Masterclass in Machine Learning

Graph clustering and the Stocahstic Bloc Model

January 2022

https://jchiquet.github.io/MAP573

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 pollinator, 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.

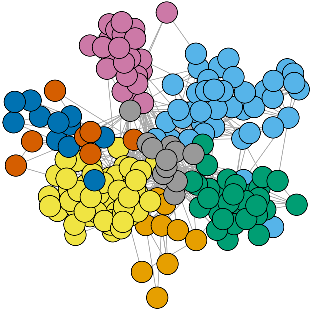
```
data("frenchblog2007", package = "missSBM")
blog <- frenchblog2007 %>%  delete_vertices(which(degree(frenchblog2007) <= 1))
summary(blog)

## IGRAPH 6fb607c 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

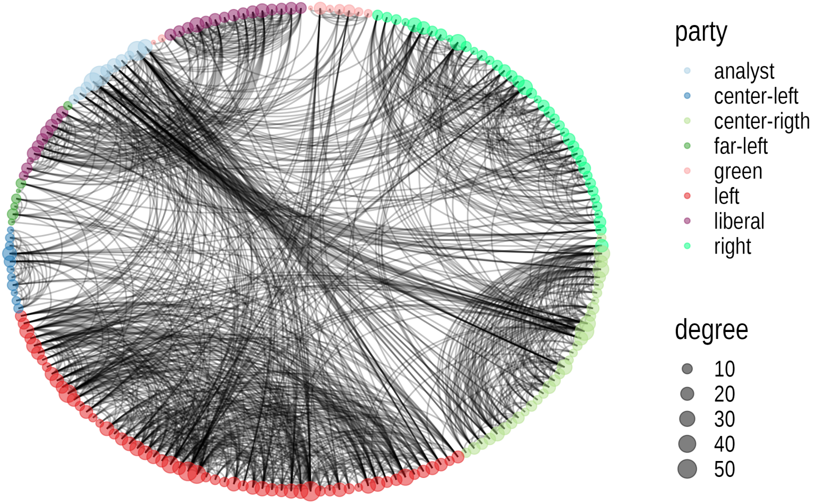
Vizualization: graph view

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
 )
```

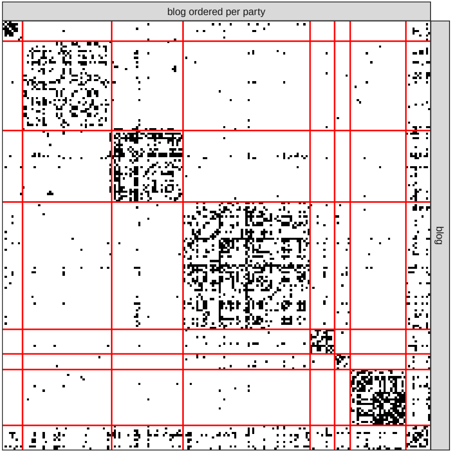


Vizualization: graph view (advanced)



Vizualization: matrix view

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



Questions

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 a predefined classification
- Same remark holds for any kind of clusteringa and unsupervised leaning problem

Objective

Our objective is to automatically find a partitioning of the node, i.e. a clustering, that groups together nodes with similar connectivity pattern. This is known as graph clustering.

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

Principle of graph partionning

Definition (Partition)

A decomposition $\mathcal{C} = \{C_1, \ldots, C_K\}$ of the vertices $\mathcal{V}$ such that

- $C_k \cap C_{k'} = \emptyset$ for any $k \neq k'$
- $\bigcup_k C_k = \mathcal{V}$

Goal of graph partionning

Form a partition of the vertices with unsupervised approach where the $\mathcal{C}$ is composed by "cohesive" sets of vertices, for instance,

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

Outline

Principle

Input: n individuals with p attributes

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 $\{\{1,\ldots,n\}\}$

Algorithm 1: Agglomerative hierarchical clustering

Ingredients

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

Dissimilarity measures

Standards

Use standard distances on adjacency matrix:

