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# Clustering: from modeling to visualizing Mapping clusters as spherical Gaussians

Christophe Biernacki, Vincent Vandewalle, Matthieu Marbac

► **To cite this version:**

Christophe Biernacki, Vincent Vandewalle, Matthieu Marbac. Clustering: from modeling to visualizing Mapping clusters as spherical Gaussians. SFC 2023 - Rencontres de la Société Francophone de Classification, Jul 2023, Strasbourg, France. hal-04370886

**HAL Id: hal-04370886**

**<https://inria.hal.science/hal-04370886v1>**

Submitted on 3 Jan 2024

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# Gaussian Based Visualization of Gaussian and Non-Gaussian Based Clustering

**C. Biernacki**

with M. Marbac-Lourdelle and V. Vandewalle

SFC'2023

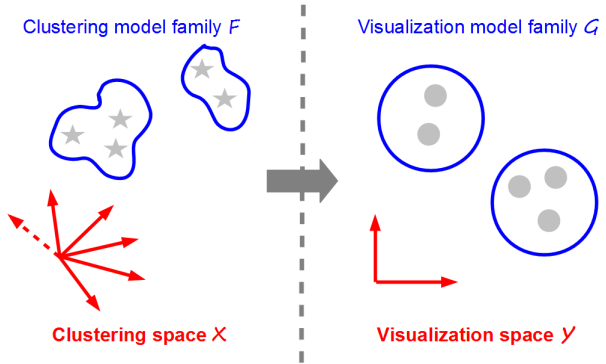
Rencontres de la Société Francophone de Classification

6-7 juillet 2023, Strasbourg, France



# Take home message

**Traditionally:** spaces for visualizing clusters are fixed for their user-convenience  
**Natural extension:** models for visualizing clusters should follow the same principle!



# Outline

**1** Clustering: from modeling to visualizing

2 Mapping clusters as spherical Gaussians

3 Numerical illustrations for complex data

4 Axes interpretability

5 Discussion

## Model-based clustering: pitch<sup>1</sup>

- **Data set:**  $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ , each  $\mathbf{x}_i \in \mathcal{X}$  with  $d_X$  variables
- **Partition (unknown):**  $\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_n)$  with binary notation  $\mathbf{z}_i = (z_{i1}, \dots, z_{iK})$
- **Statistical model:** couples  $(\mathbf{x}_i, \mathbf{z}_i)$  independently arise from the parametrized pdf

$$\underbrace{f(\mathbf{x}_i, \mathbf{z}_i)}_{\in \mathcal{F}} = \prod_{k=1}^K [\pi_k f_k(\mathbf{x}_i)]^{z_{ik}}$$

- **Estimating  $f$ :** implement the MLE principle through an EM-like algorithm
- **Estimating  $K$ :** use some information criteria as BIC, ICL, ...
- **Estimating  $\mathbf{z}$ :** use the MAP principle  $\hat{z}_{ik} = 1$  iff  $k = \arg \max_{\ell} t_{i\ell}(\hat{f})$  where

$$t_{ik}(f) = \mathbb{p}(z_{ik} = 1 | \mathbf{x}_i; f) = \frac{\pi_k f_k(\mathbf{x}_i)}{\underbrace{\sum_{\ell=1}^K \pi_{\ell} f_{\ell}(\mathbf{x}_i)}_{f(\mathbf{x}_i)}}$$

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<sup>1</sup>See for instance [McLachlan & Peel 2004], [Biernacki 2017]

## Model-based clustering: flexibility of $\mathcal{F}$ for complex $\mathcal{X}$

- **Continuous data** ( $\mathcal{X} = \mathbb{R}^{d_x}$ ): multivariate Gaussian/ $t$  distrib. [McNicholas 2016]
- **Categorical data**: product of multinomial distributions [Goodman 1974]
- **Mixing cont./cat.**: product Gaussian/multinomial [Moustaki & Papageorgiou 2005]
- **Functional data**: the discriminative functional mixture [Bouveyron *et al.* 2015]
- **Network data**: the Erdős Rényi mixture [Zanghi *et al.* 2008]
- Other kinds of data, missing data, high dimension, . . .

