Data anaysis and Unsupervised Learning
Clustering: model-based approaches

MAP 573, 2020 – Julien Chiquet

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ACCÉLÉRATEUR &
INCUBATEUR DE START-UP
ÉCOLE POLYTECHNIQUE

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

Packages required for reproducing the slides

```r
library(tidyverse)  # opinionated collection of packages for data manipulation
library(GGally)     # extension to ggplot vizualization system
library(kernlab)    # Kernel-based methods, among which spectral-clustering
library(aricode)    # fast computation of clustering measures
library(mclust)     # gaussian mixture models
library(sbm)        # Stochastic Block Models
library(igraph)     # graph manipulation
theme_set(theme_bw()) # plots themes
```

Companion data set

Morphological Measurements on Leptograpsus Crabs

Description

The crabs data frame has 200 rows and 8 columns, describing 5 morphological measurements on 50 crabs each of two colour forms and both sexes, of the species *Leptograpsus variegatus* collected at Fremantle, W. Australia.

```
crabs <- MASS::crabs %>% select(-index) %>%
  rename(sex = sex,
         species         = sp,
         frontal_lob     = FL,
         rear_width      = RW,
         carapace_length = CL,
         carapace_width  = CW,
         body_depth      = BD)
crabs %>% select(sex, species) %>% summary() %>% knitr::kable("latex")
```

	sex	species
	F:100	B:100
	M:100	O:100

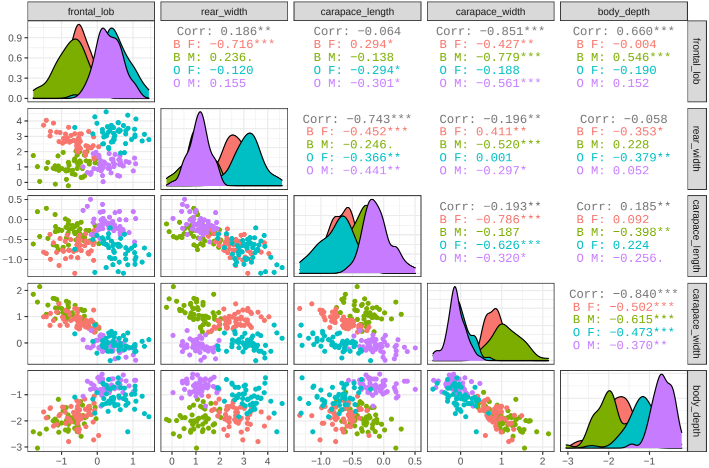
Remove size effect I

```
attributes <- select(crabs, -sex, -species) %>% as.matrix()
u1 <- eigen(cov(attributes))$vectors[, 1, drop = FALSE]
attributes_rank1 <- attributes %*% u1 %*% t(u1)
crabs_corrected <- crabs
crabs_corrected[, 3:7] <- attributes - attributes_rank1
```

⇝ Axis 1 explains a latent effect, here the size in the case at hand, common to all attributes.

```
ggpairs(crabs_corrected, columns = 3:7, aes(colour = paste(crabs$species, crabs$sex
```

Remove size effect II



Clustering: general goals

Objective: construct a map

$$f : \mathcal{D} = \{1, \ldots, n\} \mapsto \{1, \ldots, K\}$$

where K is a fixed number of clusters.

Careful! classification $\neq$ clustering

- Classification presupposes the existence of classes
- Clustering labels only elements of the dataset
  - $\rightsquigarrow$ no ground truth (no given labels)
  - $\rightsquigarrow$ discovers a structure "natural" to the data
  - $\rightsquigarrow$ not necessarily related to a known classification

Motivations

- describe large masses of data in a simplified way,
- structure a set of knowledge,
- reveal structures, hidden causes,
- use of the groups in further processing,
- ...

