

# Frugal Gaussian clustering of huge imbalanced datasets through a bin-marginal approach

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# Frugal Gaussian clustering of huge imbalanced datasets through a bin-marginal approach

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WG-MBC-2021, Athens, October 25-29, 2021



FACULTÉ DES SCIENCES D'ORSAY





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## Motivation: huge and imbalanced data sets

- huge in the sense tall data
  - $\hookrightarrow$  number of observations (high dimension setting out of scope)
  - $\hookrightarrow$  out of computer limits
  - → or within computer limits but with frugal resource consumption (green computing)
- discover new information

  - → reveal (valuable) tiny clusters: imbalanced data sets a few *abnormal* objects have to be recognized among a large amount of *normal* ones

credit card fraud detection [Chan and Stolfo 1998)], cancer recognition [Yu et al.

2012], fraudulent calls [Fawcett and Provost 1997]

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supervised approach (classification) with imbalanced data sets

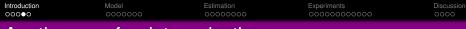
 → create artificial balanced data sets: oversampling the minority class [*Chawla et al. 2002*], undersampling the majority class [*Tahir et al. 2009*]
 → labeling could be difficult when sample size is very large

 unsupervised approach (clustering) with sample size is very large

- $\hookrightarrow$  subsampling [Fraley and Raftery 2002, Xia et al. 2019]  $\hookrightarrow$  difficult to detect very tiny clusters
- $\hookrightarrow$  computer science solutions

powerful computers or distributed architectures (MAP-reduce, ...)  $\hookrightarrow not \ frugal$ 

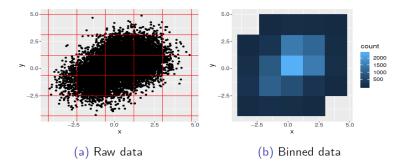
 our aim : clustering of huge and imbalanced datasets under memory contraints



## Another way for data reduction

unsupervised approach (clustering)

 $\hookrightarrow$  from raw to binned data



## Our bin-marginal approach in a nutshell

Frugal unsupervised MBC (D-dimensional Gaussian mixtures) using marginal binned data:

- 1. from raw to binned data
  - → particular version of the EM algorithm [McLachlan and Jones 1998; Cadez et al. 2002]
  - $\, \hookrightarrow \ \, \text{another dimensionality pb} \,$
- 2. from binned data to (1D-)marginal counts
  - $\hookrightarrow$  need to design a new EM algorithm but computationally intractable
- optimization of a composite likelihood (CL) [Lindsay 1988; Whitaker et al. 2020] instead of the full one → for diagonal GMM
- CL + GMM + 2D-bin [Ranalli and Rocci 2016] new in our approach: harder data reduction (1D-bin)

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## Model Based Clustering with finite GMM

Observations  $\mathbf{x} = {\mathbf{x}_i \in \mathbb{R}^D, i = 1, ..., n}$  are i.i.d. according to a *D*-dimensional Gaussian mixture with *K* components:

v

$$f(\boldsymbol{x}; \boldsymbol{\psi}) = \sum_{k=1}^{n} \pi_k \phi(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$
$$\sum_k \pi_k = 1, \quad \pi_k > 0 \quad (k = 1, \dots, K)$$

where  $\psi = (\pi_1, \dots, \pi_K, \mu_1, \dots, \mu_K, \Sigma_1, \dots, \Sigma_K)$  and  $\phi(.)$  is the *D*-variate Gaussian density

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Binned dat	a			

unobservable or too many raw data  $\boldsymbol{x}_i$  $\hookrightarrow$  vector of binned data  $\boldsymbol{n} = (n_1, \dots, n_B)$ 

▶ the original sample space is divided into a partition  $\{B_b \subset \mathbb{R}^d, b = 1, ..., B\}$ 

$$\triangleright \ n_b = \#\{\boldsymbol{x}_i \in \mathcal{B}_b\}$$

*n* arises from a multinomial model with pmf [Cadez et al. 2002]<sup>1</sup>

$$p(\boldsymbol{n}; \boldsymbol{\psi}) \propto \prod_{b=1}^{B} \left(\sum_{k=1}^{K} \pi_{k} \int_{\mathcal{B}_{b}} \phi(\boldsymbol{x}; \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}) d\boldsymbol{x}\right)^{n_{b}}$$

• trick for sample size reduction: select  $B \ll n$ 

<sup>&</sup>lt;sup>1</sup>also provide an estimate of  $\psi$  with a binned version of EM