## Model-based clustering: poor user-friendly understanding

- $n$  or  $K$  large: poor overview of partition  $\hat{z}$
- $d_X$  large: too many parameters to embrace as a whole in  $\hat{f}_k$
- Complex  $\mathcal{X}$ : specific and non trivial parameters involved in  $\hat{f}_k$

### Visualization procedures

Aim at proposing user-friendly understanding of the mathematical clustering results

## Overview of clustering visualization: mapping vs. drawing

Visualization is the achievement of two different successive steps:

- **The mapping step:**

- Performs a transformation, typically space dimension reduction of a data set or of a pdf
- It produces **no graphical output** at all (deliver just a mathematical object)

- **The drawing step:**

- Provides the final **graphical display** from the output of the previous mapping step
- Usually involves classical graphical toolboxes and tunes any graphical parameters

Mathematician is first concerned by the more challenging mapping step



## Overview of clustering visualization: individual mapping

- Aims at visualizing simultaneously the data set  $\mathbf{x}$  and its estimated partition  $\hat{\mathbf{z}}$
- Transforms  $\mathbf{x}$ , defined on  $\mathcal{X}$ , into  $\mathbf{y} = (\mathbf{y}_1, \dots, \mathbf{y}_n)$ , defined on a new space  $\mathcal{Y}$

$$M^{\text{ind}} \in \mathcal{M}^{\text{ind}} : \mathbf{x} \in \mathcal{X}^n \mapsto \mathbf{y} = M^{\text{ind}}(\mathbf{x}) \in \mathcal{Y}^n$$

- Many methods, depending on  $\mathcal{X}$  definition: PCA, MCA, MFA, FPCA, MDS...
- Some of them use  $\hat{\mathbf{z}}$  in  $M^{\text{ind}}$ : LDA, mixture entropy preservation [Scrucca 2010]
- Nearly always,  $\mathcal{Y} = \mathbb{R}^2$

Model  $\hat{f}$  is not taken into account through this approach which is focused on  $\mathbf{x}$

## Overview of clustering visualization: pdf mapping

- Aims at displaying information relative to the mapping of the  $f$  distribution
- Transforms  $f = \sum_k \pi_k f_k \in \mathcal{F}$ , into a new mixture  $g = \sum_k \pi_k g_k \in \mathcal{G}$

$$M^{\text{pdf}} \in \mathcal{M}^{\text{pdf}} : f \in \mathcal{F} \mapsto g = M^{\text{pdf}}(f) \in \mathcal{G}$$

- $\mathcal{G}$  is a pdf family defined on the space  $\mathcal{Y}$
- $M^{\text{pdf}}$  is often obtained as a by product of  $M^{\text{ind}}$  (tedious outside linear mappings)
- For large  $n$ ,  $M^{\text{ind}}$  finally displays  $M^{\text{pdf}}$
- Often, both  $\mathbf{y}$  and  $g$  are overlaid

## Summary of traditional visualization strategies<sup>2</sup>

### Controlling the mapping family $\mathcal{M}^{\text{pdf}}$

$$\boxed{\text{Strategy}_{\mathcal{M}}} : \underbrace{\mathcal{G}(\mathcal{M}^{\text{pdf}})}_{\text{uncontrolled}} = \left\{ g : g = M^{\text{pdf}}(f), f \in \mathcal{F}, M^{\text{pdf}} \in \underbrace{\mathcal{M}^{\text{pdf}}}_{\text{controlled}} \right\}$$

- Nature of  $\mathcal{G}$  can dramatically depend on the choice of  $\mathcal{M}^{\text{pdf}}$
- It can potentially lead to very different cluster shapes!
- Arguments for traditional  $\mathcal{M}^{\text{pdf}}$ : user-friendly, easy-to-compute
- Examples: linear mappings in all PCA-like methods

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<sup>2</sup>Similar thinking with  $\mathcal{M}^{\text{ind}}$

## New visualization strategy

### Controlling the pdf family $\mathcal{G}$

$$\boxed{\text{Strategy}_{\mathcal{G}}} : \underbrace{\mathcal{M}^{\text{pdf}}(\mathcal{G})}_{\text{uncontrolled}} = \left\{ M^{\text{pdf}} : g = M^{\text{pdf}}(f), f \in \mathcal{F}, g \in \underbrace{\mathcal{G}}_{\text{controlled}} \right\}$$

- It is the reversed situation where  $\mathcal{G}$  is defined instead of  $\mathcal{M}^{\text{pdf}}$
- Offer opportunity to impose directly  $\mathcal{G}$  to be a user-friendly mixture family
- $\text{Strategy}_{\mathcal{M}}$  and  $\text{Strategy}_{\mathcal{G}}$  are both valid but  $\text{Strategy}_{\mathcal{G}}$  is rarely explored!