Clustering: challenges

Clustering quality

No obvious measure to define the quality of the clusters. Ideas:

- Inner homogeneity: samples in the same group should be similar
- Outer inhomogeneity: samples in different groups should be different

Number of clusters

Choice of the number of clusters K often complex

- No ground truth in unsupervised learning!
- Several solutions might be equally good

Two general approaches

- distance-based: require a distance/dissimilarity between $\{\mathbf{x}_i\}$
- **model-based**: require assumptions on the distribution $\mathbb{P}$

Part II

Model-based method

Outline

Model-based method

1. Mixture models
   - Statistical model: latent variable
   - Expectation-Maximization algorithm
   - Example: mixture of Gaussians
2. The Stochastic Block Model (SBM)

References

Pattern recognition and machine learning,
Christopher Bishop
Chapter 9: Mixture Models and EM
http://users.isr.ist.utl.pt/~wurmd/Livros/school/

Models with Hidden Structure with Applications in Biology and Genomics,
Stéphane Robin
Master MathSV Course
https:
//www6.inra.fr/mia-paris/content/download/4587/42934/version/1/file/ModelsHiddenStruct-Biology.pdf

Classification non-supervisées,
É. Lebarbier, T. Mary-Huard
Chapitre 3 - méthode probabiliste: le modèle de mélange
https://www.agroparistech.fr/IMG/pdf/ClassificationNonSupervisee-AgroParisTech.pdf

Outline

Model-based method

1. Mixture models
   - Statistical model: latent variable
   - Expectation-Maximization algorithm
   - Example: mixture of Gaussians
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Latent variable models

Definition

A latent variable model is a statistical model that relates, for $i = 1, \ldots, n$ individuals,

- a set of manifest (observed) variables $\mathbf{X} = (X_i, i = 1, \ldots, n)$ to
- a set of latent (unobserved) variables $\mathbf{Z} = (Z_i, i = 1, \ldots, n)$.

Common assumption: conditional independence

$$\mathbb{P}((X_1, \ldots, X_n)|(Z_1, \ldots, Z_n)) = \prod_{i=1}^{n} \mathbb{P}(X_i|Z_i).$$

Famous examples

- $(Z_i, i \geq 1)$ is Markov chain: Markov models
- Z_i categorical and independent: mixture models

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Mixture models: the latent variables

When $(Z_1, \ldots, Z_n)$ are independent categorical variables, they give a natural (latent) classification of the observations $(X_1, \ldots, X_n)$ – or labels.

Notations

Let $(Z_1, \ldots, Z_n)$ be *iid* categorical variables with distribution

$$\mathbb{P}(i \in q) = \mathbb{P}(Z_i = q) = \alpha_q, \quad \text{s.t.} \sum_{q=1}^{Q} \alpha_q = 1.$$

Alternative (equivalent) notation

Let $Z_i = (Z_{i1}, \ldots, Z_{iq})$ be an indicator vector of label for i:

$$\mathbb{P}(i \in q) = \mathbb{P}(Z_{iq} = 1) = \alpha_q, \quad \text{s.t.} \sum_{q=1}^{Q} \alpha_q = 1.$$

By definition, $Z_i \sim \mathcal{M}(1, \boldsymbol{\alpha})$, with $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_Q)$.

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Mixture models: the manifest variables

A mixture model represents the presence of subpopulations within an overall population as follows:

$$\mathbb{P}(X_i) = \sum_{z_i \in \mathcal{Z}_i} \mathbb{P}(X_i, Z_i) = \sum_{Z_i \in \mathcal{Z}_i} \mathbb{P}(X_i | Z_i) \mathbb{P}(Z_i).$$

Conditional distribution of the manifest variables

We assume a parametric distribution of X in each subpopulation

$$X_i | \{Z_i = q\} \sim \mathbb{P}_{\theta_q} \qquad \left(\Leftrightarrow X_i | \{Z_{iq}\} = 1 \sim \mathbb{P}_{\theta_q} \right)$$

The specificity of each class is handled by $\{\boldsymbol{\theta}_q\}_{q=1}^{Q}$.

