

## 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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UNIVERSITE PARIS-SACLAY

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
  - $\hookrightarrow$  more and more clusters: not the focus of this talk
  - → 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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## Approaches

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 very large sample size
  - $\hookrightarrow$  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, ...)

 $\hookrightarrow \text{not frugal}$ 

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

*l*odel

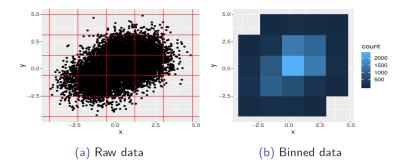
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## Another way for data reduction

### unsupervised approach (clustering)

 $\hookrightarrow$  from raw to binned data



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### Our bin-marginal approach in a nutshell Frugal unsupervised D-dim. GMM using marginal binned data:

- 1. from raw to binned data
  - → particular version of the EM algorithm [McLachlan and Jones 1998; Cadez et al. 2002]
  - $\hookrightarrow$  but we will be face to another dimensionality problem...
- from binned data to (1D-)marginal counts
   → 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 → restriction for diagonal GMM

already exists: CL + GMM + 2D-bin [Ranalli and Rocci 2016] novelty 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 model (GMM) with *K* components:

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

where  $\boldsymbol{\psi} = (\pi_1, \dots, \pi_K, \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K)$  and  $\phi(.)$  is the *D*-variate Gaussian density

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## **Binned data**

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

▶ 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

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## Curse of dimensionality for binned data

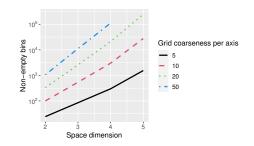
- in our case: Cartesian grid G = G<sub>1</sub> × ... × G<sub>D</sub> where G<sub>d</sub> is a univariate grid with R<sub>d</sub> + 2 cut points
   → B = ∏<sup>D</sup><sub>d=1</sub>(R<sub>d</sub> + 1) bins, representing the grid's coarseness
- works well if  $B \ll n$  and univariate context

### when D increases

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

numerical integrations.

 $\hookrightarrow$  vanishes any kind of gain

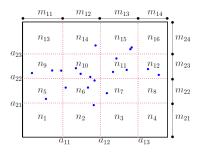


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## Marginal binned data

- ▶ 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



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 ( Full binned diagonal GMM - 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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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.

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 (Marginal-binned diag. GMM - 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

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## EM algorithm for bin-marginal model

### E-step

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

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

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

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

$$M-step$$

$$\blacktriangleright \pi_{k}^{(j+1)} = \frac{1}{n} \sum_{\boldsymbol{n}\in\mathcal{F}_{\boldsymbol{m}}} \alpha^{(j)}(\boldsymbol{n}) \sum_{b=1}^{B} n_{b} \int_{\mathcal{B}_{b}} \tau_{k}^{(j)}(\boldsymbol{x})d\boldsymbol{x}$$

both steps involve intractable computation of all crossed tables  $\mathcal{F}_m$  alternative: use of marginal composite likelihood

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## Marginal Composite Likelihood

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>)
  - $\hookrightarrow \mathbf{x}_d = (x_{1d}, \dots, x_{nd})$  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]
- $\blacktriangleright$   $\hookrightarrow$  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.:

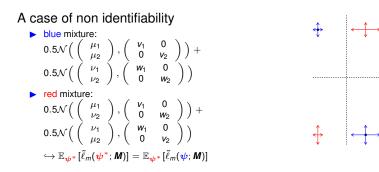
$$\tilde{\ell}_m(\psi; \boldsymbol{m}) = \sum_{d=1}^D \ell_d(\psi_d; \boldsymbol{m}_d)$$
$$= \sum_{d=1}^D \sum_{b_d=1}^{B_d} m_{db_d} \log\Big(\int_{\mathcal{B}_{b_d}^d} f_d(x_d; \psi_d) dx_d\Big).$$

 $\hookrightarrow$  diagonal mixtures only...

what about identifiability again?



## Bin-marginal CL: generic identifiability



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

generic identifiability, then consistency [Whitaker et al. 2020]

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## 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 to conciliate the partitions from each direction ?
  - $\hookrightarrow$  use the same  $\pi_1, \ldots, \pi_K$  on each direction, in a global EM

formalize more this idea now with a unique EM algorithm...

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

With  $\psi_d = (\pi_1, ..., \pi_K, \mu_{1d}, ..., \mu_{Kd}, \sigma_{1d}^2, ..., \sigma_{Kd}^2)$ 

### 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

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

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

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

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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*
  - $\hookrightarrow \ \ \mathsf{R}\text{=}50,\,100,\,200$

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

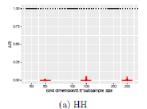
Scenario	Separation	Imbalance	Small class proportion $(\pi_1)$	Means
HH HM HL	High	High Medium Low	$     \begin{array}{r} 10^{-4} \\     10^{-3} \\     10^{-2} \end{array} $	$ \begin{aligned} \mu_1 &= (-4,-4,-4) \\ \mu_2 &= (4,4,4) \end{aligned} $
MH MM ML	Medium	High Medium Low	$     \begin{array}{r}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

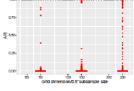
20 replications of each scenario



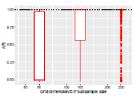
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## A zoom on some (partition quality) results...