This work: explore  $\text{Strategy}_{\mathcal{G}}$

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## Spherical Gaussians as candidates

- Users are usually familiar with **multivariate spherical Gaussians** on  $\mathcal{Y} = \mathbb{R}^{d_Y}$
- Thus a simple and “user-friendly” candidate  $g$  is a mixture of spherical Gaussians

$$g(\mathbf{y}; \boldsymbol{\mu}) = \sum_{k=1}^K \underbrace{\pi_k}_{\text{from } f} \phi_{d_Y}(\mathbf{y}; \underbrace{\boldsymbol{\mu}_k, \mathbf{I}}_?)$$

where  $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K)$  and  $\phi_{d_Y}(\cdot; \boldsymbol{\mu}_k, \mathbf{I})$  the pdf of the Gaussian distribution

- with mean  $\boldsymbol{\mu}_k = (\mu_{k1}, \dots, \mu_{kd_Y}) \in \mathbb{R}^{d_Y}$
- with covariance matrix equal to identity  $\mathbf{I}$

$g(\cdot; \boldsymbol{\mu})$  should be then linked with  $f$  in order to define a sensible  $\mathcal{G}$

$$\mathcal{G} = \{g : g(\cdot; \boldsymbol{\mu}), \boldsymbol{\mu} \in \arg \min \delta(f, g(\cdot; \boldsymbol{\mu})), f \in \mathcal{F}\}$$

## $g$ as the “clustering twin” of $f$

**Question:** how to choose  $\delta$  since generally  $\mathcal{X} \neq \mathcal{Y}$ ?

**Answer:** in our clustering context,  $\delta$  should measure the **clustering ability difference**

Kullback-Leibler divergence of clustering ability between both  $f$  and  $g(\cdot; \mu)$ <sup>3</sup>

$$\delta_{\text{KL}}(f, g(\cdot; \mu)) = \int_{\mathcal{T}} p_f(\mathbf{t}) \ln \frac{p_f(\mathbf{t})}{p_g(\mathbf{t}; \mu)} d\mathbf{t}$$

where

- $p_f$ : pdf of proba. of classification  $\mathbf{t}(f) = (\mathbf{t}_i(f))_{i=1}^n$ , with  $\mathbf{t}_i(f) = (\mathbf{t}_{ik}(f))_{k=1}^{K-1}$
- $p_g(\cdot; \mu)$ : pdf of proba. of classif.  $\mathbf{t}(g) = (\mathbf{t}_i(g))_{i=1}^n$ , with  $\mathbf{t}_i(g) = (\mathbf{t}_{ik}(g))_{k=1}^{K-1}$
- $\mathcal{T} = \{\mathbf{t} : \mathbf{t} = (t_1, \dots, t_{K-1}), t_k > 0, \sum_k t_k < 1\}$

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<sup>3</sup> $p_f$  is the reference measure

## $\mathcal{G}$ reduced to a unique distribution

- A natural requirement:  $p_g(\cdot; \mu)$  and  $g$  should be linked by a one-to-one mapping
- Currently not true since rotations and/or translations are possible
- It means: for one distribution  $f$ , there is a unique optimal distribution  $g(\cdot; \mu)$
- Additional constraints on  $g(\cdot; \mu)$ :  $d_Y = K - 1$ ,  $\mu_K = \mathbf{0}$ ,  $\mu_{kh} = 0$  ( $h > k$ ),  $\mu_{kk} \geq 0$



## Estimating the Gaussian centers (pitch)

- The Kullback-Leibler divergence  $\delta_{\text{KL}}$  has generally no closed-form
- Estimate it by the following consistent (in  $S$ ) Monte-Carlo expression

$$\hat{\delta}_{\text{KL}}(f, g(\cdot; \mu)) = \frac{1}{S} \underbrace{\sum_{s=1}^S \ln p_g(\mathbf{t}^{(s)}; \mu)}_{L(\mu; \mathbf{t})} + \text{cst}$$

with  $S$  independent draws of conditional proba.  $\mathbf{t} = (\mathbf{t}^{(1)}, \dots, \mathbf{t}^{(S)})$  from  $p_f$

