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## Model-based variable clustering

Vincent VANDEWALLE<sup>1,2</sup>, Thierry MOTTET<sup>2</sup>, Matthieu MARCBAC<sup>3</sup>

<sup>1</sup> Université Lille 2, EA 2694

<sup>2</sup> Inria

<sup>3</sup> ENSAI

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## Outline

- 1 Extension of the variable selection to variable clustering
  - Variable selection in clustering
  - Multiple Gaussian Mixture
  - Proposed Multiple Mixture Model
  - Properties of the model
- 2 Parameters estimation and model selection
  - Maximum likelihood inference
  - Penalized observed-data likelihood
  - Integrated complete-data likelihood
- 3 Numerical experiments on real data
  - Mixed data framework
  - Results on real data

## Data

$\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$  composed of  $n$  independent observations  $\mathbf{x}_i = (x_{i1}, \dots, x_{id})$  defined on  $\mathbb{R}^d$ .

## Goal

Cluster the data in  $G$  clusters.

## What variables use in clustering?

- Well-posed problem in the supervised classification setting with objective criteria: error rate, AUC, ...
- Ill-posed problem in clustering since the class variable is not known by advance. Thus what are the most relevant variables with respect to this unknown variable?
- Pragmatic solution 1: Prior choice of the practitioner among available variables (according to some focus)
- Pragmatic solution 2: Posterior analysis of the correlation between the predicted cluster (based on all the variables) and each variable

## The model based clustering solution

- Mixture models allow to perform clustering by modelling the distribution of the data as a mixture of  $G$  components each one corresponding to a cluster.
- Thus possibility to suppose that some variables do not depend (directly) on the cluster in the probabilistic model.

## Some references

- Raftery & Dean (2006): some classifying, and some redundant variables. Redundant variables independent of the cluster given the classifying variables.
- Maugis & *al.* (2009): refinement of Raftery & Dean (2006) by specifying the role of each variable.

## Advantages of these approaches

- Improve the accuracy of the clustering by decreasing the variance of the estimators
- Allow some specific interpretation of the classifying variables

## Limitations of these approaches

- Combinatorial problem to select the best model with these refined approaches
- Search too hard to perform when the number of variables is large

## Solution: use simpler models for a better search (Marbac & Serdki 2016,2017)

- Assumption of conditional independence of the classifying variables given the cluster
- Non-classifying variables are independent
- Optimisation of the integrated classification likelihood (ICL)
- Better results than previous approaches on large number of variables with moderated sample size
- The independence assumption allows to easily consider the heterogeneous data setting

## Several clustering variables

- The variables in the data can convey several clustering view points with respect to different groups of variables
- Allow to find some clustering which could be hidden by other variables

## Some references

- Galimberti & *al.* (2007): First proposition of a multiple Gaussian mixture model
- Galimberti & *al.* (2017): Refinement of the previous model with ideas similar to to Raftery & Dean (2006) et Maugis & *al.* (2009)

## Remarks

- Smart modelling of the role of each variable
- Search hard to perform when the number of variables is large
- Specific to the Gaussian setting

- $B$  independent blocks.
- block  $b$  follows a Gaussian mixture with  $G_b$  components (for  $b = 1, \dots, B$ ), with the assumption of class conditional independence of the variables
- $\omega = (\omega_j; j = 1, \dots, d)$  the repartition of the variables in blocks;  $\omega_j = b$  if variable  $j$  belongs to block  $b$ .
- The probability distribution function (pdf) of  $x_i$  is

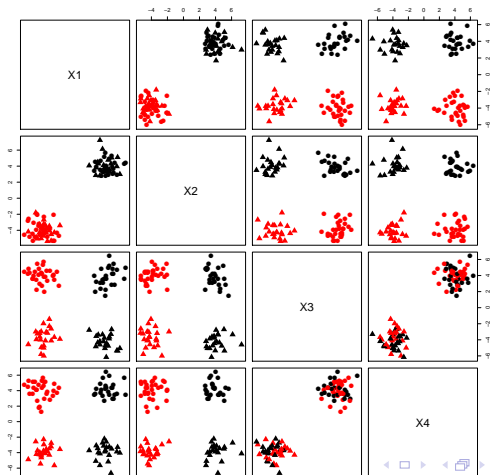
$$p(x_i | \mathbf{m}, \theta) = \prod_{b=1}^B \sum_{g=1}^{G_b} \pi_{bg} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{gj}, \sigma_{gj}^2),$$

