Thesis

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Contents

Todo list

Chapter 1

Introduction

Contents

The broad goal of this thesis is to tackle a clustering problem in the scope of mixtures model framework. More precisely, we will study the clustering of points drawn from high-dimensional Gaussian mixtures distributions. Thus, in the first part of this section we present the Gaussian mixture model and the second part we describe the well know Expectation-Maximization algorithm (EM). We will also present the limitations of this algorithm in high-dimensional setting.

1.1 The clustering problem and density estimation problem

1. Will approach this problem from a probabilistic point a view

2. CS point of view

1.2 The Gaussian mixture model

The Gaussian mixture model is an important framework for clustering problems. It assumes that the observations are drawn from a mixture distribution the components of which are Gaussian with parameters $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$:

$$\varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(x) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}_k|^{1/2}} \exp\Big(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)\Big) \tag{1.1}$$

Let $\boldsymbol{\theta}$ be the list containing all the unknown parameters of a Gaussian mixture model: the family of means $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K) \in (\mathbb{R}^p)^K$, the family of covariance matrices $\boldsymbol{\Sigma} = (\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_k) \in (\mathcal{S}_{++}^p)^K$ and the vector of cluster probabilities $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k) \in [0,1]^K$ such that $\mathbf{1}_p^\top \boldsymbol{\pi} = 1$. The density of one observation $\boldsymbol{X}_1$ is then given by:

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k \varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(\boldsymbol{x}), \qquad \forall \boldsymbol{x} \in \mathbb{R}^p, \tag{1.2}$$

where $\boldsymbol{\theta} = (\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})$.

This model can be interpreted from a latent variable perspective. Let Z be a discrete random variable taking its values in the set $[K]$ and such that $\mathbf{P}(Z = k) = \pi_k$ for every $k \in [K]$. The random variable Z indicates the cluster from which the observation $\boldsymbol{X}$ is drawn. Considering that all the conditional distributions $\boldsymbol{X}|Z = k$ are Gaussian, we get the following formula for the marginal density of X:

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{k=1}^{K} \mathbf{P}(Z = k) p_\theta(\boldsymbol{x}|Z = k) = \sum_{k=1}^{K} \pi_k \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}(\boldsymbol{x}), \qquad \forall \boldsymbol{x} \in \mathbb{R}^p. \quad (1.3)$$

In the clustering problem, the goal is to assign X to a cluster or, equivalently, to predict the cluster Z of the vector $\boldsymbol{X}$. A prediction function in such a context is $g : \mathbb{R}^p \to [K]$ such that $g(\boldsymbol{X})$ is as close as possible to Z. If we measure the risk of a prediction function g in terms of misclassification error rate $R_{\boldsymbol{\theta}}(g) = \mathbf{P}_{\boldsymbol{\theta}}(g(\boldsymbol{X}) \neq Z)$, then it is well known that the optimal (Bayes) predictor $g^*_{\boldsymbol{\theta}} \in \arg\min_g R_{\boldsymbol{\theta}}(g)$ is provided by the rule

$$g^*_{\boldsymbol{\theta}}(\boldsymbol{x}) = \arg\max_{k \in [K]} \tau_k(\boldsymbol{x}, \boldsymbol{\theta}),$$

where $\tau_k(\boldsymbol{x}, \boldsymbol{\theta}) = p_{\boldsymbol{\theta}}(Z = k|\boldsymbol{X} = \boldsymbol{x})$ stands for the conditional probability of the latent variable Z given $\boldsymbol{X}$. In the Gaussian mixture model, Bayes's rule implies that

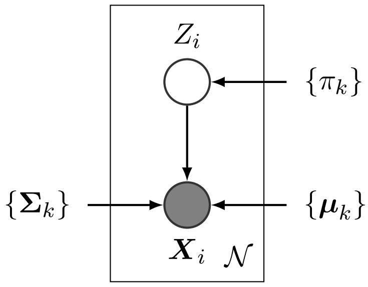
$$\tau_k(\boldsymbol{x}, \boldsymbol{\theta}) = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}|Z = k)\mathbf{P}(Z = k)}{p_{\boldsymbol{\theta}}(\boldsymbol{x})} = \frac{\pi_k \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}(\boldsymbol{x})}{\sum_{k'=1}^{K} \pi_{k'} \varphi_{\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'}}(\boldsymbol{x})} \qquad (1.4)$$

Since the true value of the parameter $\boldsymbol{\theta}$ is not available, formula (1.4) can not be directly used for solving the problem of clustering. Instead, a natural strategy is to estimate $\boldsymbol{\theta}$ by some vector $\widehat{\boldsymbol{\theta}}$, based on a sample $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ drawn from the density $p_{\boldsymbol{\theta}}$, and then to define the clustering rule by

$$\widehat{g}(\boldsymbol{x}) = g^*_{\widehat{\boldsymbol{\theta}}}(\boldsymbol{x}) = \arg\max_{k \in [K]} \tau_k(\boldsymbol{x}, \widehat{\boldsymbol{\theta}}) = \arg\max_{k \in [K]} \ \widehat{\pi}_k \varphi_{\widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\Sigma}}_k}(\boldsymbol{x}). \qquad (1.5)$$

A common approach to estimating the parameter $\boldsymbol{\theta}$ is to rely on the likelihood maximization.

Let $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ with $\boldsymbol{X}_i \in \mathbb{R}^p$ be a set of iid observations drawn from the density $p_{\boldsymbol{\theta}}$ given by (1.2). The following graphical model depicts the scheme of the observations:



The log-likelihood of the Gaussian mixture model is

$$\ell_n(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_i) = \sum_{i=1}^{n} \log \left\{ \sum_{k=1}^{K} \pi_k \varphi_{(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}(\boldsymbol{x}_i) \right\}. \tag{1.6}$$

Because of the presence in this equation of the logarithm of a sum, the maximization of the log-likelihood is a difficult nonlinear and nonconvex problem. In particular, this is not a exponential family distribution yielding simple expressions. A commonly used approach for approximately maximizing (1.6) with respect to $\boldsymbol{\theta}$ is the Expectation-Maximization (EM) Algorithm [Dempster et al., 1977] that we recall below.

Summarizing the content of this section, we can describe the following natural approach to solving the clustering problem under Gaussian mixture modeling assumption:

1.2.1 EM Algorithm

The goal of the EM algorithm is to approximate a solution of the problem (1.7). Since this optimization problem contains a nonconvex cost function, it is impossible to design a polynomial time algorithm that provably converges to the global maximum point. Instead, the EM algorithm provides a

Input: data vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$ and the number of clusters K

Output: function $\widehat{g} : \mathbb{R}^p \to [K]$

1: `Estimate` $\boldsymbol{\theta} = (\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ `by maximizing the log-likelihood:`

$$\widehat{\boldsymbol{\theta}} \in \arg\max_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \ell(\boldsymbol{\theta}|\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \arg\max_{\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}} \sum_{i=1}^{n} \log\left\{\sum_{k=1}^{K} \pi_k \varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(\boldsymbol{x}_i)\right\}. \tag{1.7}$$

2: `Output the clustering rule:`

$$\widehat{g}(\cdot) = \arg\max_{k\in[K]} \widehat{\pi}_k \varphi_{\widehat{\boldsymbol{\mu}}_k,\widehat{\boldsymbol{\Sigma}}_k}(\cdot). \tag{1.8}$$

Figure 1.1: Clustering under Gaussian mixture modeling

sequence $\{\widehat{\boldsymbol{\theta}}(t)\}_{t\in\mathbb{N}}$ of parameter values such that the cost function (*i.e.*, the log-likelihood) evaluated at these values forms an increasing sequence that converges to a local maximum.

The main idea underlying the EM algorithm is the following representation of the log-likelihood of one observation derived from the log-sum inequality:

$$\log\left\{\sum_{k=1}^{K} \pi_k \varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(\boldsymbol{x}_i)\right\} = \max_{\boldsymbol{\tau}\in[0,1]^K\ \boldsymbol{\tau}^\top\mathbf{1}_K=1} \sum_{k=1}^{K} \Big\{\tau_k \log\varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(\boldsymbol{x}_i) + \tau_k \log(\pi_k/\tau_k)\Big\}. \tag{1.9}$$

Let us denote by $\boldsymbol{\mathcal{T}} = (\tau_{i,k})$ a $n \times K$ matrix with nonnegative entries such that $\boldsymbol{\mathcal{T}}\mathbf{1}_K = \mathbf{1}_n$, that is each row of $\boldsymbol{\mathcal{T}}$ is a probability distribution on $[K]$. Combining (1.7) and (1.9), we get

$$\widehat{\boldsymbol{\theta}} \in \arg\max_{\boldsymbol{\theta}=(\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma})} \max_{\boldsymbol{\mathcal{T}}} \sum_{i=1}^{N} \sum_{k=1}^{K} \Big\{\tau_{i,k} \log\varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k}(\boldsymbol{x}_i) + \tau_{i,k} \log(\pi_k/\tau_{i,k})\Big\}. \tag{1.10}$$

The great advantage of this new representation of the log-likelihood function is that the cost function in (1.10), considered as a function of $\boldsymbol{\theta}$ and $\boldsymbol{\mathcal{T}}$, is biconcave, *i.e.*, it is concave with respect to $\boldsymbol{\theta}$ for every fixed $\boldsymbol{\mathcal{T}}$ and concave with respect to $\boldsymbol{\mathcal{T}}$ for every fixed $\boldsymbol{\theta}$. In such a situation, one can apply the alternating maximization approach to sequentially improve on an initial point. In the present context, an additional attractive feature of the cost function in (1.10) is that the two optimization problems involved in the alternating maximization procedure admit explicit solutions.

Input: data vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$ and the number of clusters K

Output: parameter estimate $\widehat{\boldsymbol{\theta}} = \{\widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\Sigma}}_k, \pi_k\}_{k\in[K]}$

1: `Initialize` $t = 0$, $\boldsymbol{\theta} = \boldsymbol{\theta}^0$.

2: **Repeat**

  3: `Update the parameter` $\boldsymbol{\mathcal{T}}$:

$$\tau_{i,k}^t = \frac{\pi_k^t \varphi_{\boldsymbol{\mu}_k^t, \boldsymbol{\Sigma}_k^t}(\boldsymbol{x}_i)}{\sum_{k'\in[K]} \pi_{k'}^t \varphi_{\boldsymbol{\mu}_{k'}^t, \boldsymbol{\Sigma}_{k'}^t}(\boldsymbol{x}_i)}.$$

  4: `Update the parameter` $\boldsymbol{\theta}$:

$$\pi_k^{t+1} = \frac{1}{n}\sum_{i=1}^n \tau_{i,k}^t, \qquad \boldsymbol{\mu}_k^{t+1} = \frac{1}{n\pi_k^{t+1}}\sum_{i=1}^n \tau_{i,k}^t \boldsymbol{x}_i,$$

$$\boldsymbol{\Sigma}_k^{t+1} = \frac{1}{n\pi_k^{t+1}}\sum_{i=1}^n \tau_{i,k}^t (\boldsymbol{x}_i - \boldsymbol{\mu}_k^{t+1})(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{t+1})^\top.$$

  5: `increment` t: $t = t + 1$.

6: **Until** `stopping rule.`

7: **Return** $\boldsymbol{\theta}^t$.

Figure 1.2: EM algorithm for Gaussian mixtures

Lemma 1. *Let us introduce the cost function*

$$F(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) = \sum_{i=1}^n \sum_{k=1}^K \Big\{\tau_{i,k} \log \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}(\boldsymbol{x}_i) + \tau_{i,k} \log(\pi_k/\tau_{i,k})\Big\}. \tag{1.11}$$

Then, the following two optimization problems

$$\widehat{\boldsymbol{\theta}}(\boldsymbol{\mathcal{T}}) \in \arg\max_{\boldsymbol{\theta}} F(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}), \qquad \widehat{\boldsymbol{\mathcal{T}}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{\mathcal{T}}} F(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) \tag{1.12}$$

has explicit solutions given by

$$\widehat{\pi}_k = \frac{1}{n}\sum_{i=1}^{n} \tau_{i,k}, \qquad \widehat{\boldsymbol{\mu}}_k = \frac{1}{n\widehat{\pi}_k}\sum_{i=1}^{n} \tau_{i,k}\boldsymbol{x}_i, \qquad \forall k \in [K], \tag{1.13}$$

$$\widehat{\boldsymbol{\Sigma}}_k = \frac{1}{n\widehat{\pi}_k}\sum_{i=1}^{n} \tau_{i,k}(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)^\top, \qquad \forall k \in [K], \tag{1.14}$$

$$\widehat{\tau}_{i,k} = \frac{\pi_k \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}(\boldsymbol{x}_i)}{\sum_{k' \in [K]} \pi_{k'} \varphi_{\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'}}(\boldsymbol{x}_i)}, \qquad \forall k \in [K],\ \forall i \in [n]. \tag{1.15}$$

Based on this result, the EM algorithm is defined as in Figure 1.2. The algorithm operates iteratively and needs a criterion to determine when the iterations should be stopped. There is no clear consensus on this point in the statistical literature, but it is a commonly used practice to stop when one of the following conditions is fulfilled:

i) The number of iterations t exceeds a pre-specified level $t_{\max}$.

ii) The increase of the log-likelihood over past t_0 iterations is not significantly different from zero: $\ell_n(\boldsymbol{\theta}^t) - \ell_n(\boldsymbol{\theta}^{t-t_0}) \le \varepsilon$ for some pre-specified values $t_0 \in \mathbb{N}$ and $\varepsilon > 0$.

EM is conceptually easy and each iteration increases the log-likelihood:

$$\ell_n(\boldsymbol{\theta}^{t+1}) \ge \ell_n(\boldsymbol{\theta}^t), \qquad \forall t \in \mathbb{N}.$$

The complexity at each step of the EM algorithm is $O(Knp^2)$ and it usually requires many iterations to converge. In a high-dimensional setting when p is large, the quadratic dependence on p may result in prohibitively large running times. However, the computation of the elements of the covariance matrices $\boldsymbol{\Sigma}_k^t$ and the mean vectors $\boldsymbol{\mu}_k^t$ can be parallelized which may lead to considerable savings in the running time.

1.3 The curse of dimensionality

Note: reecrire cette partie en commencant par le pb de la HD en stats en general, se baser sur les points de Giraud, puis une deuxieme sous section avec le cas du clustering et les pistes de resolution connues, ex: penalization, subspace clustering...

Note: Ajouter un tableau des differents types de modeles et le nombre de parametres

Note: citer

The expression "Curse of dimensionality" introduced by R.Bellman referes to the problems linked with high dimension. One can see that evaluating a function on the segment $(0, 1)$ with a step size of 0.1 is straightforward. However, evaluating the function in a grid of dimension 10 requires 10^{10} computations which can be intractable even today within a reasonable time. This is an important issue in the clustering context. In the Gaussian mixture model of K components in dimension p, the number of parameters to estimate is:

$$\nu = \underbrace{(K-1)}_{\text{Weights}} + \underbrace{Kp}_{\text{Means}} + \underbrace{Kp(p-1)^2}_{\text{Covariances Matrices}} \tag{1.16}$$

Moreover, the evaluation of $\widehat{\tau}_{i,k}$ in eq. (1.15) needs to evaluate the inverse of the covariance matrix $\widehat{\boldsymbol{\Sigma}}_k$ which is called the precision matrix. If $n << \nu$ the matrices $\widehat{\boldsymbol{\Sigma}}_k$ $k = 1, \ldots, K$ are ill conditioned and the precision matrices are prone to large numerical errors or more often singular and the problem can not be solved. In section 1.5, we tackle this challenge by studying some nice structural properties of precision matrices. However, an interesting phenomenon occurs in high dimension, Scoot and Thomson showed that high-dimensional spaces are mostly empty, Huber showed that the realizations of a p-dimensional random vector with a uniform probability distribution on the unit hypershpere lies with high probability close to the boundary of this hypershere. Therefore, the data belong mostly in a $p-1$ dimensional subspace. Therefore, in the clustering problem, different clusters may live on different subspaces

Note: cite

Note: cite

Note: attention de pas copier Bouveyron Bouveyron and Brunet [2013]

Note: subspace clustering

1.3.1 Bibliographic notes

The reader can find a more thorough study of high dimensional statistics in Giraud [2014]. The reader can refer to [Bouveyron and Brunet, 2013] to have an overview of the different Gaussian mixture models for clustering in high dimension.

1.4 Some contributions

1.5 Graphical Lasso for Gaussian mixtures

As we saw in the introduction chapter, the number of free parameters in a full GMM with K components in dimension p are $(K-1)+Kp+Kp(p+1)/2$ which means that for $K=5$ and $p=100$ we have 125704 parameters to estimate. In this high dimensional setting, the EM algorithm experiences severe performance degradation. In particular, the inversion of the covariance matrices are challenged. One way to tackle these problems is to use regularization. We will make the assumption on some structure on the inverse of the covariance matrix of a component called the precision or concentration matrix. The work presented in this chapter is inspired by [Friedman et al., 2007], [Banerjee et al., 2008], [Yuan and Lin, 2007] and [Meinshausen and Bühlmann, 2006] in which they penalize the components of the precision matrix of a Gaussian graphical model. We generalize this work to the Gaussian mixture model.

1.5.1 Introduction

We consider $\boldsymbol{X} = (\boldsymbol{X}^{(1)}, \dots, \boldsymbol{X}^{(p)})$ a random vector admitting a p-dimensional normal distribution $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Sigma}$ non-singular. One can construct an undirected graph $G = (V, E)$ with p vertices corresponding to each coordinates and, $E = (e_{i,j})_{1\leq i<j\leq p}$, the edges between the vertices describing the conditional independence relationship among $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(p)}$. If in this graph, $e_{i,j}$ is absent in E if and only if $X^{(i)}$ and $X^{(j)}$ are independent conditionally to the other variables $\{X^{(l)}\}$ with $l \neq i, j$ (noted $X^{(i)} \perp\!\!\!\perp X^{(j)} | X^{(l)}\, l \neq i, j$), then G is called the Gaussian concentration graph model for the Gaussian random vector $\boldsymbol{X}$. This property is particularly interesting in the study of the inverse of the covariance matrix. Let us denote $\boldsymbol{\Sigma}^{-1} = \boldsymbol{\Omega} = (\omega_{i,j})$ the precision matrix. The components of this matrix verify $\omega_{i,j} = 0$ if and only if $X^{(i)} \perp\!\!\!\perp X^{(j)}$ conditionally to the other variables. We recall in the following lemma this well known result

Lemma 1.5.1 (Conditional independence in Gaussian concentration graph model)**.** *Consider* $\boldsymbol{X} = (\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(p)})$ *a* p*-dimensional random vector with a multivariate normal distribution* $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$*, note* $\boldsymbol{\Sigma}^{-1} = \boldsymbol{\Omega} = (\omega_{i,j})$*, then* $X^{(i)} \perp\!\!\!\perp X^{(j)} | X^{(l)} \iff \omega_{i,j} = 0$ *with* $l \neq i, j$

Proof. This result can be found in [Edwards, 2000], consider the density of $\boldsymbol{X}$

$$\varphi_{\boldsymbol{\mu},\boldsymbol{\Sigma}}(\boldsymbol{x}) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\Big(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\Big), \tag{1.17}$$

it can be rewritten as

$$\varphi_{\boldsymbol{\mu},\boldsymbol{\Sigma}}(\boldsymbol{x}) = \exp(\alpha + \beta^T \boldsymbol{x} - \frac{1}{2}\boldsymbol{x}^T \boldsymbol{\Omega} \boldsymbol{x}), \tag{1.18}$$

with $\beta = \boldsymbol{\Omega}\boldsymbol{\mu}$ and $\alpha = \frac{1}{2}\log(|\boldsymbol{\Omega}|) - \frac{1}{2}\boldsymbol{\mu}^T\boldsymbol{\Omega}\boldsymbol{\mu} - \frac{p}{2}\log(2\pi)$. Then, the previous equation can be rewritten as

$$\exp\big(\alpha + \sum_{j=1}^{p} \beta_j \boldsymbol{x}^{(j)} - \frac{1}{2}\sum_{j=1}^{p}\sum_{(i=1)}^{p} \omega_{i,j}\boldsymbol{x}^{(j)}\boldsymbol{x}^{(i)}\big). \tag{1.19}$$

Now, for X, Y, Z three random variables, we have $X \perp\!\!\!\perp Y|Z$ iff the joint density can be factorized into two factors $f_{X,Y,Z}(x, y, z) = h(x, z)g(y, z)$ with h anf g two functions. Then, at the light of eq. (1.19), we have $X^{(i)} \perp\!\!\!\perp X^{(j)}|X^{(l)} \iff \omega_{i,j} = 0$. □

The literature on this subject focused on a first hand on the estimation of the graph structure, [Dempster, 1972] developed a greedy forward or backward search method to estimate the set of non-zero components in the concentration matrix. The forward method relies on initializing an empty set and select iteratively an edge with an MLE fit for $\mathcal{O}(p^2)$ different parameters. The procedure stops according to a suitable selection criterion. The backward method performs in the same manner by starting with all edges and performing deletions. It is obvious that such methods are computationally intractable in high dimension. In [Meinshausen and Bühlmann, 2006], the authors studied a neighborhood selection procedure with lasso. The goal is to estimate the neighborhood $ne_{X^{(i)}}$ of a node $X^{(i)}$ which is the smallest subset of $G \setminus \{X^{(i)}\}$ such that $X^{(i)} \perp\!\!\!\perp \{X^{(j)} : X^{(j)} \in G \setminus \{ne_{X^{(i)}}\}\}|X_{ne_{X^{(i)}}}$. The estimation of the neighborhood is cast as a regression problem with a lasso penalization. The authors showed that this procedure is consistent for sparse high dimensional graphs and computationally efficient. More precisely, let $\theta^{(i)} \in \mathbb{R}^p$ be the vector of coefficient of the optimal prediction,

Note: banerjee p488, consistency lies on choice of penalty

$$\theta^{(i)} = \underset{\theta:\theta_i=0}{\arg\min}\, \mathbb{E}\Big[X^{(i)} - \sum_{k=1}^{p} \theta_k X^{(k)}\Big], \tag{1.20}$$

then the components of $\theta^{(i)}$ are determined by the precision matrix, $\theta_j^{(i)} = -\omega_{i,j}/\omega_{i,i}$. Therefore, the set of neighbors of $X^{(i)} \in G$ is given by

$$ne_{X^{(i)}} = \{X^{(j)}, j \in [p] : \omega_{i,j} \neq 0\}. \tag{1.21}$$

Now, let $\mathbb{X}$ be the $n \times p$-dimensional matrix such that the column $\mathbb{X}^{(i)}$ is the n observations vector of $X^{(i)}$, given a regularization parameter $\lambda \geq 0$ carefully chosen, the Lasso estimate $\widehat{\theta}^{i,\lambda}$ of $\theta^{(i)}$ is given by

$$\widehat{\theta}^{i,\lambda} = \underset{\theta:\theta_i=0}{\arg\min}\left(\frac{1}{n}\|\mathbb{X}^{(i)} - \mathbb{X}\theta\|_2^2 + \lambda\|\theta\|_1\right). \tag{1.22}$$

The authors proved under several assumptions that

$$P(\widehat{ne}^{\lambda}_{X^{(i)}} = ne_{X^{(i)}}) \to 1 \quad \text{for}\, n \to \infty, \tag{1.23}$$

and for some $\epsilon > 0$,

$$P(\widehat{E}^{\lambda} = E) = 1 - \mathcal{O}(\exp(-cn^{\epsilon})) \quad \text{for}\, n \to \infty. \tag{1.24}$$

Therefore, this method recovers the conditional independence structure of sparse high-dimensional Gaussian concentration graph at exponential rates. However, this method performs model selection but does not estimate the parameters of the model. One could estimate the parameters of a model which has been selected by this method. Such procedure often leads to instability of the estimator since small changes on the data would change the model selected [Yuan and Lin, 2007], [Breiman, 1996]. One major difficulty of a method that would perform both tasks is to ensure that the estimator of the precision matrix is positive definite. [Yuan and Lin, 2007] proposed a penalized-likelihood method that performs model selection and parameter estimation simultaneously as well as ensuring the positive definiteness of the precision matrix. Their approach is similar to [Meinshausen and Bühlmann, 2006] as they use the ℓ_1 penalty but with the likelihood and the addition of a positive definite constraint. The log-likelihood for $\mathbf{\Omega}$ based on a centered random sample $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ of $\boldsymbol{X}$ is

Note: ajouter un mot sur la complexité

$$\frac{n}{2}\log(|\mathbf{\Omega}|) - \frac{1}{2}\sum_{i=1}^{n} \boldsymbol{X}_i^T \mathbf{\Omega} \boldsymbol{X}_i \tag{1.25}$$

and the constrained minimization problem over the set of positive definite matrices is

$$\min\Big\{ -\log(|\boldsymbol{\Omega}|) + \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{X}_i^T \boldsymbol{\Omega} \boldsymbol{X}_i \Big\} \quad \text{subject to} \quad \sum_{i\neq j} |\omega_{i,j}| \leq t, \tag{1.26}$$

with $t \geq 0$ a tuning parameter. Note that $\widehat{\boldsymbol{\mu}} = \bar{\boldsymbol{X}}$. Consider the empirical covariance matrix $\boldsymbol{S} = 1/n \sum_{i=1}^{n} \boldsymbol{X}_i^T \boldsymbol{X}_i$, the eq. (1.26) can be rewritten as

$$\min\Big\{ -\log(|\boldsymbol{\Omega}|) + \operatorname{tr}(\boldsymbol{S}\boldsymbol{\Omega}) \Big\} \quad \text{subject to} \quad \sum_{i\neq j} |\omega_{i,j}| \leq t. \tag{1.27}$$