Mixture models: likelihoods

The complete-data likelihood

It is the join distribution of (X_i, Z_i):

$$\mathbb{P}(X_i, Z_i) = \alpha_{Z_i} \mathbb{P}_{\boldsymbol{\theta}_{Z_i}}(X_i)$$

The incomplete-data likelihood

It is the marginal distribution of X_i once Z_i integrated:

$$\mathbb{P}(X_i) = \sum_{q=1}^{Q} \mathbb{P}(X_i, Z_i = q) = \sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\boldsymbol{\theta}_q}(X_i)$$

$\rightsquigarrow$ A mixture model is a sum of distributions weigthed by the proportion of each subpopulation.

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Outline

Model-based method

Intractability of the Likelihood

Maximum Likelihood Estimator

The MLE aims to maximize the (marginal) likehood of the observations:

$$L(\boldsymbol{\theta}; \mathbf{X}) = \mathbb{P}_{\boldsymbol{\theta}}((X_1, \dots, X_n)) = \int_{\mathbf{Z} \in \mathcal{Z}} \mathbb{P}_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{Z}) \mathrm{d}\mathbf{Z}$$

Integrations are summation over $\{1, \dots, Q\}$: we have Q^n terms !

Intractable summation

With mixture models, for $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_Q)$ we have

$$\log L(\boldsymbol{\theta}; \mathbf{X}) = \sum_{i=1}^{n} \log \left\{ \sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\boldsymbol{\theta}_q}(X_i) \right\}.$$

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Intractability of the Likelihood

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$\leadsto$ Direct maximization of the likelihood is impossible in practice

Bayes decision rule / Maximum *a posteriori*

Principle

Affect an individual i to the subpopulation which is the most likely according to the data:

$$\tau_{iq} = \mathbb{P}(Z_{iq} = 1 | X_i = x_i)$$

This is the posterior probability for $i \in q$.

Application of the Bayes Theorem

It is straightforward to show that

$$\tau_{iq} = \frac{\alpha_q \mathbb{P}_{\theta_q}(x_i)}{\sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\theta_q}(x_i)}$$

Principle of the EM algorithm

If $\boldsymbol{\theta}$ were known

...estimating the posterior probability $\mathbb{P}(Z_i|\mathbf{X})$ of $\mathbf{Z}$ should be easy
By means of the Bayes decision rule

If $\mathbf{Z}$ were known...

...estimating the best set of parameter $\boldsymbol{\theta}$ should be easy
This is close to usual maximum likelihood estimation

EM principle

Maximize the marginal likelihood iteratively:

1. Initialize θ
2. Compute the probability of $\mathbf{Z}$ given θ
3. Get a better θ with the new $\mathbf{Z}$
4. Iterate until convergence

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EM: the complete data log-likelihood

- Marginal likelihood is hard to work with
- Use the **"complete-data" likelihood**, where $\mathbf{Z}_i$ is known

$$
\begin{aligned}
\log L(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Z}) &= \log \prod_{i=1}^{n} \mathbb{P}(\mathbf{X}_i, \mathbf{Z}_i) \\
&= \log \prod_{i=1}^{n} \underbrace{\prod_{q=1}^{Q} \mathbb{P}(\mathbf{X}_i, (\mathbf{Z}_{i1}, \ldots, \mathbf{Z}_{iQ})^{Z_{iq}}}_{\text{a single "active" term (the one with } Z_{iq}=1)} \\
&= \log \prod_{i=1}^{n} \prod_{q=1}^{Q} \alpha_q \mathbb{P}_{\theta_q}(\mathbf{X}_i)^{Z_{iq}} \\
&= \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \log \left[\alpha_q \mathbb{P}_{\theta_q}(\mathbf{X}_i) \right]
\end{aligned}
$$

EM: the criterion

- Alright, Use the "complete-data" likelihood, **but $\mathbf{Z}_i$ is unknown!**
- **Replace the $\mathbf{Z}_i$** by its best prediction: $\mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}(\,\cdot\,)$
- Use an estimation of $\mathbb{P}_{\boldsymbol{\theta}^{(t)}}(\mathbf{Z}|\mathbf{X}))$ to estimate $\mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}(\,\cdot\,)$

