum_q \tau_{iq} = 1$ for all $i = 1, \ldots, n$.

Variational EM for SBM: the criterion

Lower bound of the loglikehood

Since $\mathbb{Q}$ is an approximation of $\mathbb{P}(\mathbf{Z}|\mathbf{Y})$, the Kullback-Leibler divergence is non-negative and

$$\log L(\boldsymbol{\theta}; \mathbf{Y}) \geq \mathbb{E}_{\mathbb{Q}}[\log L(\boldsymbol{\theta}, \mathbf{Y}, \mathbf{Z})] + \mathcal{H}(\mathbb{Q}) = J(\mathbb{Q}, \boldsymbol{\theta}).$$

For the SBM,

$$J(\mathbb{Q}, \boldsymbol{\theta}) = \sum_{i,q} \tau_{iq} \log \alpha_q + \sum_{i<j,q,\ell} \tau_{iq}\tau_{j\ell} \log b(X_{ij}; \pi_{q\ell}) - \sum_{i,q} \tau_{iq} \log(\tau_{iq}),$$

$\rightsquigarrow$ we optimize the loglikelihood lower bound $J(\mathbb{Q}, \boldsymbol{\theta}) = J(\boldsymbol{\tau}, \boldsymbol{\theta})$ in $(\boldsymbol{\tau}, \boldsymbol{\theta})$.

E and M steps for SBM

Variational E-step

Maximizing $J(\boldsymbol{\tau})$ for fixed $\boldsymbol{\theta}$, we find a fixed-point relationship:

$$\hat{\tau}_{iq} \propto \alpha_q \prod_j \prod_\ell b(Y_{ij}, \pi_{q\ell})^{\hat{\tau}_{j\ell}}$$

M-step

Maximizing $J(\boldsymbol{\theta})$ for fixed $\boldsymbol{\tau}$, we find,

$$\hat{\alpha}_q = \frac{1}{n} \sum_i \hat{\tau}_{iq}, \quad \hat{\pi}_{q\ell} = \frac{\sum_{i \neq j} \hat{\tau}_{iq} \hat{\tau}_{j\ell} Y_{ij}}{\sum_{i \neq j} \hat{\tau}_{iq} \hat{\tau}_{j\ell}}.$$

Model selection

We use our lower bound of the loglikelihood to compute an approximation of the ICL

$$\text{vICL}(Q) = \mathbb{E}_{\hat{\mathbb{Q}}}[\log L(\hat{\boldsymbol{\theta}}); \mathbf{Y}, \mathbf{Z}] - \frac{1}{2}\left(\frac{Q(Q+1)}{2}\log\frac{n(n-1)}{2} + (Q-1)\log(n)\right),$$

where

$$\mathbb{E}_{\hat{\mathbb{Q}}}[\log L(\hat{\boldsymbol{\theta}}; \mathbf{Y}, \mathbf{Z})] = J(\hat{\boldsymbol{\tau}}, \hat{\boldsymbol{\theta}}) - \mathcal{H}(\hat{\mathbb{Q}}).$$

The variational BIC is just

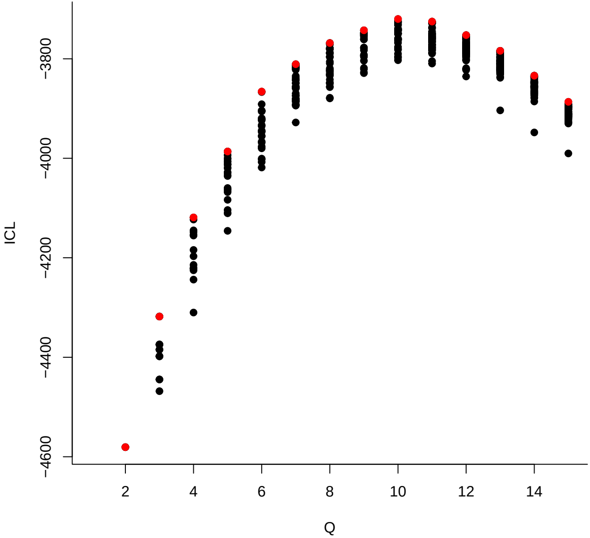
$$\text{vBIC}(Q) = J(\hat{\boldsymbol{\tau}}, \hat{\boldsymbol{\theta}}) - \frac{1}{2}\left(\frac{Q(Q+1)}{2}\log\frac{n(n-1)}{2} + (Q-1)\log(n)\right).$$