Since the whole problem is convex, the Lagrangian form is given by

$$\mathcal{L}(\lambda, \boldsymbol{\Omega}) = -\log(|\boldsymbol{\Omega}|) + \operatorname{tr}(\boldsymbol{S}\boldsymbol{\Omega}) + \lambda \sum_{i\neq j} |\omega_{i,j}|, \tag{1.28}$$

with λ the tuning parameter. A non-negative garrote-type estimator is provided in [Yuan and Lin, 2007] but can be only applied when a good estimator of $\boldsymbol{\Omega}$ is available. Therefore, we will continue our study of the Lasso-type estimator, the authors provided an asymptotic result

Note: regarder de plus pres

Theorem 1.5.1 (Theorem 1 from [Yuan and Lin, 2007]). *If $\sqrt{n}\lambda \to \lambda_0 \geq 0$ as $n \to \infty$, the lasso-type estimator is such that*

$$\sqrt{n}(\widehat{\boldsymbol{\Omega}} - \boldsymbol{\Omega}) \to \arg\min_{\boldsymbol{U}=\boldsymbol{U}^T}(V),$$

in distribution where

$$V(\boldsymbol{U}) = \operatorname{tr}(\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{U}\boldsymbol{\Sigma}) + \operatorname{tr}(\boldsymbol{U}\boldsymbol{W}) + \lambda_0 \sum_{i\neq j} \big\{ u_{i,j}\operatorname{sign}(\omega_{i,j}) I(\omega_{i,j} \neq 0) + |u_{i,j}| I(\omega_{i,j} = 0) \big\}$$

in which $\boldsymbol{W}$ is a random symmetric $p \times p$ matrix such that $\operatorname{vec}(\boldsymbol{W}) \sim \mathcal{N}(0, \Lambda)$, and Λ is such that

$$\operatorname{cov}(w_{i,j}, w_{i',j'}) = \operatorname{cov}(X^{(i)}X^{(j)}, X^{(i')}X^{(j')}).$$

Note: mettre un commentair sur ce resultat et aspect algorithmique

Unfortunately, the computational complexity of interior point methods for maximizing eq. (1.28) is $\mathcal{O}(p^6)$ and at each steps, we have to compute and store a Hessian matrix of size $\mathcal{O}(p^2)$. These prohibitive complexities led the research on more specialized methods. [Banerjee et al., 2008] worked on the same approach, solving a maximum likelihood problem with an ℓ_1 penalty and focusing on the computation complexity by proposing an iterative block coordinate descent algorithm. The problem to maximize is similar to eq. (1.28)

$$\widehat{\mathbf{\Omega}} = \arg\max_{\mathbf{\Omega}\succ 0}\{\log(|\mathbf{\Omega}|) - \mathrm{tr}(\boldsymbol{S}\mathbf{\Omega}) - \lambda\|\mathbf{\Omega}\|_1\}. \tag{1.29}$$

Note that the ℓ_1 norm of a matrix $\mathbf{\Omega}$ can be expressed as

$$\|\mathbf{\Omega}\|_1 = \max_{\|\boldsymbol{U}\|_\infty \leq 1} \mathrm{tr}(\mathbf{\Omega}\boldsymbol{U}), \tag{1.30}$$

injecting this in eq. (1.29) gives

$$\max_{\mathbf{\Omega}\succ 0} \min_{\|\boldsymbol{U}\|_\infty \leq \lambda} \big\{ \log(|\mathbf{\Omega}|) - \mathrm{tr}(\mathbf{\Omega}(\boldsymbol{S}+\boldsymbol{U}))\big\}. \tag{1.31}$$

After exchanging the min and the max, we solve the problem for $\mathbf{\Omega}$ by setting the gradient to 0 which gives $(\mathbf{\Omega}^{-1})^T - (\boldsymbol{S}+\boldsymbol{U})^T = 0$ then $\mathbf{\Omega} = (\boldsymbol{S}+\boldsymbol{U})^{-1}$. The dual problem is then

$$\min_{\|\boldsymbol{U}\|_\infty} \{-\log(|\boldsymbol{S}+\boldsymbol{U}|) - p\}, \tag{1.32}$$

or by setting $\boldsymbol{W} = \boldsymbol{S}+\boldsymbol{U}$,

$$\widehat{\mathbf{\Sigma}} = \widehat{\mathbf{\Omega}^{-1}} = \arg\max \log(|\boldsymbol{W}|) \quad \text{s.t} \quad \|\boldsymbol{W}-\boldsymbol{S}\|_\infty \leq \lambda. \tag{1.33}$$

We observe the presence of a log-barrier adding the implicit constraint $(\boldsymbol{S}+\boldsymbol{U}) \succ 0$. Furthermore, the dual problem estimates the covariance matrix... To solve this maximization problem, the authors proposed a Block Coordinate Descent Algorithm described in fig. 1.3. For any symmetric matrix $\boldsymbol{A}$,

Note: pourquoi $\Sigma_{kk} = S_{kk} + \lambda$?, p488

Note: citer les theoremes et choix du param

Input: Matrix $\boldsymbol{S}$, parameter λ and threshold ε

Output: Estimate of $\boldsymbol{W}$

Initialize $\boldsymbol{W}^{(0)} := \boldsymbol{S} + \lambda I$

repeat

  for $j = 1, \ldots, p$ **do**

    (a) Let $\boldsymbol{W}^{(j-1)}$ denote the current iterate. Solve the quadratic program

$$\widehat{\mathbf{y}} := \arg\min_{\mathbf{y}} \{\mathbf{y}^T (\boldsymbol{W}^{(j-1)}_{\backslash j \backslash j})^{-1} \mathbf{y} : \|\mathbf{y} - \boldsymbol{S}_j\|_\infty \leq \lambda\}.$$

    (b) Update the rule: $\boldsymbol{W}^{(j)}$ is $\boldsymbol{W}^{(j-1)}$ with column/row $\boldsymbol{W}_j$ replaced by $\widehat{\mathbf{y}}$.

  end for

  Let $\widehat{\boldsymbol{W}}^{(0)} := \boldsymbol{W}^{(p)}$.

until convergence occurs when

$$\mathrm{tr}\big((\widehat{\boldsymbol{W}}^{(0)})^{-1}\boldsymbol{S}\big) - p + \lambda\big\|(\widehat{\boldsymbol{W}}^{(0)})^{-1}\big\|_1 \leq \varepsilon.$$

Figure 1.3: Block Coordinate Descent Algorithm

let $\boldsymbol{A}_{\backslash k \backslash j}$ be the matrix produced by removing column k and row j to $\boldsymbol{A}$. Let $\boldsymbol{A}_j$ the j^{th} column of $\boldsymbol{A}$ with the element $\boldsymbol{A}_{jj}$ removed. They proved that the Block Coordinate Descent algorithm converges, achieving an ε-suboptimal solution to eq. (1.33) and each iterates produce a strictly positive definite matrix. For a fixed number of sweeps K, the complexity of this algorithm is $\mathcal{O}(Kp^4)$. They provide also another algorithm using Nesterov's first order method which has a $\mathcal{O}(p^{4.5}/\epsilon)$ complexity for $\varepsilon > 0$ the desired accuracy. It is interesting to note that the dual problem of line 6 in fig. 1.3 is

$$\min_{\boldsymbol{x}} \boldsymbol{x}^T \boldsymbol{W}^{(j-1)}_{\backslash j \backslash j} \boldsymbol{x} - \boldsymbol{S}_j^T \boldsymbol{x} + \lambda \|\boldsymbol{x}\|_1, \tag{1.34}$$

and strong duality holds, it can best casted as

$$\min_{\boldsymbol{x}} \|\boldsymbol{Q}\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda \|\boldsymbol{x}\|_1, \tag{1.35}$$

with $\boldsymbol{Q} = (\boldsymbol{W}^{(j-1)}_{\backslash j \backslash j})^{1/2}$ and $\boldsymbol{b} := \frac{1}{2}\boldsymbol{Q}^{-1}\boldsymbol{S}_j$. Therefore, we recover the Lasso problem, more precisely, the algorithm can be interpreted as a sequence of iterative Lasso problems. This approach is similar to another paper that we would like to mention [Friedman et al., 2007]. The authors proposed a faster algorithm based on the Block Coordinate Descent algorithm from [Banerjee et al., 2008] called Graphical Lasso. They estimate the matrix $\boldsymbol{W} = \boldsymbol{\Omega}^{-1}$ by performing iterative permutations of the columns of this matrix to make the target column the last for a coupled Lasso problem. The matrices $\boldsymbol{W}$ and $\boldsymbol{S}$ will be presented as following

$$\boldsymbol{W} = \begin{bmatrix} \boldsymbol{W}_{11} & \boldsymbol{w}_{12} \\ \boldsymbol{w}_{21} & w_{22} \end{bmatrix}, \quad \boldsymbol{S} = \begin{bmatrix} \boldsymbol{S}_{11} & \boldsymbol{s}_{12} \\ \boldsymbol{s}_{21} & s_{22} \end{bmatrix}, \tag{1.36}$$

and the Graphical Lasso algorithm is described in fig. 1.4. The Lasso problem can be solved via a coordinate descent, the reader can refer to [Friedman et al., 2007] for the procedure. In this problem, the algorithm estimates $\widehat{\boldsymbol{\Sigma}}$

and returns also $\boldsymbol{B} = (\boldsymbol{b}^{(1)}, \ldots, \boldsymbol{b}^{(p)})$, the matrix where each column is the solution of the Lasso problem in eq. (1.35) for each column of $\boldsymbol{W}$. It is easy to recover $\boldsymbol{\Omega}$ since

$$\boldsymbol{W} = \begin{bmatrix} \boldsymbol{W}_{11} & \boldsymbol{w}_{12} \\ \boldsymbol{w}_{21} & w_{22} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\Omega}_{11} & \boldsymbol{\omega}_{12} \\ \boldsymbol{\omega}_{21} & \omega_{22} \end{bmatrix} = \begin{bmatrix} I_{p-1} & 0 \\ 0 & 1 \end{bmatrix}, \tag{1.37}$$

and

$$\begin{aligned} \boldsymbol{\omega}_{12} &= -\boldsymbol{W}_{11}^{-1}\boldsymbol{w}_{12}\omega_{22} \\ \omega_{22} &= 1/(w_{22} - \boldsymbol{w}_{12}^T\boldsymbol{W}_{11}^{-1}\boldsymbol{w}_{12}). \end{aligned}$$

Therefore, for $j = 1, \ldots, p$, the permuted target components of $\boldsymbol{\Omega}$ are

$$\begin{aligned} \boldsymbol{\omega}_{12} &= -\boldsymbol{b}^{(j)}\widehat{\omega}_{22} \\ \omega_{22} &= 1/(w_{22} - \boldsymbol{w}_{12}^T\boldsymbol{b}^{(j)}). \end{aligned}$$

In what follows, we will adapt these methods on a Gaussian mixture models, more precisely we will assume that each clusters present a sparse Gaussian concentration graph. We will rely on the Graphical Lasso for estimating the precision matrix and derive a EM algorithm.

1.5.2 Graphical Lasso on Gaussian mixtures

In this section, we present our contribution. We consider a Gaussian mixture model of K components and our task is to estimate the parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_K)$ with $\theta_k = (\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Omega}_k)$ where $\boldsymbol{\Omega}_k$ is the precision matrix regarding the k^{th} component of the mixture. We denote $\varphi_{(\boldsymbol{\mu}_k, \boldsymbol{\Omega}_k)}$ the Gaussian density of mean $\boldsymbol{\mu}_k$ and precision matrix $\boldsymbol{\Omega}_k$. The penalized log-likelihood is

$$\ell_n^{pen}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}_i) - pen(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log \left\{ \sum_{k=1}^{K} \pi_k \varphi_{(\boldsymbol{\mu}_k, \boldsymbol{\Omega}_k)}(\boldsymbol{x}_i) \right\} - pen(\boldsymbol{\theta}). \tag{1.39}$$

Input: Matrix $\boldsymbol{S}$, parameter λ and threshold ε
Output: Estimate of $\boldsymbol{W}$ and $\boldsymbol{B}$ a matrix of parameters.
Initialize $\boldsymbol{W}^{(0)} := \boldsymbol{S} + \lambda I$ and $\boldsymbol{B} = 0_{p\times p}$. The diagonal of $\boldsymbol{W}$ remained unchanged in what follows.
repeat
  for $j = 1, \dots, p$ **do**
    (a) Let $\boldsymbol{W}^{(j-1)}$ denote the current iterate. Solve the Lasso problem in eq. (1.35)

$$\widehat{\boldsymbol{x}}^{(j-1)} = \arg\min_{\boldsymbol{x}} \frac{1}{2}\|(\boldsymbol{W}_{11}^{(j-1)})^{1/2}\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda\|\boldsymbol{x}\|_1, \tag{1.38}$$

with $\boldsymbol{b} := (\boldsymbol{W}_{11}^{(j-1)})^{-1/2}\boldsymbol{s}_{12}$.
    (b) Update: $\boldsymbol{W}^{(j)}$ is $\boldsymbol{W}^{(j-1)}$ with $\boldsymbol{w}_{12} = \boldsymbol{W}_{11}^{(j-1)}\widehat{\boldsymbol{x}}^{(j-1)}$.
    (c) Save the parameter $\boldsymbol{x}^{(j-1)}$ in the j^{th} column of $\boldsymbol{B}$.
    (d) Permute the columns and rows of $\boldsymbol{W}^{(j-1)}$ such that the j^{th} column is $\boldsymbol{w}_{12}$, the next target.
  end for
  Let $\widehat{\boldsymbol{W}}^{(0)} := \boldsymbol{W}^{(p)}$.
until convergence occurs.

Figure 1.4: Graphical Lasso

We suppose that each component of the mixture has a sparse Gaussian concentration graph. Therefore, in the scope of [Banerjee et al., 2008] and [Friedman et al., 2007], we consider an ℓ_1 regularization $pen(\theta_k) = \sum_{k=1}^{K} \lambda_k ||\mathbf{\Omega}_k||_{1,1}$ with $\lambda_k > 0$. The penalization of the log-likelihood concerns only the precision matrices $\mathbf{\Omega}_k$. Regarding the other parameters $(\pi_k, \boldsymbol{\mu}_k)$, our algorithm is the same as EM and we can use the same iteration technique as in lemma 1 to maximize the following cost function

$$F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) = \sum_{k=1}^{K} \left(\sum_{i=1}^{n} \Big\{ \tau_{i,k} \log \varphi_{\boldsymbol{\mu}_k, \mathbf{\Omega}_k}(\boldsymbol{x}_i) + \tau_{i,k} \log(\pi_k / \tau_{i,k}) \Big\} - \lambda_k ||\mathbf{\Omega}_k||_{1,1} \right). \tag{1.40}$$

The maximization of this function over $\boldsymbol{\theta}$ and $\boldsymbol{\mathcal{T}}$ leads to the two following optimization problems

Note: ajouter les domaines

$$\widehat{\boldsymbol{\theta}}(\boldsymbol{\mathcal{T}}) \in \arg\max_{\boldsymbol{\theta}} F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}), \qquad \widehat{\boldsymbol{\mathcal{T}}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{\mathcal{T}}} F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}). \tag{1.41}$$

For a given $\widehat{\boldsymbol{\mathcal{T}}}$, estimates of $(\pi_1, \ldots, \pi_K$ and $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$ obtained by the first optimization problem in eq. (1.41) are the same as in the EM algorithm

$$\widehat{\pi}_k = \frac{1}{n} \sum_{i=1}^{n} \widehat{\tau}_{i,k}, \quad \text{and} \quad \widehat{\boldsymbol{\mu}}_k = \frac{1}{n\widehat{\pi}_k} \sum_{i=1}^{n} \widehat{\tau}_{i,k} \boldsymbol{x}_i, \qquad \forall k \in [K] \tag{1.42}$$

And for a given $\widehat{\boldsymbol{\theta}}$, the estimate of $\boldsymbol{\mathcal{T}}$ obtained by the second optimization problem is

$$\widehat{\tau}_{i,k} = \frac{\widehat{\pi}_k \varphi_{\widehat{\boldsymbol{\mu}}_k, \widehat{\mathbf{\Omega}}_k}(\boldsymbol{x}_i)}{\sum_{k' \in [K]} \widehat{\pi}_{k'} \varphi_{\widehat{\boldsymbol{\mu}}_{k'}, \widehat{\mathbf{\Omega}}_{k'}}(\boldsymbol{x}_i)} = p_{\boldsymbol{\theta}}(Z = k | \boldsymbol{X} = \boldsymbol{x}_i), \qquad \forall k \in [K],\ \forall i \in [n]. \tag{1.43}$$

However, due to the penality $\lambda_k ||\mathbf{\Omega}_k||_{1,1}$, the estimation of $\mathbf{\Omega}_k$ is not straightforward.

We introduce the weighted empirical covariance matrix

$$\mathbf{\Sigma}_{n,k} = \frac{1}{n} \frac{\sum_{i=1}^{n} \tau_{i,k} (\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)^\top}{\sum_{i=1}^{n} \tau_{i,k}} \tag{1.44}$$

The Gaussian density in equation (1.40) can be expanded as follows

$$
\begin{aligned}
F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) = & \sum_{k=1}^{K} \Bigg(\sum_{i=1}^{n} \Big\{ \tau_{i,k} \Big(-\frac{p}{2}\log(2\pi) + \frac{1}{2}\log|\boldsymbol{\Omega}_k| \\
& - \frac{1}{2}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Omega}_k (\boldsymbol{x}_i - \boldsymbol{\mu}_k) \Big) + \tau_{i,k}\log(\pi_k/\tau_{i,k}) \Big\} - \lambda_k ||\boldsymbol{\Omega}_k||_{1,1} \Bigg) \\
= & -\frac{np}{2}\log(2\pi) + \sum_{k=1}^{K} \Bigg(\frac{n\pi_k}{2}\log|\boldsymbol{\Omega}_k| \\
& + \sum_{i=1}^{n} \Big\{ -\frac{\tau_{i,k}}{2}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Omega}_k (\boldsymbol{x}_i - \boldsymbol{\mu}_k) + \tau_{i,k}\log(\pi_k/\tau_{i,k}) \Big\} - \lambda_k ||\boldsymbol{\Omega}_k||_{1,1} \Bigg).
\end{aligned}
$$

The opposite minimization problem regarding each $\boldsymbol{\Omega}_k$ is

$$
\boldsymbol{\Omega}_k \in \arg\min_{\boldsymbol{\Omega} \succeq 0} \Big\{ -\frac{n\pi_k}{2}\log|\boldsymbol{\Omega}| + \frac{1}{2}\sum_{i=1}^{n} \tau_{i,k}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Omega} (\boldsymbol{x}_i - \boldsymbol{\mu}_k) + \lambda_k ||\boldsymbol{\Omega}||_{1,1} \Big\} \tag{1.45}
$$

Using the well-known commutativity property of the trace operator and dividing by $n\pi_k$

$$
\boldsymbol{\Omega}_k \in \arg\min_{\boldsymbol{\Omega} \succeq 0} \Big\{ -\frac{1}{2}\log|\boldsymbol{\Omega}| + \frac{1}{2} tr(\boldsymbol{\Sigma}_{n,k}\boldsymbol{\Omega}) + \frac{\lambda_k}{n\pi_k} ||\boldsymbol{\Omega}||_{1,1} \Big\} \tag{1.46}
$$

Our algorithm solves a graphical lasso problem within each cluster. We use a block coordinate ascent algorithm [Mazumder, 2012] to solve this convex problem as in the graphical lasso implementation in R, see `http://statweb.stanford.edu/~tibs/glasso/` The alternating maximization procedure is summarized in the following algorithm

1.6 Estimating the number of clusters

In this chapter, we will focus on the open problem of estimating the number of clusters. Most of current clustering methods such that K-Means, Expectation-Maximisation with Gaussian mixture model or hierarchical clustering need a this parameter in input. Different methods are being used to

Input: data vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$ and the number of clusters K

Output: parameter estimate $\widehat{\boldsymbol{\theta}} = \{\widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\Omega}}_k, \widehat{\pi}_k\}_{k\in[K]}$

1: `Initialize` $t = 0$, $\boldsymbol{\theta} = \boldsymbol{\theta}^0$.

2: **Repeat**

3: `Update the parameter` $\boldsymbol{\mathcal{T}}$:

$$\tau_{i,k}^t = \frac{\pi_k^t \varphi_{\boldsymbol{\mu}_k^t, \boldsymbol{\Omega}_k^t}(\boldsymbol{x}_i)}{\sum_{k'\in[K]} \pi_{k'}^t \varphi_{\boldsymbol{\mu}_{k'}^t, \boldsymbol{\Omega}_{k'}^t}(\boldsymbol{x}_i)}.$$

4: `Update the parameter` $\boldsymbol{\theta}$:

$$\pi_k^{t+1} = \frac{1}{n}\sum_{i=1}^n \tau_{i,k}^t,$$

$$\boldsymbol{\mu}_k^{t+1} = \frac{1}{n\pi_k^{t+1}}\sum_{i=1}^n \tau_{i,k}^t \boldsymbol{x}_i$$

$$\boldsymbol{\Sigma}_{n,k} = \frac{1}{n^2\pi_k^{t+1}}\sum_{i=1}^n \tau_{i,k}^{t+1}(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k^{t+1})(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k^{t+1})^\top$$

$$\boldsymbol{\Omega}_k^{t+1} \in \arg\min_{\boldsymbol{\Omega}\succeq 0}\Big\{ -\frac{1}{2}\log|\boldsymbol{\Omega}| + \frac{1}{2}tr(\boldsymbol{\Sigma}_{N,k}\boldsymbol{\Omega}) + \frac{\lambda_k}{n\pi_k^{t+1}}||\boldsymbol{\Omega}||_{1,1}\Big\}$$

5: `increment` t: $t = t + 1$.

6: **Until** `stopping rule.`

7: **Return** $\boldsymbol{\theta}^t$.

Figure 1.5: Graphical lasso algorithm for Gaussian mixtures

perform a selection of the best model according to a criterion, unfortunately with a computational cost. In this work, we will try to tackle this challenge.

1.6.1 Introduction and related work

In previous models, we knew the number of components K in the Gaussian mixture. In reality this parameter is unknown. Several methods exists to select the number of clusters

1.6.2 Bayesian Information Criterion (BIC)

A common method to select the number of clusters is to use the Bayesian Information Criterion given by:

$$BIC(K) = -\log \ell_n(\widehat{\boldsymbol{\theta}}^K) + K.\log(n) \tag{1.47}$$

And select the model which minimizes the BIC. This can be done by running EM algorithm over a large number of models which is computationally expensive.

1.6.3 Silhouette method

Elbow method

Gap Statistic

1.6.4 Our First method

The idea is to add a regularization term on the estimation of the $n \times K$ matrix $\boldsymbol{\mathcal{T}}$, the estimate of the number of clusters K will be the number of non-empty columns of $\boldsymbol{\mathcal{T}}$.