$$
\begin{aligned}
\mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\big(\log L(\boldsymbol{\theta};\mathbf{X},\mathbf{Z})\big) &= \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\Big(\sum_{i=1}^{n}\sum_{q=1}^{Q} Z_{iq}\log\big[\alpha_q \mathbb{P}_{\theta_q}(\mathbf{X}_i)\big]\Big) \\
&= \sum_{i=1}^{n}\sum_{q=1}^{Q} \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\big(Z_{iq}\big)\log\big[\alpha_q \mathbb{P}_{\theta_q}(\mathbf{X}_i)\big] \\
&= \sum_{i=1}^{n}\sum_{q=1}^{Q} \tau_{iq}\log\big[\alpha_q \mathbb{P}_{\theta_q}(\mathbf{X}_i)\big] \\
&\triangleq Q\big(\boldsymbol{\theta}|\boldsymbol{\theta}'\big)
\end{aligned}
$$

Formal algorithm

Initialization: start from a good guess either of $\mathbf{Z}$ or $\boldsymbol{\theta}$, then iterate 1-2

1. Expectation step

Calculate the expected value of the loglikelihood under the current $\boldsymbol{\theta}$

$$Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right) = \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}^{(t)}}\left[\log L(\boldsymbol{\theta};\mathbf{X},\mathbf{Z})\right] \qquad (\textit{needs } \mathbb{P}_{\boldsymbol{\theta}^{(t)}}(\mathbf{Z}|\mathbf{X}))$$

2. Maximization step

Find the parameters that maximize this quantity

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right)$$

Stop when $\|\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\| < \varepsilon$ or $\|Q^{(t+1)} - Q^{(t)}\| < \varepsilon$

(Basic) Convergence analysis I

Theorem

At each step of the EM algorithm, the loglikelihood increases. EM thus reaches a local optimum.

Proof

By definition of conditional probability $\mathbb{P}(\mathbf{Z}|\mathbf{X})$, one has

$$\log L(\mathbf{X};\boldsymbol{\theta}) = \log L(\mathbf{X},\mathbf{Z};\boldsymbol{\theta}) - \log L(\mathbf{Z}|\mathbf{X};\boldsymbol{\theta})$$

We then apply the expectation $\mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\big(\,\cdot\,\big)$ both side

$$\log L(\mathbf{X}) = \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\big(\log L(\mathbf{X},\mathbf{Z};\boldsymbol{\theta})\big) - \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}'}\big(\log L(\mathbf{Z}|\mathbf{X};\boldsymbol{\theta})\big)$$

Indeed, the marginal likelihood does not depend on $\mathbf{Z}$.

continue...

(Basic) Convergence analysis II

We recognize two important quantities: the criterion Q and what we call the entropy of $\mathcal{H}$ of $\mathbb{P}(\mathbf{Z}|\mathbf{X})$:

$$\log L(\mathbf{X}) = Q(\boldsymbol{\theta}|\boldsymbol{\theta}') + \mathcal{H}(\boldsymbol{\theta}, \boldsymbol{\theta}')$$

To prove that $\log L$ is increased by EM, we consider two successive iteration with parameter $\boldsymbol{\theta}'$ and $\boldsymbol{\theta}''$ and study there difference:

$$\begin{aligned}\log L(\mathbf{X}; \boldsymbol{\theta}'') - \log L(\mathbf{X}; \boldsymbol{\theta}') &= Q(\boldsymbol{\theta}''|\boldsymbol{\theta}') - Q(\boldsymbol{\theta}'|\boldsymbol{\theta}') \\ &+ \mathcal{H}(\boldsymbol{\theta}'', \boldsymbol{\theta}') - \mathcal{H}(\boldsymbol{\theta}', \boldsymbol{\theta}')\end{aligned}$$

1. First $Q(\boldsymbol{\theta}''|\boldsymbol{\theta}') - Q(\boldsymbol{\theta}'|\boldsymbol{\theta}') \geq 0$ by definition of the maximization step.
2. Second we need to prove that $\mathcal{H}(\boldsymbol{\theta}'', \boldsymbol{\theta}') - \mathcal{H}(\boldsymbol{\theta}', \boldsymbol{\theta}') \geq 0$