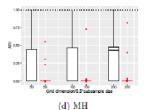


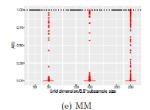


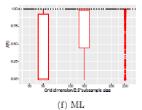
(b) HM









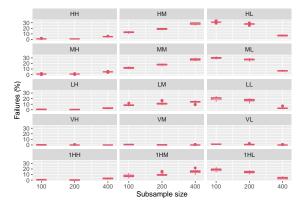


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### Results (subsampling failures)

### 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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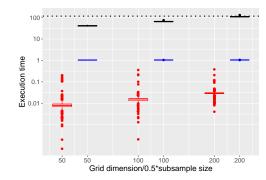
## Results (computation time)

## time vs grid/subsample size

- 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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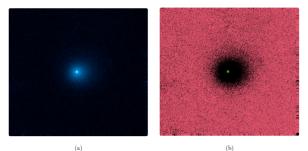
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## Real imbalanced datasets

- 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

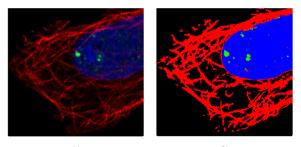
## Results: Image segmentation Comet (R=400, K=3)

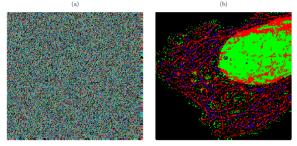




(c)

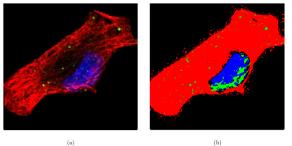
## Results: Image segmentation Cell-1 (R=20, K=4)







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



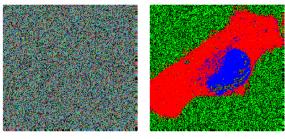
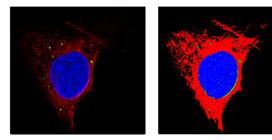


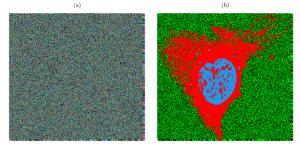
Figure 7: Cell-2 segmentation: a) Original image: b) Worst and host segmentation obtained with hin-

(d)

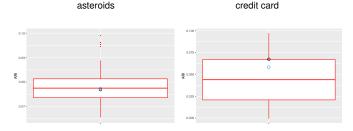
(c)

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





### Results: asteroids and credit card



subsampled EM (red boxplots), bin-marginal CL-EM (black circle) and full dataset EM (blue circle)

- two known clusters
- ARI very low for all methods, included the full dataset one, but it is not the concern of this
  experiment
- despite the loss of information, binned method behave similarly than full dataset and subsampling
- subsampling has high variability (dependency to the drawn subsample)

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## Sum-up

clustering of huge and imbalanced datasets under memory contraints:

- bin marginal composite likelihood (bmCL) approach allows to answer:
  - $\hookrightarrow$  memory requirements
  - $\hookrightarrow \ \ \text{tractability of EM algorithm}$
  - $\, \hookrightarrow \ \, \text{recovery of tiny classes} \,$
  - $\,\,\hookrightarrow\,\,$  not very sensitive to grid coarseness

### subsampling

- $\, \hookrightarrow \ \, \text{easy to implement} \,$
- $\,\hookrightarrow\,\,$  pb to recover tiny clusters
- $\, \hookrightarrow \ \, \text{high variability} \,$
- $\hookrightarrow\,$  number of subsamples (in clustering, no information on the tiny cluster)?

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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
  - $\rightarrow$  prone to slow convergence, open algorithmic question
  - $\leftrightarrow$  hybrid method bmCL / subsampling?
- preliminary study, seminal for further researches
  - $\rightarrow$  how to deal with frugality while increasing number of clusters
  - $\leftrightarrow$  strategy when many (tiny) clusters
  - $\hookrightarrow$  grid definition as a model choice?
  - $\rightarrow$  specific criterion for selecting the number of clusters and grid definition (remind: likelihood value is intractable)

Discussion

Thank you for your attention!

## Identifiability (main steps)

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

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

▶ 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<sup>\*</sup> at a up to a relabeling whatever the grid is

$$\begin{aligned} \pi \sum_{k=1}^{K} \Phi(\frac{a_1 - \mu_k}{\sigma_k}) &= \sum_{k=1}^{K^*} \pi^* \Phi(\frac{a_1 - \mu_k^*}{\sigma_k^*}) \\ \pi \sum_{k=1}^{K} \Phi(\frac{a_2 - \mu_k}{\sigma_k}) &= \sum_{k=1}^{K^*} \pi^* \Phi(\frac{a_2 - \mu_k^*}{\sigma_k^*}) \\ \vdots \\ \pi \sum_{k=1}^{K} \Phi(\frac{a_3 - \mu_k}{\sigma_k}) &= \sum_{k=1}^{K^*} \pi^* \Phi(\frac{a_3 - \mu_k^*}{\sigma_k^*}) \end{aligned}$$

- ▶ 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

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

where  $z_{ik} = 1$  observation *i* in cluster *k* E-step

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