Example: French politcal blogosphere

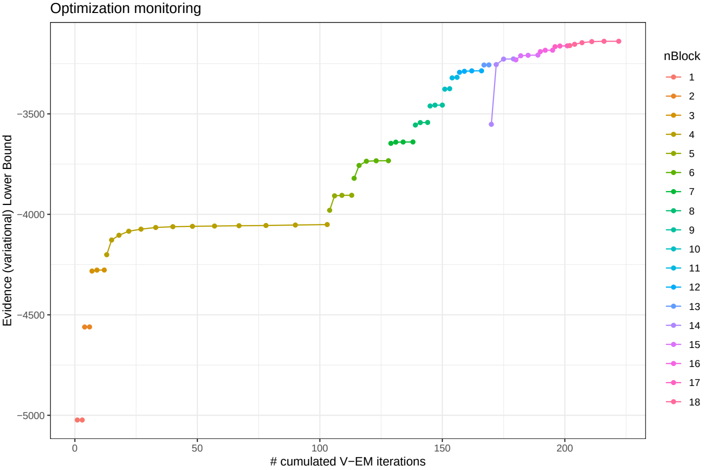
```r
my_sbm <-
  blog %>% as_adj(sparse = FALSE) %>%
   sbm::estimateSimpleSBM(estimOptions = list(plot = FALSE))
```

```r
my_sbm

## Fit of a Simple Stochastic Block Model -- bernoulli variant
## =====================================================================
## Dimension = ( 192 ) - ( 10 ) blocks and no covariate(s).
## =====================================================================
## * Useful fields
##   $nbNodes, $modelName, $dimLabels, $nbBlocks, $nbCovariates, $nbDyads
##   $blockProp, $connectParam, $covarParam, $covarList, $covarEffect
##   $expectation, $indMemberships, $memberships
## * R6 and S3 methods
##   $rNetwork, $rMemberships, $rEdges, plot, print, coef
## * Additional fields
##   $probMemberships, $loglik, $ICL, $storedModels,
## * Additional methods
##   predict, fitted, $setModel, $reorder
```

Example: model exploration (vICL)

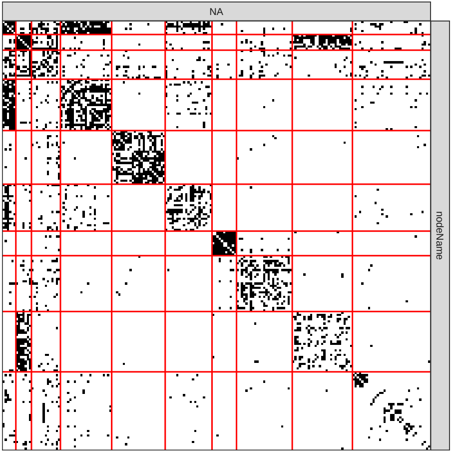


Example: monitoring convergence (ELBO)



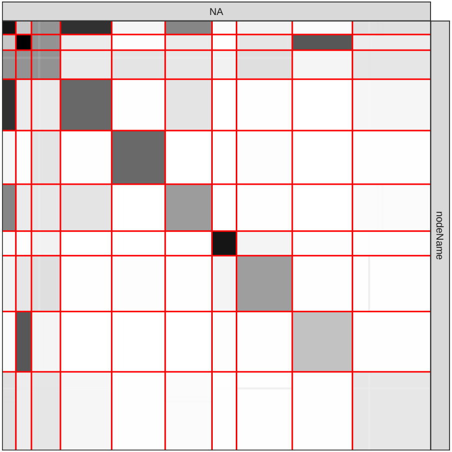
Vizualisation: matrix view

```
plot(my_sbm, dimLabels = list(row = "blogs", col = "blogs"))
```