- It is the normalized (observed-data) log-likelihood function of a mixture model
- But, by construction, all the conditional probabilities are fixed in this mixture
- Thus, just maximize the normalized complete-data log-likelihood  $L_{\text{comp}}(\mu; \mathbf{t})$ :
  - $K = 2$ : this maximization is straightforward
  - $K > 2$ : use a standard [Quasi-Newton algorithm](#) with different random initializations, for avoiding possible local optima

## From a multivariate to a bivariate Gaussian mixture

- $g$  is defined on  $\mathbb{R}^{K-1}$  but it is **more convenient to be on  $\mathbb{R}^2$**
- **Just apply LDA** on  $g$  to display this distribution on its most discriminative map
- It leads to the bivariate spherical Gaussian mixture  $\tilde{g}$

$$\tilde{g}(\tilde{\mathbf{y}}; \tilde{\boldsymbol{\mu}}) = \sum_{k=1}^K \pi_k \phi_2(\tilde{\mathbf{y}}; \tilde{\boldsymbol{\mu}}_k, I),$$

where  $\tilde{\mathbf{y}} \in \mathbb{R}^2$ ,  $\tilde{\boldsymbol{\mu}} = (\tilde{\boldsymbol{\mu}}_1, \dots, \tilde{\boldsymbol{\mu}}_K)$  and  $\tilde{\boldsymbol{\mu}}_k \in \mathbb{R}^2$

- Use the **% of inertia** of LDA to measure the quality of the mapping from  $g$  to  $\tilde{g}$

### Remark

If  $\mathcal{X} = \mathbb{R}^d$  and  $f$  is a Gaussian mixture with isotropic covariance matrices, then **the proposed mapping is equivalent to applying a LDA to the centers of  $f$**

## Overall accuracy of the mapping between $f$ and $\tilde{g}$

Use the following **difference between the normalized entropies** of  $f$  and  $\tilde{g}$

$$\delta_E(f, \tilde{g}) = -\frac{1}{\ln K} \sum_{k=1}^K \left\{ \int_{\mathcal{X}} t_k(\mathbf{x}; f) \ln t_k(\mathbf{x}; f) d\mathbf{x} - \int_{\mathbb{R}^2} t_k(\tilde{\mathbf{y}}; \tilde{g}) \ln t_k(\tilde{\mathbf{y}}; \tilde{g}) d\tilde{\mathbf{y}} \right\}$$

- Such a quantity can be **easily estimated** by empirical values
- Its meaning is particularly relevant:
  - $\delta_E(f, \tilde{g}) \approx 0$ : the component overlap conveyed by  $\tilde{g}$  (over  $f$ ) is accurate
  - $\delta_E(f, \tilde{g}) \approx 1$ :  $\tilde{g}$  strongly underestimates the component overlap of  $f$
  - $\delta_E(f, \tilde{g}) \approx -1$ :  $\tilde{g}$  strongly overestimates the component overlap of  $f$

$\delta_E(f, \tilde{g})$  permits to **evaluate the bias of the visualization**

## Drawing $\tilde{g}$

- **Cluster centers:** the locations of  $\tilde{\mu}_1, \dots, \tilde{\mu}_K$  are materialized by vectors
- **Cluster spread:** the 95% confidence level displayed by a black border
- **Cluster overlap:** iso-probability curves of the MAP classification for different levels
- **Mapping accuracy:**  $\delta_E(f, \tilde{g})$  and also % of inertia by axis

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## House of Representatives Congressmen: data<sup>4</sup> and model