(Basic) Convergence analysis III

$$\begin{aligned}\mathcal{H}(\boldsymbol{\theta}'', \boldsymbol{\theta}') - \mathcal{H}(\boldsymbol{\theta}', \boldsymbol{\theta}') &= -\mathbb{E}_{\boldsymbol{\theta}'}\left(\log L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}'') - \log L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}')\right) \\ &= -\mathbb{E}_{\boldsymbol{\theta}'}\left(\log \frac{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}'')}{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}')}\right)\end{aligned}$$

We then use the Jensen inequality: if ϕ is convex, then $\phi(\mathbb{E}(X)) \leq \mathbb{E}(\phi(X))$. Since $\log$ is concave,

$$\begin{aligned}\mathcal{H}(\boldsymbol{\theta}'', \boldsymbol{\theta}') - \mathcal{H}(\boldsymbol{\theta}', \boldsymbol{\theta}') &= -\mathbb{E}_{\boldsymbol{\theta}'}\left(\log \frac{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}'')}{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}')}\right) \\ &\geq -\log \mathbb{E}_{\boldsymbol{\theta}'}\left(\frac{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}'')}{L(\mathbf{Z}|\mathbf{X}; \boldsymbol{\theta}')}\right) \\ &= -\log \int_{\mathcal{Z}}\left(\frac{L(\mathbf{z}|\mathbf{X}; \boldsymbol{\theta}'')}{\mathbb{P}(\mathbf{z}|\mathbf{X}; \boldsymbol{\theta}')}\mathbb{P}(\mathbf{z}|\mathbf{X}; \boldsymbol{\theta}')\mathrm{d}\mathbf{z}\right) \\ &= -\log(1) = 0\end{aligned}$$

Choosing the number of component

Reminder: Bayesian Information Criterion

The BIC is a model selection criterion which penalizes the adjustement to the data by the number of parameter in model $\mathcal{M}$ as follows:

$$\mathrm{BIC}(\mathcal{M}) = \log L(\hat{\boldsymbol{\theta}}; \mathbf{X}) - \frac{1}{2}\log(n)\mathrm{df}(\mathcal{M}).$$

Integrated Classification Criterion

It is an adaptation working with the complete-data likelihood:

$$\begin{aligned}\mathrm{ICL}(\mathcal{M}) &= \log L(\hat{\boldsymbol{\theta}}; \mathbf{X}, \hat{\mathbf{Z}}) + \frac{1}{2}\log(n)\mathrm{df}(\mathcal{M}) \\ &= \mathrm{BIC} - \mathcal{H}(\mathbb{P}(\hat{\mathbf{Z}}|\mathbf{X}),\end{aligned}$$

where the entropy $\mathcal{H}$ measures the separability of the subpopulations.

$\rightsquigarrow$ We choose $\mathcal{M}(Q)$ that maximizes either BIC or ICL

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Popular model: Gaussian Multivariate mixture models

The distribution of X_i conditional on the label of i is assumed to be a multivariate Gaussian distribution with unknown parameters:

$$X_i | i \in q \sim \mathcal{N}(\boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q)$$

Complete Likelihood $(\mathbf{X}, \mathbf{Z})$

The model complete loglikelihood is

$$\log L(\boldsymbol{\mu}, \boldsymbol{\Sigma}; \mathbf{X}, \mathbf{Z}) = \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \left(\log \alpha_q - \frac{1}{2} \log \det(\boldsymbol{\Sigma}_q) - \frac{1}{2} \|\mathbf{x}_i - \boldsymbol{\mu}_q\|^2_{\boldsymbol{\Sigma}_q^{-1}}) \right) + c$$

$\rightsquigarrow$ Implementation of the univariate case during the today's lab.