We consider a maximum number of clusters M, we note the convex set $A = \{\tau \in \mathbb{R}^M : \sum_{k=1}^{M} \tau_k = 1, \tau_k \geq 0 \quad \forall k \in [M]\}$ and the "indicator" function $\chi_A(.)$ defined by:

$$\chi_A(x) = \begin{cases} 0 & \text{if } x \in A, \\ \infty & \text{if } x = 0 \end{cases}$$

We note $\boldsymbol{\mathcal{T}}_{.,k}$ the k^{th} column and $\boldsymbol{\mathcal{T}}_{i,.}$ the i^{th} line of $\boldsymbol{\mathcal{T}}$. We will estimate $\boldsymbol{\mathcal{T}}$ using the same equation 1.40, 1.41 with a regularization term:

$$\begin{aligned} F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) = &\sum_{k=1}^{K} \left(\sum_{i=1}^{n} \left\{ \tau_{i,k} \log \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Omega}_k}(\boldsymbol{x}_i) + \tau_{i,k} \log(\pi_k / \tau_{i,k}) \right\} - \lambda_k ||\boldsymbol{\Omega}_k||_{1,1} \right) \\ &+ \sum_{k=1}^{K} ||\boldsymbol{\mathcal{T}}_{.,k}||_2 + \sum_{i=1}^{n} \chi_A(\boldsymbol{\mathcal{T}}_{i,.}) \end{aligned}$$

Removing the penalization on $\boldsymbol{\Omega}$:

$$\begin{aligned} F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) = &\sum_{k=1}^{K} \left(\sum_{i=1}^{n} \left\{ \tau_{i,k} \log \varphi_{\boldsymbol{\mu}_k, \boldsymbol{\Omega}_k}(\boldsymbol{x}_i) + \tau_{i,k} \log(\pi_k / \tau_{i,k}) \right\} \right. \\ &+ \sum_{k=1}^{K} ||\boldsymbol{\mathcal{T}}_{.,k}||_2 + \sum_{i=1}^{n} \chi_A(\boldsymbol{\mathcal{T}}_{i,.}) \end{aligned}$$

and the optimization problem:

$$\widehat{\boldsymbol{\mathcal{T}}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{\mathcal{T}}} F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}}) \tag{1.48}$$

Unfortunately, the regularization term prevents to derive explicit solution as in previous chapters. Furthermore, we cant separate the objective function since we optimize along columns and lines of $\boldsymbol{\mathcal{T}}$. The objective function $F^{pen}(\boldsymbol{\theta}, \boldsymbol{\mathcal{T}})$ rewritten $F^{pen}_{\boldsymbol{\theta}}(\boldsymbol{\mathcal{T}})$ can be split into two terms:

$$F^{pen}_{\boldsymbol{\theta}}(\boldsymbol{\mathcal{T}}) = f(\boldsymbol{\mathcal{T}}) + g(\boldsymbol{\mathcal{T}}) \tag{1.49}$$

with:

$$f(\boldsymbol{\mathcal{T}}) = \sum_{k=1}^{K}\left(\sum_{i=1}^{n}\left\{\tau_{i,k}\log\varphi_{\boldsymbol{\mu}_k,\boldsymbol{\Omega}_k}(\boldsymbol{x}_i) + \tau_{i,k}\log(\pi_k/\tau_{i,k})\right\} + \sum_{k=1}^{K}||\boldsymbol{\mathcal{T}}_{.,k}||_2\right.$$
$$g(\boldsymbol{\mathcal{T}}) = \sum_{i=1}^{n}\chi_A(\boldsymbol{\mathcal{T}}_{i,.})$$

f is convex and differentiable on its domain, g is also convex but not smooth. We will tackle this problem by using a proximal method:

$$\begin{aligned}\boldsymbol{\mathcal{T}}^{k+1} =& \mathbf{prox}_{\lambda g}(\boldsymbol{\mathcal{T}}^k - \lambda\nabla f(\boldsymbol{\mathcal{T}}^k)) \ = \qquad P_A(\boldsymbol{\mathcal{T}}^k - \lambda\nabla f(\boldsymbol{\mathcal{T}}^k))\\ =& \underset{\boldsymbol{\mathcal{T}}:\forall K, \boldsymbol{\mathcal{T}}^k\in A}{\arg\min}\left(||\boldsymbol{\mathcal{T}} - (\boldsymbol{\mathcal{T}}^k - \lambda\nabla f(\boldsymbol{\mathcal{T}}^k))||_2^2\right)\end{aligned}$$

The gradient of f on $\boldsymbol{\mathcal{T}}$ is given by:

$$\begin{aligned}\Big[\nabla_{\boldsymbol{\mathcal{T}}} f(\boldsymbol{\mathcal{T}})\Big]_{i,j} =& \left[\frac{\partial f}{\partial \boldsymbol{\mathcal{T}}_{ij}}(\boldsymbol{\mathcal{T}})\right]_{i,j}\\ =& \log(\varphi_{\boldsymbol{\mu}_j,\boldsymbol{\Omega}_j}(x_i)) + \log(\frac{\pi_j}{\tau_{i,j}}) + \frac{\tau_{i,j}}{||\boldsymbol{\mathcal{T}}_{.,j}||_2} - 1\end{aligned}$$

We will use FISTA to accelerate the convergence

We use the algorithm of last chapter with the new estimation procedure of $\boldsymbol{\mathcal{T}}$

1.6.5 Sparse Weights Vector Estimation

We fit a model with an arbitrarily large number of components K and penalyze the weights vector $\boldsymbol{\pi}$. The penalized negative log-likelihood is:

$$\ell_n(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\log\left\{\sum_{j=1}^{K}\pi_k\varphi_{(\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)}(\boldsymbol{x}_i)\right\} + \lambda\sum_{j=1}^{K-1}\pi_j^{1/\gamma} \quad \gamma\geq 1 \qquad (1.50)$$

Input:

Output: parameter estimate $\boldsymbol{\mathcal{T}}$

1: `Initialize` $t_1 = 1$ `and` $\boldsymbol{\xi}^0$ `with`

$$\xi^0_{i,k} = \frac{\pi^0_k \varphi_{\boldsymbol{\mu}^0_k, \boldsymbol{\Omega}^0_k}(\boldsymbol{x}_i)}{\sum_{k' \in [K]} \pi^0_{k'} \varphi_{\boldsymbol{\mu}^0_{k'}, \boldsymbol{\Omega}^0_{k'}}(\boldsymbol{x}_i)}$$

2: **Repeat**

$$\boldsymbol{\mathcal{T}}^k = \underset{\boldsymbol{\mathcal{T}}: \forall K, \boldsymbol{\mathcal{T}}^k \in A}{\arg\min} \left(||\boldsymbol{\mathcal{T}} - (\boldsymbol{\xi}^k - \lambda \nabla f(\boldsymbol{\xi}^k))||_2^2 \right)$$

$$t^{k+1} = \frac{1 + \sqrt{1 + 4 * (t^k)^2}}{2}$$

$$\boldsymbol{\xi}^{k+1} = \boldsymbol{\mathcal{T}}^k + \left(\frac{t^k - 1}{t^{k+1}} \right) (\boldsymbol{\mathcal{T}}^k - \boldsymbol{\mathcal{T}}^{k-1})$$

Figure 1.6: $\boldsymbol{\mathcal{T}}$ estimation with FISTA

Such that:

$$\sum_j^{K-1} \pi_j \leq 1 \quad \text{and} \quad \pi_K = 1 - \sum_j^{K-1} \pi_j \tag{1.51}$$

and $\sum_j^{K-1} \pi_j^{1/\gamma}$ is not convex, to rectify it let note $\alpha_j = \pi^{1/\gamma}$, then:

$$\widehat{\boldsymbol{\alpha}} \in \underset{\boldsymbol{\alpha} \in \mathbb{R}^{K-1}}{\arg\min} \left\{ -\frac{1}{n} \sum_{i=1}^n \log \left\{ \sum_{j=1}^K \alpha_j^\gamma \varphi_{(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}(\boldsymbol{x}_i) \right\} + \lambda \sum_{j=1}^{K-1} \alpha_j \right\} \quad \gamma \geq 1, \tag{1.52}$$

such that: $\sum_j^{K-1} \alpha_j^\gamma \leq 1$ and $\alpha_K^\gamma = 1 - \sum_j^{K-1} \alpha_j^\gamma$. We denote $f_{\boldsymbol{\theta}}(\boldsymbol{\alpha})$ this cost function.

If we note A the $K-1$ dimensional unit sphere and χ_A the indicator function of A (0 in A, ∞ elsewhere), the minimization problem can be rewritten as

$$\widehat{\boldsymbol{\alpha}} \in \underset{\boldsymbol{\alpha} \in \mathbb{R}^{K-1}}{\arg\min} \{ f_{\boldsymbol{\theta}}(\boldsymbol{\alpha}) + \chi_A(\boldsymbol{\alpha}) \}. \tag{1.53}$$

Input: data vectors $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n \in \mathbb{R}^p$ and the number of clusters K

Output: parameter estimate $\widehat{\boldsymbol{\theta}} = \{\widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\Omega}}_k, \widehat{\pi}_k\}_{k\in[K]}$

1: `Initialize` $t = 0$, $\boldsymbol{\theta} = \boldsymbol{\theta}^0$.

2: **Repeat**

3: `Update the parameter` $\boldsymbol{\mathcal{T}}$ `with previous algorithm`

4: `Update the parameter` $\boldsymbol{\theta}$:

$$\pi_k^{t+1} = \frac{1}{n}\sum_{i=1}^{n} \tau_{i,k}^{t},$$

$$\boldsymbol{\mu}_k^{t+1} = \frac{1}{n\pi_k^{t+1}}\sum_{i=1}^{n} \tau_{i,k}^{t}\boldsymbol{x}_i$$

$$\boldsymbol{\Sigma}_{n,k} = \frac{1}{n^2\pi_k^{t+1}}\sum_{i=1}^{n} \tau_{i,k}^{t+1}(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k^{t+1})(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k^{t+1})^\top$$

$$\boldsymbol{\Omega}_k^{t+1} \in \arg\min_{\boldsymbol{\Omega}\succeq 0}\Big\{ -\frac{1}{2}\log|\boldsymbol{\Omega}| + \frac{1}{2}tr(\boldsymbol{\Sigma}_{N,k}\boldsymbol{\Omega}) + \frac{\lambda_k}{n\pi_k^{t+1}}||\boldsymbol{\Omega}||_{1,1}\Big\}$$

5: `increment` t: $t = t + 1$.

6: **Until** `stopping rule.`

7: **Return** $\boldsymbol{\theta}^t$.

Figure 1.7: Graphical lasso algorithm for Gaussian mixtures with cluster number discovery

To solve this minimization problem, we can use a proximal gradient method and Nesterov acceleration for the following iterative procedure:

$$\widehat{\alpha}^{t+1} = \operatorname{prox}_{\chi_A}(\boldsymbol{\alpha}^t - h\nabla f_{\boldsymbol{\theta}}(\boldsymbol{\alpha}^t)) \tag{1.54}$$

$$= \arg\min_{x\in\mathbb{R}^{K-1}} \left\{\chi_A(x) + \frac{1}{2}||x - (\boldsymbol{\alpha}^t - h\nabla f_{\boldsymbol{\theta}}(\boldsymbol{\alpha}^t))||^2\right\} \tag{1.55}$$

$$= P_A(\boldsymbol{\alpha}^t - h\nabla f_{\boldsymbol{\theta}}(\boldsymbol{\alpha}^t)). \tag{1.56}$$

This iteration procedure gives us the following algorithm

Input: $\boldsymbol{\theta}$

Output: parameter estimate $\widehat{\boldsymbol{\pi}} = (\boldsymbol{\alpha}_1^\gamma, ..., \boldsymbol{\alpha}_{K-1}^\gamma, 1 - \sum_{j=1}^{K-1} \boldsymbol{\alpha}_j^\gamma)^t$

1: `Initialize` $t = 0$, $s_0 = 1$ `and` $\boldsymbol{\xi}^0 = (\boldsymbol{\pi}_1^{1/\gamma}, ..., \boldsymbol{\pi}_{K-1}^{1/\gamma})$

2: **Repeat**

3:

$$\boldsymbol{\alpha}^t = P_A(\xi^t - h\nabla f_{\boldsymbol{\theta}}(\xi^t)) \tag{1.57}$$

$$s_{t+1} = \frac{1 + \sqrt{1 + 4 * s_t^2}}{2} \tag{1.58}$$

$$\boldsymbol{\xi}^{t+1} = \boldsymbol{\alpha}^t + \left(\frac{s_t - 1}{s_{t+1}}\right)(\boldsymbol{\alpha}^t - \boldsymbol{\alpha}^{t-1}) \tag{1.59}$$

5: `increment` t: $t = t + 1$.

6: **Until** `stopping rule.`

Figure 1.8: Estimation of α

and the final algorithm for estimating the gaussian mixture with a penalized weight vector is

Input: data vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$ and a large number of clusters K

Output: parameter estimate $\widehat{\boldsymbol{\theta}} = \{\widehat{\boldsymbol{\mu}}_k, \widehat{\boldsymbol{\Sigma}}_k, \widehat{\pi}_k\}_{k\in[K]}$ Initialize $t = 0$, $\boldsymbol{\theta} = \boldsymbol{\theta}^0$

1: `Initialize` $t = 0$, $\boldsymbol{\theta} = \boldsymbol{\theta}^0$

2: **Repeat**

3: `Update the parameter` $\boldsymbol{\mathcal{T}}$

$$\tau_{i,k}^t = \frac{\pi_k^t \varphi_{\boldsymbol{\mu}_k^t, \boldsymbol{\Omega}_k^t}(\boldsymbol{x}_i)}{\sum_{k'\in[K]} \pi_{k'}^t \varphi_{\boldsymbol{\mu}_{k'}^t, \boldsymbol{\Omega}_{k'}^t}(\boldsymbol{x}_i)}. \tag{1.60}$$

4: `Update parameters` $\boldsymbol{\mu}, \boldsymbol{\Sigma}$.

$$\boldsymbol{\mu}_k^{t+1} = \frac{1}{n\pi_k^{t+1}} \sum_{i=1}^n \tau_{i,k}^t \boldsymbol{x}_i, \tag{1.61}$$

$$\boldsymbol{\Sigma}_k^{t+1} = \frac{1}{n\pi_k^{t+1}} \sum_{i=1}^n \tau_{i,k}^t (\boldsymbol{x}_i - \boldsymbol{\mu}_k^{t+1})(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{t+1})^\top. \tag{1.62}$$

5: `Update the parameter` π `with previous algorithm`

6: `increment` t: $t = t + 1$

7: **Until** `stopping rule.`

Figure 1.9: Algorithm for estimating sparse weights vector on GMM

Ci-dessous, les résultats de l'algorithme d'estimation parcimonieuse des poids du mélange sur des données simulées. En vert notre algorithme et en rouge la méthode EM+BIC. En abscisse le nombre de vrais clusters, K. En ordonnée, le logarithme de l'erreur $\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1$. Pour chaque K, 50 simulations ont été effectuées. Nous représentons les premiers et troisièmes quartiles ainsi que la médiane.

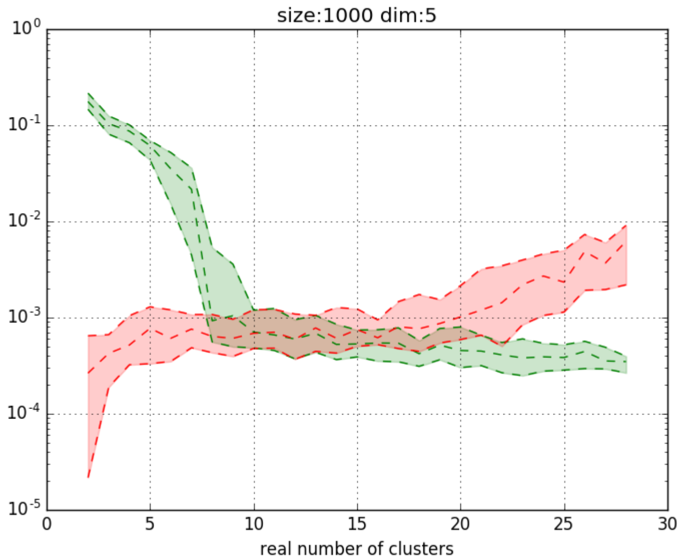


Figure 1.10: Vert: Notre algorithme. Rouge: EM+BIC

1.7 structural analysis on Σ approach

We consider a multivariate Gaussian distribution with mean $\boldsymbol{\mu}^*$ and covariance $\boldsymbol{\Sigma}^*$ and $Y_1, \ldots, Y_N \in \mathbb{R}^p$ iid drawn from this distribution. We would like to estimate $\boldsymbol{\mu}^*$ and $\boldsymbol{\Sigma}^*$. We know that $\widehat{\boldsymbol{\mu}}_n = \bar{Y}_n$, then wlog we consider $\mu^* = 0$, the problem is to estimate $\boldsymbol{\Sigma}^*$. We will study the precision matrix and consider that Σ^{-1} is sparse. We note $\Sigma^{-1} = \Omega$, Y_n the n-th random variable and Y_n^i the i-th component of this vector. If $\Sigma_{ij}^{-1} = 0 \Rightarrow Y^i \perp\!\!\!\perp Y^j$ conditionally to $Y^{l \neq \{i,j\}}$. Thus, it makes sense to impose a L_1 penalty on Σ^{-1} to increase its sparsity.

1.7.1 Graphical Lasso

Let consider a multivariate normal distribution with parameters μ^*, Σ^* with density;

$$\mathcal{N}(x|\mu^*, \Sigma^*) = \frac{1}{(2\pi)^{d/2}|\Sigma^*|^{1/2}} \exp^{-\frac{1}{2}(x-\mu^*)^T\Sigma^{-1*}(x-\mu^*)} \tag{1.63}$$

We consider $\mu = 0$. Given N datapoints $X_1, \ldots, X_N$ and $X_i \in \mathbb{R}^d$, the log-likelihood is given by:

$$\begin{aligned} \mathcal{L}(\Sigma) &= \log\left(\prod_{n=1}^{N} \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp^{-\frac{1}{2}(x_n)^T\Sigma^{-1}(x_n)}\right) \\ &= -\frac{dN}{2}\log 2\pi - \frac{N}{2}\sum_{n=1}^{N}\log|\Sigma^*| - \frac{1}{2}\sum_{n=1}^{N} x_n^T\Sigma^{*,-1}x_n \end{aligned} \tag{1.64}$$

Note that $x_n^T\Sigma^{*,-1}x_n = tr(x_n^T\Sigma^{*,-1}x_n)$, and therefore:

$$\sum_{n=1}^{N} x_n^T\Sigma^{*,-1}x_n = tr\big(\sum_{n=1}^{N} x_n^T\Sigma^{*,-1}x_n\big) = tr\Big(\big[\sum_{n=1}^{N} x_n^T x_n\big]\Sigma^{*,-1}\Big) = tr(S_N\Sigma^*) \tag{1.65}$$

Where S_N is the empirical covariance matrix. We can replace that in the log-likelihood expression:

$$\mathcal{L}(\Sigma) = -\frac{dN}{2}\log 2\pi - \frac{N}{2}\sum_{n=1}^{N}\log|\Sigma^*| - \frac{1}{2}tr(S_N\Sigma^*) \tag{1.66}$$

Finally:

$$\mathcal{L}(\Sigma) = C + \frac{N}{2}\log|\Sigma^{-1}| - \frac{1}{2}tr(S_n\Sigma^{-1}) \tag{1.67}$$

Where C is a constant (dependent on N). Thus, considering the sparsity of the precision matrix $\Omega = \Sigma^{-1}$, we impose a penalization to the maximum likelihood estimator of Ω

$$\widehat{\Omega} \in argmin\big\{\log|\Omega| - tr(S_N\Omega) - \lambda||\Omega||_1\big\} \tag{1.68}$$

A reason to use the L_1 penalization instead of the ridge is that for an L_p penalization, the problem is convex for $p \geq 1$ and we have parsimonious property for $p \leq 1$. This is a convex optimization problem, however the complexity is $O(p^3)$ (Source, high dim & var select Buhlmann 2006 ? Wassermann)

1.7.2 Column-Wise Lasso

We consider a gaussian vector $Y \in \mathbb{R}^d$, $Y \sim \mathcal{N}(0, \Sigma)$. We can write $Y = (Y^1, Y^{2:d})$. With this decomposition we can write the covariance matrix as following:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \Sigma_{12} \, \Sigma_{12}^T & \Sigma_{22} \end{pmatrix} \tag{1.69}$$

and according to theorem[?]: If Σ_{22} is inversible, then:

$$\begin{aligned} \mathbf{E}[Y^1|Y^{2:d}] &= \Sigma_{12}\Sigma_{22}^{-1}Y^{2:d} \\ Var[Y^1|Y^{2:d}] &= \sigma_1^2 - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^T \end{aligned} \tag{1.70}$$

We have the following identity:

$$\begin{pmatrix} \omega_{11} & \Omega_{12} \, \Omega_{12}^T & \Omega_{22} \end{pmatrix} \begin{pmatrix} \sigma_1^2 & \Sigma_{12} \, \Sigma_{12}^T & \Sigma_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \, 0 & I_{p-1} \end{pmatrix} \tag{1.71}$$

Which gives the following equations:

$$\begin{cases} \omega_{11}\sigma_1^2 + \Omega_{12}\Sigma_{12}^T & = 1 \qquad (*) \\ \omega_{11}\Sigma_{12} + \Omega_{12}\Sigma_{22} & = 0 \qquad (**) \\ \Omega_{12}^T\Sigma_{12} + \Omega_{22}\Sigma_{22} & = I_{p-1} \quad (***) \end{cases} \tag{1.72}$$

With (**) we have $-\omega_{11}\Sigma_{12}\Sigma_{22}^{-1} = \Omega_{12}$ and injected to (*) we have:

$$\begin{cases} \mathbf{E}[Y^1|Y^{2:d}] & = -\frac{1}{\omega_{11}}\Omega_{12}Y^{2:d} \\ Var[Y^1|Y^{2:d}] & = \frac{1}{\omega_{11}} \end{cases} \tag{1.73}$$

Finally, $Y^1 - \mathbf{E}[Y^1|Y^{2:d}]$ is a gaussian vector of $\mathbb{R}^{d-1}$, centered, independent of $Y^{2:d}$ and of covariance matrix $\sigma_1^2 - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^T$. If we denote $\xi^1 \sim \mathcal{N}(0, 1)$ we have $Y^1 - \mathbf{E}[Y^1|Y^{2:d}] = \frac{1}{\sqrt{\omega_{11}}}\xi^1$.

Therefore, for $Y_1, \dots, Y_n$ iid of law $\mathcal{N}(0, \Sigma^*)$ we have:

$$\begin{aligned} Y_i^1 &= -\tfrac{1}{\omega_{11}^*}\Omega_{12}Y_i^{2:d} + \tfrac{1}{\sqrt{\omega_{11}^*}}\xi_i^1 \\ &= -\textstyle\sum_{j=2}^d \tfrac{w_{ij}^*}{\omega_{11}^*}Y_i^j + \tfrac{1}{\sqrt{\omega_{11}^*}}\xi_i^1 \end{aligned} \tag{1.74}$$

and

$$\beta_1^{*T} Y_i = \frac{1}{\sqrt{\omega_{11}^*}}\xi_i^1 \Rightarrow \beta_1^{*T}\boldsymbol{Y} = \frac{1}{\sqrt{\omega_{11}^*}}\boldsymbol{\xi}^1 \tag{1.75}$$

with

$$\beta_1^* = \frac{1}{\sqrt{\omega_{11}^*}}\left[w_{11}^* \; w_{12} \vdots w_{1d}\right] \in \mathbb{R}^d \quad \text{and} \quad \boldsymbol{Y} = \left[verifier\ \right] \tag{1.76}$$

1.8 Overview

Chapter 2

Optimal KL-Aggregation in Density Estimation

Contents

We study the maximum likelihood estimator of density of n independent observations, under the assumption that it is well approximated by a mixture with a large number of components. The main focus is on statistical properties with respect to the Kullback-Leibler loss. We establish risk bounds taking the form of sharp oracle inequalities both in deviation and in expectation. A simple consequence of these bounds is that the maximum likelihood estimator attains the optimal rate $((\log K)/n)^{1/2}$, up to a possible logarithmic correction, in the problem of convex aggregation when the number K of components is larger than $n^{1/2}$. More importantly, under the additional assumption that the Gram matrix of the components satisfies the compatibility condition, the obtained oracle inequalities yield the optimal rate in the sparsity scenario. That is, if the weight vector is (nearly) D-sparse, we get the rate $(D \log K)/n$. As a natural complement to our oracle inequalities, we introduce the notion of nearly-D-sparse aggregation and establish matching lower bounds for this type of aggregation.

2.1 Introduction

Assume that we observe n independent random vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n \in \mathcal{X}$ drawn from a probability distribution P^* that admits a density function f^* with respect to some reference measure ν. The goal is to estimate the unknown density by a mixture density. More precisely, we assume that for a given family of mixture components $f_1, \ldots, f_K$, the unknown density of the observations f^* is well approximated by a convex combination $f_{\boldsymbol{\pi}}$ of these components, where

$$f_{\boldsymbol{\pi}}(\boldsymbol{x}) = \sum_{j=1}^{K} \pi_j f_j(\boldsymbol{x}), \quad \boldsymbol{\pi} \in \mathbb{B}_+^K = \Big\{\boldsymbol{\pi} \in [0,1]^K : \sum_{j=1}^{K} \pi_j = 1\Big\}. \tag{2.1}$$

The assumption that the component densities $\mathcal{F} = \{f_j : j \in [K]\}$ are known essentially means that they are chosen from a dictionary obtained on the basis of previous experiments or expert knowledge.

We focus on the problem of estimation of the density function $f_{\boldsymbol{\pi}}$ and the weight vector $\boldsymbol{\pi}$ from the simplex $\mathbb{B}_+^K$ under the sparsity scenario: the ambient dimension K can be large, possibly larger than the sample size n, but most entries of $\boldsymbol{\pi}$ are either equal to zero or very small.

Our goal is to investigate the statistical properties of the Maximum Likelihood Estimator (MLE), defined by

$$\widehat{\boldsymbol{\pi}} \in \arg\min_{\boldsymbol{\pi}\in\Pi} \Big\{ -\frac{1}{n}\sum_{i=1}^{n} \log f_{\boldsymbol{\pi}}(\boldsymbol{X}_i) \Big\}, \tag{2.2}$$

where the minimum is computed over a suitably chosen subset Π of $\mathbb{B}_+^K$. In the present work, we will consider sets $\Pi = \Pi_n(\mu)$, depending on a parameter $\mu > 0$ and the sample $\{\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n\}$, defined by

$$\Pi_n(\mu) = \Big\{ \boldsymbol{\pi} \in \mathbb{B}_+^K : \min_{i\in[n]} \sum_{j=1}^{K} \pi_j f_j(\boldsymbol{X}_i) \geq \mu \Big\}. \tag{2.3}$$

Note that the objective function in (2.2) is convex and the same is true for set (2.3). Therefore, the MLE $\widehat{\boldsymbol{\pi}}$ can be efficiently computed even for large K by solving a problem of convex programming. To ease notation, very often, we will omit the dependence of $\Pi_n(\mu)$ on μ and write Π_n instead of $\Pi_n(\mu)$.

The quality of an estimator $\widehat{\boldsymbol{\pi}}$ can be measured in various ways. For instance, one can consider the Kullback-Leibler divergence

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) = \begin{cases} \int_{\mathcal{X}} f^*(\boldsymbol{x}) \, \log \frac{f^*(\boldsymbol{x})}{f_{\widehat{\boldsymbol{\pi}}}(\boldsymbol{x})} \, \nu(d\boldsymbol{x}), & \text{if } P^*\big(f^*(\boldsymbol{X})/f_{\widehat{\boldsymbol{\pi}}}(\boldsymbol{X}) = 0\big) = 0, \\ +\infty, & \text{otherwise,} \end{cases} \tag{2.4}$$

which has the advantage of bypassing identifiability issues. One can also consider the (well-specified) setting where $f^* = f_{\boldsymbol{\beta}^*}$ for some $\boldsymbol{\beta}^* \in \mathbb{B}_+^K$ and measure the quality of estimation through a distance between the vectors $\widehat{\boldsymbol{\pi}}$ and $\boldsymbol{\pi}^*$ (such as the ℓ_1-norm $\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1$ or the Euclidean norm $\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_2$).