## Curse of dimensionality for binned data

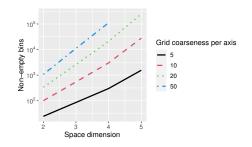
- in our case: Cartesian grid G = G<sub>1</sub> × ... × G<sub>D</sub> where G<sub>d</sub> is a univariate grid with R<sub>d</sub> + 2 cut points
   → B = ∏<sup>D</sup><sub>d=1</sub>(R<sub>d</sub> + 1) bins, representing the grid's coarseness
- works well if  $B \ll n$  and univariate context

#### when D increases

the number of non-empty bins depends exponentially on the dimension D $\rightarrow$  impossible to obtain a manageable amount of binned data

 $\hookrightarrow$  several *D*-dimensional numerical integrations.

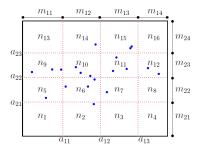
 $\hookrightarrow$  vanishes any kind of gain





## Marginal binned data

- work with the 1-D binned data on each direction separately
- ► marginal counts: m = {m<sub>1</sub>,..., m<sub>D</sub>} for each direction d = 1,..., D, m<sub>d</sub> = (m<sub>d1</sub>,..., m<sub>dB<sub>d</sub></sub>), component m<sub>db<sub>d</sub></sub> is the count of observations x<sub>id</sub> in the b<sub>d</sub>-th bin of the d-th dimension



 $\hookrightarrow$  store  $\sum_{d=1}^{D} B_d$  values instead of  $\prod_{d=1}^{D} B_d$ 

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## Bin-marginal model

#### bin-marginal pdf

$$p_m(\boldsymbol{m}; \boldsymbol{\psi}) = \sum_{\boldsymbol{n}' \in \mathcal{F}_{\boldsymbol{m}}} p(\boldsymbol{n}'; \boldsymbol{\psi}),$$

where  $\mathcal{F}_m$  is the set of tables n' sharing the same marginals m.

#### issues

- $\hookrightarrow$  identifiability
- $\hookrightarrow$  mathematical complexity of the likelihood
- $\hookrightarrow$  optimization of the likelihood

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## Identifiability

- GMM identifiable up to a label permutation [Yakowitz and Spragings 1968] (raw data)
- as so far, no reference for the binned case

Proposition (<u>Full</u> binned Gaussian diagonal mixtures - ABK 2021)

Under hypothesis of diagonal covariance matrices, binned D-variate mixtures of at most  $K_{max}$  components are identifiable if  $R_d > 4K_{max} - 3$ , d = 1, ..., D.

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## Identifiability

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the proof relies on an existing result

#### Proposition (11.5 - Valiant 2012)

Given the linear combination of K univariate Gaussian densities  $f(x) = \sum_{k=1}^{K} \pi_k \phi(x; \mu_k, \sigma_k^2)$ , such that either  $\mu_i \neq \mu_j$  or  $\sigma_i^2 \neq \sigma_j^2$  for  $i \neq j$  and for all  $k \ \pi_k \neq 0$ , the number of solutions to f(x) = 0 is at most 2(K - 1).

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## Identifiability

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Proposition ( Full binned Gaussian diagonal mixtures - ABK 2021)

Under hypothesis of diagonal covariance matrices, binned D-variate mixtures of at most  $K_{max}$  components are identifiable if  $R_d > 4K_{max} - 3$ , d = 1, ..., D.

Proposition (Marginal-binned Gaussian diagonal mixtures - ABK 2021)

Bin-marginal D-variate mixtures of at most  $K_{max}$  components are identifiable if binned D-variate mixtures are identifiable. So, under diagonal covariance matrices hypothesis, identifiability is achieved if  $R_d > 4K_{max} - 3$ , d = 1, ..., D.