- $\mathbf{m} = (G_1, \dots, G_B, \omega)$  defines the model
- $\Omega_b = \{j : \omega_j = b\}$  the subset of variables belonging to block  $b$
- $\theta = (\pi, \mu, \sigma)$  model parameters
  - $\pi = (\pi_{bg}; b = 1, \dots, B; g = 1, \dots, G_b)$  the proportions with  $0 < \pi_{bg}$  and  $\sum_{g=1}^{G_b} \pi_{bg} = 1$
  - $\mu = (\mu_{gj}; g = 1, \dots, G_{\omega_j}; j = 1, \dots, d)$  the means
  - $\sigma = (\sigma_{gj}; g = 1, \dots, G_{\omega_j}; j = 1, \dots, d)$  the standard deviations
- $\phi(\cdot | \mu_{gj}, \sigma_{gj}^2)$  the pdf of the Gaussian distribution with mean  $\mu_{gj}$  and variance  $\sigma_{gj}^2$ .



Illustration :

- $n = 100$  from a MGMM with  $B = 2$  blocks of two variables.
- Variable 1 and 2 belong to block 1 and variables 3 and 4 in block 2
- Each block follows a bi-component Gaussian mixture (*i.e.*,  $G_b = 2$ ) with equal proportions (*i.e.*,  $\pi_{bg} = 1/2$ ) and  $\mu_{1j} = 4$ ,  $\mu_{2j} = -4$  and  $\sigma_{gj} = 1$ .



## Remarks

- Different partitions explained by subsets of variables.
- Generalizes approaches used for variable selection in model-based clustering (if  $B = 2$  and  $G_1 = 1$  then variables belonging to block 1 are not relevant for the clustering, while variables belonging to block 2 are relevant)
- MGMM permits **variable selection** and **multiple partitions** explained by **subsets of variables** (variables classification).
- Sparse model: number of parameters  $\nu_m = \sum_{b=1}^B (G_b - 1) + 2G_b \text{card}(\Omega_b)$
- Better model search expected than in the model of Galimberti & *al.* (2017)
- Natural extension to the heterogeneous data setting

## Identifiability

Model identifiability is directly obtained from the identifiability of Gaussian mixture with local independence (Teicher, 1963, 1967).

## Observed-data likelihood for sample $\mathbf{x}$ and model $\mathbf{m}$

$$\ell(\boldsymbol{\theta}|\mathbf{m}, \mathbf{x}) = \sum_{b=1}^B \sum_{i=1}^n \ln \left( \sum_{g=1}^{G_b} \pi_{bg} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{gj}, \sigma_{gj}^2) \right).$$

## Observed-data likelihood for sample $\mathbf{x}$ and model $\mathbf{m}$

- $B$  independent mixtures
- $\mathbf{z} = (\mathbf{z}_{ib}; i = 1, \dots, n; b = 1, \dots, B)$  vectors of the component memberships
- $\mathbf{z}_{ib} = (z_{ib1}, \dots, z_{ibG_b})$  where  $z_{ibg} = 1$  if observation  $i$  arose from component  $g$  for block  $b$ , and  $z_{ibg} = 0$  otherwise

## Completed-data likelihood for sample $\mathbf{x}$ and model $\mathbf{m}$

$$\ell(\boldsymbol{\theta}|\mathbf{m}, \mathbf{x}, \mathbf{z}) = \sum_{b=1}^B f_{\pi_b} + \sum_{j=1}^d f_j(\omega_j),$$

$$f_{\pi_b} = \sum_{i=1}^n \sum_{g=1}^{G_b} z_{ibg} \ln \pi_{bg} \text{ and } f_j(\omega_j) = \sum_{i=1}^n \sum_{g=1}^{G_{\omega_j}} z_{i\omega_j g} \ln \phi(x_{ij} | \mu_{\omega_j g}, \sigma_{\omega_j g}^2).$$

## EM algorithm

Starting from the initial value  $\theta^{[0]}$ , iteration  $[r]$  is composed of two steps:

**E-step** Computation of the fuzzy partitions  $t_{ibg}^{[r]} := \mathbb{E}[Z_{ibg} | \mathbf{x}_i, \mathbf{m}, \theta^{[r-1]}]$ , hence

$$t_{ibg}^{[r]} = \frac{\pi_{bg}^{[r-1]} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{gj}, \sigma_{gj}^2)}{\sum_{k=1}^{G_b} \pi_{bk}^{[r-1]} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{kj}, \sigma_{kj}^2)},$$