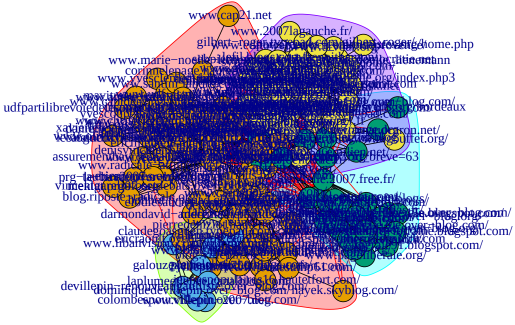
- Euclidean distance: $x_{ij} = \sqrt{\sum_{ij}(A_{ik} - A_{jk})^2}$
- Manhattan distance: $x_{ij} = \sum_{ij} |A_{ik} - A_{jk})|$
- etc. . .

Graph-specific

For instance, Modularity (studied during tutorial)

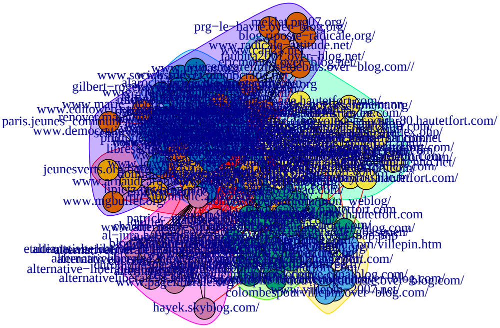
Examples of graph partionning I

```r
hc <- cluster_fast_greedy(blog)
plot(hc, blog)
```



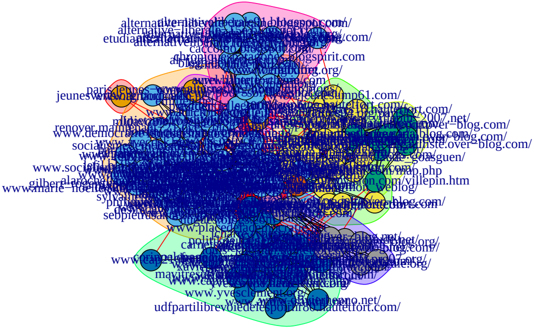
Examples of graph partionning II

```r
hc <- cluster_louvain(blog)
plot(hc, blog)
```



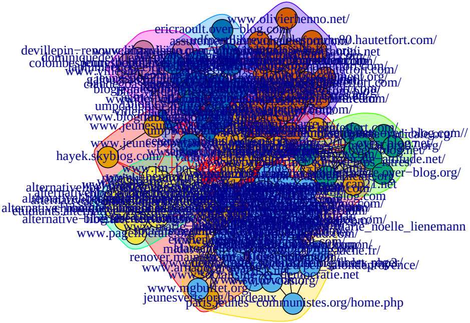
Examples of graph partionning III

```r
hc <- cluster_edge_betweenness(blog)
plot(hc, blog)
```



Examples of graph partionning IV

```r
hc <- cluster_walktrap(blog)
plot(hc, blog)
```



Outline

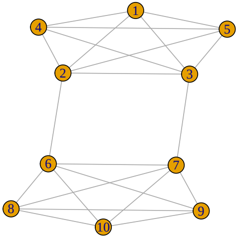
Graph-cut

Definition

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

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

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



Min-cut

Idea

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

Based on this principle, the normalized cut consider the connectivity between group 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