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## EM algorithm for bin-marginal model

#### complete log-likelihood

$$\ell^{c}(\psi; \mathbf{x}, \mathbf{z}) = \sum_{k=1}^{K} \sum_{i=1}^{n} z_{ik} \log(\pi_{k} \phi(\mathbf{x}_{i}, \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}))$$

where z gathers all  $z_{ik} = \mathbf{1}_{observation} i$  in cluster k

## EM algorithm for bin-marginal model

#### E-step

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• expectation respectively to  $p(\mathbf{x}, \mathbf{z} | \mathbf{m}; \psi^{(j)})$ 

$$Q_{m}(\boldsymbol{\psi},\boldsymbol{\psi}^{(j)}) = \mathbb{E}_{\boldsymbol{\psi}^{(j)}}[\ell^{c}(\boldsymbol{\psi};\mathbf{X},\mathbf{Z})|\boldsymbol{m}]$$

$$= \sum_{\boldsymbol{n}\in\mathcal{F}_{\boldsymbol{m}}} \alpha^{(j)}(\boldsymbol{n}) \sum_{k=1}^{K} \sum_{b=1}^{B} n_{b} \int_{\mathcal{B}_{b}} \tau_{k}^{(j)}(\boldsymbol{x}) \log[\pi_{k}\phi(\boldsymbol{x};\boldsymbol{\mu}_{k},\boldsymbol{\Sigma}_{k})]d\boldsymbol{x}$$

$$\alpha^{(j)}(\boldsymbol{n}) = \frac{p(\boldsymbol{n};\boldsymbol{\psi}^{(j)})}{\sum_{\boldsymbol{n}'\in\mathcal{F}_{\boldsymbol{m}}} p(\boldsymbol{n}';\boldsymbol{\psi}^{(j)})} \text{ and } \tau_{k}^{(j)}(.) = \frac{\pi_{k}^{(j)}\phi(.;\boldsymbol{\mu}_{k}^{(j)},\boldsymbol{\Sigma}_{k}^{(j)})}{f(.;\boldsymbol{\psi}^{(j)})}.$$
-step

 $\hookrightarrow$  both steps involve the computation of all crossed tables ( $\mathcal{F}_{\textit{m}}$ ): intractable

 $\hookrightarrow$  alternative: use of marginal composite likelihood

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Let **x** be a *D*-dimensional sample with *n* observations  $\mathbf{x}_i = (x_{i1}, \dots, x_{iD}), i = 1, \dots, n$ , generated by a GMM with parameter  $\psi$ 

- ► pseudo-likelihood only relying on the likelihood of the marginals L<sub>d</sub>(ψ<sub>d</sub>; x<sub>d</sub>)
  - $\rightarrow x_d = (x_{1d}, \dots, x_{nd})$  the component *d* of the dataset
  - $\hookrightarrow$  with parameter  $\psi_d = (\pi_1, \dots, \pi_K, \mu_{1d}, \dots, \mu_{Kd}, \sigma_{1d}^2, \dots, \sigma_{Kd}^2)$

$$\tilde{L}(\psi; \mathbf{x}) = \prod_{d=1}^{D} L_d(\psi_d; \mathbf{x}_d)$$

- the estimator ψ̃ maximizing L̃(ψ; x) is consistent and asymptotically normal [Molenberghs and Verbeke 2005]
- ▶  $\hookrightarrow$  EM algorithm with CL for HMM [Gao and Song 2011]
  - $\hookrightarrow$  CL on bivariate-binned data [Ranalli and Rocci 2016]

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## Bin-marginal Composite Likelihood (bmCL)

our proposal: combine memory reduction (bin-marginal)

$$\log p_m(\boldsymbol{m}; \boldsymbol{\psi}) = \log \sum_{\boldsymbol{n'} \in \mathcal{F}_{\boldsymbol{m}}} p(\boldsymbol{n'}; \boldsymbol{\psi})$$

and computational advantages of 1D-marginal CL

 $\hookrightarrow$  we aim at maximizing the bin-marginal composite log-lik.:

$$\tilde{\ell}_m(\psi; \boldsymbol{m}) = \sum_{d=1}^D \ell_d(\psi_d; \boldsymbol{m}_d)$$
$$= \sum_{d=1}^D \sum_{b_d=1}^{B_d} m_{db_d} \log\Big(\int_{\mathcal{B}_{b_d}^d} f_d(x_d; \psi_d) dx_d\Big).$$

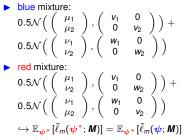
 $\hookrightarrow$  diagonal mixtures only...

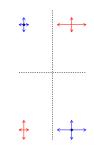
 $\hookrightarrow$  identifiability ?