The main contributions of the present work are the following:

(a) We demonstrate that in the mixture model there is no need to introduce sparsity favoring penalty in order to get optimal rates of estimation under the Kullback-Leibler loss in the sparsity scenario. In fact, the constraint that the weight vector belongs to the simplex acts as a sparsity inducing penalty. As a consequence, there is no need to tune a parameter accounting for the magnitude of the penalty.

(b) We show that the maximum likelihood estimator of the mixture density simultaneously attains the optimal rate of aggregation for the Kullback-Leibler loss for at least three types of aggregation: model-selection, convex and D-sparse aggregation.

(c) We introduce a new type of aggregation, termed *nearly D-sparse aggregation* that extends and unifies the notions of convex and D-sparse aggregation. We establish strong lower bounds for the nearly D-sparse aggregation and demonstrate that the maximum likelihood estimator attains this lower bound up to logarithmic factors.

2.1.1 Related work

The results developed in the present work aim to gain a better understanding (a) of the statistical properties of the maximum likelihood estimator over a high-dimensional simplex and (b) of the problem of aggregation of density estimators under the Kullback-Leibler loss. Various procedures of aggregation[1] for density estimation have been studied in the literature with respect to different loss functions. [Catoni, 1997, Yang, 2000, Juditsky et al., 2008] investigated different variants of the progressive mixture rules, also known as mirror averaging [Yuditskiĭ et al., 2005, Dalalyan and Tsybakov, 2012], with respect to the Kullback-Leibler loss and established model selection type oracle inequalities[2] in expectation. Same type of guarantees, but holding with

[1] We refer the interested reader to [Tsybakov, 2014] for an up to date introduction into aggregation of statistical procedures.

[2] This means that they prove that the expected loss of the aggregate is almost as small as the loss of the best element of the dictionary $\{f_1, \ldots, f_K\}$.

high probability, were recently obtained in [Bellec, 2014, Butucea et al., 2016] for the procedure termed Q-aggregation, introduced in other contexts by [Dai et al., 2012, Rigollet, 2012].

Aggregation of estimators of a probability density function under the L_2-loss was considered in [Rigollet and Tsybakov, 2007], where it was shown that a suitably chosen unbiased risk estimate minimizer is optimal both for convex and linear aggregation. The goal in the present work is to go beyond the settings of the aforementioned papers in that we want simultaneously to do as well as the best element of the dictionary, the best convex combination of the dictionary elements but also the best sparse convex combination. Note that the latter task was coined D-aggregation in [Lounici, 2007] (see also [Bunea et al., 2007]). In the present work, we rename it in D-sparse aggregation, in order to make explicit its relation to sparsity.

Key differences between the latter work and ours are that we do not assume the sparsity index to be known and we are analyzing an aggregation strategy that is computationally tractable even for large K. This is also the case of [Bunea et al., 2010, Bertin et al., 2011], which are perhaps the most relevant references to the present work. These papers deal with the L_2-loss and investigate the lasso and the Dantzig estimators, respectively, suitably adapted to the problem of density estimation. Their methods handle dictionary elements $\{f_j\}$ which are not necessarily probability density functions, but has the drawback of requiring the choice of a tuning parameter. This choice is a nontrivial problem in practice. Instead, we show here that the optimal rates of sparse aggregation with respect to the Kullback-Leibler loss can be attained by procedure which is tuning parameter free.

Risk bounds for the maximum likelihood and other related estimators in the mixture model have a long history [Li and Barron, 1999, Li, 1999, Rakhlin et al., 2005]. For the sake of comparison we recall here two elegant results providing non-asymptotic guarantees for the Kullback-Leibler loss.

Theorem 2.1.1 (Theorem 5.1 in [Li, 1999]). *Let $\mathcal{F}$ be a finite dictionary of cardinality K of density functions such that $\max_{f\in\mathcal{F}} \|f^*/f\|_\infty \le V$. Then, the maximum likelihood estimator over $\mathcal{F}$, $\widehat{f}_{\mathcal{F}}^{\rm ML} \in \arg\max_{f\in\mathcal{F}} \sum_{i=1}^n \log f(\boldsymbol{X}_i)$, satisfies the inequality*

$$\mathbf{E}_{f^*}\big[\mathrm{KL}\big(f^*||\widehat{f}_{\mathcal{F}}^{\rm ML}\big)\big] \le \big(2+\log V\big)\bigg(\min_{f\in\mathcal{F}} \mathrm{KL}(f^*||f) + \frac{2\log K}{n}\bigg). \tag{2.5}$$

Inequality (2.5) is an inexact oracle inequality in expectation that quantifies the ability of $\widehat{f}_{\mathcal{F}}^{\rm ML}$ to solve the problem of model-selection aggregation. The adjective inexact refers to the fact that the "bias term" $\min_{f\in\mathcal{F}} \mathrm{KL}(f^*||f)$ is multiplied by factor strictly larger than one. It is noteworthy that the remainder term $\frac{2\log K}{n}$ corresponds to the optimal rate of model-selection aggregation [Juditsky and Nemirovski, 2000, Tsybakov, 2003]. In relation with Theorem 2.1.1, it is worth mentioning a result of [Yang, 2000] and [Catoni, 1997], see also Theorem 5 in [Lecué, 2006] and Corollary 5.4 in [Juditsky et al., 2008], establishing a risk bound similar to (2.5) without the extra factor $2+\log V$ for the so called mirror averaging aggregate.

Theorem 2.1.2 (page 226 in [Rakhlin et al., 2005]). *Let $\mathcal{F}$ be a finite dictionary of cardinality K of density functions and let $\mathcal{C}_k = \big\{f_{\boldsymbol{\pi}} : \|\boldsymbol{\pi}\|_0 \le k\big\}$ be the set of all the mixtures of at most k elements of $\mathcal{F}$ ($k \in [K]$). Assume that f^* and the densities f_k from $\mathcal{F}$ are bounded from below and above by some positive constants m and M, respectively. Then, there is a constant C depending only on m and M such that, for any tolerance level $\delta \in (0,1)$, the maximum likelihood estimator over $\mathcal{C}_k$, $\widehat{f}_{\mathcal{C}_k}^{\rm ML} \in \arg\max_{f\in\mathcal{C}_k} \sum_{i=1}^n \log f(\boldsymbol{X}_i)$, satisfies the inequality*

$$\mathrm{KL}\big(f^*||\widehat{f}_{\mathcal{C}_k}^{\rm ML}\big) \le \min_{f\in\mathcal{C}_k} \mathrm{KL}(f^*||f) + C\Big(\frac{\log(K/\delta)}{n}\Big)^{1/2} \tag{2.6}$$

with probability at least $1 - \delta$*.*

This result is remarkably elegant and can be seen as an exact oracle inequality in deviation for D-sparse aggregation (for $D = k$). Furthermore, if we choose $k = K$ in Theorem 2.1.2, then we get an exact oracle inequality for convex aggregation with a rate-optimal remainder term [Tsybakov, 2003]. However, it fails to provide the optimal rate for D-sparse aggregation.

Closing this section, we would like to mention the recent work [Xia and Koltchinskii, 2016], where oracle inequalities for estimators of low rank density matrices are obtained. They share a common feature with those obtained in this work: the adaptation to the unknown sparsity or rank is achieved without any additional penalty term. The constraint that the unknown parameter belongs to the simplex acts as a sparsity inducing penalty.

2.1.2 Additional notation

In what follows, for any $i \in [n]$, we denote by $\boldsymbol{Z}_i$ the K-dimensional vector $[f_1(\boldsymbol{X}_i), \ldots, f_K(\boldsymbol{X}_i)]^\top$ and by $\mathbf{Z}$ the $n \times K$ matrix $[\boldsymbol{Z}_1^\top, \ldots, \boldsymbol{Z}_n^\top]^\top$. We also define $\ell(u) = -\log u$, $u \in (0, +\infty)$, so that the MLE $\widehat{\boldsymbol{\pi}}$ is the minimizer of the function

$$L_n(\boldsymbol{\pi}) = \frac{1}{n}\sum_{i=1}^{n} \ell\big(\boldsymbol{Z}_i^\top \boldsymbol{\pi}\big). \tag{2.7}$$

For any set of indices $J \subseteq [K]$ and any $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K)^\top \in \mathbb{R}^K$, we define $\boldsymbol{\pi}_J$ as the K-dimensional vector whose j-th coordinate equals π_j if $j \in J$ and 0 otherwise. We denote the cardinality of any $J \subseteq [K]$ by $|J|$. For any set $J \subset \{1, \ldots, K\}$ and any constant $c \geq 0$, we introduce the compatibility constants [van de Geer and Bühlmann, 2009] of a $K \times K$ positive semidefinite matrix $\mathbf{A}$,

$$\kappa_{\mathbf{A}}(J,c) = \inf\left\{\frac{c^2|J|\|\mathbf{A}^{1/2}\boldsymbol{v}\|_2^2}{(c\|\boldsymbol{v}_J\|_1 - \|\boldsymbol{v}_{J^c}\|_1)^2} : \boldsymbol{v}\in\mathbb{R}^K, \|\boldsymbol{v}_{J^c}\| < c\|\boldsymbol{v}_J\|_1\right\}, \tag{2.8}$$

$$\bar{\kappa}_{\mathbf{A}}(J,c) = \inf\left\{\frac{|J|\|\mathbf{A}^{1/2}\boldsymbol{v}\|_2^2}{\|\boldsymbol{v}_J\|_1^2} : \boldsymbol{v}\in\mathbb{R}^K, \|\boldsymbol{v}_{J^c}\|_1 < c\|\boldsymbol{v}_J\|_1\right\}. \tag{2.9}$$

The risk bounds established in the present work involve the factors $\kappa_{\mathbf{A}}(J,3)$ and $\bar{\kappa}_{\mathbf{A}}(J,1)$. One can easily check that $\bar{\kappa}_{\mathbf{A}}(J,3) \le \kappa_{\mathbf{A}}(J,3) \le \frac{9}{4}\bar{\kappa}_{\mathbf{A}}(J,1)$. We also recall that the compatibility constants of a matrix $\mathbf{A}$ are bounded from below by the smallest eigenvalue of $\mathbf{A}$.

Let us fix a function $f_0 : \mathcal{X} \to \mathbb{R}$ and denote $\bar{f}_k = f_k - f_0$ and $\bar{\boldsymbol{Z}}_i = [\bar{f}_1(\boldsymbol{X}_i),\dots,\bar{f}_K(\boldsymbol{X}_i)]^\top$ for $i\in[n]$. In the results of this work, the compatibility factors are used for the empirical and population Gram matrices of vectors $\bar{\boldsymbol{Z}}_k$, that is when $\mathbf{A} = \widehat{\boldsymbol{\Sigma}}_n$ and $\mathbf{A} = \boldsymbol{\Sigma}$ with

$$\widehat{\boldsymbol{\Sigma}}_n = \frac{1}{n}\sum_{i=1}^n \bar{\boldsymbol{Z}}_i\bar{\boldsymbol{Z}}_i^\top, \qquad \boldsymbol{\Sigma} = \mathbf{E}[\bar{\boldsymbol{Z}}_1\bar{\boldsymbol{Z}}_1^\top]. \tag{2.10}$$

The general entries of these matrices are $(\widehat{\boldsymbol{\Sigma}}_n)_{k,l} = {}^1\!/\!_n\sum_{i=1}^n \bar{f}_k(\boldsymbol{X}_i)\bar{f}_l(\boldsymbol{X}_i)$ and $(\boldsymbol{\Sigma})_{k,l} = \mathbf{E}[\bar{f}_k(\boldsymbol{X}_1)\bar{f}_l(\boldsymbol{X}_1)]$, respectively. We assume that there exist positive constants m and M such that for all densities f_k with $k\in[K]$, we have

$$\forall x\in\mathcal{X}, \quad m \le f_k(x) \le M. \tag{2.11}$$

We use the notation $V = M/m$. It is worth mentioning that the set of dictionaries satisfying simultaneously this boundedness assumption and the aforementioned compatibility condition is not empty. For instance, one can consider the functions $f_k(x) = 1 + {}^1\!/\!_2\sin(2\pi kx)$ for $k\in[K]$. These functions are probability densities w.r.t. the Lebesgue measure on $\mathcal{X} = [0,1]$. They are bounded from below and from above by $1/2$ and $3/2$, respectively. Taking $f_0(x) = 1$, the corresponding Gram matrix is $\boldsymbol{\Sigma} = {}^1\!/\!_8\mathbf{I}_K$, which has all eigenvalues equal to $1/8$.

2.1.3 Agenda

The rest of the paper is organized as follows. In Section 2.2, we state our main theoretical contributions and discuss their consequences. Possible relaxations of the conditions, as well as lower bounds showing the tightness of the established risk bounds, are considered in Section 2.3. A brief summary of the paper and some future directions of research are presented in Section 2.4. The proofs of all theoretical results are postponed to Section 2.5 and Section 2.6.

2.2 Oracle inequalities in deviation and in expectation

In this work, we prove several non-asymptotic risk bounds that imply, in particular, that the maximum likelihood estimator is optimal in model-selection aggregation, convex aggregation and D-sparse aggregation (up to log-factors). In all the results of this section we assume the parameter μ in (2.3) to be equal to 0.

Theorem 2.2.1. *Let $\mathcal{F}$ be a set of $K \geq 4$ densities satisfying the boundedness condition (2.11). Denote by $f_{\widehat{\boldsymbol{\pi}}}$ the mixture density corresponding to the maximum likelihood estimator $\widehat{\boldsymbol{\pi}}$ over Π_n defined in (2.7). There are constants $c_1 \leq 32V^3$, $c_2 \leq 288M^2V^6$ and $c_3 \leq 128M^2V^6$ such that, for any*

$\delta \in (0, 1/2)$, *the following inequalities hold*

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{\substack{J\subset[K]\\ \boldsymbol{\pi}\in\mathbb{B}_+^K}} \bigg\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + c_1\Big(\frac{\log(K/\delta)}{n}\Big)^{1/2}\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{c_2|J|\log(K/\delta)}{n\kappa_{\widehat{\boldsymbol{\Sigma}}_n}(J,3)}\bigg\}, \tag{2.12}$$

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{J\subset[K]} \inf_{\substack{\boldsymbol{\pi}\in\mathbb{B}_+^K\\ \boldsymbol{\pi}_{J^c}=0}} \bigg\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{c_3|J|\log(K/\delta)}{n\bar{\kappa}_{\widehat{\boldsymbol{\Sigma}}_n}(J,1)}\bigg\} \tag{2.13}$$

with probability at least $1-\delta$.

The proof of this and the subsequent results stated in this section are postponed to Section 2.5. Comparing the two inequalities of the above theorem, one can notice two differences. First, the term proportional to $\|\boldsymbol{\pi}_{J^c}\|_1$ is absent in the second risk bound, which means that the risk of the MLE is compared to that of the best mixture with a weight sequences supported by J. Hence, this risk bound is weaker than the first one provided by (2.12). Second, the compatibility factor $\bar{\kappa}_{\widehat{\boldsymbol{\Sigma}}_n}(J,1)$ in (2.13) is larger that its counterpart $\kappa_{\widehat{\boldsymbol{\Sigma}}_n}(J,3)$ in (2.12). This entails that in the cases where the oracle is expected to be sparse, the remainder term of the bound in (2.12) is slightly looser than that of (2.13).

A first and simple consequence of Theorem 2.1.1 is obtained by taking $J=\varnothing$ in the right hand side of the first inequality. Then, $\|\boldsymbol{\pi}_{J^c}\|_1 = \|\boldsymbol{\pi}\|_1 = 1$ and we get

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{\boldsymbol{\pi}\in\mathbb{B}_+^K} \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + c_1\Big(\frac{\log(K/\delta)}{n}\Big)^{1/2}. \tag{2.14}$$

This implies that for every dictionary $\mathcal{F}$, without any assumption on the smallness of the coherence between its elements, the maximum likelihood estimator achieves the optimal rate of convex aggregation, up to a possible[3]

[3] In fact, the optimal rate of convex aggregation when $K \geq n^{1/2}$ is of order

logarithmic correction, in the high-dimensional regime $K \geq n^{1/2}$. In the case of regression with random design, an analogous result has been proved by Lecué and Mendelson [2013] and Lecué [2013]. One can also remark that the upper bound in (2.14) is of the same form as the one of Theorem 2.1.2 stated in section 2.1.1 above.

The main compelling feature of our results is that they show that the MLE adaptively achieves the optimal rate of aggregation not only in the case of convex aggregation, but also for the model-selection aggregation and D-(convex) aggregation. For handling these two cases, it is more convenient to get rid of the presence of the compatibility factor of the empirical Gram matrix $\widehat{\boldsymbol{\Sigma}}_n$. The latter can be replaced by the compatibility factor of the population Gram matrix, as stated in the next result.

Theorem 2.2.2. *Let $\mathcal{F}$ be a set of K densities satisfying the boundedness condition (2.11). Denote by $f_{\widehat{\boldsymbol{\pi}}}$ the mixture density corresponding to the maximum likelihood estimator $\widehat{\boldsymbol{\pi}}$ over Π_n defined in (2.7). There are constants $c_4 \leq 32V^3 + 4$, $c_5 \leq 4.5M^2(8\,V^3+1)^2$ and $c_6 \leq 2M^2(8\,V^3+1)^2$ such that, for any $\delta \in (0, 1/2)$, the following inequalities hold*

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{\substack{J\subset[K]\\ \boldsymbol{\pi}\in\mathbb{B}_+^K}} \bigg\{\mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + c_4\Big(\frac{\log(K/\delta)}{n}\Big)^{1/2}\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{c_5|J|\log(K/\delta)}{n\kappa_{\boldsymbol{\Sigma}}(J,3)}\bigg\}, \tag{2.15}$$

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{J\subset[K]} \inf_{\substack{\boldsymbol{\pi}\in\mathbb{B}_+^K\\ \boldsymbol{\pi}_{J^c}=0}} \bigg\{\mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{c_6|J|\log(K/\delta)}{n\bar{\kappa}_{\boldsymbol{\Sigma}}(J,1)}\bigg\} \tag{2.16}$$

with probability at least $1-2\delta$.

$\big(\log(K/n^{1/2})/n\big)^{1/2}$. Therefore, even the $\log K$ term is optimal whenever $K \geq Cn^{1/2+\alpha}$ for some $\alpha > 0$.

The main advantage of the upper bounds provided by Theorem 2.2.2 as compared with those of Theorem 2.2.1 is that the former is deterministic, whereas the latter involves the compatibility factor of the empirical Gram matrix which is random. The price to pay for getting rid of randomness in the risk bound is the increased values of the constants c_4, c_5 and c_6. Note, however, that this price is not too high, since obviously $1 \le M \le L$ and, therefore, $c_4 \le 1.25c_1$, $c_5 \le 1.56c_2$ and $c_6 \le 1.56c_3$. In addition, the absence of randomness in the risk bound allows us to integrate it and to convert the bound in deviation into a bound in expectation.

Theorem 2.2.3 (Bound in Expectation)**.** *Let $\mathcal{F}$ be a set of K densities satisfying the boundedness condition* (2.11)*. Denote by $f_{\widehat{\boldsymbol{\pi}}}$ the mixture density corresponding to the maximum likelihood estimator $\widehat{\boldsymbol{\pi}}$ over Π_n defined in* (2.7)*. There are constants $c_7 \le 20V^3 + 8$, $c_8 \le M^2(22V^3 + 3)^2$ and $c_9 \le M^2(15V^3 + 2)^2$ such that*

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \le \inf_{\substack{J\subset[K]\\ \boldsymbol{\pi}\in\mathbb{B}_+^K}} \left\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + c_7\Big(\frac{\log K}{n}\Big)^{1/2}\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{c_8|J|\log K}{n\kappa_{\boldsymbol{\Sigma}}(J,3)} \right\}, \tag{2.17}$$

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \le \inf_{J\subset[K]} \inf_{\substack{\boldsymbol{\pi}\in\mathbb{B}_+^K\\ \boldsymbol{\pi}_{J^c}=0}} \left\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{c_9|J|\log K}{n\bar{\kappa}_{\boldsymbol{\Sigma}}(J,1)} \right\}. \tag{2.18}$$

In inequality (2.18), upper bounding the infimum over all sets J by the infimum over the singletons, we get

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \le \inf_{j\in[K]} \left\{ \mathrm{KL}(f^*||f_j) + \frac{c_9\log K}{n\bar{\kappa}_{\boldsymbol{\Sigma}}(J,1)} \right\}. \tag{2.19}$$

This implies that the maximum likelihood estimator $f_{\widehat{\pi}}$ achieves the rate $\frac{\log K}{n}$ in model-selection type aggregation. This rate is known to be optimal in the model of regression [Rigollet, 2012]. If we compare this result with Theorem 2.1.1 stated in Section 2.1.1, we see that the remainder terms of these two oracle inequalities are of the same order (provided that the compatibility factor is bounded away from zero), but inequality (2.19) has the advantage of being exact.

We can also apply (2.18) to the problem of convex aggregation with small dictionary, that is for K smaller than $n^{1/2}$. Upper bounding $|J|$ by $|K|$, we get

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \leq \inf_{\boldsymbol{\pi}\in\mathbb{B}_+^K} \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{c_9 K\log K}{n\bar{\kappa}_{\boldsymbol{\Sigma}}([K],1)}. \tag{2.20}$$

Assuming, for instance, the smallest eigenvalue of $\boldsymbol{\Sigma}$ bounded away from zero (which is a quite reasonable assumption in the context of low dimensionality), the above upper bound provides a rate of convex aggregation of the order of $\frac{K\log K}{n}$. Up to a logarithmic term, this rate is known to be optimal for convex aggregation in the model of regression.

Finally, considering all the sets J of cardinal smaller than D (with $D \leq K$) and setting $\bar{\kappa}_{\boldsymbol{\Sigma}}(D,1) = \inf_{J:|J|\leq D} \bar{\kappa}_{\boldsymbol{\Sigma}}(J,1)$, we deduce from (2.18) that

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \leq \inf_{\boldsymbol{\pi}\in\mathbb{B}_+^K:\|\boldsymbol{\pi}\|_0\leq D} \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{c_9 D\log K}{n\bar{\kappa}_{\boldsymbol{\Sigma}}(D,1)}. \tag{2.21}$$

According to [Rigollet and Tsybakov, 2011, Theorem 5.3], in the regression model, the optimal rate of D-sparse aggregation is of order $(D/n)\log(K/D)$, whenever $D = o(n^{1/2})$. Inequality (2.21) shows that the maximum likelihood estimator over the simplex achieves this rate up to a logarithmic factor. Furthermore, this logarithmic inflation disappears when the sparsity D is such that, asymptotically, the ratio $\frac{\log D}{\log K}$ is bounded from above by a constant $\alpha < 1$. Indeed, in such a situation the optimal rate $\frac{D\log(K/D)}{n} = \frac{D\log K}{n}(1 - \frac{\log D}{\log K})$ is of the same order as the remainder term in (2.21), that is $\frac{D\log K}{n}$.

2.3 Discussion of the conditions and possible extensions

In this section, we start by announcing lower bounds for the Kullback-Leibler aggregation in the problem of density estimation. Then we discuss the implication of the risk bounds of the previous section to the case where the target is the weight vector $\boldsymbol{\pi}$ rather than the mixture density $f_{\boldsymbol{\pi}}$. Finally, we present some extensions to the case where the boundedness assumption is violated.

2.3.1 Lower bounds for nearly-D-sparse aggregation

As mentioned in previous section, the literature is replete with lower bounds on the minimax risk for various types of aggregation. However most of them concern the regression setting either with random or with deterministic design. Lower bounds of aggregation for density estimation were first established by Rigollet [2006] for the L_2-loss. In the case of Kullback-Leibler aggregation in density estimation, the only lower bounds we are aware are those established by Lecué [2006] for model-selection type aggregation. It is worth emphasizing here that the results of the aforementioned two papers provide weak lower bounds. Indeed, they establish the existence of a dictionary for which the minimax excess risk is lower bounded by the suitable quantity. In contrast with this, we establish here strong lower bounds that hold for every dictionary satisfying the boundedness and the compatibility conditions.

Let $\mathcal{F} = \{f_1, \ldots, f_K\}$ be a dictionary of density functions on $\mathcal{X} = [0, 1]$. We say that the dictionary $\mathcal{F}$ satisfies the boundedness and the compatibility assumptions if for some positive constants m, M and κ, we have $m \leq f_j(x) \leq$

M for all $j \in [K]$, $x \in \mathcal{X}$. In addition, we assume in this subsection that all the eigenvalues of the Gram matrix $\mathbf{\Sigma}$ belong to the interval $[\varkappa_*, \varkappa^*]$, with $\varkappa_* > 0$ and $\varkappa^* < \infty$.