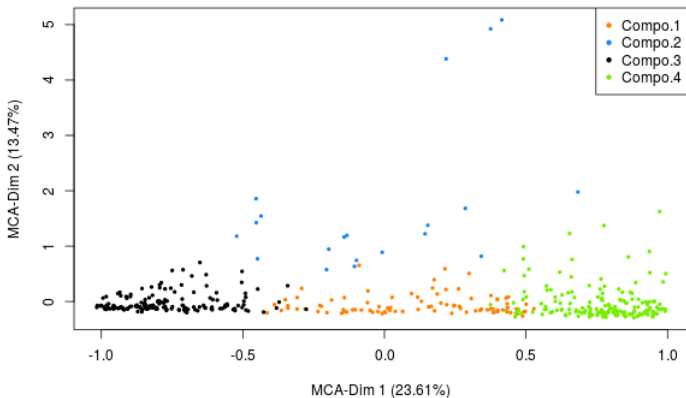
- Votes of the  $n = 435$  U.S. Congressmen on the  $d_X = 16$  key votes
- **Categorical data**: for each vote, three levels are considered (yea, nay, ?)
- Data clustered by a mixture of product of multinomial distributions [Goodman 1974]
- $K = 4$  selected by BIC [Schwarz 1974]
- Use the R package Rmixmod [Lebret et al. 2015]
- Complex output: 435 individual memberships,  $192 = 16 \times 3 \times 4$  parameters

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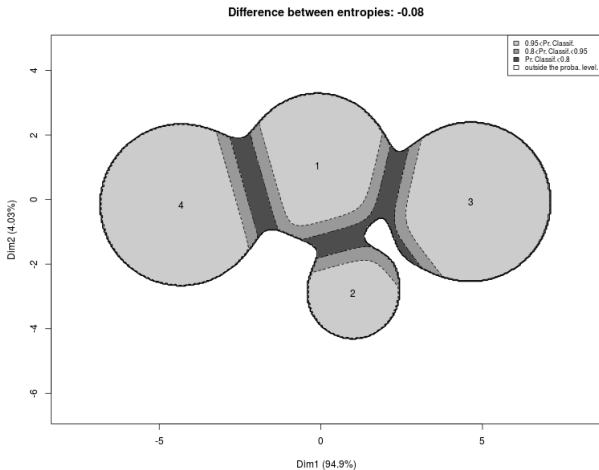
<sup>4</sup>[Schlimmer (1987)]

## House of Representatives Congressmen: standard MCA visualization

First map of the MCA (R package FactoMineR [Lê *et al.* 2008]): difficult to interpret



# House of Representatives Congressmen: Gaussian visualization



Mapping of  $f$  on this graph is accurate because  $\delta_E(f, \tilde{g}) = 0.01$



## Contraceptive method choice: data<sup>5</sup> and model

- Subset of the 1987 National Indonesia Contraceptive Prevalence Survey
- **Mixed data**: 1473 Indian women with two numerical variables (age and number of children) and eight categorical variables (education level, education level of the husband, religion, occupation, occupation of the husband, standard-of-living index and media exposure)
- Clustered by a mixture  $f$  assuming that variables are independent within components
- Model selection is done by the BIC criterion which detects six components
- Use the R package Rmixmod [Lebret *et al.* 2015]

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<sup>5</sup>[Lim *et al.* 2000]

## Contraceptive method choice: estimated parameters

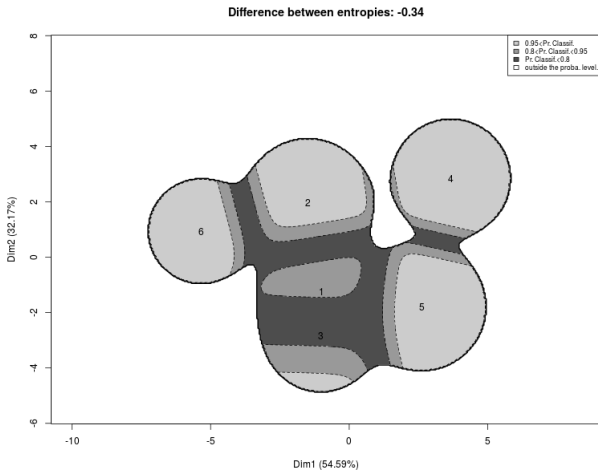
|             | Age  |          | Number of children |          |
|-------------|------|----------|--------------------|----------|
|             | Mean | Variance | Mean               | Variance |
| Component 1 | 35   | 30       | 4                  | 4        |
| Component 2 | 35   | 22       | 3                  | 2        |
| Component 3 | 40   | 42       | 5                  | 9        |
| Component 4 | 25   | 10       | 1                  | 1        |
| Component 5 | 24   | 13       | 2                  | 1        |
| Component 6 | 45   | 7        | 5                  | 8        |