## Bin-marginal CL: generic identifiability

#### A case of non identifiability





Identifiability except on the set of null measure composed by mixtures having two equal proportions with two components sharing the same projection

 $\hookrightarrow \text{generic identifiability, then consistency} \ [\textit{Whitaker et al. 2020}]$ 

A naive EM algorithm for bin-marginal CL

on each direction d: work with  $m_d$ 

- ► associate the missing vectors (x<sub>d</sub>, z<sub>d</sub>), where z<sub>d</sub> is n × K indicator membership matrix for x<sub>d</sub>.
- run 1D EM algorithm separately
- how two conciliate the partitions from each direction ?
  - $\hookrightarrow$  use the same  $\pi_1, \ldots, \pi_K$  on each direction, in a global EM

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## EM algorithm for bin-marginal CL (bmCL)

With 
$$\psi_d = (\pi_1, \dots, \pi_K, \mu_{1d}, \dots, \mu_{Kd}, \sigma_{1d}^2, \dots, \sigma_{Kd}^2)$$
  
**bmCL E-step**

$$\tilde{Q}_m(\psi,\psi^{(j)}) = \sum_{d=1}^D \int_{\mathcal{X}_d \times \mathcal{Z}_d} \ell_d^c(\psi_d; \boldsymbol{x}_d, \boldsymbol{z}_d) f(\boldsymbol{x}_d, \boldsymbol{z}_d | \boldsymbol{m}_d; \psi_d^{(j)}) d\boldsymbol{x}_d d\boldsymbol{z}_d.$$

bmCL M-step straightforward

$$\tau_{kd}^{(j)}(.) = \frac{\pi_k^{(j)}\phi(.;\mu_{kd}^{(j)},\sigma_{kd}^{2(j)})}{f(.;\psi_d^{(j)})}$$

$$\pi_{k}^{(j+1)} = \frac{\sum_{d=1}^{D} \sum_{b_{d}=1}^{B_{d}} m_{db_{d}} \int_{\mathcal{B}_{b_{d}}^{d}} \tau_{kd}^{(j)}(x_{d}) dx_{d}}{Dn}; \quad \mu_{kd}^{(j+1)} = \frac{\sum_{b_{d}=1}^{B_{d}} m_{db_{d}} \int_{\mathcal{B}_{b_{d}}^{d}} x_{d} \tau_{kd}^{(j)}(x_{d}) dx_{d}}{\sum_{b_{d}=1}^{B_{d}} m_{db_{d}} \int_{\mathcal{B}_{b_{d}}^{d}} \tau_{kd}^{(j)}(x_{d}) dx_{d}}$$

• estimated partition:  $\widehat{\mathbf{z}} = \arg \max_k \frac{\widehat{\pi}_k \phi(.:\widehat{\mu}_k, \widehat{\Sigma}_k^2)}{f(.:\widehat{\psi})}$ 

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## Numerical experiment on simulated data

- ability to recognize the minority class
- comparison with two competitors (estimation with Rmixmod)
  - $\hookrightarrow$  classic estimation with the full dataset
  - $\hookrightarrow$  a subsampling strategy
- clustering quality measured by the ARI score and time, under same memory constraints:
  - $\,\hookrightarrow\,$  bin marginal: grid coarseness R  $\,\hookrightarrow\,$  2R memory space
  - $\hookrightarrow$  subsampling: 100 different subsamples of size 2*R*
  - $\hookrightarrow \ \ \mathsf{R}{=}50,\,100,\,200$

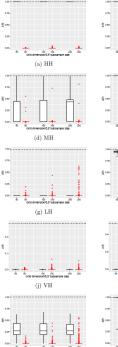
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## Experimental settings: 1M obs from 3D 2-classes mixtures

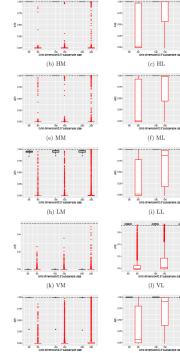
Scenario	Separation	Imbalance	Small class proportion $(\pi_1)$	Means
HH HM HL	High	High Medium Low	$     10^{-4} \\     10^{-3} \\     10^{-2}   $	
MH MM ML	Medium	High Medium Low	$     \begin{array}{r} 10^{-4} \\     10^{-3} \\     10^{-2} \end{array} $	
LH LM LL	Low	High Medium Low	$     10^{-4} \\     10^{-3} \\     10^{-2}   $	
VH VM VL	Very low	High Medium Low	$     10^{-4} \\     10^{-3} \\     10^{-2}   $	$ \begin{aligned} \mu_1 &= (-1, -1, -1) \\ \mu_2 &= (1, 1, 1) \end{aligned} $
1HH 1HM 1HL	One separated component	High Medium Low	$10^{-4}$ $10^{-3}$ $10^{-2}$	$ \begin{aligned} \mu_1 &= (-1, -1, -4) \\ \mu_2 &= (1, 1, 4) \end{aligned} $

