

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

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To cite this version:

Filippo Antonazzo, Christophe Biernacki, Christine Keribin. Frugal Gaussian clustering of huge imbalanced datasets through a bin-marginal approach. Doctoral. France. 2021. hal-03505670

HAL Id: hal-03505670 <https://hal.science/hal-03505670v1>

Submitted on 31 Dec 2021

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

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Séminaire de statistique du laboratoire de mathématiques d'Avignon November 29, 2021

EACULTÉ DES SCIENCES **D'ORSAY**

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Motivation: huge and imbalanced data sets

- \blacktriangleright huge in the sense tall data
	- \leftrightarrow number of observations (high dimension setting out of scope)
	- \leftrightarrow out of computer limits
	- \rightarrow or within computer limits but with frugal resource consumption (*green computing*)
- ▶ discover new information
	- ,→ more and more clusters: not the focus of this talk
	- \leftrightarrow 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*]

Approaches

▶ supervised approach (classification) with imbalanced data sets

- \rightarrow create artificial balanced data sets: oversampling the minority class [*Chawla et al. 2002*], undersampling the majority class [*Tahir et al. 2009*] \hookrightarrow labeling could be difficult when sample size is very large
- \triangleright unsupervised approach (clustering) with very large sample size
	- ,→ subsampling [*Fraley and Raftery 2002, Xia et al. 2019*] \hookrightarrow difficult to detect very tiny clusters
	- \leftrightarrow 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)

 \rightarrow from raw to binned data

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*]
	- \rightarrow but we will be face to another dimensionality problem...
- 2. from binned data to (1D-)marginal counts \hookrightarrow need to design a new EM algorithm but computationally intractable.
- 3. optimization of a composite likelihood (CL) [*Lindsay 1988; Whitaker et al. ²⁰²⁰*] instead of the full one \hookrightarrow 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 $\mathbf{x} = \{ \boldsymbol{x}_i \in \mathbb{R}^D, i = 1, \dots, n \}$ are i.i.d. according to a *D*-dimensional Gaussian mixture model (GMM) with *K* components:

 \overline{K}

$$
f(\mathbf{x}; \psi) = \sum_{k=1}^{K} \pi_k \phi(\mathbf{x}; \mu_k, \Sigma_k)
$$

$$
\sum_{k} \pi_k = 1, \quad \pi_k > 0 \quad (k = 1, \dots, K)
$$

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

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Binned data

unobservable or too many raw data *xⁱ* \hookrightarrow vector of binned data $\boldsymbol{n} = (n_1, \ldots, n_B)$

 \triangleright the original sample space is divided into a partition $\{\mathcal{B}_b \subset \mathbb{R}^d, b = 1, \ldots, B\}$

$$
\blacktriangleright \; n_b = \#\{\bm{x}_i \in \mathcal{B}_b\}
$$

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

$$
p(\boldsymbol{n};\boldsymbol{\psi}) \propto \prod_{b=1}^{B} \Big(\sum_{k=1}^{K} \pi_k \int_{\mathcal{B}_b} \phi(\boldsymbol{x};\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) d\boldsymbol{x}\Big)^{n_b}.
$$

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

¹also provide an estimate of ψ with a binned version of EM

Curse of dimensionality for binned data

- \triangleright in our case: Cartesian grid $G = G_1 \times \ldots \times G_n$ where G_d is a univariate grid with $R_d + 2$ cut points \hookrightarrow $B = \prod_{d=1}^D (R_d + 1)$ bins, representing the grid's coarseness
- ▶ works well if *B* ≪ *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 ,→ 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: $m = \{m_1, \ldots, m_D\}$ for each direction $d = 1, \ldots, D$, $m_d = (m_{d1}, \ldots, m_{dB_d})$, component m_{db_d} is the count of observations x_{id} in the b_d -th bin of the *d*-th dimension

$$
\left| \text{ store } \sum_{d=1}^{D} B_d \text{ values instead of } \prod_{d=1}^{D} B_d \right|
$$

Bin-marginal model

 \blacktriangleright bin-marginal pdf

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

where F*^m* is the set of tables *n* ′ sharing the same marginals *m*.

\blacktriangleright issues

- \leftrightarrow identifiability
- \rightarrow mathematical complexity of the likelihood
- \rightarrow optimization of the likelihood

Identifiability

- ▶ GMM identifiable up to a label permutation *[Yakowitz and Spragings 1968]* (raw data)
- \triangleright 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 Kmax components are identifiable if $R_d > 4K_{max} - 3$, $d = 1, \ldots, D$.