For every $\gamma \in (0,1)$ and any $D \in [K]$, we define the set of nearly-D-sparse convex combinations of the dictionary elements $f_j \in \mathcal{F}$ by

$$\mathcal{H}_{\mathcal{F}}(\gamma, D) = \Big\{ f_{\boldsymbol{\pi}} : \boldsymbol{\pi} \in \mathbb{B}_+^K \text{ such that } \min_{J:|J| \le D} \|\boldsymbol{\pi}_{J^c}\|_1 \le \gamma \Big\}. \tag{2.22}$$

In simple words, $f_{\boldsymbol{\pi}}$ belongs to $\mathcal{H}_{\mathcal{F}}(\gamma, D)$ if it admits a γ-approximately D-sparse representation in the dictionary $\mathcal{F}$. We are interested in bounding from below the minimax excess risk

$$\mathcal{R}\big(\mathcal{H}_{\mathcal{F}}(\gamma, D)\big) = \inf_{\widehat{f}} \sup_{f^*} \Big\{ \mathbf{E}[\mathrm{KL}(f^* || \widehat{f}\,)] - \inf_{f_{\boldsymbol{\pi}} \in \mathcal{H}_{\mathcal{F}}(\gamma, D)} \mathrm{KL}(f^* || f_{\boldsymbol{\pi}}) \Big\}, \tag{2.23}$$

where the inf is over all possible estimators of f^* and the sup is over all density functions over $[0,1]$. Note that the estimator $\widehat{f}$ is not necessarily a convex combination of the dictionary elements. Furthermore, it is allowed to depend on the parameters γ and D characterizing the class $\mathcal{H}_{\mathcal{F}}(\gamma, D)$. It follows from (2.17), that if the dictionary satisfies the boundedness and the compatibility condition, then

$$\mathcal{R}\big(\mathcal{H}_{\mathcal{F}}(\gamma, D)\big) \le C \Big\{ \Big(\frac{\gamma^2 \log K}{n} \Big)^{1/2} + \frac{D \log K}{n} \Big\} \bigwedge \Big(\frac{\log K}{n} \Big)^{1/2}, \tag{2.24}$$

for some constant C depending only on m, M and $\varkappa_*$. Note that the last term accounts for the following phenomenon: If the sparsity index D is larger than a multiple of $\sqrt{n}$, then the sparsity bears no advantage as compared to the ℓ_1 constraint. The next result implies that this upper bound is optimal, at least up to logarithmic factors.

Theorem 2.3.1. *Assume that* $\log(1 + eK) \le n$. *Let* $\gamma \in (0,1)$ *and* $D \in [K]$ *be fixed. There exists a constant* A *depending only on* m, M, $\varkappa_*$ *and* $\varkappa^*$ *such* *that $\mathcal{R}(\mathcal{H}_{\mathcal{F}}(\gamma, D))$ is larger than*

$$A\bigg\{\bigg[\frac{\gamma^2}{n}\log\bigg(1+\frac{K}{\gamma\sqrt{n}}\bigg)\bigg]^{1/2}+\frac{D\log(1+K/D)}{n}\bigg\}\bigwedge\bigg[\frac{1}{n}\log\bigg(1+\frac{K}{\sqrt{n}}\bigg)\bigg]^{1/2}. \tag{2.25}$$

This is the first result providing lower bounds on the minimax risk of aggregation over nearly-D-sparse aggregates. To the best of our knowledge, even in the Gaussian sequence model, such a result has not been established to date. It has the advantage of unifying the results on convex and D-sparse aggregation, as well as extending them to a more general class. Let us also stress that the condition $\log(1 + eK) \leq n$ is natural and unavoidable, since it ensures that the right hand side of (2.24) is smaller than the trivial bound $\log V$.

2.3.2 Weight vector estimation

The risk bounds carried out in the previous section for the problem of density estimation in the Kullback-Leibler loss imply risk bounds for the problem of weight vector estimation. Indeed, under the boundedness assumption (2.11), the Kullback-Leibler divergence between two mixture densities can be shown to be equivalent to the squared Mahalanobis distance between the weight vectors of these mixtures with respect to the Gram matrix. In order to go from the Mahalanobis distance to the Euclidean one, we make use of the restricted eigenvalue

$$\kappa_{\boldsymbol{\Sigma}}^{\mathrm{RE}}(s,c) = \inf_{\boldsymbol{v}\in\Delta(s,c)} \|\boldsymbol{\Sigma}^{1/2}\boldsymbol{v}\|_2^2, \tag{2.26}$$

with $\Delta(s,c) := \{\boldsymbol{v} : \exists\, J \subset [K] \text{ s.t. } |J| \leq s,\ \|\boldsymbol{v}_{J^c}\|_1 \leq c\|\boldsymbol{v}_J\|_1 \text{ and } \|\boldsymbol{v}_J\|_2 = 1\}$. This strategy leads to the next result.

Proposition 1. *Let $\mathcal{F}$ be a set of $K \geq 4$ densities satisfying condition (2.11). Denote by $f_{\widehat{\boldsymbol{\pi}}}$ the mixture density corresponding to the maximum likelihood estimator $\widehat{\boldsymbol{\pi}}$ over Π_n defined in (2.7). Let $\boldsymbol{\pi}^*$ the weight-vector of the best mixture density: $\boldsymbol{\pi}^* \in \arg\min_{\boldsymbol{\pi}} \mathrm{KL}(f^*||f_{\boldsymbol{\pi}})$, and let J^* be the support of $\boldsymbol{\pi}^*$. There are constants $c_{10} \leq M^2(64V^3+8)$ and $c_{11} \leq 4M^2(8V^3+1)$ such that, for any $\delta \in (0, 1/2)$, the following inequalities hold*

$$\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1 \leq \frac{c_{10}|J^*|}{\bar{\kappa}_{\boldsymbol{\Sigma}}(J^*, 1)} \Big(\frac{\log(K/\delta)}{n}\Big)^{1/2}, \tag{2.27}$$

$$\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_2 \leq \frac{c_{11}}{\kappa_{\boldsymbol{\Sigma}}^{\mathrm{RE}}(|J^*|, 1)} \Big(\frac{2|J^*|\log(K/\delta)}{n}\Big)^{1/2}, \tag{2.28}$$

$$\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_2^2 \leq \frac{c_{11}}{\kappa_{\boldsymbol{\Sigma}}^{\mathrm{RE}}(|J^*|, 1)} \Big(\frac{2\log(K/\delta)}{n}\Big)^{1/2} \tag{2.29}$$

with probability at least $1 - 2\delta$.

In simple words, this result tells us that the wight estimator $\widehat{\boldsymbol{\pi}}$ attains the minimax rate of estimation $|J^*|(\frac{\log(K)}{n})^{1/2}$ over the intersection of the ℓ_1 and ℓ_0 balls, when the error is measured by the ℓ_1-norm, provided that the compatibility factor of the dictionary $\mathcal{F}$ is bounded away from zero. The optimality of this rate—up to logarithmic factors—follows from the fact that the error of estimation of each nonzero coefficients of $\boldsymbol{\pi}^*$ is at least $cn^{-1/2}$ (for some $c > 0$), leading to a sum of the absolute values of the errors at least of the order $|J^*|n^{-1/2}$. The logarithmic inflation of the rate is the price to pay for not knowing the support J^*. It is clear that this reasoning is valid only when the sparsity $|J^*|$ is of smaller order than $n^{1/2}$. Indeed, in the case $|J^*| \geq cn^{1/2}$, the trivial bound $\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1 \leq 2$ is tighter than the one in (2.27).

Concerning the risk measured by the Euclidean norm, we underline that there are two regimes characterized by the order between upper bounds in (2.28) and (2.29). Roughly speaking, when the signal is highly sparse in the sense that $|J^*|$ is smaller than $(n/\log K)^{1/2}$, then the smallest bound is given by (2.28) and is of the order $\frac{|J^*|\log(K)}{n}$. This rate is can be compared to the rate $\frac{|J^*|\log(K/|J^*|)}{n}$, known to be optimal in the Gaussian sequence model. In the second regime corresponding to mild sparsity, $|J^*| > (n/\log K)^{1/2}$, the smallest bound is the one in (2.29). The latter is of order $(\frac{\log(K)}{n})^{1/2}$, which is known to be optimal in the Gaussian sequence model. For various results providing lower bounds in regression framework we refer the interested reader to [Raskutti et al., 2011, Rigollet and Tsybakov, 2011, Wang et al., 2014].

2.3.3 Extensions to the case of vanishing components

In the previous sections we have deliberately avoided any discussion of the role of the parameter μ, present in the search space $\Pi_n(\mu)$ of the problem (2.2)-(2.3). In fact, when all the dictionary elements are separated from zero by a constant m, a condition assumed throughout previous sections, choosing any value of $\mu \leq m$ is equivalent to choosing $\mu = 0$. Therefore, the choice of this parameter does not impact the quality of estimation. However, this parameter might have strong influence in practice both on statistical and computational complexity of the maximum likelihood estimator. A first step in understanding the influence of μ on the statistical complexity is made in the next paragraphs.

Let us consider the case where the condition $\min_x \min_j f_j(x) \geq m > 0$ fails, but the upper-boundedness condition $\max_x \max_j f_j(x) \leq M$ holds true. In such a situation, we replace the definition $V = M/m$ by $V = M/\mu$. We also define the set $\Pi^*(\mu) = \big\{\boldsymbol{\pi} \in \mathbb{B}_+^K : P^*\big(f_{\boldsymbol{\pi}}(\boldsymbol{X}) \geq \mu\big) = 1\big\}$. In order to keep mathematical formulae simple, we will only state the equivalent of (2.13) in the case of $m = 0$. All the other results of the previous section can be extended in a similar way.

Proposition 2. *Let $\mathcal{F}$ be a set of $K \geq 2$ densities satisfying the boundedness* *condition* $\sup_{\boldsymbol{x}\in\mathcal{X}} f_j(\boldsymbol{x}) \leq M$*. Denote by* $f_{\widehat{\boldsymbol{\pi}}}$ *the mixture density corresponding to the maximum likelihood estimator* $\widehat{\boldsymbol{\pi}}$ *over* $\Pi_n(\mu)$ *defined in* (2.7)*. There is a constant* $\bar{c} \leq 128M^2V^4$ *such that, for any* $\delta \in (0, 1/2)$*,*

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \inf_{J\subset[K]} \inf_{\substack{\boldsymbol{\pi}\in\Pi^*(\mu)\\ \boldsymbol{\pi}_{J^c}=0}} \left\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{\bar{c}|J|\log(K/\delta)}{n\bar{\kappa}_{\widehat{\boldsymbol{\Sigma}}_n}(J,1)} \right\} + \int_{\mathcal{X}} (\log\mu - \log f_{\widehat{\boldsymbol{\pi}}})_+ f^* d\nu \tag{2.30}$$

on an event of probability at least $1-\delta$*. Furthermore, if* $\inf_{\boldsymbol{x}\in\mathcal{X}} f^*(\boldsymbol{x}) \geq \mu$*, then, on the same event, we have*

$$\|f^* - f_{\widehat{\boldsymbol{\pi}}}\|^2_{L^2(P^*)} \leq 2M^2 \inf_{J\subset[K]} \inf_{\substack{\boldsymbol{\pi}\in\Pi^*(\mu)\\ \boldsymbol{\pi}_{J^c}=0}} \left\{ \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \frac{\bar{c}|J|\log(K/\delta)}{n\bar{\kappa}_{\widehat{\boldsymbol{\Sigma}}_n}(J,1)} \right\}. \tag{2.31}$$

The last term present in the first upper bound, $\int_{\mathcal{X}} (\log\mu - \log f_{\widehat{\boldsymbol{\pi}}})_+ f^* d\nu$ is the price we pay for considering densities that are not lower bounded by a given constant. A simple, non-random upper bound on this term is $\int_{\mathcal{X}} \max_{k\in[K]}(\log\mu - \log f_k)_+ f^* d\nu$. Providing a tight upper bound on this kind or remainder terms is an important problem which lies beyond the scope of the present work.

2.4 Conclusion

In this paper, we have established exact oracle inequalities for the maximum likelihood estimator of a mixture density. This oracle inequality clearly highlights the interplay of three sources of error: misspecification of the model of mixture, departure from D-sparsity and stochastic error of estimating D nonzero coefficients. We have also proved a lower bound that show that the remainder terms of our upper bounds are optimal, up to logarithmic terms. This lower bound is valid not only for the maximum likelihood estimator, but for any estimator of the density function. As a consequence, the maximum likelihood estimator has a nearly optimal excess risk in the minimax sense.

In all the results of the present paper, we have assumed that the components of the mixture model are deterministic. From a practical point of view, it might be reasonable to choose these components in a data driven way, using, for instance, a hold-out sample. This question, as well as the problem of tuning the parameter μ , constitute interesting and challenging avenues for future research.

2.5 Proofs of results stated in previous sections

This section collects the proofs of the theorems and claims stated in previous sections.

2.5.1 Proof of Theorem 2.2.1

The main technical ingredients of the proof are a strong convexity argument and a control of the maximum of an empirical process. The corresponding results are stated in Lemma 2.5.2 and Proposition 2.5.1, respectively, deferred to Section 2.5.6. We denote by $\bar{\mathbf{Z}}$ the $n \times K$ matrix $[\bar{\boldsymbol{Z}}_1, \ldots, \bar{\boldsymbol{Z}}_K]$.

Since $\widehat{\boldsymbol{\pi}}$ is a minimizer of $L_n(\cdot)$, see (2.2) and (2.7), we know that $L_n(\widehat{\boldsymbol{\pi}}) \leq L_n(\boldsymbol{\pi})$ for every π. However, this inequality can be made sharper using the (local) strong convexity of the function $\ell(u) = -\log(u)$. Indeed, Lemma 2.5.2 below shows that

$$\frac{1}{n}\sum_{i=1}^{n} \ell(f_{\widehat{\boldsymbol{\pi}}}(\boldsymbol{X}_i)) \leq \frac{1}{n}\sum_{i=1}^{n} \ell(f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)) - \frac{1}{2M^2 n}\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2. \tag{2.32}$$

On the other hand, if we set $\varphi(\pi, \boldsymbol{x}) = \int (\log f_{\boldsymbol{\pi}}) f^* d\nu - \log f_{\boldsymbol{\pi}}(\boldsymbol{x})$, we have $\mathbf{E}_{f^*}[\varphi(\boldsymbol{\pi}, \boldsymbol{X}_i)] = 0$ and

$$\ell(f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)) = \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) - \int_{\mathcal{X}} f^* \log f^* d\nu + \varphi(\pi, \boldsymbol{X}_i). \tag{2.33}$$

Combining inequalities (2.32) and (2.33), we get

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) - \frac{1}{2M^2 n}\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 + \frac{1}{n}\sum_{i=1}^{n}\big(\varphi(\boldsymbol{\pi}, \boldsymbol{X}_i) - \varphi(\widehat{\boldsymbol{\pi}}, \boldsymbol{X}_i)\big). \tag{2.34}$$

The next step of the proof consists in establishing a suitable upper bound on the noise term $\Phi_n(\boldsymbol{\pi}) - \Phi_n(\widehat{\boldsymbol{\pi}})$ where

$$\Phi_n(\boldsymbol{\pi}) = \frac{1}{n}\sum_{i=1}^{n}\varphi(\boldsymbol{\pi}, \boldsymbol{X}_i). \tag{2.35}$$

According to the mean value theorem, setting $\zeta_n := \sup_{\bar{\boldsymbol{\pi}} \in \boldsymbol{\Pi}_n} \big\|\nabla\Phi_n(\bar{\boldsymbol{\pi}})\big\|_\infty$, for every vector $\boldsymbol{\pi} \in \boldsymbol{\Pi}_n$, it holds that

$$|\Phi_n(\widehat{\boldsymbol{\pi}}) - \Phi_n(\boldsymbol{\pi})| \leq \sup_{\bar{\boldsymbol{\pi}} \in \boldsymbol{\Pi}_n} \big\|\nabla\Phi_n(\bar{\boldsymbol{\pi}})\big\|_\infty \|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1 = \zeta_n \|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1. \tag{2.36}$$

This inequality, combined with (2.34), yields

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) - \frac{1}{2M^2 n}\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 + \zeta_n\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1. \tag{2.37}$$

Using the Gram matrix $\widehat{\boldsymbol{\Sigma}}_n = {}^1\!/_n \bar{\mathbf{Z}}^\top \bar{\mathbf{Z}}$, the quantity $\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2$ can be rewritten as

$$\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 = n\|\widehat{\boldsymbol{\Sigma}}_n^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2. \tag{2.38}$$

We proceed with applying the following result [Bellec et al., 2016, Lemma 2].

Lemma 2.5.1 (Bellec et al. [2016], Lemma 2)**.** *For any pair of vectors $\boldsymbol{\pi}, \boldsymbol{\pi}' \in \mathbb{R}^K$, for any pair of scalars $\mu > 0$ and $\gamma > 1$, for any $K \times K$ symmetric matrix $\mathbf{A}$ and for any set $J \subset [p]$, the following inequality is true*

$$2\mu\gamma^{-1}(\|\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}}\|_1 + \gamma\|\boldsymbol{\pi}\|_1 - \gamma\|\widehat{\boldsymbol{\pi}}\|_1) - \|\mathbf{A}(\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}})\|_2^2 \leq 4\mu\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{(\gamma+1)^2\mu^2|J|}{\gamma^2\kappa_{\mathbf{A}^2}(J, c_\gamma)}, \tag{2.39}$$

where $c_\gamma = (\gamma + 1)/(\gamma - 1)$.

Choosing $\mathbf{A} = \widehat{\mathbf{\Sigma}}_n^{1/2}/(\sqrt{2}\,M)$, $\mu = \zeta_n$ and $\gamma = 2$ (thus $c_\gamma = 3$) we get the inequality

$$\zeta_n\|\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}}\|_1 - \|\mathbf{A}(\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}})\|_2^2 \le 4\zeta_n\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{9\zeta_n^2|J|}{4\kappa_{\mathbf{A}^2}(J,3)}, \qquad \forall J \in \{1,\ldots,p\}. \tag{2.40}$$

One can check that $\kappa_{\mathbf{A}^2}(J,3) = \kappa_{\widehat{\mathbf{\Sigma}}_n}(J,3)/(2M^2)$. Combining the last inequality with (2.37), we arrive at

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \le \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + 4\zeta_n\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{9M^2\zeta_n^2|J|}{2\kappa_{\widehat{\mathbf{\Sigma}}_n}(J,3)}. \tag{2.41}$$

Since the last inequality holds for every $\boldsymbol{\pi}$, we can insert an $\inf_{\boldsymbol{\pi}}$ in the right hand side. Furthermore, in view of Proposition 2.5.1 below, with probability larger than $1-\delta$, ζ_n is bounded from above by $8V^3(\frac{\log(K/\delta)}{n})^{1/2}$. This completes the proof of (2.12).

To prove (2.13), we follow the same steps as above up to inequality (2.37). Then, we remark that for every $\boldsymbol{\pi}$ in the simplex satisfying $\boldsymbol{\pi}_{J^c} = 0$, it holds

$$\|(\widehat{\boldsymbol{\pi}}-\boldsymbol{\pi})_{J^c}\|_1 = \|\widehat{\boldsymbol{\pi}}_{J^c}\|_1 = 1-\|\widehat{\boldsymbol{\pi}}_J\|_1 = \|\boldsymbol{\pi}_J\|_1-\|\widehat{\boldsymbol{\pi}}_J\|_1 \le \|(\widehat{\boldsymbol{\pi}}-\boldsymbol{\pi})_J\|_1. \tag{2.42}$$

Therefore, $\|\widehat{\mathbf{\Sigma}}_n^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 \ge$ we have with probability at least $1-\delta$

$$\begin{aligned}
\zeta_n\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1 - \frac{1}{2M^2n}\|\mathbf{Z}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 &\le 2\zeta_n\|(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})_J\|_1 - \frac{1}{2M^2}\|\widehat{\mathbf{\Sigma}}_n^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 \\
&\le 2\zeta_n\|(\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}})_J\|_1 - \frac{\bar{\kappa}_{\widehat{\mathbf{\Sigma}}_n}(J,1)\|(\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}})_J\|_1^2}{2M^2|J|} \\
&\le \frac{2\zeta_n^2M^2|J|}{\bar{\kappa}_{\widehat{\mathbf{\Sigma}}_n}(J,1)}.
\end{aligned} \tag{2.43}$$

Replacing the right hand term in (2.37) and taking the infimum, we get the claim of the corollary. Since, in view of Proposition 2.5.1 below, with probability larger than $1-\delta$, ζ_n is bounded from above by $8V^3(\frac{\log(K/\delta)}{n})^{1/2}$, we get the claim of (2.13).

2.5.2 Proof of Theorem 2.2.2

Let us denote $\boldsymbol{v} = \widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}$. According to (2.37) and (2.38), we have

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \zeta_n\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1 - \frac{1}{2M^2}\|\widehat{\boldsymbol{\Sigma}}_n^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 \tag{2.44}$$

$$\leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \zeta_n\|\boldsymbol{v}\|_1 - \frac{1}{2M^2}\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{v}\|_2^2 + \frac{1}{2M^2}\boldsymbol{v}^\top(\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n)\boldsymbol{v}. \tag{2.45}$$

As $\boldsymbol{v}$ is the difference of two vectors lying on the simplex, we have $\|\boldsymbol{v}\|_1 \leq 2$. Let $\|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty = \max_{j,j'}|(\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n)_{j,j'}|$ stand for the largest (in absolute values) element of the matrix $\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n$. We have

$$\boldsymbol{v}^\top(\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n)\boldsymbol{v} \leq \|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty\|\boldsymbol{v}\|_1^2 \leq 2\|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty\|\boldsymbol{v}\|_1. \tag{2.46}$$

Setting $\bar{\zeta}_n = \zeta_n + M^{-2}\|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty$, we get

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + \bar{\zeta}_n\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_1 - \frac{1}{2M^2}\|\boldsymbol{\Sigma}^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2. \tag{2.47}$$

Following the same steps as those used for obtaining (2.41), we arrive at

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + 4\bar{\zeta}_n\|\boldsymbol{\pi}_{J^c}\|_1 + \frac{9\bar{\zeta}_n^2M^2|J|}{2\kappa_{\boldsymbol{\Sigma}}(J,3)}. \tag{2.48}$$

The last step consists in evaluating the quantiles of the random variable $\bar{\zeta}_n$. To this end, one checks that the Hoeffding inequality combined with the union bound yields

$$\mathbf{P}\Big\{\|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty > t\Big\} \leq K(K-1)\exp(-2nt^2/M^4), \qquad \forall t > 0. \tag{2.49}$$

In other terms, for every $\delta \in (0,1)$, we have

$$\mathbf{P}\Big\{\|\boldsymbol{\Sigma} - \widehat{\boldsymbol{\Sigma}}_n\|_\infty \leq M^2\Big(\frac{\log(K^2/\delta)}{2n}\Big)^{1/2}\Big\} \geq 1 - \delta. \tag{2.50}$$

Note that for $\delta \leq 1$, we have $\log(K^2/\delta) \leq 2\log(K/\delta)$. Combining with Proposition 2.5.1, this implies that $\bar{\zeta}_n \leq (8V^3+1)\big(\frac{\log(K/\delta)}{n}\big)^{1/2}$ with probability larger than $1-2\delta$. This completes the proof of (2.15). The proof of (2.16) is omitted since it repeats the same arguments as those used for proving (2.13).

2.5.3 Proof of Theorem 2.2.3

According to (2.48), for any $\boldsymbol{\pi} \in \Pi$ and any $J \subset \{1, \ldots, K\}$, we have

$$\mathbf{E}[\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}})] \leq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}}) + 4\|\boldsymbol{\pi}_{J^c}\|_1 \mathbf{E}[\bar{\zeta}_n] + \frac{9M^2|J|}{2\kappa_{\boldsymbol{\Sigma}}(J,3)} \mathbf{E}[\bar{\zeta}_n^2]. \tag{2.51}$$

Recall now that $\bar{\zeta}_n = \zeta_n + M^{-2}\|\widehat{\boldsymbol{\Sigma}}_n - \boldsymbol{\Sigma}\|_\infty$ and, according to Proposition 2.5.1, we have

$$\mathbf{E}[\zeta_n] \leq 4V^3\Big(\frac{2\log(2K^2)}{n}\Big)^{1/2} \qquad \text{and} \qquad \mathbf{Var}[\zeta_n] \leq \frac{V^2}{2n}. \tag{2.52}$$

Using Theorem 2.6.2, one easily checks that

$$\mathbf{E}[\|\widehat{\boldsymbol{\Sigma}}_n - \boldsymbol{\Sigma}\|_\infty] \leq M^2\Big(\frac{\log(2K^2)}{2n}\Big)^{1/2}. \tag{2.53}$$

This implies that

$$\mathbf{E}[\bar{\zeta}_n] \leq (8V^3+1)\Big(\frac{\log(2K^2)}{2n}\Big)^{1/2}. \tag{2.54}$$

Similarly, in view of the Efron-Stein inequality, we have $\mathbf{Var}[\|\widehat{\boldsymbol{\Sigma}}_n - \boldsymbol{\Sigma}\|_\infty] \leq \frac{M^4}{2n}$. This implies that

$$\mathbf{E}[\bar{\zeta}_n^2] \leq (\mathbf{E}[\bar{\zeta}_n])^2 + \big\{(\mathbf{Var}[\zeta_n])^{1/2} + M^{-2}(\mathbf{Var}[\|\widehat{\boldsymbol{\Sigma}}_n - \boldsymbol{\Sigma}\|_\infty])^{1/2}\big\}^2 \tag{2.55}$$

$$\leq (8V^3+1)^2\frac{\log(2K^2)}{2n} + \frac{(V+1)^2}{2n} \tag{2.56}$$

$$\leq 1.615(8V^3+1)^2\frac{\log K}{n}. \tag{2.57}$$

Combining (2.54), (2.57) and (2.51), we get the desired result.