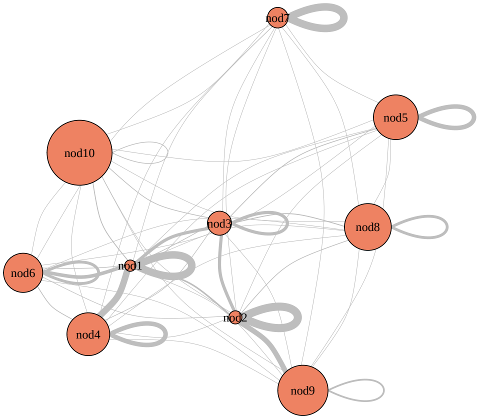
Vizualisation: expected value

```
plot(my_sbm, "expected", dimLabels = list(row = "blogs", col = "blogs"))
```



Vizualisation: mesoscopic view

```
plot(my_sbm, "meso")
```

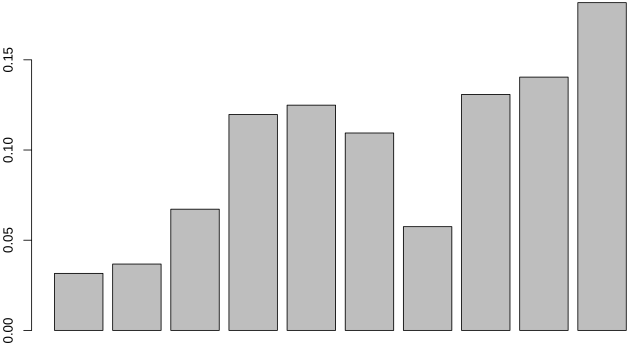


Accessing field I

```r
aricode::ARI(my_sbm$memberships, party)

## [1] 0.4650112
```

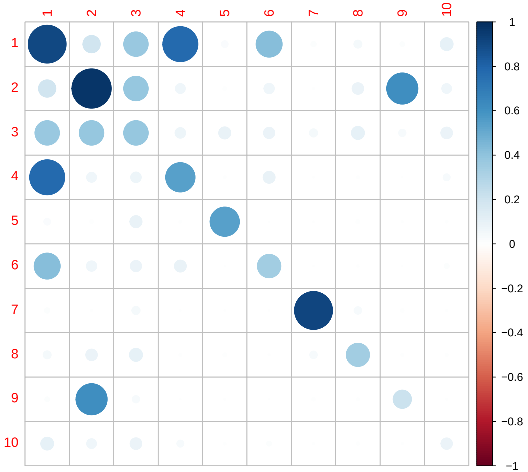
```r
barplot(my_sbm$blockProp)
```

Accessing field II




```
corrplot(my_sbm$connectParam$mean)
```

Accessing field III



etc... see documentation and website

Outline

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

(Y_{ij}) independent and

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

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

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: $Y_{ij} \mid \{i \in \bullet, j \in \bullet\} \sim^{\text{ind}} \mathcal{N}(\mu_{\bullet\bullet}, \sigma^2)$, [?]
3. More generally,

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

Latent Block Models aka Bipartite SBM

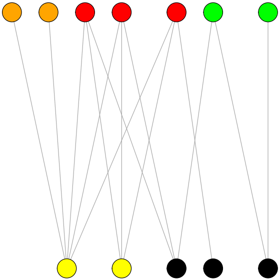
Let Y_{ij} be a bi-partite network. Individuals in row and cols are not the same.

Latent variables : bi-clustering

- Nodes $i = 1, \dots, n_1$ partitionned into K_1 clusters, nodes $j = 1, \dots, n_2$ 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

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

Latent Block Model : illustration



Latent Block Model

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

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

To go further...

- Group GroßBM : https://github.com/GrossSBM/ sbm;
- Documentation of package sbm:
  https://grosssbm.github.io/sbm/
- missSBM SBM with missing data
  https://github.com/GrossSBM/misssbm
  Slides : https:
  //grosssbm.github.io/slideshow-missSBM/slides.html