**Table:** Parameters of the continuous variables for the Contraceptive method choice.

|             | education level | husband's education level | religion | occupation | husband's occupation | standard-of-living index | media exposure |
|-------------|-----------------|---------------------------|----------|------------|----------------------|--------------------------|----------------|
| Component 1 | 3               | 3                         | 2        | 2          | 3                    | 4                        | 1              |
| Component 2 | 4               | 4                         | 2        | 2          | 1                    | 4                        | 1              |
| Component 3 | 1               | 2                         | 2        | 2          | 3                    | 3                        | 1              |
| Component 4 | 4               | 4                         | 2        | 2          | 1                    | 4                        | 1              |
| Component 5 | 3               | 3                         | 2        | 2          | 3                    | 3                        | 1              |
| Component 6 | 4               | 4                         | 2        | 2          | 1                    | 4                        | 1              |

**Table:** Modes of the categorical variables for the Contraceptive method choice.

## Contraceptive method choice: Gaussian visualization



Mapping of  $f$  on this graph is accurate because  $\delta_E(f, \tilde{g}) = 0.04$

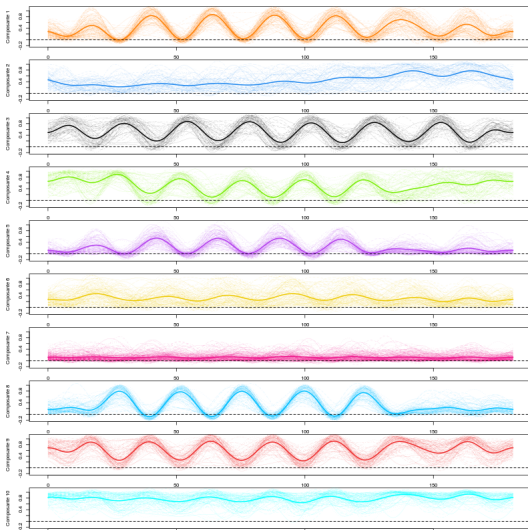
## Bike sharing system: data<sup>6</sup> and model

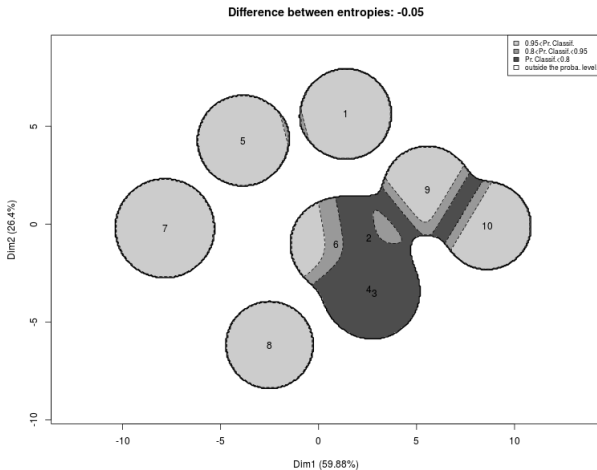
- Station occupancy data collected over the course of one month on the bike sharing system in Paris
- Data collected over 5 weeks, between February, 24 and March, 30, 2014, on 1 189 bike stations
- **Functional data**: station status information (available bikes/docks) downloaded every hour from the open-data APIs of JCDecaux company
- The final data set contains 1 189 loading profiles, one per station, sampled at 1 448 time points
- Model: profiles of the stations were projected on a basis of 25 Fourier functions
- Model-based clustering of these functional data [Bouveyron *et al.* 2015] with the R package FunFEM [Bouveyron 2015]
- Retain 10 clusters

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<sup>6</sup>[Bouveyron *et al.* (2015)]

## Bike sharing system: cluster of curves visualization





Mapping of  $f$  on this graph is accurate because  $\delta_E(f, \tilde{g}) = -0.03$