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Identifiability

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Proposition ( Full binned diagonal GMM - ABK 2021)
```
Under hypothesis of diagonal covariance matrices, binned D-variate mixtures of at most Kmax components are identifiable if $R_d > 4K_{\text{max}} - 3$, $d = 1, \ldots, D$.

 \triangleright 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)*.*

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 Kmax components are identifiable if $R_d > 4K_{max} - 3$, $d = 1, \ldots, D$.

Proposition (Marginal-binned diag. GMM - ABK 2021)

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

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EM algorithm for bin-marginal model

▶ complete log-likelihood

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

where z gathers all $z_{ik} = 1$ ^Iobservation *i* in cluster *k*

 \sim

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EM algorithm for bin-marginal model

E-step

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

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

\n
$$
= \sum_{\mathbf{n} \in \mathcal{F}_m} \alpha^{(j)}(\mathbf{n}) \sum_{k=1}^K \sum_{b=1}^B n_b \int_{\mathcal{B}_b} \tau_k^{(j)}(\mathbf{x}) \log[\pi_k \phi(\mathbf{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)] d\mathbf{x}
$$

\n
$$
\mathbf{\Delta}^{(j)}(\mathbf{n}) = \frac{p(\mathbf{n}; \psi^{(j)})}{\sum_{\mathbf{n'} \in \mathcal{F}_m} p(\mathbf{n'}; \psi^{(j)})} \text{ and } \tau_k^{(j)}(.) = \frac{\pi_k^{(j)} \phi(.; \boldsymbol{\mu}_k^{(j)}, \boldsymbol{\Sigma}_k^{(j)})}{f(.; \psi^{(j)})}.
$$

\n**M-step**

$$
\blacktriangleright \pi_k^{(j+1)} = \frac{1}{n} \sum_{\mathbf{n} \in \mathcal{F}_m} \alpha^{(j)}(\mathbf{n}) \sum_{b=1}^B n_b \int_{\mathcal{B}_b} \tau_k^{(j)}(\mathbf{x}) d\mathbf{x}
$$

both steps involve intractable computation of all crossed tables 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 $\mathbf{x}_i = (x_{i1}, \ldots, x_{iD}), i = 1, \ldots, n$, generated by a GMM with parameter ψ

- ▶ pseudo-likelihood only relying on the likelihood of the marginals $L_d(\psi_d; \mathbf{x}_d)$
	- \rightarrow $\mathbf{x}_d = (x_{1d}, \dots, x_{nd})$ the component *d* of the dataset
	- \hookrightarrow with parameter $\psi_d = (\pi_1, \ldots, \pi_K, \mu_{1d}, \ldots, \mu_{Kd}, \sigma_{1d}^2, \ldots, \sigma_{Kd}^2)$

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

- **Example 1** the estimator $\tilde{\psi}$ maximizing $\tilde{L}(\psi; \mathbf{x})$ is consistent and asymptotically normal [*Molenberghs and Verbeke 2005*]
- ▶ ,→ EM algorithm with CL for HMM [*Gao and Song 2011*]
	- ,→ CL on bivariate-binned data [*Ranalli and Rocci 2016*]

Bin-marginal Composite Likelihood (bmCL)

▶ **our proposal**: combine memory reduction (bin-marginal)

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

and computational advantages of 1D-marginal CL

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

$$
\tilde{\ell}_m(\psi; \mathbf{m}) = \sum_{d=1}^D \ell_d(\psi_d; \mathbf{m}_d)
$$

=
$$
\sum_{d=1}^D \sum_{b_d=1}^{B_d} m_{db_d} \log \Big(\int_{B_{b_d}^d} f_d(x_d; \psi_d) dx_d \Big).
$$

 \leftrightarrow diagonal mixtures only...

what about identifiability again?

Bin-marginal CL: generic identifiability

A case of non identifiability ▶ blue mixture: 0.5 $\mathcal{N}\Big(\left(\begin{array}{c} \mu_1 \ \mu_2 \end{array} \right.$ $\left(\begin{array}{cc} \mathsf{v}_1 & \mathsf{0} \ \mathsf{0} & \mathsf{v}_2 \end{array} \right) +$ 0.5 $\mathcal{N}\Big(\left(\begin{array}{c} \nu_1 \ \nu_2 \end{array} \right)$ $\Bigg),\left(\begin{array}{cc} w_1 & 0 \\ 0 & w_2 \end{array}\right)\Bigg)$ ▶ red mixture: 0.5 $\mathcal{N}\Big(\left(\begin{array}{c} \mu_1 \ \nu_2 \end{array} \right)$ $\left(\begin{array}{cc} {\sf v}_1 & {\sf 0} \ {\sf 0} & {\sf w}_2 \end{array}\right)\big)+$ 0.5 $\mathcal{N}\Big(\left(\begin{array}{c} \nu_1 \ \mu_2 \end{array} \right.$ $\Bigg), \left(\begin{array}{cc} w_1 & 0 \ 0 & v_2 \end{array}\right) \Bigg)$ $\hookrightarrow \mathbb{E}_{\boldsymbol{\psi}^{*}}[\tilde{\ell}_{m}(\boldsymbol{\psi}^{*};\boldsymbol{M})]=\mathbb{E}_{\boldsymbol{\psi}^{*}}[\tilde{\ell}_{m}(\boldsymbol{\psi};\boldsymbol{M})]$

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*

- \blacktriangleright associate the missing vectors (x_d, z_d) , where z_d is $n \times K$ indicator membership matrix for x*^d* .