Mixture of Gaussians

Calculs in the univariate case: complete likelihood

The distribution of X_i conditional on the label of i is assumed to be a univariate Gaussian distribution with unknown parameters:

$$X_i | Z_{iq} = 1 \sim \mathcal{N}(\mu_q, \sigma_q^2)$$

complete Likelihood $(\mathbf{X}, \mathbf{Z})$

The model complete loglikelihood is

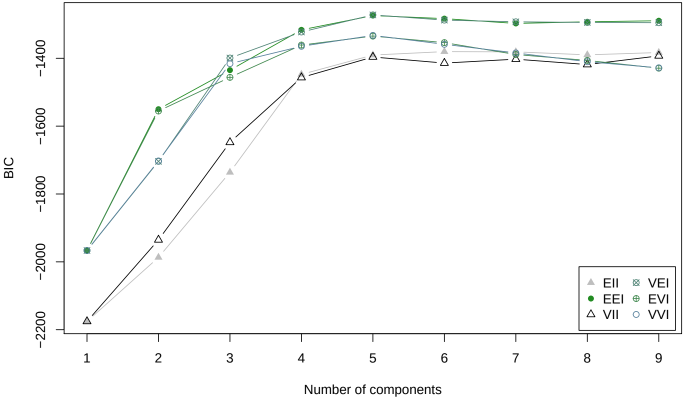
$$\log L(\boldsymbol{\mu}, \boldsymbol{\sigma}^2; \mathbf{X}, \mathbf{Z}) = \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \left(\log \alpha_q - \log \sigma_q - \log(\sqrt{2\pi}) - \frac{1}{2\sigma_q^2}(x_i - \mu_q)^2 \right)$$

Gaussian mixture model in R I

The package `Mclust` is a great reference
See https://cran.r-project.org/web/packages/mclust/vignettes/mclust.html

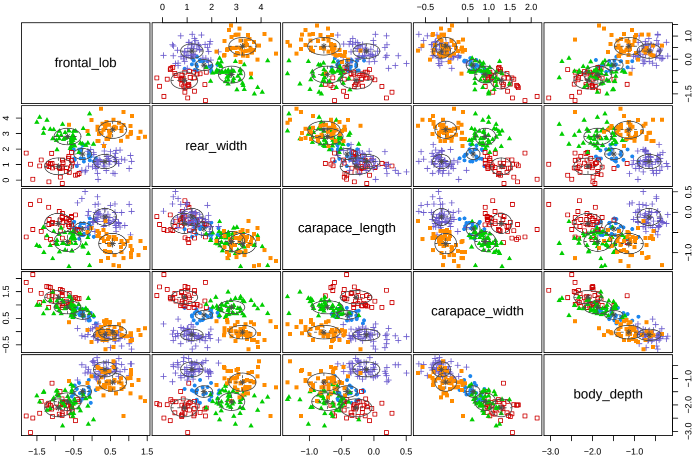
```
classes <- paste(crabs_corrected$sex, crabs_corrected$species, sep="-")
GMM <- crabs_corrected %>%
  select(-sex, -species) %>%
  Mclust(modelNames = c("EII", "EEI", "VII", "VEI", "EVI", "VVI"))
plot(GMM, 'BIC')
```

Gaussian mixture model in R II




```r
plot(GMM, 'classification')
```

Gaussian mixture model in R III



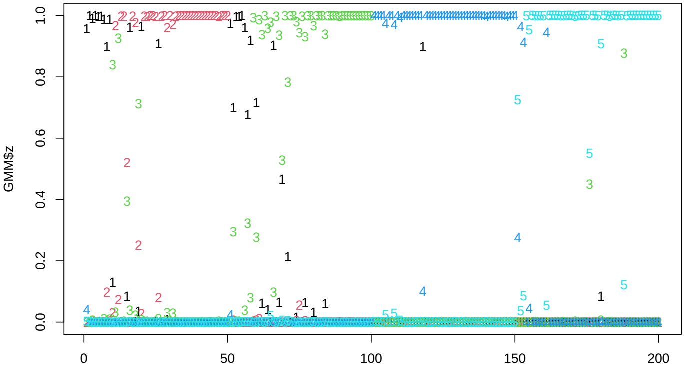
Gaussian mixture model in R IV

```
kmeans_cl <- crabs_corrected %>% select(-sex, -species) %>% as.matrix() %>%
  kmeans(centers = 4, nstart = 100) %>% pluck("cluster")
ward_cl <- crabs_corrected %>% select(-sex, -species) %>% dist() %>%
  hclust(method = "ward.D2") %>% cutree(4)
aricode::ARI(GMM$classification, classes)

## [1] 0.764725

aricode::ARI(GMM$classification, kmeans_cl)

## [1] 0.8230122

aricode::ARI(GMM$classification, ward_cl)

## [1] 0.7670297
```