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

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,

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

so that

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

Solving Min-cut for 2 clusters

Normalized graph-cut $\Leftrightarrow$ integer programming problem

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

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

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

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

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)
```

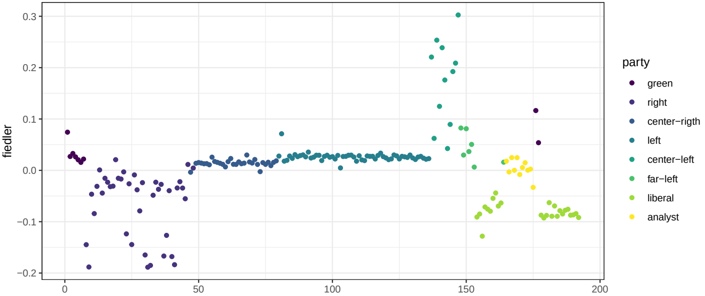
Bi-partionning and the Fiedler vector

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

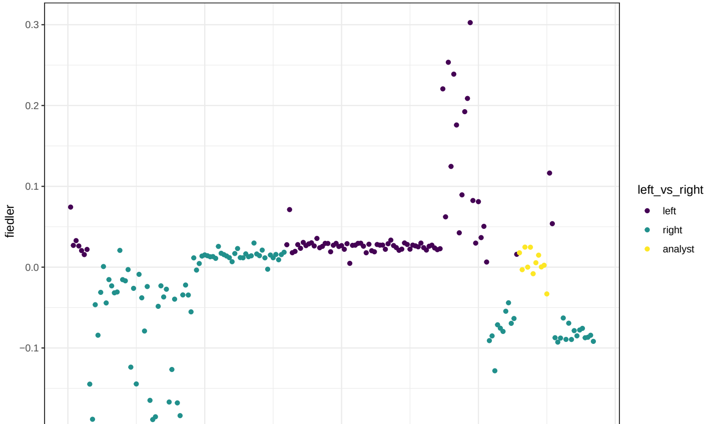
$\rightarrow$ can be used to compute a bi-partition of a graph.

```
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)
```



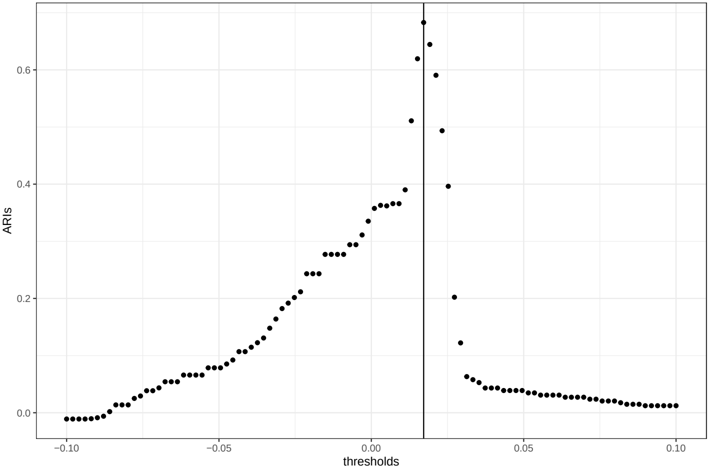
Example on a simplied left/right view

```
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 $i \in q$

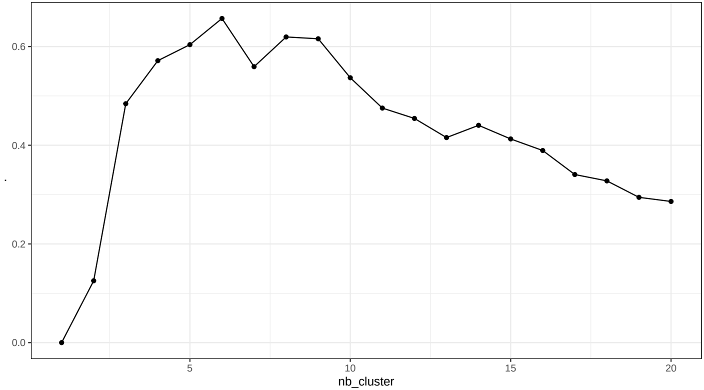
Implementation of normalized spectral clustering

```
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:

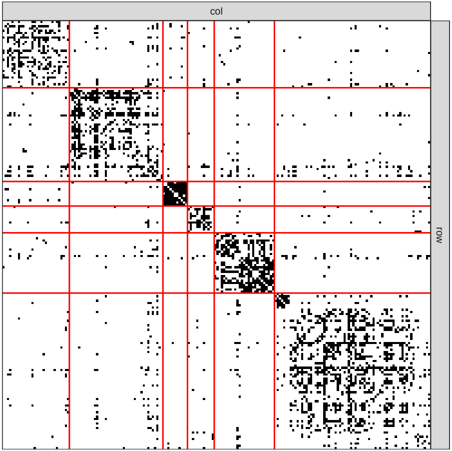
```
nb_cluster <- 1:20
map(nb_cluster, ~spectral_clustering(blog, .)) %>%
  map_dbl(ARI, party) %>% qplot(nb_cluster, y = .) + geom_line() + theme_bw()
```



Application to the French blogosphere (2)

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

```
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.