2.5.4 Proof of Proposition 1

Using the strong convexity of the function $u \mapsto \log u$ over the interval $[m, M]$ and the fact that $\boldsymbol{\pi}^*$ minimizes the convex function $\boldsymbol{\pi} \mapsto \mathrm{KL}(f^*||f_{\boldsymbol{\pi}})$, we get

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol{\pi}}}) \geq \mathrm{KL}(f^*||f_{\boldsymbol{\pi}^*}) + \frac{1}{2M^2}\|\widehat{\boldsymbol{\Sigma}}_n^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*)\|_2^2. \tag{2.58}$$

Combining with (2.47), in which we replace $\boldsymbol{\pi}$ by $\boldsymbol{\pi}^*$, we get

$$\|\boldsymbol{\Sigma}^{1/2}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*)\|_2^2 \leq 2M^2\bar{\zeta}_n\|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1. \tag{2.59}$$

Let us set $\boldsymbol{v} = \widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*$. If $\boldsymbol{v} = 0$, then the claims are trivial. In the rest of this proof, we assume $\|\boldsymbol{v}\|_1 > 0$. In view of (2.42), we have $\|\boldsymbol{v}\|_1 \leq 2\|\boldsymbol{v}_{J^*}\|_1$. Therefore, using the definition of the compatibility factor, we get

$$\|\boldsymbol{v}\|_1^2 \leq 4\|\boldsymbol{v}_{J^*}\|_1^2 \leq \frac{4|J^*|\,\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{v}\|_2^2}{\bar{\kappa}(J^*,1)} \leq \frac{8|J^*|\,M^2\bar{\zeta}_n\|\boldsymbol{v}\|_1}{\bar{\kappa}(J^*,1)}. \tag{2.60}$$

We have already checked that $\bar{\zeta}_n \leq (8V^3+1)\big(\frac{\log(K/\delta)}{n}\big)^{1/2}$ with probability larger than $1-2\delta$. Dividing both sides of inequality (2.60) by $\|\boldsymbol{v}\|_1$ and using the aforementioned upper bound on $\bar{\zeta}_n$, we get the desired bound on $\|\boldsymbol{v}\|_1 = \|\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*\|_1$.

In order to bound the error $\boldsymbol{v} = \widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}^*$ in the Euclidean norm, we denote by $\widehat{J}$ the set of $D = |J^*|$ indices corresponding to D largest entries of the vector $(|v_1|,\ldots,|v_K|)$. Since $\|\boldsymbol{v}\|_1 \leq 2\|\boldsymbol{v}_{J^*}\|_1$, we clearly have $\|\boldsymbol{v}\|_1 \leq 2\|\boldsymbol{v}_{\widehat{J}}\|_1$. Therefore,

$$\begin{aligned}
\|\boldsymbol{v}\|_2^2 &= \|\boldsymbol{v}_{\widehat{J}}\|_2^2 + \|\boldsymbol{v}_{\widehat{J}^c}\|_2^2 &\quad(2.61)\\
&\leq \|\boldsymbol{v}_{\widehat{J}}\|_2^2 + \|\boldsymbol{v}_{\widehat{J}^c}\|_\infty\|\boldsymbol{v}_{\widehat{J}^c}\|_1 &\quad(2.62)\\
&\leq \|\boldsymbol{v}_{\widehat{J}}\|_2^2 + \frac{\|\boldsymbol{v}_{\widehat{J}}\|_1}{D}\|\boldsymbol{v}_{\widehat{J}^c}\|_1 &\quad(2.63)\\
&\leq \|\boldsymbol{v}_{\widehat{J}}\|_2^2 + \frac{1}{D}\|\boldsymbol{v}_{\widehat{J}}\|_1^2 \leq 2\|\boldsymbol{v}_{\widehat{J}}\|_2^2. &\quad(2.64)
\end{aligned}$$

Combining this inequality with the definition of the restricted eigenvalue and inequality (2.59) above, we arrive at

$$\begin{aligned}
\|\boldsymbol{v}_{\widehat{J}}\|_2^2 &\leq \frac{\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{v}\|_2^2}{\kappa^{\mathrm{RE}}(D,1)} \leq \frac{2M^2\bar{\zeta}_n\|\boldsymbol{v}\|_1}{\kappa^{\mathrm{RE}}(D,1)} &\quad(2.65)\\
&\leq \frac{4M^2\bar{\zeta}_n(\|\boldsymbol{v}_{\widehat{J}}\|_1 \wedge 1)}{\kappa^{\mathrm{RE}}(D,1)} \leq \frac{4M^2\,\bar{\zeta}_n(\sqrt{D}\|\boldsymbol{v}_{\widehat{J}}\|_2 \wedge 1)}{\kappa^{\mathrm{RE}}(D,1)}. &\quad(2.66)
\end{aligned}$$

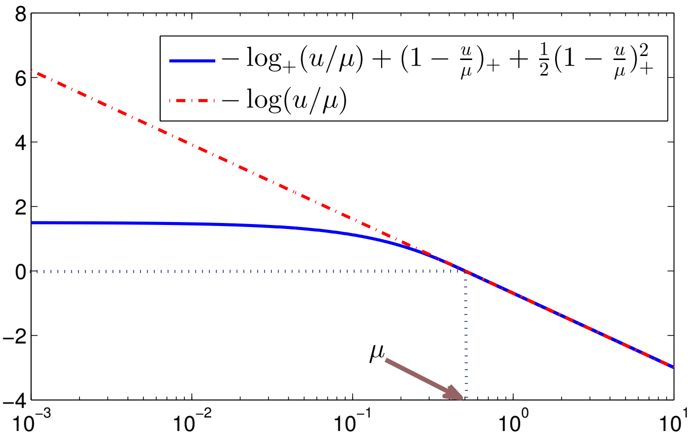


Figure 2.1: The plot of the function $u \mapsto \bar\ell(u)$, used in the proof of Proposition 2, superposed on the plot of the function $u \mapsto \ell(u) = -\log u$. We see that the former is a strongly convex surrogate of the latter.

Dividing both sides by $\|\boldsymbol{v}_{\widehat J}\|_2$, taking the square and using (2.64), we get

$$\|\boldsymbol{v}\|_2 \le \sqrt{2}\,\|\boldsymbol{v}_{\widehat J}\|_2 \le \frac{4\sqrt{2}M^2|J^*|^{1/2}\,\bar\zeta_n}{\kappa^{\rm RE}(|J^*|,1)} \bigwedge \frac{2\sqrt{2}M\bar\zeta_n^{1/2}}{\kappa^{\rm RE}(|J^*|,1)^{1/2}}. \tag{2.67}$$

This inequality, in conjunction with the upper bound on $\bar\zeta_n$ used above, completes the proof of the second claim.

2.5.5 Proof of Proposition 2

We repeat the proof of Theorem 2.2.1 with some small modifications. First of all, we replace the function $\ell(u) = -\log(u)$ by the function

$$\bar\ell(u) = \begin{cases} -\log(u/\mu), & \text{if } u \ge \mu, \\ (1-\frac{u}{\mu}) + \frac{1}{2}(1-\frac{u}{\mu})^2, & \text{if } u \in (0,\mu). \end{cases} \tag{2.68}$$

One easily checks that this function is twice continuously differentiable with a second derivative satisfying $M^{-2} \le \bar\ell''(u) \le \mu^{-2}$ for every $u \in (0, M)$.

Furthermore, since $\bar\ell(u) = \ell(u/\mu)$ for every $u \geq \mu$, we have $\bar L_n(\widehat{\boldsymbol\pi}) = L_n(\widehat{\boldsymbol\pi})$, where we have used the notation $\bar L_n(\boldsymbol\pi) = \frac{1}{n}\sum_{i=1}^n \bar\ell(f_{\boldsymbol\pi}(\boldsymbol X_i))$. Therefore, similarly to (2.32), we get

$$\frac{1}{n}\sum_{i=1}^n \bar\ell(f_{\widehat{\boldsymbol\pi}}(\boldsymbol X_i)) \leq \frac{1}{n}\sum_{i=1}^n \bar\ell(f_{\boldsymbol\pi}(\boldsymbol X_i)) - \frac{1}{2M^2 n}\|\bar{\mathbf Z}(\widehat{\boldsymbol\pi} - \boldsymbol\pi)\|_2^2, \tag{2.69}$$

for every $\boldsymbol\pi \in \Pi^*(\mu)$. Let us define $\bar\varphi(\boldsymbol\pi, \boldsymbol x) = \bar\ell(f_{\boldsymbol\pi}(\boldsymbol x)) - \int \bar\ell(f_{\boldsymbol\pi}) f^* d\nu$ and $\bar\Phi_n(\boldsymbol\pi) = \frac{1}{n}\sum_{i=1}^n \bar\varphi(\boldsymbol\pi, \boldsymbol X_i)$. We have

$$\begin{aligned}
\int \bar\ell(f_{\widehat{\boldsymbol\pi}})\, f^* d\nu &\leq \int \bar\ell(f_{\boldsymbol\pi})\, f^* d\nu - \frac{1}{2M^2 n}\|\bar{\mathbf Z}(\widehat{\boldsymbol\pi} - \boldsymbol\pi)\|_2^2 \\
&\quad + \frac{1}{n}\sum_{i=1}^n \big(\varphi(\boldsymbol\pi, \boldsymbol X_i) - \varphi(\widehat{\boldsymbol\pi}, \boldsymbol X_i)\big) \qquad (2.70)\\
&\leq \int \bar\ell(f_{\boldsymbol\pi})\, f^* d\nu - \frac{1}{2M^2 n}\|\bar{\mathbf Z}(\widehat{\boldsymbol\pi} - \boldsymbol\pi)\|_2^2 \\
&\quad + \underbrace{\sup_{\boldsymbol\pi \in \Pi_n(0)} \|\nabla\bar\Phi_n(\boldsymbol\pi)\|_\infty}_{:=\xi_n} \|\widehat{\boldsymbol\pi} - \boldsymbol\pi\|_1. \qquad (2.71)
\end{aligned}$$

Notice that $\boldsymbol\pi \in \Pi^*(\mu)$ implies that $\bar\ell(f_{\boldsymbol\pi}) = \log\mu - \log f_{\boldsymbol\pi}$ and that $\bar\ell(f_{\widehat{\boldsymbol\pi}}) \geq \log\mu - \log f_{\widehat{\boldsymbol\pi}} - (\log\mu - \log f_{\widehat{\boldsymbol\pi}})_+$. Therefore, along the lines of the proof of (2.13) (see, namely, (2.43)), we get

$$\mathrm{KL}(f^*||f_{\widehat{\boldsymbol\pi}}) \leq \mathrm{KL}(f^*||f_{\boldsymbol\pi}) + \frac{2\xi_n^2 M^2 |J|}{\bar\kappa_{\widehat{\boldsymbol\Sigma}_n}(J,1)} + \int_{\mathcal X} (\log\mu - \log f_{\widehat{\boldsymbol\pi}})_+ f^* d\nu. \tag{2.72}$$

We can repeat now the arguments of Proposition 2.5.1 with some minor modifications. First of all, we rewrite ξ_n as $\xi_n = \max_{l=1,\ldots,K} \xi_{l,n}$ with $\xi_{l,n} = \sup_{\boldsymbol\pi\in\Pi_n(0)} |\partial_l \bar\Phi_n(\boldsymbol\pi)|$. One checks that the bounded difference inequality and the Efron-Stein inequality can be applied with an additional factor 2, since for $F_l(\mathbf X) = \sup_{\boldsymbol\pi\in\Pi_n(0)} |\partial_l \bar\Phi_n(\boldsymbol\pi)|$, we have

$$|F_l(\mathbf X) - F_l(\mathbf X')| \leq \frac{2M}{n\mu} = \frac{2V}{n}. \tag{2.73}$$

Therefore, for every $l \in [K]$, with probability larger than $1 - (\delta/K)$, we have $\xi_{l,n} \leq \mathbf E[\xi_{l,n}] + V(\frac{2\log(K/\delta)}{n})^{1/2}$ and $\mathbf{Var}[\xi_n] \leq (2V)^2/n$. By the union bound, we obtain that with probability larger than $1-\delta$, $\xi_n \le \max_l \mathbf{E}[\xi_{l,n}] + V(\frac{2\log(K/\delta)}{n})^{1/2}$. Thus, to upper bound $\mathbf{E}[\xi_{l,n}]$, we use the symmetrization argument:

$$\mathbf{E}[\xi_{l,n}] \le 2\mathbf{E}\bigg[\sup_{\boldsymbol{\pi}\in\Pi_n(0)}\bigg|\frac{1}{n}\sum_{i=1}^n \epsilon_i \bar{\ell}'(f_{\boldsymbol{\pi}}(\boldsymbol{X}_i))f_l(\boldsymbol{X}_i)\bigg|\bigg] \tag{2.74}$$

$$\le 2M\mathbf{E}\bigg[\sup_{\boldsymbol{\pi}\in\Pi_n(0)}\bigg|\frac{1}{n}\sum_{i=1}^n \epsilon_i \bar{\ell}'(f_{\boldsymbol{\pi}}(\boldsymbol{X}_i))\bigg|\bigg] \tag{2.75}$$

$$\le \frac{2M}{\mu}\mathbf{E}\bigg[\bigg|\frac{1}{n}\sum_{i=1}^n \epsilon_i\bigg|\bigg] + 2M\mathbf{E}\bigg[\sup_{\boldsymbol{\pi}\in\Pi_n(0)}\bigg|\frac{1}{n}\sum_{i=1}^n \epsilon_i[\bar{\ell}'(f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)) - \bar{\ell}'(0)]\bigg|\bigg], \tag{2.76}$$

where the second inequality comes from [Boucheron et al., 2013, Th. 11.5]. Note that the function $\bar{\ell}'$, the derivative of $\bar{\ell}$ defined in (2.68), is by construction Lipschitz with constant $1/\mu^2$. Therefore, in view of the contraction principle,

$$\mathbf{E}[\xi_{l,n}] \le \frac{2M}{\mu}\mathbf{E}\bigg[\bigg(\frac{1}{n}\sum_{i=1}^n \epsilon_i\bigg)^2\bigg]^{1/2} + \frac{4M}{\mu^2}\mathbf{E}\bigg[\sup_{\boldsymbol{\pi}\in\Pi_n(0)}\frac{1}{n}\sum_{i=1}^n \epsilon_i f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)\bigg] \tag{2.77}$$

$$\le \frac{2M}{\mu\sqrt{n}} + \frac{4M}{\mu^2}\mathbf{E}\bigg[\sup_{k\in[K]}\frac{1}{n}\sum_{i=1}^n \epsilon_i f_k(\boldsymbol{X}_i)\bigg] \tag{2.78}$$

$$\le \frac{2M}{\mu\sqrt{n}} + \frac{8M^2}{\mu^2}\Big(\frac{\log K}{2n}\Big)^{1/2} \le \frac{2V^2(1+2\sqrt{2\log K})}{\sqrt{n}}. \tag{2.79}$$

As a consequence, we proved that with probability larger than $1-\delta$, we have $\xi_n \le 8V^2(\frac{\log K}{n})^{1/2}$. This completes the proof of the first inequality. In order to prove the second one, we simply change the way we have evaluated the term $\int \bar{\ell}(f_{\widehat{\boldsymbol{\pi}}})f^*$ in the left hand side of (2.70). Since $\bar{\ell}$ is strongly convex with a second order derivative bounded from below by $1/M^2$, we have $\bar{\ell}(f_{\widehat{\boldsymbol{\pi}}}) \ge \bar{\ell}(f^*) + \bar{\ell}'(f^*)(f_{\widehat{\boldsymbol{\pi}}} - f^*) + \frac{1}{2M^2}(f_{\widehat{\boldsymbol{\pi}}} - f^*)^2$. Since f^* is always larger than μ, the derivative $\bar{\ell}'(f^*)$ equals $1/f^*$. Integrating over $\mathcal{X}$, we get the second inequality of the proposition.

2.5.6 Auxiliary results

We start by a general convex result based on the strong convexity of the $-log$ function to derive a bound on the estimated log-likelihood.

Lemma 2.5.2. *Let us assume that* $M = \max_{j\in[K]} \|f_j\|_\infty < \infty$*. Then, for any* $\boldsymbol{\pi} \in \mathbb{B}_+^K$*, it holds that*

$$L_n(\widehat{\boldsymbol{\pi}}) \leq L_n(\boldsymbol{\pi}) - \frac{1}{2M^2 n}\|\bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2. \tag{2.80}$$

Proof. Recall that $\widehat{\boldsymbol{\pi}}$ minimizes the function L_n defined in (2.7) over Π_n. Furthermore, the function $u \mapsto \ell(u)$ is clearly strongly convex with a second order derivative bounded from below by $1/M^2$ over the set $u \in (0, M]$. Therefore, for every $\widehat{u} \in (0, M]$, the function $\widetilde{\ell}$ given by:

$$\widetilde{\ell}(u) = \ell(u) - \frac{1}{2M^2}(\widehat{u} - u)^2, \quad u \in (0, M], \tag{2.81}$$

is convex. This implies that the mapping

$$\boldsymbol{\pi} \mapsto \widetilde{L}_n(\boldsymbol{\pi}) = L_n(\boldsymbol{\pi}) - \frac{1}{2M^2 n}\|\mathbf{Z}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})\|_2^2 \tag{2.82}$$

is convex over the set $\boldsymbol{\pi} \in \mathbb{B}_+^K$. This yields[4]

$$\widetilde{L}_n(\boldsymbol{\pi}) - \widetilde{L}_n(\widehat{\boldsymbol{\pi}}) \geq \sup_{\boldsymbol{v}\in\partial \widetilde{L}_n(\widehat{\boldsymbol{\pi}})} \boldsymbol{v}^\top(\boldsymbol{\pi} - \widehat{\boldsymbol{\pi}}), \qquad \forall \boldsymbol{\pi} \in \mathbb{B}_+^K. \tag{2.83}$$

Using the Karush-Kuhn-Tucker conditions and the fact that $\widehat{\boldsymbol{\pi}}$ minimizes L_n, we get $\mathbf{0}_K \in \partial L_n(\widehat{\boldsymbol{\pi}}) = \partial \widetilde{L}_n(\widehat{\boldsymbol{\pi}})$. This readily gives $\widetilde{L}_n(\boldsymbol{\pi}) - \widetilde{L}_n(\widehat{\boldsymbol{\pi}}) \geq 0$, for any $\boldsymbol{\pi} \in \mathbb{B}_+^K$. The last step is to remark that $\mathbf{Z}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi}) = \bar{\mathbf{Z}}(\widehat{\boldsymbol{\pi}} - \boldsymbol{\pi})$, since both $\widehat{\boldsymbol{\pi}}$ and $\boldsymbol{\pi}$ have entries summing to one. □

The core of our results lies in the following proposition which bound the deviations of the empirical process part.

[4] We denote by ∂g the sub-differential of a convex function g.

Proposition 2.5.1 (Supremum of Empirical Process)**.** *For any* $\boldsymbol{\pi} \in \mathbb{B}_+^K$ *and* $\boldsymbol{x} \in \mathcal{X}$*, define* $\varphi(\pi, \boldsymbol{x}) = \int (\log f_{\boldsymbol{\pi}}) f^* - \log f_{\boldsymbol{\pi}}(\boldsymbol{x})$ *and consider* $\Phi_n(\boldsymbol{\pi}) = \frac{1}{n}\sum_{i=1}^n \varphi(\boldsymbol{\pi}, \boldsymbol{X}_i)$*. If* $K \geq 2$*, then for any* $\delta \in (0,1)$*, with probability at least* $1-\delta$*, we have*

$$\zeta_n = \sup_{\boldsymbol{\pi}\in\Pi_n} \big\|\nabla\Phi_n(\boldsymbol{\pi})\big\|_\infty \leq 8V^3\Big(\frac{\log(K/\delta)}{n}\Big)^{1/2}. \tag{2.84}$$

Furthermore, we have $\mathbf{E}[\zeta_n] \leq 4V^3\big(\frac{2\log(2K^2)}{n}\big)^{1/2}$ *and* $\mathbf{Var}[\zeta_n] \leq V^2/(2n)$*.*

Proof. To ease notation, let us denote $g_{\boldsymbol{\pi},l}(x) = \frac{f_l(x)}{f_{\boldsymbol{\pi}}(x)} - \mathbf{E}\big[\frac{f_l(\boldsymbol{X})}{f_{\boldsymbol{\pi}}(\boldsymbol{X})}\big]$ and

$$F(\mathbf{X}) = \sup_{\boldsymbol{\pi}\in\Pi_n} \big\|\nabla\Phi_n(\boldsymbol{\pi})\big\|_\infty = \sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]} \Big|\frac{1}{n}\sum_{i=1}^n g_{\boldsymbol{\pi},l}(\boldsymbol{X}_i)\Big|, \tag{2.85}$$

where $\mathbf{X} = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n)$. To derive a bound on F, we will use the McDiarmid concentration inequality that requires the bounded difference condition to hold for F. For some $i_0 \in [n]$, let $\mathbf{X}' = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}'_{i_0}, \ldots, \boldsymbol{X}_n)$ be a new sample obtained from $\mathbf{X}$ by modifying the i_0-th element $\boldsymbol{X}_i$ and by leaving all the others unchanged. Then, we have

$$F(\mathbf{X}) - F(\mathbf{X}') = \sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]} \Big|\frac{1}{n}\sum_{i=1}^n g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}_i\big)\Big| - \sup_{(\boldsymbol{\pi},l)\in\Pi\times[K]} \Big|\frac{1}{n}\sum_{i=1}^n g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}'_i\big)\Big| \tag{2.86}$$

$$\leq \sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]} \Big|\frac{1}{n}\sum_{i=1}^n g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}_i\big) - \frac{1}{n}\sum_{i=1}^n g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}'_i\big)\Big| \tag{2.87}$$

$$= \sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]} \Big|\frac{1}{n}\Big(g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}_{i_0}\big) - g_{\boldsymbol{\pi},l}\big(\boldsymbol{X}'_{i_0}\big)\Big)\Big| \leq \frac{V}{n}, \tag{2.88}$$

where the last inequality is a direct consequence of assumption (2.11). Therefore, using the McDiarmid concentration inequality recalled in Theorem 2.6.3 below, we check that the inequality

$$F(\mathbf{X}) \leq \mathbf{E}(F(\mathbf{X})) + V\sqrt{\frac{\log(1/\delta)}{2n}} \tag{2.89}$$

holds with probability at least $1-\delta$. Furthermore, in view of the Efron-Stein inequality, we have

$$\mathbf{Var}[\zeta_n] = \mathbf{Var}[F(\mathbf{X})] \le \frac{V^2}{2n}. \tag{2.90}$$

Let us denote $\mathcal{G} := \{(f_l/f_{\boldsymbol{\pi}}) - 1, (\boldsymbol{\pi}, l) \in \Pi_n \times [K]\}$ and $\mathfrak{R}_{n,q}(\mathcal{G})$ the Rademacher complexity of $\mathcal{G}$ given by

$$\mathfrak{R}_n(\mathcal{G}) = \mathbf{E}_\epsilon\bigg[\sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]}\bigg|\frac{1}{n}\sum_{i=1}^n \epsilon_i\Big(\frac{f_l(\boldsymbol{X}_i)}{f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)} - 1\Big)\bigg|\bigg], \tag{2.91}$$

with $\epsilon_1, \ldots, \epsilon_n$ independent and identically distributed Rademacher random variables independent of $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$. Using the symmetrization inequality (see, for instance, Theorem 2.1 in Koltchinskii [2011]) we have

$$\mathbf{E}[F(\mathbf{X})] = \mathbf{E}[\zeta_n] \le 2\mathbf{E}[\mathfrak{R}_n(\mathcal{G})]. \tag{2.92}$$

Lemma 2.5.3. *The Rademacher complexity defined in (2.91) satisfies*

$$\mathfrak{R}_n(\mathcal{G}) \le 4V^3\sqrt{\frac{\log K}{n}}. \tag{2.93}$$

Proof. The proof relies on the contraction principle of Ledoux and Talagrand [1991] that we recall in Section 2.6.3 for the convenience. We apply this principle to the random variables $X_{i,(\boldsymbol{\pi},l)} = f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)/f_l(\boldsymbol{X}_i) - 1$ and to the function $\psi(x) = (1+x)^{-1} - 1$. Clearly ψ is Lipschitz on $[\frac{1}{V} - 1, V - 1]$ with the Lipschitz constant equal to V^2 and $\psi(0) = 0$. Therefore

$$\begin{aligned}
\mathfrak{R}_n(\mathcal{G}) &\le \mathbf{E}_\epsilon\bigg[\sup_{(\boldsymbol{\pi},l)}\frac{1}{n}\sum_{i=1}^n \epsilon_i\psi(\boldsymbol{X}_{i,(\boldsymbol{\pi},l)})\bigg] + \mathbf{E}_\epsilon\bigg[\sup_{(\boldsymbol{\pi},l)}\frac{1}{n}\sum_{i=1}^n \epsilon_i(-\psi)(\boldsymbol{X}_{i,(\boldsymbol{\pi},l)})\bigg] \\
&\le 2V^2\mathbf{E}_\epsilon\bigg[\sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]}\frac{1}{n}\sum_{i=1}^n \epsilon_i\boldsymbol{X}_{i,(\boldsymbol{\pi},l)}\bigg] \\
&= 2V^2\mathbf{E}_\epsilon\bigg[\sup_{(\boldsymbol{\pi},l)\in\Pi_n\times[K]}\frac{1}{n}\sum_{i=1}^n \epsilon_i\bigg(\frac{f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)} - 1\bigg)\bigg].
\end{aligned} \tag{2.94}$$

Expanding $f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)$ we obtain

$$\begin{aligned}\mathbf{E}_\epsilon\left[\sup_{(\boldsymbol{\pi},l)}\frac{1}{n}\sum_{i=1}^{n}\epsilon_i\left(\frac{f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)}-1\right)\right] &= \mathbf{E}_\epsilon\left[\sup_{(\boldsymbol{\pi},l)}\sum_{k=1}^{K}\frac{\pi_k}{n}\sum_{i=1}^{n}\epsilon_i\left(\frac{f_k(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)}-1\right)\right]\\ &= \mathbf{E}_\epsilon\left[\max_{k,l\in[K]}\frac{1}{n}\sum_{i=1}^{n}\epsilon_i\left(\frac{f_k(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)}-1\right)\right].\end{aligned} \tag{2.95}$$

We apply now Theorem 2.6.2 with $s=(k,l)$, $N=K^2$, $a=-V$, $b=V$ and $Y_{i,s}=\epsilon_i\big(\frac{f_k(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)}-1\big)$. This yields

$$\mathbf{E}_\epsilon\left[\max_{k,l\in[K]}\frac{1}{n}\sum_{i=1}^{n}\epsilon_i\left(\frac{f_k(\boldsymbol{X}_i)}{f_l(\boldsymbol{X}_i)}-1\right)\right]\le 2V\Big(\frac{\log K^2}{2n}\Big)^{1/2}. \tag{2.96}$$

This completes the proof of the lemma. □

Combining inequalities (2.89,2.92) and Lemma 2.5.3, we get that the inequality

$$F(\mathbf{X})\le 8V^3\Big(\frac{\log K}{n}\Big)^{1/2}+V\Big(\frac{\log(1/\delta)}{2n}\Big)^{1/2} \tag{2.97}$$

holds with probability at least $1-\delta$. Noticing that $V\ge 1$ and, for $K\ge 2$, $\delta\in(0,K^{-1/31})$ we have $8\sqrt{\log K}+\sqrt{(1/2)\log(1/\delta)}\le 8\sqrt{\log(K/\delta)}$, we get the first claim of the proposition. The second claim is a direct consequence of Lemma 2.5.3 and (2.92). □

2.6 Proof of the lower bound for nearly-D-sparse aggregation

We prove the minimax lower bound for estimation in Kullback-Leibler risk using the following slightly adapted version of Theorem 2.5 from Tsybakov [2009]. Throughout this section, we denote by $\lambda_{\min,\boldsymbol{\Sigma}}(k)$ and $\lambda_{\max,\boldsymbol{\Sigma}}(k)$, respectively, the smallest and the largest eigenvalue of all $k\times k$ principal minors of the matrix $\boldsymbol{\Sigma}$.