The posterior probabilities

```
matplot(GMM$z)
```

Gaussian mixture model in R V



The model parameters:

Gaussian mixture model in R VI

```
str(GMM$parameters, max.level = 1)

## List of 3
##  $ pro     : num [1:5] 0.114 0.175 0.222 0.261 0.228
##  $ mean    : num [1:5, 1:5] -0.256 1.681 -0.414 0.626 -1.493 ...
##   ..- attr(*, "dimnames")=List of 2
##  $ variance:List of 6
```

Outline

Model-based method

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

Model-based method

A mathematical model: Erdös-Rényi graph

Definition

Let $\mathcal{V} = 1, \dots, n$ 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

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

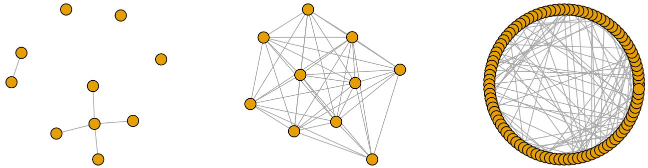
Proposition (degree distribution)

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

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

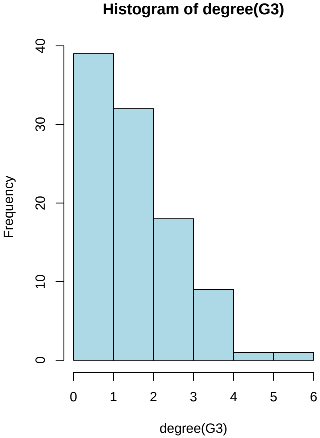
Erdös-Rényi - example

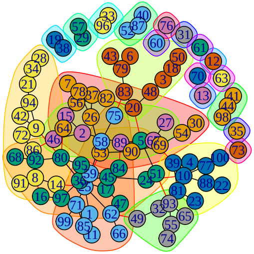
```
G1 <- igraph::sample_gnp(10, 0.1)
G2 <- igraph::sample_gnp(10, 0.9)
G3 <- igraph::sample_gnp(100, .02)
par(mfrow=c(1,3))
plot(G1, vertex.label=NA) ; plot(G2, vertex.label=NA)
plot(G3, vertex.label=NA, layout=layout.circle)
```