## French political blogosphere: data<sup>7</sup> and model

- **Not oriented network data:** a single day snapshot of over 1 100 political blogs automatically extracted the October, 14th, 2006 and manually classified by the “Observatoire Présidentielle” project.
- Nodes represent hostnames (= a set of pages) and edges represent hyperlinks between different hostnames
- Gather different communities organization due to the existence of several political parties and commentators
- Assumption: authors of these blogs tend to link, by political affinities, blogs with similar political positions
- Use the graph clustering via Erdős–Rényi mixture proposed by [Zanghi et al. 2008]
- Use the R package mixer
- As proposed by these authors, we consider  $K = 6$  components

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<sup>7</sup>[Zanghi et al. 2008]

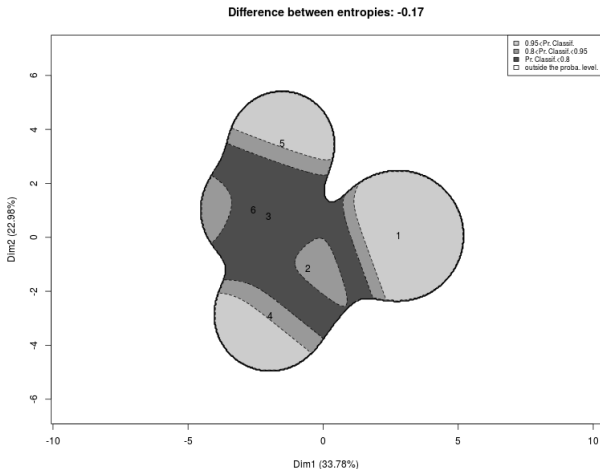
## French political blogosphere: confusion matrix

|                         | Comp. 1 | Comp. 2 | Comp. 3 | Comp. 4 | Comp. 5 | Comp. 6 |
|-------------------------|---------|---------|---------|---------|---------|---------|
| Cap21                   | 2       | 0       | 0       | 0       | 0       | 0       |
| Commentateurs Analystes | 10      | 0       | 0       | 1       | 0       | 0       |
| FN - MNR - MPF          | 2       | 0       | 0       | 0       | 0       | 0       |
| Les Verts               | 7       | 0       | 0       | 0       | 0       | 0       |
| PCF - LCR               | 7       | 0       | 0       | 0       | 0       | 0       |
| PS                      | 31      | 0       | 0       | 0       | 26      | 0       |
| Parti Radical de Gauche | 11      | 0       | 0       | 0       | 0       | 0       |
| UDF                     | 1       | 1       | 0       | 30      | 0       | 0       |
| UMP                     | 2       | 25      | 11      | 2       | 0       | 0       |
| liberaux                | 0       | 1       | 0       | 0       | 0       | 24      |

**Table:** Confusion matrix between the component memberships and the political party memberships.



## French political blogosphere: Gaussian visualization



The graph slightly over-represents the component overlaps:  $\delta_E(f, \tilde{g}) = -0.216$

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## Correspondence between new axis 1<sup>8</sup> and initial features

We measure the overlap strength of each feature  $j$  by the following **entropy ratio**:

$$\bar{E}_j = \frac{E_j}{\sum_{j=1}^d E_j} \in [0, 1]$$

where  $E_j$  corresponds to the **marginal entropy** of axis 1 **re-estimated** without feature  $j$

- The larger is  $\bar{E}_j$ , the more discriminant is feature  $j$  on axis 1
- Since axis 1 is the most discriminant axis,  $\bar{E}_j$  measures the contribution of feature  $j$  to the mixture overlap on axis 1

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<sup>8</sup>The same principle could be applied to all other new axes.

## Prostate cancer data<sup>10</sup>: definition

- **Individuals:** 506 patients with prostatic cancer grouped on clinical criteria into two Stages 3 and 4 of the disease
- **Variables:**  $d = 12$  pre-trial variates were measured on each patient, composed by **eight continuous** variables (age, weight, systolic blood pressure, diastolic blood pressure, serum haemoglobin, size of primary tumour, index of tumour stage and histologic grade, serum prostatic acid phosphatase) and **four categorical** variables with various numbers of levels (performance rating, cardiovascular disease history, electrocardiogram code, bone metastases)
- Some **missing data:** 62 missing values ( $\approx 1\%$ )

Use the Rmixture package<sup>9</sup> to estimate the mixture...