Theorem 2.6.1. *For some integer $L \geq 4$ assume that $\mathcal{H}_{\mathcal{F}}(\gamma, D)$ contains L elements $f_{\boldsymbol{\pi}^{(1)}}, \ldots, f_{\boldsymbol{\pi}^{(L)}}$ satisfying the following two conditions.*

(i) $\mathrm{KL}(f_{\boldsymbol{\pi}^{(j)}}||f_{\boldsymbol{\pi}^{(k)}}) \geq 2s > 0$, *for all pairs (j,k) such that $1 \leq j < k \leq L$.*

(ii) For product densities f_ℓ^n defined on $\mathcal{X}^n$ by $f_\ell^n(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = f_{\boldsymbol{\pi}^{(\ell)}}(\boldsymbol{x}_1) \times \ldots \times f_{\boldsymbol{\pi}^{(\ell)}}(\boldsymbol{x}_n)$ it holds

$$\max_{\ell \in [L]} \mathrm{KL}(f_\ell^n || f_1^n) \leq \frac{\log L}{16}. \tag{2.98}$$

Then

$$\inf_{\widehat{f}} \sup_{f \in \mathcal{H}_{\mathcal{F}}(\gamma, D)} \mathbf{P}_f\big(\mathrm{KL}(f||\widehat{f}) \geq s\big) \geq 0.17. \tag{2.99}$$

To establish the bound claimed in Theorem 2.3.1, we will split the problem into two parts, corresponding to the following two subsets of $\mathcal{H}_{\mathcal{F}}(\gamma, D)$

$$\begin{aligned}
\mathcal{H}_{\mathcal{F}}(0, D) \quad &= \big\{ f_{\boldsymbol{\pi}} : \boldsymbol{\pi} \in \mathbb{B}_+^K \text{ s.t. } \exists\, J \subset [K] \text{ with } \|\boldsymbol{\pi}_{J^c}\|_1 = 0 \text{ and } |J| \leq D \big\}, \\
\mathcal{H}_{\mathcal{F}}(\gamma, 1) \quad &= \big\{ f_{\boldsymbol{\pi}} : \boldsymbol{\pi} \in \mathbb{B}_+^K \text{ s.t. } \pi_1 = 1 - \gamma \text{ and } \textstyle\sum_{j=2}^K \pi_j = \gamma \big\}.
\end{aligned} \tag{2.100}$$

We will show that over $\mathcal{H}_{\mathcal{F}}(0, D)$, we have a lower bound of order $\log(1 + K/D)/n$ while over $\mathcal{H}_{\mathcal{F}}(\gamma, 1)$, a lower bound of order $\big[\frac{\gamma^2}{n} \log\big(1 + K/(\gamma\sqrt{n})\big)\big]^{1/2}$ holds true. Therefore, the lower bound over $\mathcal{H}_{\mathcal{F}}(\gamma, D)$ is larger than the average of these bounds.

For any $M \geq 1$ and $k \in [M-1]$, let Ω_k^M be the subset of $\{0,1\}^M$ defined by

$$\Omega_k^M := \Big\{ \boldsymbol{\omega} \in \{0,1\}^M : \|\boldsymbol{\omega}\|_1 = k \Big\}. \tag{2.101}$$

Before starting, we remind here a version of the Varshamov-Gilbert lemma (see, for instance, [Rigollet and Tsybakov, 2011, Lemma 8.3]) which will be helpful for deriving our lower bounds.

Lemma 2.6.1. *Let $M \geq 4$ and $k \in [M/2]$ be two integers. Then there exist a subset $\Omega \subset \Omega_k^M$ and an absolute constant C_1 such that*

$$\|\boldsymbol{\omega} - \boldsymbol{\omega}'\|_1 \geq \frac{k+1}{4} \quad \forall \boldsymbol{\omega}, \boldsymbol{\omega}' \in \Omega \text{ s.t. } \boldsymbol{\omega} \neq \boldsymbol{\omega}' \tag{2.102}$$

and $L = |\Omega|$ *satisfies* $L \geq 4$ *and*

$$\log L \geq C_1 k \log\Big(1 + \frac{eM}{k}\Big). \tag{2.103}$$

We will also use the following lemma that allows us to relate the KL-divergence $\mathrm{KL}(f_{\boldsymbol{\pi}}||f_{\boldsymbol{\pi}'})$ to the Euclidean distance between the weight vectors $\boldsymbol{\pi}$ and $\boldsymbol{\pi}'$.

Lemma 2.6.2. *If the dictionary* $\mathcal{F}$ *satisfies the boundedness assumption* (2.11), *then for any* $f_{\boldsymbol{\pi}}, f_{\boldsymbol{\pi}'} \in \mathcal{H}_{\mathcal{F}}(\gamma, D)$ *we have*

$$\frac{1}{2V^2M}\,\|\boldsymbol{\Sigma}^{1/2}(\boldsymbol{\pi}'-\boldsymbol{\pi})\|_2^2 \leq \mathrm{KL}(f_{\boldsymbol{\pi}}||f_{\boldsymbol{\pi}'}) \leq \frac{V^2}{2m}\,\|\boldsymbol{\Sigma}^{1/2}(\boldsymbol{\pi}'-\boldsymbol{\pi})\|_2^2. \tag{2.104}$$

Proof. Using the Taylor expansion, one can check that for any $u \in [1/L, L]$, we have $(1-u) + \frac{1}{2V^2}(u-1)^2 \leq -\log u \leq (1-u) + \frac{V^2}{2}(u-1)^2$. Therefore,

$$\frac{1}{2V^2}\int_{\mathcal{X}}\Big(\frac{f_{\boldsymbol{\pi}'}}{f_{\boldsymbol{\pi}}} - 1\Big)^2 f_{\boldsymbol{\pi}}\,d\nu \leq \mathrm{KL}(f_{\boldsymbol{\pi}}||f_{\boldsymbol{\pi}'}) \leq \frac{V^2}{2}\int_{\mathcal{X}}\Big(\frac{f_{\boldsymbol{\pi}'}}{f_{\boldsymbol{\pi}}} - 1\Big)^2 f_{\boldsymbol{\pi}}\,d\nu. \tag{2.105}$$

Since $\mathcal{F}$ satisfies the boundedness assumption, we get

$$\frac{1}{2MV^2}\int_{\mathcal{X}}\big(f_{\boldsymbol{\pi}'} - f_{\boldsymbol{\pi}}\big)^2 d\nu \leq \mathrm{KL}(f_{\boldsymbol{\pi}}||f_{\boldsymbol{\pi}'}) \leq \frac{V^2}{2m}\int_{\mathcal{X}}\big(f_{\boldsymbol{\pi}'} - f_{\boldsymbol{\pi}}\big)^2 d\nu. \tag{2.106}$$

The claim of the lemma follows from these inequalities and the fact that $\int_{\mathcal{X}}\big(f_{\boldsymbol{\pi}'} - f_{\boldsymbol{\pi}}\big)^2 d\nu = \|\boldsymbol{\Sigma}^{1/2}(\boldsymbol{\pi}'-\boldsymbol{\pi})\|_2^2$. □

2.6.1 Lower bound on $\mathcal{H}_{\mathcal{F}}(0, D)$

We show that the lower bound $({}^{D}\!/_{n})\log(1 + {}^{eK}\!/_{D}) \wedge \big(({}^{1}\!/_{n})\log(1 + {}^{K}\!/_{\sqrt{n}})\big)^{1/2}$ holds when we consider the worst case error for f^* belonging to the set $\mathcal{H}_{\mathcal{F}}(0, D)$.

Proposition 3. *If* $\log(1 + eK) \leq n$ *then, for the constant*

$$C_2 = \frac{C_1 m \bar{\kappa}_{\boldsymbol{\Sigma}}(2D, 0)}{2^9V^2M(C_1 m \vee 4V^2\lambda_{\max,\boldsymbol{\Sigma}}(2D))} \geq \frac{C_1 m \varkappa_*}{2^9V^2M(C_1 m \vee 4V^2\varkappa^*)}, \tag{2.107}$$

we have

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(0,D)} \mathbf{P}_f\left(\mathrm{KL}(f\|\widehat{f}) \geq C_2\,\frac{D\log(1+\frac{K}{D})}{n}\bigwedge\left(\frac{\log\left(1+\frac{K}{\sqrt{n}}\right)}{n}\right)^{1/2}\right) \geq 0.17. \tag{2.108}$$

Proof. We assume that $D \leq K/2$. The case $D > K/2$ can be reduced to the case $D = K/2$ by using the inclusion $\mathcal{H}_{\mathcal{F}}(0, K/2) \subset \mathcal{H}_{\mathcal{F}}(0, D)$. Let us set $A_1 = 4 \vee 16V^2\lambda_{\max,\mathbf{\Sigma}}(2D)/(C_1 m)$ and denote by d the largest integer such that

$$d \leq D \quad \text{and} \quad d^2 \log\left(1 + \frac{eK}{d}\right) \leq A_1 n. \tag{2.109}$$

According to Lemma 2.6.1, there exists a subset $\Omega = \{\boldsymbol{\omega}^{(\ell)} : \ell \in [L]\}$ of Ω_d^K of cardinality $L \geq 4$ satisfying $\log L \geq C_1 d \log(1 + eK/d)$ such that for any pair of distinct elements $\boldsymbol{\omega}^{(\ell)}, \boldsymbol{\omega}^{(\ell')} \in \Omega$ we have $\|\boldsymbol{\omega}^{(\ell)} - \boldsymbol{\omega}^{(\ell')}\|_1 \geq d/4$. Using these binary vectors $\boldsymbol{\omega}^{(\ell)}$, we define the set $\mathcal{D} = \{\boldsymbol{\pi}^{(1)}, \ldots, \boldsymbol{\pi}^{(L)}\} \subset \mathbb{B}_+^K$ as follows:

$$\boldsymbol{\pi}^{(1)} = \boldsymbol{\omega}^{(1)}/d, \quad \boldsymbol{\pi}^{(\ell)} = (1-\varepsilon)\boldsymbol{\pi}^{(1)} + \varepsilon\boldsymbol{\omega}^{(\ell)}/d, \quad \ell = 2, \ldots, L. \tag{2.110}$$

Clearly, for every $\varepsilon \in [0, 1]$, the vectors $\boldsymbol{\pi}^{(\ell)}$ belong to $\mathbb{B}_+^K$. Furthermore, for any pair of distinct values $\ell, \ell' \in [L]$, we have $\|\boldsymbol{\pi}^{(\ell)} - \boldsymbol{\pi}^{(\ell')}\|_q^q = (\varepsilon/d)^q\|\boldsymbol{\omega}^{(\ell)} - \boldsymbol{\omega}^{(\ell')}\|_1 \geq (\varepsilon/d)^q d/4$. In view of Lemma 2.6.2, this yields

$$\mathrm{KL}(f_{\boldsymbol{\pi}^{(\ell)}}\|f_{\boldsymbol{\pi}^{(\ell')}}) \geq \frac{\bar{\kappa}_{\mathbf{\Sigma}}(2d, 0)}{4V^2 M d}\|\boldsymbol{\pi}^{(\ell)} - \boldsymbol{\pi}^{(\ell')}\|_1^2 \geq \frac{\bar{\kappa}_{\mathbf{\Sigma}}(2D, 0)}{64V^2 M} \times \frac{\varepsilon^2}{d}. \tag{2.111}$$

Let us choose

$$\varepsilon^2 = \frac{d^2\log(1 + eK/d)}{nA_1}. \tag{2.112}$$

It follows from (2.109) that $\varepsilon \leq 1$. Inserting this value of ε in (2.111), we get

$$\mathrm{KL}(f_{\boldsymbol{\pi}^{(\ell)}}\|f_{\boldsymbol{\pi}^{(\ell')}}) \geq 2C_2\,\frac{d\log(1 + eK/d)}{n}. \tag{2.113}$$

This inequality shows that condition (i) of Theorem 2.6.1 is satisfied with $s = C_2\,({}^{d}/{}_{n})\log(1+eK/d)$. For the second condition of the same theorem, we have

$$\max_{\ell\in[L]} \mathrm{KL}(f_\ell^n || f_1^n) = n \max_{\ell} \mathrm{KL}(f_{\boldsymbol{\pi}^{(\ell)}} || f_{\boldsymbol{\pi}^{(1)}}) \tag{2.114}$$

$$\leq \frac{nV^2\lambda_{\max,\boldsymbol{\Sigma}}(2d)}{2m} \max_{\ell} \|\boldsymbol{\pi}^{(\ell)} - \boldsymbol{\pi}^{(1)}\|_2^2 \tag{2.115}$$

$$\leq \frac{nV^2\lambda_{\max,\boldsymbol{\Sigma}}(2D)}{m} \times \frac{\varepsilon^2}{d}, \tag{2.116}$$

since one can check that $\|\boldsymbol{\pi}^{(\ell)} - \boldsymbol{\pi}^{(1)}\|_2^2 \leq (\varepsilon/d)^2 \|\boldsymbol{\omega}^{(\ell)} - \boldsymbol{\omega}^{(1)}\|_1 \leq 2\varepsilon^2/d$. Therefore, using the definition of ε, we get

$$\max_{\ell\in[L]} \mathrm{KL}(f_\ell^n || f_1^n) \leq \frac{nV^2\lambda_{\max,\boldsymbol{\Sigma}}(2D)}{m} \times \frac{C_1 dm \log(1+eK/d)}{16nV^2\lambda_{\max,\boldsymbol{\Sigma}}(2D)} \tag{2.117}$$

$$= \frac{C_1 d \log(1+eK/d)}{16} \leq \frac{\log L}{16}. \tag{2.118}$$

Theorem 2.6.1 implies that

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(0,D)} \mathbf{P}_f\left(\mathrm{KL}(f||\widehat{f}) \geq C_2 \frac{d\log(1+eK/d)}{n}\right) \geq 0.17. \tag{2.119}$$

We use the fact that d is the largest integer satisfying (2.109). Therefore, either $d+1 > D$ or

$$(d+1)^2 \log\left(1 + \frac{eK}{d+1}\right) \leq A_1 n. \tag{2.120}$$

If $d \geq D$, then the claim of the proposition follows from (2.119), since $d\log(1+eK/d) \geq D\log(1+eK/D)$. On the other hand, if (2.120) is true, then

$$d\log(1+eK/d) \geq \frac{1}{2}(d+1)\log(1+eK/(d+1))$$

$$\geq \frac{1}{2}\big(A_1 n \log(1+eK/(d+1))\big)^{1/2}. \tag{2.121}$$

In addition, $d^2\log(1+eK/d) \le A_1 n$ implies that $(d+1)^2 \le A_1 n$. Combining the last two inequalities, we get the inequality $d\log(1+eK/d) \ge {}^1\!/_2\big(A_1 n\log(1+eK/\sqrt{A_1 n})\big)^{1/2} \ge \big(n\log(1+eK/\sqrt{n})\big)^{1/2}$. Therefore, in view of (2.119), we get the claim of the proposition. $\square$

2.6.2 Lower bound on $\mathcal{H}_{\mathcal{F}}(\gamma, 1)$

Next result shows that the lower bound $\frac{\gamma^2}{n}\log\big(1+\frac{K}{\gamma\sqrt{n}}\big)$ holds for the worst case error when f^* belongs to the set $\mathcal{H}_{\mathcal{F}}(\gamma,1)$.

Proposition 4. *Assume that*

$$\Big(\frac{\log(1+eK)}{n}\Big)^{1/2} \le 2\gamma. \tag{2.122}$$

Then, for the constant $C_3 = \frac{C_1 m\bar{\kappa}_{\mathbf{\Sigma}}(2D,0)}{2^{12}V^4 M\lambda_{\max,\mathbf{\Sigma}}(2D)}$, *it holds that*

$$\inf_{\widehat{f}}\ \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,1)} \mathbf{P}_f\bigg(\mathrm{KL}(f\|\widehat{f}) \ge C_3\Big\{\frac{\gamma^2}{n}\log\Big(1+\frac{K}{\gamma\sqrt{n}}\Big)\Big\}^{1/2}\bigg) \ge 0.17. \tag{2.123}$$

Proof. Let $C > 2$ be a constant the precise value of which will be specified later. Denote by d the largest integer satisfying

$$d\sqrt{\log(1+eK/d)} \le C\gamma\sqrt{n}. \tag{2.124}$$

Note that $d \ge 1$ in view of the condition $(\frac{\log(1+eK)}{n})^{1/2} \le 2\gamma$ of the proposition. This readily implies that $d \le C\gamma\sqrt{n}$ and, therefore,

$$\frac{\gamma}{d} \ge C^{-1}\Big\{\frac{1}{n}\log\Big(1+\frac{eK}{C\gamma\sqrt{n}}\Big)\Big\}^{1/2} \ge 2C^{-2}\Big\{\frac{1}{n}\log\Big(1+\frac{K}{\gamma\sqrt{n}}\Big)\Big\}^{1/2}. \tag{2.125}$$

Let us first consider the case $d \le (K-1)/2$. According to Lemma 2.6.1, there exists a subset $\Omega \subset \Omega_d^{K-1}$ of cardinality L satisfying $\log L \ge C_1\log\big(1+\frac{e(K-1)}{d}\big)$ and $\|\boldsymbol{\omega}^{(\ell)} - \boldsymbol{\omega}^{(\ell')}\|_1 \ge d/4$ for any pair of distinct elements $\boldsymbol{\omega}, \boldsymbol{\omega}'$ taken from Ω. With these binary vectors in hand, we define the set $\mathcal{D} \subset \mathbb{B}_+^K$ of cardinality L as follows:

$$\mathcal{D} = \Big\{ \boldsymbol{\pi} = \big(1-\gamma, \gamma\boldsymbol{\omega}/d\big) : \quad \omega \in \Omega \Big\}. \tag{2.126}$$

It is clear that all the vectors of $\mathcal{D}$ belong to $\mathcal{H}_{\mathcal{F}}(\gamma, 1)$. Let us fix now an element of $\mathcal{D}$ and denote it by $\boldsymbol{\pi}^1$, the corresponding element of Ω being denoted by $\boldsymbol{\omega}^1$. We have

$$\max_{\boldsymbol{\pi}\in\mathcal{D}} \mathrm{KL}(f_{\boldsymbol{\pi}}^n || f_{\boldsymbol{\pi}^1}^n) \le \frac{nV^2}{2m} \max_{\boldsymbol{\pi}\in\mathcal{D}} \|\boldsymbol{\Sigma}^{1/2}(\boldsymbol{\pi}-\boldsymbol{\pi}^1)\|_2^2 \tag{2.127}$$

$$\le \frac{nV^2 \lambda_{\max,\boldsymbol{\Sigma}}(2d)\gamma^2}{2md^2} \max_{\boldsymbol{\omega}\in\Omega} \|\boldsymbol{\omega}-\boldsymbol{\omega}^1\|_2^2 \tag{2.128}$$

$$\le \frac{nV^2 \lambda_{\max,\boldsymbol{\Sigma}}(2d)\gamma^2}{md}. \tag{2.129}$$

The definition of d yields $(d+1)\sqrt{\log(1+eK/(d+1))} > C\gamma\sqrt{n}$, which implies that

$$\begin{aligned} \frac{\gamma^2}{d} &\le 2(d+1)\frac{\gamma^2}{(d+1)^2} \\ &\le 2(d+1)\frac{\log\big(1+eK/(d+1)\big)}{nC^2} \\ &\le \frac{4d\log\big(1+e(K-1)/d\big)}{nC^2}. \end{aligned} \tag{2.130}$$

Combined with eq. (2.129), this implies that

$$\max_{\boldsymbol{\pi}\in\mathcal{D}} \mathrm{KL}(f_{\boldsymbol{\pi}}^n || f_{\boldsymbol{\pi}^1}^n) \le \frac{nV^2\lambda_{\max,\boldsymbol{\Sigma}}(2d)}{m} \times \frac{4d\log\big(1+e(K-1)/d\big)}{nC^2} \tag{2.131}$$

$$= \frac{4V^2\lambda_{\max,\boldsymbol{\Sigma}}(2d)}{mC^2} \times d\log\big(1+e(K-1)/d\big). \tag{2.132}$$

Choosing

$$C^2 = 2 \vee \frac{64V^2\lambda_{\max,\boldsymbol{\Sigma}}(2d)}{C_1 m}$$

we get that $\max_{\boldsymbol{\pi}\in\mathcal{D}} \mathrm{KL}(f_{\boldsymbol{\pi}}^n || f_{\boldsymbol{\pi}^1}^n) \le \frac{1}{16} C_1 d \log\big(1+e(K-1)/d\big) \le \frac{\log L}{16}$.

