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Clustering: from modeling to visualizing Mapping clusters as spherical Gaussians

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Gaussian Based Visualization of Gaussian and Non-Gaussian Based Clustering

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Working Group on Model-Based Clustering

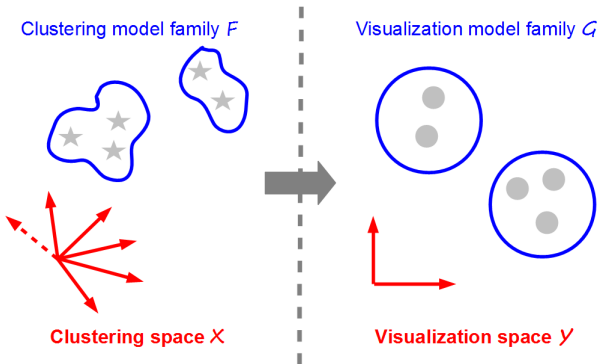
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Take home message

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: pitch¹

- **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

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

¹See 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^{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^{pdf} is often obtained as a by product of M^{ind} (tedious outside linear mappings)
- For large n , M^{ind} finally displays M^{pdf}
- Often, both \mathbf{y} and g are overlaid

Summary of traditional visualization strategies²

Controlling the mapping family \mathcal{M}^{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}^{pdf}
- It can potentially lead to very different cluster shapes!
- Arguments for traditional \mathcal{M}^{pdf} : user-friendly, easy-to-compute
- Examples: linear mappings in all PCA-like methods

²Similar thinking with \mathcal{M}^{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}^{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 δ since generally $\mathcal{X} \neq \mathcal{Y}$?

Answer: in our clustering context, δ should measure the **clustering ability difference**

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

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

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 $\mathbf{t}_i(g) = (\mathbf{t}_{ik}(g))_{k=1}^{K-1}$
- $\mathcal{T} = \{\mathbf{t} : \mathbf{t} = (t_1, \dots, t_{K-1}), t_k > 0, \sum_k t_k < 1\}$

³ 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 δ_{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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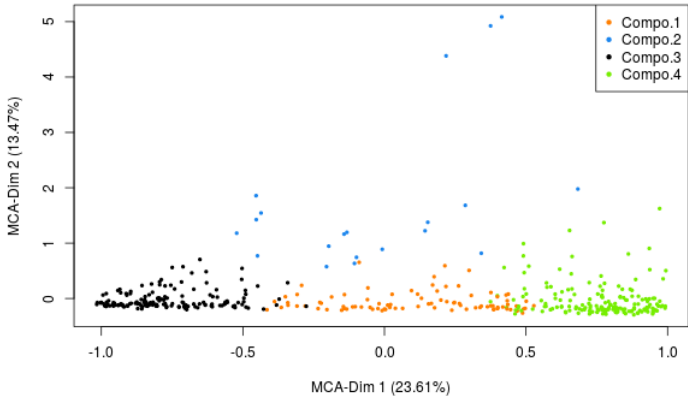
House of Representatives Congressmen: data⁴ and model

- 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

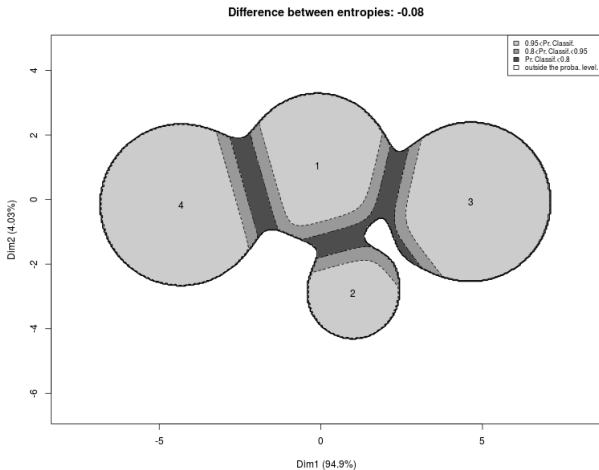
⁴[Schlimmer (1987)]

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: data⁵ 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]

⁵[Lim *et al.* 2000]

Contraceptive method choice: estimated parameters

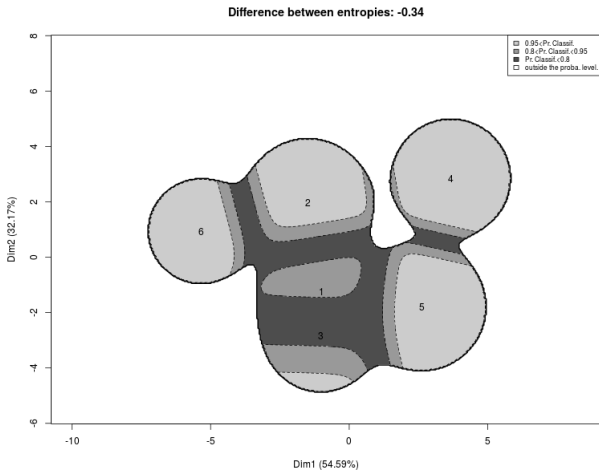
	Age		Number of children	
	Mean	Variance	Mean	Variance
Component 1	35	30	4	4
Component 2	35	22	3	2
Component 3	40	42	5	9
Component 4	25	10	1	1
Component 5	24	13	2	1
Component 6	45	7	5	8