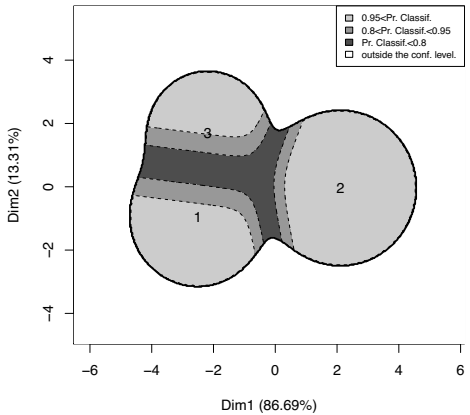
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<sup>9</sup><https://cran.r-project.org/web/packages/RMixtureComp/index.html>

<sup>10</sup>Byar DP, Green SB (1980): Bulletin Cancer, Paris 67:477-488

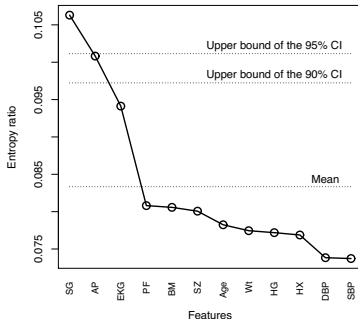
# Prostate cancer data: visualization<sup>11</sup>

Difference between entropies: 0.13



<sup>11</sup>Biernacki, C., Marbac, M., Vandewalle, V. Gaussian-Based Visualization of Gaussian and Non-Gaussian-Based Clustering. J Classif (2020).

## Prostate cancer data: axis 1 interpretation

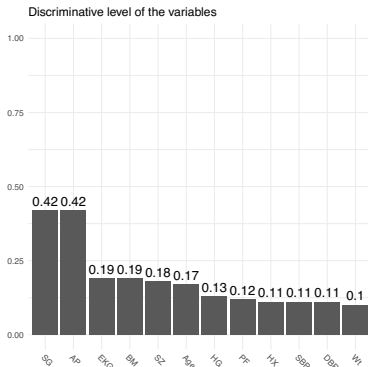


- Features SG (and AP) are the most discriminant features
- Thus axis 1 can be interpreted as a “SG/AP axis”



## Prostate cancer data: validation of axis 1 interpretation

In the Rmixcomp package, there exists an estimation of the feature importance (which is independent of the Gaussian-based visualization)



We remark that Rmixcomp feature importance and visualization interpretation are in accordance. . .

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## Conclusion

- Generic method for visualizing the results of **any** model-based clustering result
- Very easy to understand output since “Gaussian-like”
- Permit visualization for any type of data, because only based on proba. of classif.
- Can be used after **any** existing package of model-based clustering
- The overall accuracy of the visualization is also provided

R package on the CRAN: [ClusVis](#)

## Extensions

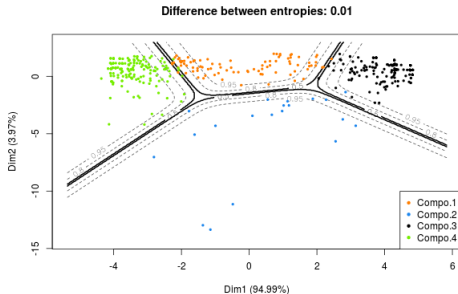
- Possibility to explore other pdf visualizations than Gaussians
- However, should keep in mind simple visualizations are targeted
- Possibility to [compare/select pdf candidates](#) through  $\delta_{KL}$  or  $\delta_E$

## About individual visualization

- Theoretically, impossible to obtain individual visualization from pdf visualization
- However, we can propose a **pseudo scatter plot** of  $\mathbf{x}$  as follows

$$\mathbf{x}_i \mapsto \mathbf{t}_i(\mathbf{f}) = \mathbf{t}_i(\mathbf{g}) \xrightarrow{\text{bijection}} \mathbf{y}_i \in \mathbb{R}^{K-1} \xrightarrow{\text{LDA}} \tilde{\mathbf{y}}_i \in \mathbb{R}^2$$

- $\tilde{\mathbf{y}}$  allows only to visualize the classification position of  $\mathbf{x}$
- Example for the congressmen data set



- **Caution:** do not overlay pdf and individual plots since  $\tilde{\mathbf{y}} = (\tilde{\mathbf{y}}_1, \dots, \tilde{\mathbf{y}}_n)$  is not necessarily drawn from a Gaussian mixture