- \triangleright run 1D EM algorithm separately
- ▶ how to conciliate the partitions from each direction ?
	- \rightarrow use the same π_1, \ldots, π_K on each direction, in a global EM

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

EM algorithm for bin-marginal CL (bmCL)

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

▶ **bmCL E-step**

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

▶ **bmCL M-step** straightforward

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

$$
\pi_k^{(j+1)} = \frac{\sum_{d=1}^D\sum_{b_d=1}^{B_d}m_{db_d}\int_{\mathcal{B}_{b_d}^d}\tau_{kd}^{(j)}(x_d)dx_d}{Dn};\ \ \mu_{kd}^{(j+1)} = \frac{\sum_{b_d=1}^{B_d}m_{db_d}\int_{\mathcal{B}_{b_d}^d}x_d\tau_{kd}^{(j)}(x_d)dx_d}{\sum_{b_d=1}^{B_d}m_{db_d}\int_{\mathcal{B}_{b_d}^d}\tau_{kd}^{(j)}(x_d)dx_d}
$$

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

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Numerical experiment on simulated data

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

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

20 replications of each scenario

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

 (b) HM

 (a) HH

Results (subsampling failures)

subsampling failures

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

Results (computation time)

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

Real imbalanced datasets

- ▶ image segmentation, fraud detection, hazardous asteroid detection
- \blacktriangleright three variables

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

 (c)

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

 (d)

 (c)

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

Floring 7: Call 9 commentations a) Outstand income b) Women and hast commentation obtained with him

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:
	- \leftrightarrow memory requirements
	- \leftrightarrow tractability of EM algorithm
	- \leftrightarrow recovery of tiny classes
	- \leftrightarrow not very sensitive to grid coarseness

\blacktriangleright subsampling

- \leftrightarrow easy to implement
- \leftrightarrow pb to recover tiny clusters
- \leftrightarrow high variability
- \rightarrow number of subsamples (in clustering, no information on the tiny cluster)?

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

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Thank you for your attention!

Identifiability (main steps)

▶ work with binned univariate mixtures of at most *Kmax* components: pmf reduces to

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

 \blacktriangleright if *G* has *R* cut points, (a_1, \ldots, a_R) then it is needed to prove that the system has only the trivial solution $\psi=\psi^*$ at a up to a relabeling whatever the grid is

$$
\left\{\begin{array}{c} \pi\sum_{k=1}^K\Phi\left(\frac{a_1-\mu_k}{\sigma_k}\right)=\sum_{k=1}^{K^*}\pi^*\Phi\left(\frac{a_1-\mu_k^*}{\sigma_k^*}\right)\\ \pi\sum_{k=1}^K\Phi\left(\frac{a_2-\mu_k}{\sigma_k}\right)=\sum_{k=1}^{K^*}\pi^*\Phi\left(\frac{a_2-\mu_k^*}{\sigma_k^*}\right)\\ \vdots\\ \pi\sum_{k=1}^K\Phi\left(\frac{a_R-\mu_k}{\sigma_k}\right)=\sum_{k=1}^{K^*}\pi^*\Phi\left(\frac{a_R-\mu_k^*}{\sigma_k^*}\right)\end{array}\right.
$$

- ▶ deduce with [*Prop. 11.5 Valiant 2012*] that binned univariate mixtures of at most *Kmax* Gaussian distributions are identifiable if the binning grid has $R > 4K_{max} - 3$ cut points.
- \blacktriangleright induction for D-variate mixtures

EM algorithm for bin-marginal data ▶ complete log-likelihood

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

where $z_{ik} = 1$ ^Iobservation *i* in cluster *k* \blacktriangleright E-step

$$
Q_m(\psi, \psi^{(j-1)}) = \mathbb{E}_{\psi^{(j-1)}}[\ell^c(\psi; \mathbf{X}, \mathbf{Z}) | \mathbf{m}]
$$

\n
$$
= \sum_{\mathbf{n} \in \mathcal{F}_m} p(\mathbf{n} | \mathbf{m}; \psi^{(j-1)}) \mathbb{E}_{\psi^{(j-1)}}[\ell^c(\psi; \mathbf{X}, \mathbf{Z}) | \mathbf{n}]
$$

\n
$$
= \sum_{\mathbf{n} \in \mathcal{F}_m} \alpha^{(j-1)}(\mathbf{n}) \mathbb{E}_{\psi^{(j-1)}}[\ell^c(\psi; \mathbf{X}, \mathbf{Z}) | \mathbf{n}]
$$

\n
$$
= \sum_{\mathbf{n} \in \mathcal{F}_m} \alpha^{(j-1)}(\mathbf{n}) \sum_{k=1}^K \sum_{b=1}^B n_b \int_{\mathcal{B}_b} \tau_k^{(j-1)}(\mathbf{x})
$$

\n
$$
\times \log[\pi_k \phi(\mathbf{x}; \mu_k, \mathbf{\Sigma}_k)] d\mathbf{x}
$$