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



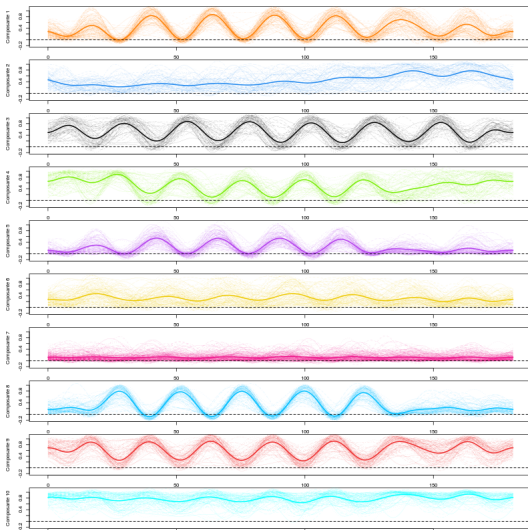
Mapping of f on this graph is accurate because $\delta_E(f, \tilde{g}) = 0.04$

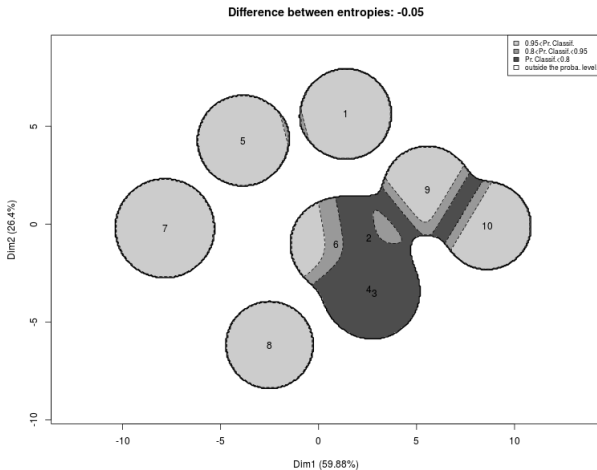
Bike sharing system: data⁶ and model

- 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

⁶[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: data⁷ 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

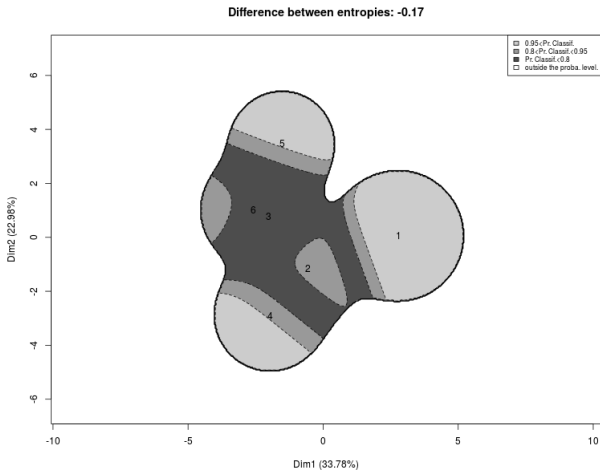
⁷[Zanghi et al. 2008]

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 1⁸ 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

⁸The same principle could be applied to all other new axes.

Prostate cancer data¹⁰: 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 ($\approx 1\%$)

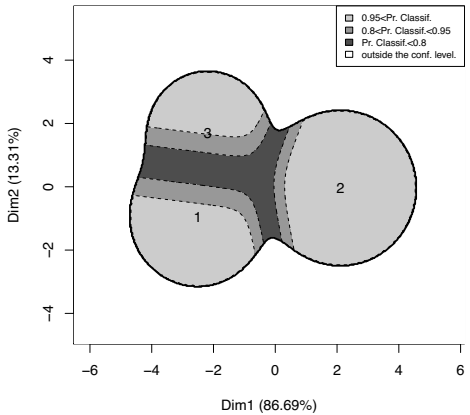
Use the Rmixture package⁹ to estimate the mixture...

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

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

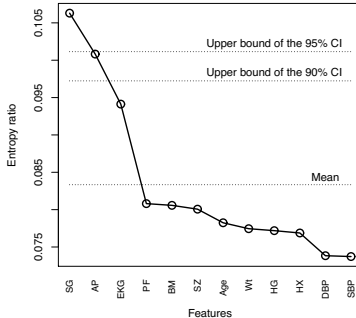
Prostate cancer data: visualization¹¹

Difference between entropies: 0.13



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

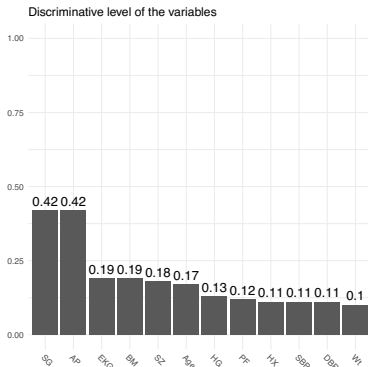
Prostate cancer data: axis 1 interpretation



- 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

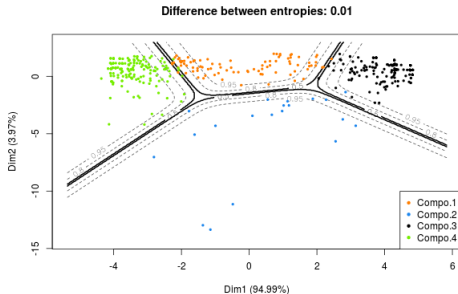
- Possibility to explore other pdf visualizations than Gaussians
- However, should keep in mind simple visualizations are targeted
- Possibility to [compare/select pdf candidates](#) through δ_{KL} or δ_E

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