**M-step** Maximization of the expected value of the complete-data log-likelihood over the parameters,

$$\pi_{bg}^{[r]} = \frac{n_{bg}^{[r]}}{n}, \mu_{gj}^{[r]} = \frac{1}{n_{\omega_{jg}}^{[r]}} \sum_{i=1}^n t_{i\omega_{jg}}^{[r]} x_{ij} \text{ and } \sigma_{gj}^{[r]} = \frac{1}{n_{\omega_{jg}}^{[r]}} \sum_{i=1}^n t_{i\omega_{jg}}^{[r]} (x_{ij} - \mu_{\omega_{jg}}^{[r]})^2.$$

## Remarks

- Independence between the  $B$  blocks of variables permits to maximize the observed-data log-likelihood on each block separately.
- Possible modification to perform the block estimation and the parameter inference simultaneously.

## Model collection $\mathcal{M}$

$$\mathcal{M} = \{\mathbf{m} : \omega_j \leq B_{\max} \text{ and } G_b \leq G_{\max}; j = 1, \dots, d; b = 1, \dots, B_{\max}\},$$

where  $B_{\max}$  is the maximum number of blocks and  $G_{\max}$  is the maximum number of components within block.

## Model selection

Model selection often achieved by searching the model  $\mathbf{m}^*$  maximizing the BIC criterion which is defined by

$$\text{BIC}(\mathbf{m}) = \max_{\theta_{\mathbf{m}}} \ell_{\text{pen}}(\theta_{\mathbf{m}} | \mathbf{m}, \mathbf{x})$$

where

$$\ell_{\text{pen}}(\theta_{\mathbf{m}} | \mathbf{m}, \mathbf{x}) = \ell(\theta_{\mathbf{m}} | \mathbf{m}, \mathbf{x}) - \frac{\nu_{\mathbf{m}}}{2} \ln n.$$

## Remark

$$(\mathbf{m}^*, \hat{\theta}_{\mathbf{m}^*}) = \arg \max_{(\mathbf{m}, \theta_{\mathbf{m}})} \ell_{\text{pen}}(\theta_{\mathbf{m}} | \mathbf{m}, \mathbf{x})$$

Combinatorial model selection through a modified the EM algorithm for  $B$  and  $(G_1, \dots, G_B)$  fixed : choice of  $\mathbf{m} \Leftrightarrow$  choice of  $\omega$

The EM algorithm to achieve  $\arg \max_{(\omega, \theta)} \ell_{pen}(\theta_{\mathbf{m}} | \mathbf{m}, \mathbf{x})$ , starting from  $(\omega^{[0]}, \theta^{[0]})$  is at iteration  $[r]$ :

**E-step** Computation of the fuzzy partitions  $t_{ibg}^{[r]} := \mathbb{E}[Z_{ibg} | \mathbf{x}_i, \mathbf{m}, \theta^{[r-1]}]$ , hence

$$t_{ibg}^{[r]} := \frac{\pi_{bg}^{[r-1]} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{gj}, \sigma_{gj}^2)}{\sum_{k=1}^{G_b} \pi_{bk}^{[r-1]} \prod_{j \in \Omega_b} \phi(x_{ij} | \mu_{kj}, \sigma_{kj}^2)},$$

**M-step** Maximization of the expected value of the complete-data log-likelihood over the parameters,

$$\pi_{bg}^{[r]} = \frac{n_{bg}^{[r]}}{n}, \omega_j^{[r]} = \arg \max_{b'=1, \dots, B} \Delta_{jb'}^{[r]}, \mu_{gj}^{[r]} = \frac{1}{n_{\omega_j^{[r]}g}^{[r]}} \sum_{i=1}^n t_{i\omega_j^{[r]}g}^{[r]} x_{ij}$$

$$\sigma_{gj}^{[r]} = \frac{1}{n_{\omega_j^{[r]}g}^{[r]}} \sum_{i=1}^n t_{i\omega_j^{[r]}g}^{[r]} (x_{ij} - \mu_{\omega_j^{[r]}j}^{[r]})^2,$$

with  $\Delta_{jb}^{[r]} = \max_{(\mu_{gj}, \sigma_{gj}^2; g=1, \dots, G_b)} \sum_{i=1}^n \sum_{g=1}^{G_b} z_{ibg} \ln \phi(x_{ij} | \mu_{gj}, \sigma_{gj}^2) - G_b \ln n$ .