Erdös-Rény - limitations: very homegeneous

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

## [1] 5.499004
## [1] 13
```





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

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

Model-based method

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.

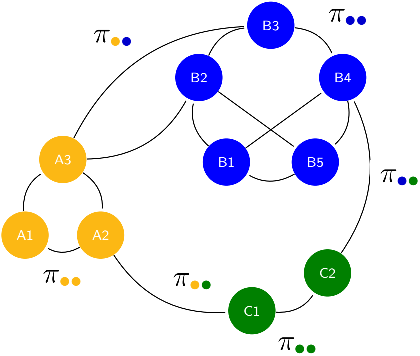
The conditional distribution of the edges

Connexion probabilities depend on the node class belonging:

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

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

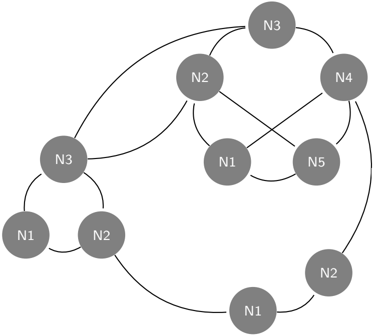
Let n nodes divided into

- $\mathcal{Q} = \{{\color{orange}\bullet}, {\color{blue}\bullet}, {\color{green}\bullet}\}$ 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

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

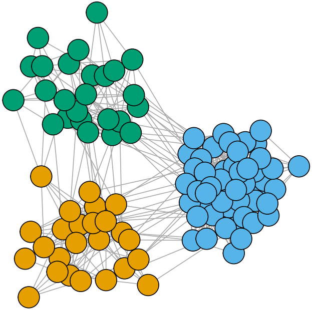
$$Z_i = \mathbf{1}_{\{i \in \bullet\}} \sim^{\text{iid}} \mathcal{M}(1, \alpha), \quad \forall \bullet \in \mathcal{Q},$$

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

Stochastic block models – examples of topology

Community network

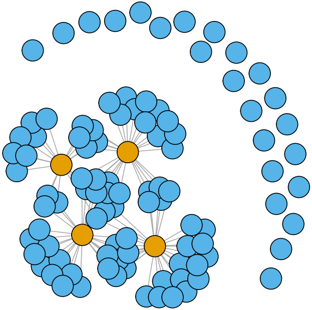
```
pi <- matrix(c(0.3,0.02,0.02,0.02,0.3,0.02,0.02,0.02,0.3),3,3)
communities <- igraph::sample_sbm(100, pi, c(25, 50, 25))
plot(communities, vertex.label=NA, vertex.color = rep(1:3,c(25, 50, 25)))
```



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 $i = 1, \dots, n$.

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

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

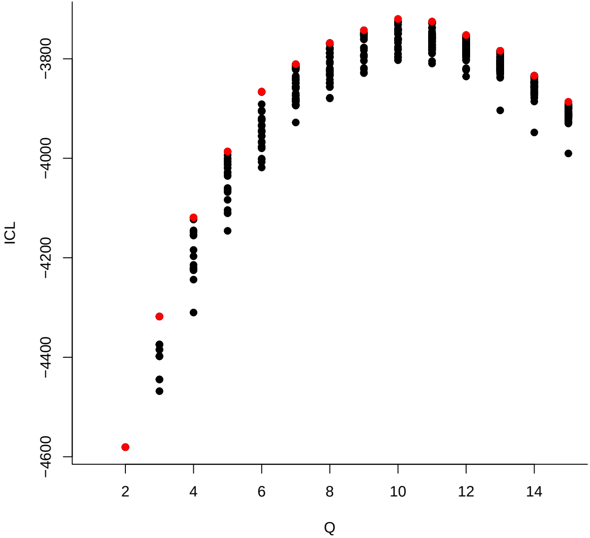
The variational BIC is just

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

Example on the French blogsphere (I)

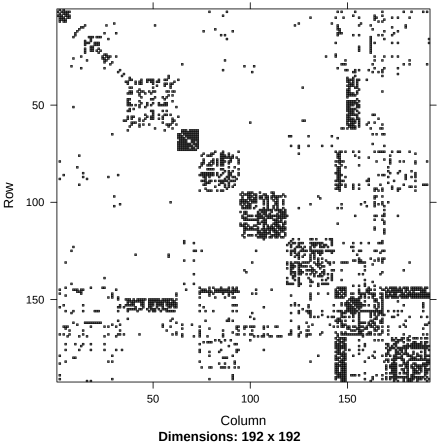
```r
library(blockmodels)
library(sand)

adj_blog <- upgrade_graph(fblog) %>%
    as_adjacency_matrix() %>%
    as.matrix()

mySBM_collection <- BM_bernoulli(
  "SBM_sym",
  adj_blog, verbosity = 0,
  plotting = "figures/ICL_fblog.pdf"
)
mySBM_collection$estimate()
```

Example on the French blogsphere (II)



Example on the French blogsphere (III)

```r
library(Matrix)
clusters <-
  apply(mySBM_collection$memberships[[10]]$Z, 1, which.max)
image(Matrix(adj_blog[order(clusters), order(clusters)]))
```



Example on the French blogsphere (IV) I

```
library(RColorBrewer); pal <- brewer.pal(10, "Set3")

g <- graph_from_adjacency_matrix(
  adj_blog,
  mode = "undirected",
  weighted = TRUE,
  diag = FALSE
)
V(g)$class <- clusters
V(g)$size <- 5
V(g)$frame.color <- "white"
V(g)$color <- pal[V(g)$class]
V(g)$label <- ""
E(g)$arrow.mode <- 0

par(mar =c(0,0,0,0))
plot(g, edge.width=E(g)$weight)
```

Example on the French blogsphere (IV) II