#### 20 replications of each scenario





(m) 1HH



(n) 1HM

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(o) 1HL

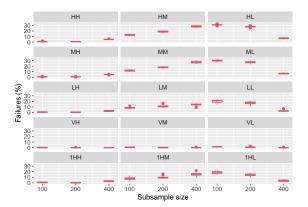
#### quality vs memory

- bmCL (black) mostly outperforms subsampling (red), even with coarser grid,
- some difficulties only with very little separation and small proportion
- in general, bmCL approaches full data set results (dotted), with drastically less amount of memory

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#### subsampling failures

- ▶ probability of failure ≯ if separation ≯ and if imbalance ratio ↘
- astonishing... but
- if subsampling does not fail, it works badly



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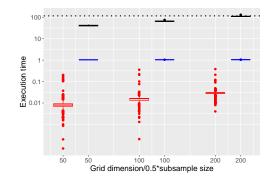
## Results

#### time vs grid/subsample size equal memory occupancy

- subsampling EM (red)
  - bin-marginal CL-EM (black)

expected CL-EM time after
 optimization in language C++ (blue)
 full dataset (dotted line)

- remarkable improvement relatively to full data set



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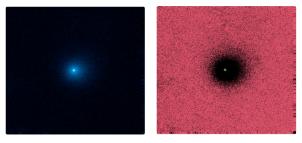
## Real imbalanced datasets

- image segmentation, fraud detection, hazardous asteroid detection
- three variables

Dataset	n	D	Small class proportion
Cell-1	101,430	3	unknown
Cell-2	65,536	3	unknown
Cell-3	685,020	3	unknown
Comet	1,083,681	3	unknown
Asteroids	932,341	3	0.002
Credit card	$284,\!807$	3	0.0014

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 Results: Image segmentation Comet (R=400, K=3)



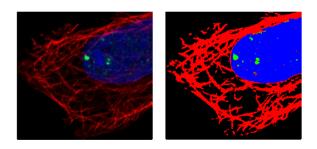


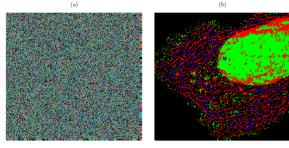




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 Results: Image segmentation Cell-1 (R=20, K=4)

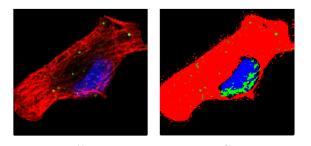


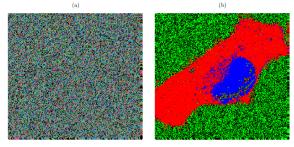


(d)

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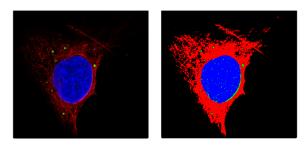
## Results: Image segmentation Cell-2 (R=20, K=4)

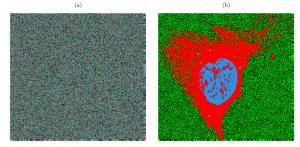




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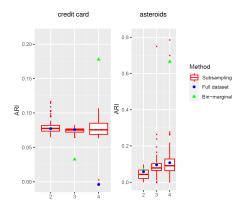
 Results: Image segmentation Cell-3 (R=20, K=4)





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## Results: credit card and asteroids



- two known clusters
- Clustering for K = 2, 3, 4, then clusters of highest proportions are grouped (mixture of mixtures)
- despite the loss of information, binned method seems to behave better than full GMM and subsampling
- the tiny class contains the abnormal objects (no false negative) but low ARI (false positive)

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## Sum-up

Introduction

clustering of huge and imbalanced datasets under memory contraints:

- bin marginal composite likelihood (bmCL) approach allows to answer:
  - $\hookrightarrow$  memory requirements
  - $\, \hookrightarrow \, \text{ tractability of EM algorithm} \,$
  - $\, \hookrightarrow \ \, \text{recovery of tiny classes}$

#### subsampling

- $\,\,\hookrightarrow\,\,$  easy to implement
- $\,\, \hookrightarrow \,\,$  pb to recover tiny clusters
- $\, \hookrightarrow \ \, \text{high variability} \,$
- $\hookrightarrow$  number of subsamples?