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

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

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

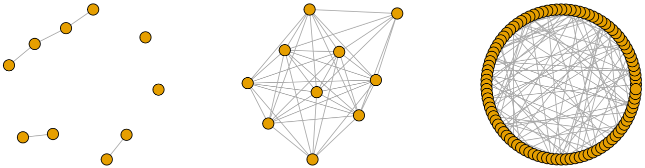
Proposition (degree distribution)

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

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

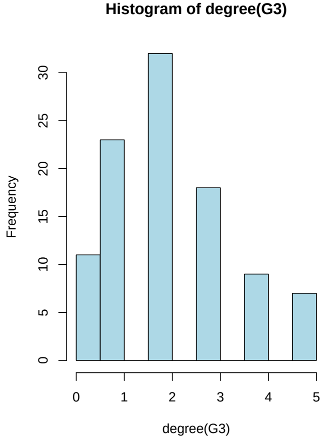
Erdös-Rényi - example

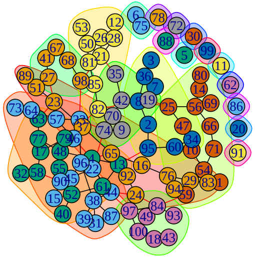
```
G1 <- igraph::sample_gnp(10, 0.1)
G2 <- igraph::sample_gnp(10, 0.9)
G3 <- igraph::sample_gnp(100, .02)
par(mfrow=c(1,3))
plot(G1, vertex.label=NA) ; plot(G2, vertex.label=NA)
plot(G3, vertex.label=NA, layout=layout.circle)
```



Erdös-Rény - limitations: very homegeneous

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

## [1] 5.649385
## [1] 13
```





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,

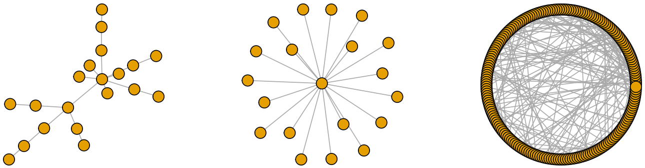
1. At t a new node V_t is added
2. V_t is connected to $i \in V_{t-1}$ with probability

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

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

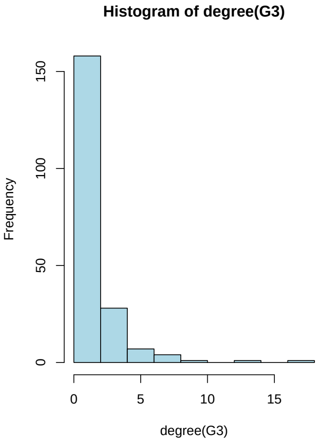
Preferential attachment - example

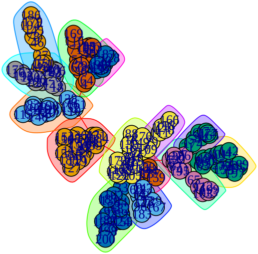
```
G1 <- igraph::sample_pa(20, 1, directed=FALSE)
G2 <- igraph::sample_pa(20, 5, directed=FALSE)
G3 <- igraph::sample_pa(200, directed=FALSE)
par(mfrow=c(1,3))
plot(G1, vertex.label=NA) ; plot(G2, vertex.label=NA)
plot(G3, vertex.label=NA, layout=layout.circle)
```



Preferential attachment - limitations

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

## [1] 6.117387
## [1] 14
```





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 $\mathcal{Q} = \{1, \ldots, Q\}$ 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.