## Integrated complete-data likelihood

$$p(\mathbf{x}, \mathbf{z}|\mathbf{m}) = \int p(\mathbf{x}, \mathbf{z}|\mathbf{m}, \boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{m})d\boldsymbol{\theta}.$$

## Assumptions

- Independence between the prior distributions
- Standard conjugate priors
- Closed form of the complete-data integrated likelihood

## MICL (maximum integrated complete-data likelihood) criterion

$$\text{MICL}(\mathbf{m}) = \ln p(\mathbf{x}, \mathbf{z}_m^*|\mathbf{m}) \text{ with } \mathbf{z}_m^* = \arg \max_{\mathbf{z}_m} \ln p(\mathbf{x}, \mathbf{z}|\mathbf{m}).$$

Thus

$$(\mathbf{m}^*, \mathbf{z}_{m^*}^*) = \arg \max_{(\mathbf{m}, \mathbf{z}_m)} \ln p(\mathbf{x}, \mathbf{z}|\mathbf{m}).$$

## Motivations

- Criteria based on the integrated complete-data likelihood are popular for model-based clustering
- Take into account the clustering purpose : model the data distribution and provide well-separated components

## Optimisation of MICL over $(\mathbf{z}, \omega)$ for $B$ and $G_1, \dots, G_B$ fixed

Starting at the initial value  $\omega^{[0]}$ , each  $\omega_j$  is uniformly sampled among  $\{1, \dots, B\}$ , the algorithm at iteration  $[r]$  is

**Partition step:** find  $\mathbf{z}^{[r]}$  such that for  $b = 1, \dots, B$

$$p(\mathbf{x}_{\{j|\omega_j^{[r]}=b\}}, \mathbf{z}_b^{[r]} | \mathbf{m}^{[r]}) \geq p(\mathbf{x}_{\{j|\omega_j^{[r]}=b\}}, \mathbf{z}_b^{[r-1]} | \mathbf{m}^{[r]}).$$

**Model step:** find  $\omega^{[r+1]}$  such that for  $j = 1, \dots, d$

$$\omega_j^{[r+1]} = \arg \max_{b \in \{1, \dots, B\}} p(\mathbf{x}_j, \mathbf{z}_b^{[r]} | \omega_j = b)$$



## Mixed dataset

- $\mathbf{x}_i = (x_{i1}, \dots, x_{id})$  is a vector of mixed variables (continuous, binary, count or categorical)
- local independence within block  $\Rightarrow$  extension to the mixed data analysis

## Subset of the 1987 National Indonesia Contraceptive Prevalence Survey

1473 Indian women described by

- One continuous variable (AGE: age)
- One integer variable (Chi: number of children)
- Seven categorical variables (EL: education level, ELH: education level of the husband, Rel: religion, Oc: occupation, OcH: occupation of the husband, SLI: standard-of-living index and ME: media exposure).

## Results obtained by the BIC criterion

Analysis with :

- maximum of three blocks :  $B_{\max} = 3$
- maximum of six components :  $G_{\max} = 6$

Age	Chi	EL	ELH	Rel	Oc	OcH	SLI	ME	$G_1$	$G_2$	BIC
1	1	2	2	2	1	2	2	2	6	3	-16078
1	1	2	2	2	1	2	2	2	5	3	-16081
1	1	2	2	2	2	2	2	2	4	3	-16088

**Table:** Best three models according to the BIC: block repartition, number of components per block and BIC values.

Adjusted Rand Index computed on the partitions obtained by blocks 1 and 2 equal to 0.01.

## Results obtained by the MICL criterion

Age	Chi	EL	ELH	Rel	Oc	OcH	SLI	ME	$G_1$	$G_2$	BIC
1	1	1	1	1	2	1	1	1	4	1	-16293
1	1	1	1	1	2	1	1	1	5	1	-16301
1	1	1	1	1	1	1	1	1	4	.	-16307

**Table:** Best three models according to the MICL: block repartition, number of components per block and MICL values.

## Conclusion

- Proposition of model-based clustering with several class variables, each one explaining the heterogeneity of a block of variables:
  - Find groups of variables producing the same clustering of the individuals
  - Interpret the clustering produced for each group of variables
- Model search performed simultaneously with parameters estimation
- Proposed model can be used in the heterogeneous data settings