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- bmCL clearly outperforms subsampling under same memory constraint, and is frugal compared to full sample but
  - $\,\,\hookrightarrow\,\,$  generates a lot of missing data
  - $\,\hookrightarrow\,$  prone to slow convergence, open algorithmic question
  - $\hookrightarrow$  hybrid method bmCL / subsampling?
- preliminary study, seminal for further researches
  - $\hookrightarrow$  how to deal with frugality while increasing number of clusters
  - $\hookrightarrow$  strategy when many (tiny) clusters
  - $\hookrightarrow$  grid definition as a model choice?
  - $\hookrightarrow\,$  specific criterion for selecting the number of clusters and grid definition

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Thank you for your attention!

## Identifiability (main steps)

work with binned univariate mixtures of at most K<sub>max</sub> components: pmf reduces to

$$orall oldsymbol{\psi}, oldsymbol{\psi}^* \in \Psi: \ \ oldsymbol{
ho}(oldsymbol{n};oldsymbol{\psi}) = oldsymbol{
ho}(oldsymbol{n};oldsymbol{\psi}^*) \ orall oldsymbol{G}, oldsymbol{n} \ \Rightarrow oldsymbol{\psi} = oldsymbol{\psi}^*$$

▶ if G has R cut points, (a<sub>1</sub>,..., a<sub>R</sub>) then it is needed to prove that the system has only the trivial solution ψ = ψ\* at a up to a relabeling whatever the grid is

$$\begin{aligned} \pi \sum_{k=1}^{K} \Phi(\frac{a_{1}-\mu_{k}}{\sigma_{k}}) &= \sum_{k=1}^{K^{*}} \pi^{*} \Phi(\frac{a_{1}-\mu_{k}}{\sigma_{k}^{*}}) \\ \pi \sum_{k=1}^{K} \Phi(\frac{a_{2}-\mu_{k}}{\sigma_{k}}) &= \sum_{k=1}^{K^{*}} \pi^{*} \Phi(\frac{a_{2}-\mu_{k}}{\sigma_{k}^{*}}) \\ \vdots \\ \pi \sum_{k=1}^{K} \Phi(\frac{a_{R}-\mu_{k}}{\sigma_{k}}) &= \sum_{k=1}^{K^{*}} \pi^{*} \Phi(\frac{a_{R}-\mu_{k}^{*}}{\sigma_{k}^{*}}) \end{aligned}$$

- ▶ deduce with [Prop. 11.5 Valiant 2012] that binned univariate mixtures of at most K<sub>max</sub> Gaussian distributions are identifiable if the binning grid has R > 4K<sub>max</sub> - 3 cut points.
- induction for D-variate mixtures

## EM algorithm for bin-marginal data

complete log-likelihood

$$\ell^{c}(\psi; \mathbf{x}, \mathbf{z}) = \sum_{k=1}^{K} \sum_{i=1}^{n} Z_{ik} \log(\pi_{k} \phi(\mathbf{x}_{i}, \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}))$$

where  $z_{ik} = \mathbb{1}_{observation i}$  in cluster k • E-step

$$\begin{aligned} Q_{m}(\psi,\psi^{(j-1)}) &= \mathbb{E}_{\psi^{(j-1)}}[\ell^{c}(\psi;\mathbf{X},\mathbf{Z})|\boldsymbol{m}] \\ &= \sum_{\boldsymbol{n}\in\mathcal{F}_{m}} p(\boldsymbol{n}|\boldsymbol{m};\psi^{(j-1)})\mathbb{E}_{\psi^{(j-1)}}[\ell^{c}(\psi;\mathbf{X},\mathbf{Z})|\boldsymbol{n}] \\ &= \sum_{\boldsymbol{n}\in\mathcal{F}_{m}} \alpha^{(j-1)}(\boldsymbol{n})\mathbb{E}_{\psi^{(j-1)}}[\ell^{c}(\psi;\mathbf{X},\mathbf{Z})|\boldsymbol{n}] \\ &= \sum_{\boldsymbol{n}\in\mathcal{F}_{m}} \alpha^{(j-1)}(\boldsymbol{n})\sum_{k=1}^{K}\sum_{b=1}^{B} n_{b} \int_{\mathcal{B}_{b}} \tau_{k}^{(j-1)}(\boldsymbol{x}) \\ &\times \log[\pi_{k}\phi(\boldsymbol{x};\boldsymbol{\mu}_{k},\boldsymbol{\Sigma}_{k})]d\boldsymbol{x} \end{aligned}$$