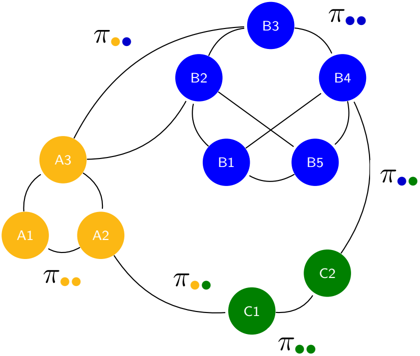
The conditional distribution of the edges

Connexion probabilities depend on the node class belonging:

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

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

Stochastic Block Model: the big picture



Stochastic Block Model

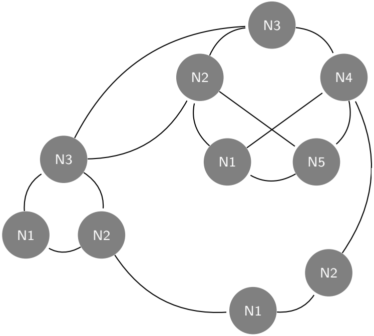
Let n nodes divided into

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

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

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

Stochastic Block Model: unknown parameters



Stochastic Block Model

Let n nodes divided into

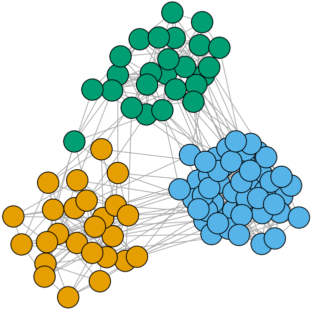
- $\mathcal{Q} = \{\color{orange}{\bullet}, \color{blue}{\bullet}, \color{green}{\bullet}\}$, card$(\mathcal{Q})$ known
- $\alpha_{\bullet} = ?$,
- $\pi_{\color{orange}{\bullet}\color{blue}{\bullet}} = ?$

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

Stochastic block models – examples of topology

Community network

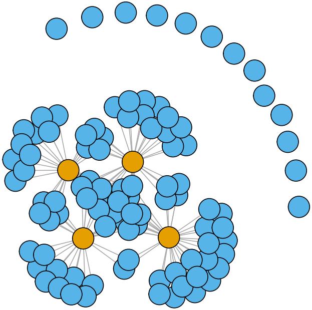
```
pi <- matrix(c(0.3,0.02,0.02,0.02,0.3,0.02,0.02,0.02,0.3),3,3)
communities <- igraph::sample_sbm(100, pi, c(25, 50, 25))
plot(communities, vertex.label=NA, vertex.color = rep(1:3,c(25, 50, 25)))
```



Stochastic block models – examples of topology

Star network

```
pi <- matrix(c(0.05,0.3,0.3,0),2,2)
star <- igraph::sample_sbm(100, pi, c(4, 96))
plot(star, vertex.label=NA, vertex.color = rep(1:2,c(4,96)))
```



Degree distributions

Conditional degree distribution

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

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

Conditional degree distribution

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

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

Likelihoods

Complete-data loglikelihood

$$\log L(\mathbf{X}, \mathbf{Z}) = \sum_{i,q} Z_{iq} \log \alpha_q + \sum_{i<j,q,\ell} Z_{iq} Z_{j\ell} \log \pi_{q\ell}^{X_{ij}} (1 - \pi_{q\ell})^{1-X_{ij}}.$$

Conditional expectation of the complete-data loglikelihood

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

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

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

Outline

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

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

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

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

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

Revisting the EM algorithm II

Let

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

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 $\mathbb{P}(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}^{(t)})$

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

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

Variational approximation for SBM

Problem for SBM

$\mathbb{P}(\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}^{(t)})$ 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 $\mathbb{P}(\mathbf{Z}|\mathbf{X})$, the Kullback-Leibler divergence is non-negative and

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

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:

$$\hat{\tau}_{iq} \propto \alpha_q \prod_j \prod_\ell b(X_{ij}, \pi_{q\ell})^{\hat{\tau}_{j\ell}} \tag{1}$$

M-step

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

$$\hat{\alpha}_q = \frac{1}{n} \sum_i \hat{\tau}_{iq}, \quad \hat{\pi}_{q\ell} = \frac{\sum_{i \neq j} \hat{\tau}_{iq} \hat{\tau}_{j\ell} X_{ij}}{\sum_{i \neq j} \hat{\tau}_{iq} \hat{\tau}_{j\ell}}. \tag{2}$$

Model selection

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

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

where

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

The variational BIC is just

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