Furthermore, for any $\boldsymbol{\pi}, \boldsymbol{\pi}' \in \mathcal{D}$, in view of Lemma 2.6.2 and (2.125), we have

$$\begin{aligned}
\mathrm{KL}(f_{\boldsymbol{\pi}}||f_{\boldsymbol{\pi}'}) &\geq \frac{\bar{\kappa}_{\boldsymbol{\Sigma}}(2d,0)}{4V^2Md}\big\|\boldsymbol{\pi}-\boldsymbol{\pi}'\big\|_1^2 = \frac{\bar{\kappa}_{\boldsymbol{\Sigma}}(2d,0)\gamma^2}{4V^2Md^3}\big\|\boldsymbol{\omega}-\boldsymbol{\omega}'\big\|_1^2 && (2.133)\\
&\geq \frac{\bar{\kappa}_{\boldsymbol{\Sigma}}(2d,0)}{64V^2M}\times\frac{\gamma^2}{d} && (2.134)\\
&\geq \frac{\bar{\kappa}_{\boldsymbol{\Sigma}}(2d,0)}{32V^2MC^2}\times\Big\{\frac{\gamma^2}{n}\log\Big(1+\frac{K}{\gamma\sqrt{n}}\Big)\Big\}^{1/2}. && (2.135)
\end{aligned}$$

Since $\frac{\bar{\kappa}_{\boldsymbol{\Sigma}}(2d,0)}{32V^2MC^2} = 2C_3$, this implies that Theorem 2.6.1 can be applied, which leads to the inequality

$$\inf_{\widehat{f}}\sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,1)}\mathbf{P}_f\bigg(\mathrm{KL}(f||\widehat{f})\geq C_3\Big\{\frac{\gamma^2}{n}\log\Big(1+\frac{K}{\gamma\sqrt{n}}\Big)\Big\}^{1/2}\bigg)\geq 0.17. \qquad (2.136)$$

To complete the proof of the proposition, we have to consider the case $d > (K-1)/2$. In this case, we can repeat all the previous arguments for $d = K/2$ and get the desired inequality. $\square$

2.6.3 Lower bound holding for all densities

Now that we have lower bounds in probability for $\mathcal{H}_{\mathcal{F}}(0, D)$ and $\mathcal{H}_{\mathcal{F}}(\gamma, 1)$, we can derive a lower bound in expectation for $\mathcal{H}_{\mathcal{F}}(\gamma, D)$. In particular, to prove Theorem 2.3.1, we will use the inequality

$$\mathcal{R}\big(\mathcal{H}_{\mathcal{F}}(\gamma,D)\big)\geq\inf_{\widehat{f}}\sup_{f^*\in\mathcal{H}_{\mathcal{F}}(0,D)\cup\mathcal{H}_{\mathcal{F}}(\gamma,1)}\mathbf{E}[\mathrm{KL}(f^*||\widehat{f})]. \qquad (2.137)$$

Proof of Theorem 2.3.1. To ease notation, let us define

$$r(n,K,\gamma,D)=\bigg[\frac{\gamma^2}{n}\log\bigg(1+\frac{K}{\gamma\sqrt{n}}\bigg)\bigg]^{1/2}+\frac{D\log(1+K/D)}{n}\bigwedge\bigg(\frac{\log(1+K/\sqrt{n})}{n}\bigg)^{1/2}. \qquad (2.138)$$

We first consider the case where the dominating term is the first one, that is

$$\bigg[\frac{\gamma^2}{n}\log\bigg(1+\frac{K}{\gamma\sqrt{n}}\bigg)\bigg]^{1/2}\geq\frac{3D\log(1+K/D)}{n}. \qquad (2.139)$$

On the one hand, since $D \geq 1$, we have

$$\frac{3D\log(1+K/D)}{n} \geq \frac{\log(1+eK)}{n}. \tag{2.140}$$

On the other hand, using the inequality $\log(1+x) \leq x$, we get

$$\left[\frac{\gamma^2}{n}\log\left(1+\frac{K}{\gamma\sqrt{n}}\right)\right]^{1/2} \leq \frac{\gamma}{\sqrt{n}}\left[\log(1+eK)+\log\left(1+\frac{1}{e^2\gamma^2 n}\right)\right]^{1/2} \tag{2.141}$$

$$\leq \gamma\left[\frac{\log(1+eK)}{n}\right]^{1/2} + \frac{\gamma}{\sqrt{n}}\left[\frac{1}{e^2\gamma^2 n}\right]^{1/2} \tag{2.142}$$

$$\leq \gamma\left[\frac{\log(1+eK)}{n}\right]^{1/2} + \frac{\log(1+eK)}{2n}. \tag{2.143}$$

Combining (2.139), (2.140) and (2.143), we get

$$\left(\frac{\log(1+eK)}{n}\right)^{1/2} \leq 2\gamma. \tag{2.144}$$

This implies that we can apply Proposition 4, which yields

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,D)} \mathbf{P}_f\left(\mathrm{KL}(f||\widehat{f}) \geq C_3\left\{\frac{\gamma^2}{n}\log\left(1+\frac{K}{\gamma\sqrt{n}}\right)\right\}^{1/2}\right) \geq 0.17. \tag{2.145}$$

In view of (2.139), this implies that

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,D)} \mathbf{P}_f\left(\mathrm{KL}(f||\widehat{f}) \geq \frac{3}{4}C_3\, r(n,K,\gamma,D)\right) \geq 0.17. \tag{2.146}$$

We now consider the second case, where the dominating term in the rate is the second one, that is

$$\left[\frac{\gamma^2}{n}\log\left(1+\frac{K}{\gamma\sqrt{n}}\right)\right]^{1/2} \leq \frac{3D\log(1+K/D)}{n} \bigwedge \left(\frac{\log(1+K/\sqrt{n})}{n}\right)^{1/2}. \tag{2.147}$$

In view of Proposition 3, we have

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,D)} \mathbf{P}_f\left(\mathrm{KL}(f||\widehat{f}) \geq C_2\,\frac{D\log(1+\frac{K}{D})}{n} \bigwedge \left(\frac{\log\left(1+\frac{K}{\sqrt{n}}\right)}{n}\right)^{1/2}\right) \geq 0.17. \tag{2.148}$$

In view of (2.147), we get

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,D)} \mathbf{P}_f\Big(\mathrm{KL}(f||\widehat{f}) \geq \frac{1}{4}C_2\, r(n,K,\gamma,D)\Big) \geq 0.17. \tag{2.149}$$

Thus, we have proved that $\log(1+eK) \leq n$ implies that

$$\inf_{\widehat{f}} \sup_{f\in\mathcal{H}_{\mathcal{F}}(\gamma,D)} \mathbf{P}_f\big(\mathrm{KL}(f||\widehat{f}) \geq C_4\, r(n,K,\gamma,D)\big) \geq 0.17, \tag{2.150}$$

for some constant $C_4 > 0$, whatever the relation between γ and D. The desired lower bound follows now from the Tchebychev inequality $\mathbf{E}\big[\mathrm{KL}(f||\widehat{f})\big] \geq C_4\, r(n,K,\gamma,D)\mathbf{P}_f\big(\mathrm{KL}(f||\widehat{f}) \geq C_4\, r(n,K,\gamma,D)\big)$. $\square$

Appendix A: Concentration inequalities

This section contains some well-known results, which are recalled here for the sake of the self-containedness of the paper.

Theorem 2.6.2. *For each $s = 1,\dots,N$, let $Y_{1,s},\dots,Y_{n,s}$ be n independent and zero mean random variables such that for some real numbers a, b we have $\mathbf{P}(Y_{i,s} \in [a,b]) = 1$ for all $i \in [n]$ and $s \in [N]$. Then, we have*

$$\mathbf{E}\Big[\max_{s\in[N]} \frac{1}{n}\sum_{i=1}^{n} Y_{i,s}\Big] \leq (b-a)\Big(\frac{\log N}{2n}\Big)^{1/2}, \tag{2.151}$$

$$\mathbf{E}\Big[\max_{s\in[N]} \Big|\frac{1}{n}\sum_{i=1}^{n} Y_{i,s}\Big|\Big] \leq (b-a)\Big(\frac{\log(2N)}{2n}\Big)^{1/2}. \tag{2.152}$$

Proof. We denote $Z_s = \frac{1}{n}\sum_{i=1}^{n} Y_{i,s}$ for $s = 1,\dots,N$ and $Z_s = -\frac{1}{n}\sum_{i=1}^{n} Y_{i,s}$ for $s = N+1,\dots,2N$. For every $s \in [2N]$, the logarithmic moment generating function $\psi_s(\lambda) = \log \mathbf{E}[e^{\lambda Z_s}]$ satisfies

$$\psi_s(\lambda) = \log\big(\prod_i \mathbf{E}[e^{\lambda Y_{i,s}/n}]\big) = \sum_{i=1}^{n} \log \mathbf{E}[e^{\lambda Y_{i,s}/n}] \leq \frac{\lambda^2(b-a)^2}{8n}, \tag{2.153}$$

where the last inequality is a consequence of the Hoeffding lemma (see, for instance, Lemma 2.2 in [Boucheron et al., 2013]). This means that Z_s is sub-Gaussian with variance-factor $\nu = (b-a)^2/4n$. Therefore, Theorem 2.5 from [Boucheron et al., 2013] yields $\mathbf{E}[\max_s Z_s] \leq \sqrt{2\nu \log(2N)}$, which completes the proof. □

We group and state together the bounded differences and the Efron-Stein inequalities (Boucheron et al. [2013], Theorems 6.2 and 3.1, respectively).

Theorem 2.6.3. *Assume that a function f satisfies the bounded difference condition: there exist constants c_i, $i = 1, \dots, n$ such that for all $i = 1, \dots, n$, all $X = (X_1, \dots, X_i, \dots, X_n)$ and $X' = (X_1, \dots, X_i', \dots, X_n)$ where only the i^{th} vector is changed*

$$|f(X) - f(X')| \leq c_i. \tag{2.154}$$

Denote

$$\nu = \sum_{i=1}^{n} c_i^2. \tag{2.155}$$

Let $Z = f(X_1, \dots, X_n)$ where X_i are independent. Then, for every $\delta \in (0,1)$,

$$\mathbf{P}\Big\{ Z \leq \mathbf{E}Z + \Big(\frac{\nu \log(1/\delta)}{2}\Big)^{1/2} \Big\} \geq 1 - \delta, \qquad \textit{and} \qquad \mathbf{Var}[Z] \leq \frac{\nu}{2}. \tag{2.156}$$

Next we state the contraction principle of [Ledoux and Talagrand, 1991]; a proof can be found in (Boucheron et al. [2013], Theorem 11.6).

Theorem 2.6.4. *Let $x_1, \dots, x_n$ be vectors whose real-valued components are indexed by $\boldsymbol{\mathcal{T}}$, that is, $x_i = (x_{i,s})_{s \in \boldsymbol{\mathcal{T}}}$. For each $i = 1, \dots, n$ let $\varphi_i : \mathbb{R} \to \mathbb{R}$ be a 1-Lipschitz function such that $\varphi_i(0) = 0$. Let $\epsilon_1, \dots, \epsilon_n$ be independent Rademacher random variables, and let $\Psi : [0, \infty) \to \mathbb{R}$ be a non-decreasing* *convex function. Then*

$$\mathbf{E}\left[\Psi\left(\frac{1}{2}\sup_{s\in\boldsymbol{\mathcal{T}}}\left|\sum_{i=1}^{n}\epsilon_i\varphi_i(x_{i,s})\right|\right)\right] \leq \mathbf{E}\left[\Psi\left(\sup_{s\in\boldsymbol{\mathcal{T}}}\left|\sum_{i=1}^{n}\epsilon_i x_{i,s}\right|\right)\right] \tag{2.157}$$

$$\mathbf{E}\left[\Psi\left(\sup_{s\in\boldsymbol{\mathcal{T}}}\sum_{i=1}^{n}\epsilon_i\varphi_i(x_{i,s})\right)\right] \leq \mathbf{E}\left[\Psi\left(\sup_{s\in\boldsymbol{\mathcal{T}}}\sum_{i=1}^{n}\epsilon_i x_{i,s}\right)\right]. \tag{2.158}$$

Chapter 3

Experimental Results for the KL-aggregation

Contents

In this section we propose an efficient algorithm for performing the KL-aggregation (see Chapter 2) and describe its implementation. We also compare its performance with different alternative methods. For the sake of simplicity, the comparison with the other methods is done in the univariate case only. The implementation of our algorithm and its behavior are the same in the multivariate setting.

3.1 Introduction

Before anything else, we remind the reader the problem setting and the estimator considered. We observe n independent random vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n \in \mathcal{X}$ drawn from a probability distribution P^* that admits a density function f^* with respect to the Lebesgue measure. Given a family of mixture components $f_1, \ldots, f_K$, we assumed that this unknown density is well approximated by a convex combination $f_{\boldsymbol{\pi}}$ of these components:

$$f_{\boldsymbol{\pi}}(\boldsymbol{x}) = \sum_{j=1}^{K} \pi_j f_j(\boldsymbol{x}), \quad \boldsymbol{\pi} \in \mathbb{B}_+^K = \Big\{\boldsymbol{\pi} \in [0,1]^K : \sum_{j=1}^{K} \pi_j = 1\Big\}. \tag{3.1}$$

The component densities $\mathcal{F} = \{f_j : j \in [K]\}$ are assumed to be given by previous experiments or expert knowledge. The problem of construction of this family is an open problem that we try to address in section ?. The objective of this chapter is to expose and study experimentally the algorithm implemented for computing the Maximum Likelihood Estimator (MLE), defined by

Note: en parler

$$\widehat{\boldsymbol{\pi}} \in \mathop{\arg\min}_{\boldsymbol{\pi} \in \mathbb{B}_+^K} \Big\{ -\frac{1}{n} \sum_{i=1}^{n} \log f_{\boldsymbol{\pi}}(\boldsymbol{X}_i) \Big\}. \tag{3.2}$$

One can note that this problem is convex as the composition of $-\log$ and a linear function is convex. Furthermore, the feasible space is also convex. This problem can be solved via a Primal-Dual interior point method. But we opted for an approach based on the accelerated proximal gradient descent method because of its suitability to the problems in high-dimensions with sparsity assumption [Beck and Teboulle, 2009].

Input: $\boldsymbol{\pi} \in \mathbb{R}^p$.

Output: The projection $\boldsymbol{\pi}^{proj}$ of $\boldsymbol{\pi}$ onto the probability simplex.

1: `Sort` $\boldsymbol{\pi}$ `into` $\boldsymbol{u}$ `:` $u_1 \geq u_2 \geq \cdots \geq u_p$.

2: `Find` $\rho = \max\{1 \leq j \leq p : u_j + \frac{1}{j}(1 - \sum_{i=1}^{j} u_i) > 0\}$.

3: `Define` $\lambda = \frac{1}{\rho}(1 - \sum_{i=1}^{\rho} u_i)$.

4: `Construct` $\boldsymbol{\pi}^{proj}$ s.t. $\boldsymbol{\pi}_i^{proj} = \max\{\pi_i + \lambda, 0\}$, $i = 1, \dots, p$.

Figure 3.1: Projection procedure onto the probability simplex

3.2 Implementation

We can see that eq. (3.2) is equivalent to

$$\arg\min_{\boldsymbol{\pi} \in \mathbb{R}^K} \Big\{ -\frac{1}{n} \sum_{i=1}^{n} \log f_{\boldsymbol{\pi}}(\boldsymbol{X}_i) + \chi_{\mathbb{B}_+^K}(\boldsymbol{\pi}) \Big\}, \tag{3.3}$$

where $\chi_{\mathbb{B}_+^K}$ is the indicator function

$$\chi_{\mathbb{B}_+^K}(\boldsymbol{\pi}) = \begin{cases} 0, & \text{if } \boldsymbol{\pi} \in \mathbb{B}_+^K, \\ +\infty, & \text{otherwise.} \end{cases}$$

This problem can be decomposed into

$$\min_{\boldsymbol{\pi}} \Big\{ \ell(\boldsymbol{\pi}) + g(\boldsymbol{\pi}) \Big\}, \tag{3.4}$$

where $\ell(\boldsymbol{\pi}) = -\frac{1}{n} \sum_{i=1}^{n} \log f_{\boldsymbol{\pi}}(\boldsymbol{X}_i)$ and $g(\boldsymbol{\pi}) = \chi_{\mathbb{B}_+^K}(\boldsymbol{\pi})$. One can note that this problem is convex but not smooth since ℓ is differentiable but g is not. One way to tackle this minimization is to consider the proximal operator

$$\text{prox}_{\lambda g}(\boldsymbol{\pi}) = \arg\min_{\boldsymbol{u}} \Big\{ g(\boldsymbol{u}) + \frac{1}{2\lambda} \|\boldsymbol{u} - \boldsymbol{\pi}\|_2^2 \Big\}, \tag{3.5}$$

where $\lambda > 0$ is a scale parameter for the function g. One can interpret $\text{prox}_{\lambda g}(\boldsymbol{\pi})$ as a point that compromises between minimizing g and being near to $\boldsymbol{\pi}$. Note that in our context, $g(.) = \chi_{\mathbb{B}_+^K}(.)$, therefore

$$\begin{aligned}\operatorname{prox}_{\lambda g}(\boldsymbol{\pi}) &= \arg\min_{\boldsymbol{u}} \left\{\chi_{\mathbb{B}_+^K}(\boldsymbol{u}) + \frac{1}{2\lambda}\|\boldsymbol{u}-\boldsymbol{\pi}\|_2^2\right\}, \\ &= \arg\min_{\boldsymbol{u}\in\mathbb{B}_+^K} \left\{\|\boldsymbol{u}-\boldsymbol{\pi}\|_2^2\right\}, \\ &= \boldsymbol{\Pi}_{\mathbb{B}_+^K}(\boldsymbol{\pi})\end{aligned}$$

where $\boldsymbol{\Pi}_{\mathbb{B}_+^K}(\boldsymbol{\pi})$ is the Euclidean projection of $\boldsymbol{\pi}$ into the probability simplex. The reader can find in [Parikh and Boyd, 2014] a detailed study of proximal algorithms. A particularly interesting procedure for our problem is the proximal gradient method that solves eq. (3.4). This method is iterative and the $(k+1)^{th}$ step is

$$\boldsymbol{\pi}^{k+1} := \operatorname{prox}_{\lambda^k g}(\boldsymbol{\pi}^k - \lambda^k \nabla f(\boldsymbol{\pi}^k)), \tag{3.6}$$

where $\lambda^k > 0$ is a step size. This step size can be found via a line-search method [Parikh and Boyd, 2014]. However, if ∇f is L-Lipschitz, we can chose a fixed $\lambda^k \in (0, 1/L)$. In this setting, one can show that this method converges with a rate of $\mathcal{O}(1/k)$. This rate is known to be sub-optimal. To improve this slow rate, accelerated versions of the proximal gradient method have been developed [Nesterov, 2007, Beck and Teboulle, 2009] that achieve optimal $\mathcal{O}(1/k^2)$ rate under the L-Lipschitz condition on ∇f. These optimization methods rely on the proximal operator and Nesterov's accelerated gradient method [Nesterov, 1983]. A version of this accelerated method is

$$\begin{cases}\boldsymbol{\xi}^k & := \boldsymbol{\pi}^k + \omega^k(\boldsymbol{\pi}^k - \boldsymbol{\pi}^{k-1}), \\ \boldsymbol{\pi}^{k+1} & := \operatorname{prox}_{\lambda^k g}(\boldsymbol{\xi}^k - \lambda^k \nabla f(\boldsymbol{\xi}^k)),\end{cases}$$

where ω^k is defined by $\omega^1 := 1$ and

$$\omega^k := \frac{2(\omega^{k-1}-1)}{1+\sqrt{1+(\omega^{k-1})^2}}.$$

This method has been coined Fast Iterative Shrinkage-Thresholding Algorithm (FISTA) in [Beck and Teboulle, 2009]. Our procedure is a special case of this algorithm that can be called "Accelerated projected gradient descent" since the proximal is the projection into $\mathbb{B}_+^K$. A procedure for the projection onto the probability simplex can be found in [Duchi et al., 2008] and a simple proof in [Wang et al., 2013]. The procedure for this projector is given in Figure 3.1. Finally, the complete procedure for our algorithm is given in Figure 3.2.

Input: A gradient step λ.
Output: parameter estimate $\widehat{\boldsymbol{\pi}}$.
`1:  Initialize` $t_0 = 1$ `and` $\boldsymbol{\pi}_0 = (1/K, \dots, 1/K)$`,`
for $k \geq 0$, until convergence occurs, **do**
    (a) $\boldsymbol{\pi}_k = \boldsymbol{\Pi}_{\mathbb{B}_+^K}\big(\xi_k - \lambda \nabla f_{\xi_k}(\xi_k)\big)$,
    (b) $t_{k+1} = \frac{1+\sqrt{1+4t_k^2}}{2}$,
    (c) $\xi_{k+1} = \boldsymbol{\pi}_k + \big(\frac{t_k - 1}{t_{k+1}}\big)(\boldsymbol{\pi}_k - \boldsymbol{\pi}_{k-1})$.
end for.

Figure 3.2: FISTA for the estimation of $\boldsymbol{\pi}$.

A nice property of this method is that it provides a sparse solution of this minimization problem which fits with our goal of selecting elements of the dictionary. General Primal-Dual interior points methods do not offer this feature.

3.3 Alternative methods considered

In this section we briefly describe several estimators of the density which are compared to our estimator. Note that although we used the algorithm EM in our experiments, we do not described it in this section since it is already done in Chapter 1.

3.3.1 SPADES

A method combining the dictionary approach and the ℓ_1-penalty (and, therefore, very close in spirit to our method) have been proposed by [Bunea et al., 2010]. They studied the linear combinations (as opposed to convex combinations studied in the previous chapter) of functions $\{f_1, \ldots, f_M\}$ with $f_j \in L_2(\mathbb{R}^d)$, $j = 1, \ldots, M$:

$$f_\lambda(x) = \sum_{j=1}^{M} \lambda_j f_j(x), \quad \lambda = (\lambda_1, \ldots, \lambda_M) \in \mathbb{R}^M. \tag{3.7}$$

They suggested the following estimator $\widehat{\lambda}$ called SPADES:

$$\widehat{\lambda} = \underset{\lambda \in \mathbb{R}^M}{\arg\min} \Big\{ -\frac{2}{n} \sum_{i=1}^{n} f_\lambda(\boldsymbol{X}_i) + \|f_\lambda\|^2 + 2 \sum_{j=1}^{M} \omega_j |\lambda_j| \Big\}. \tag{3.8}$$

It could be interesting to include SPADES in our experimental evaluation, but we did not manage to find an easy-to-use implementation of it, and it turned out that our implementation was quite slow. Furthermore, the SPADES is conceptually close to the Adaptive Dantzig (AD) [Bertin et al., 2011] procedure described in the next subsection. Therefore, we opted for excluding SPADES from our experiments but including AD.

3.3.2 Adaptive Dantzig density estimation

The Adaptive Dantzig estimator of a density has been introduced in [Bertin et al., 2011]. This method is similar to ours as it constructs an estimator of the unknown density from a linear mixture of functions taken from a dictionary. The key idea of this estimator is to minimize the ℓ_1-norm of the weight vector of the linear combination under an adaptive Dantzig constraint. This constraint comes from concentration inequalities. We recall here some material about the Dantzig selector. It has been introduced by [Candes and Tao, 2007] in the linear regression model

$$\boldsymbol{Y} = \boldsymbol{A}\boldsymbol{\lambda}_0 + \boldsymbol{\epsilon} \tag{3.9}$$

where $\boldsymbol{Y} \in \mathbb{R}^n$, $\boldsymbol{A}$ is a n by M matrix, $\boldsymbol{\epsilon} \in \mathbb{R}^n$ is the noise vector and $\boldsymbol{\lambda}_0 \in \mathbb{R}^M$ the unknown regression parameter to estimate. The Dantzig estimator is then defined as the solution of the problem

$$\text{minimize } \|\boldsymbol{\lambda}\|_1 \quad \text{subject to} \quad \|\boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{\lambda} - \boldsymbol{Y})\|_\infty \leq \eta, \tag{3.10}$$

where η is a regularization parameter. Statistical properties of this estimator were established in [Bickel et al., 2009]. They considered the non-parametric regression framework

$$Y_i = f_0(x_i) + \epsilon_i, \quad i = 1, \dots, n \tag{3.11}$$

where f is an unknown function, the design points $(x_i)_{i=1,\dots,n}$ are known and $(\epsilon_i)_{i=1,\dots,n}$ is a noise vector. One can estimate f_0 as a weighted sum $f_{\boldsymbol{\lambda}_0}$ of elements of a dictionary $D = (\varphi_m)_{m=1,\dots,M}$

$$f_{\boldsymbol{\lambda}_0} = \sum_{i=1}^{M} \lambda_{0,m}\varphi_m. \tag{3.12}$$

One easily checks that the model in 3.11 coincides with model in eq. (3.9) if we choose as design matrix $\boldsymbol{A} = (\varphi_m(x_i))$. The goal of [Bertin et al., 2011] was to estimate an unknown density f_0 with respect to a known measure dx on $\mathbb{R}$ by using the observation of n-sample $X_1, \dots, X_n$ and to build a linear combination f_λ of elements of the dictionary D as in eq. (3.12). It follows from the strong law of large numbers that

$$\widehat{\beta}_m = \frac{1}{n}\sum_{i=1}^{n} \varphi_m(X_i)$$

converges almost surely to the scalar product of f_0 and φ_m:

$$\int \varphi_m(x) f_0(x) dx = \beta_{0,m}, \tag{3.13}$$

and the Gram matrix associated to the dictionary D

$$G_{m,m'} = \int \varphi_m(x)\varphi_{m'}(x) dx \quad \text{with} \quad 1 \le m, m' \le M. \tag{3.14}$$

The scalar product of $f_{\boldsymbol{\lambda}}$ and φ_m is therefore

$$\int \varphi_m(x) f_{\boldsymbol{\lambda}}(x) dx = \sum_{m'=1}^{M} \lambda_{m'} \int \varphi_{m'}(x)\varphi_m(x) dx = (\boldsymbol{G\lambda})_m. \tag{3.15}$$

The Dantzig estimate $\widehat{\boldsymbol{\lambda}}^D$ is then obtained by solving the following constrained minimization problem

$$\begin{cases} \text{minimize} & \|\boldsymbol{\lambda}\|_1 \\ \text{subject to} & |(\boldsymbol{G\lambda})_m - \widehat{\beta}_m| \le \eta_{\gamma,m} \quad m \in \{1, \dots, M\}, \end{cases}$$

where, for a constant $\gamma > 0$,

$$\eta_{\gamma,m} = \sqrt{\frac{2\tilde{\sigma}_m^2 \gamma \log M}{n}} + \frac{2\|\varphi_m\|_\infty \gamma \log M}{3n}, \tag{3.16}$$

with

$$\tilde{\sigma}_m^2 = \widehat{\sigma}_m^2 + 2\|\varphi_m\|_\infty \sqrt{\frac{2\widehat{\sigma}_m^2 \gamma \log M}{n}} + \frac{8\|\varphi_m\|_\infty^2 \gamma \log M}{n}, \tag{3.17}$$

and

$$\widehat{\sigma}_m^2 = \frac{1}{n(n-1)} \sum_{i=2}^{n} \sum_{j=1}^{i-1} (\varphi_m(X_i) - \varphi_m(X_j)). \tag{3.18}$$

Note that $\eta_{\gamma,m}$ depends on the data which explains the name *Adaptive Dantzig*. [Bertin et al., 2011] derived the form of $\eta_{\gamma,m}$ from sharp concentration inequalities (see Theorem 1 of [Bertin et al., 2011]). More precisely, if we consider $\boldsymbol{\lambda}_0 = (\lambda_{0,m})_{m=1,\dots,M}$ such that the projection of f_0 on the space spanned by D is

$$\mathbf{P}_D f_0 = \sum_{m=1}^{M} \lambda_{0,m}\varphi_m, \tag{3.19}$$

then $(\boldsymbol{G\lambda}_0)_m = \beta_{0,m}$ and the parameter $\eta_{\gamma,m}$ can be seen as the smallest quantity such that, for $\gamma > 1$, we have $|\beta_{0,m} - \widehat{\beta}_m| \leq \eta_{\gamma,m}$ with high probability. Note that the assumption $\gamma > 1$ is an almost necessary condition to have a theoretical control on the quadratic error $\mathbf{E}\|\widehat{f}^D - f_0\|_2^2$. Therefore, we will follow the choice of $\gamma = 1.01$ made by the authors in our experiments. The pseudo code of the procedure is given in Figure 3.3. In what follows, the Adaptive Dantzig density estimator is noted $\widehat{f}^{AD}$ and the abbreviation AD is used in the plots.

1: **Input:** A sample $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n \in \mathbb{R}^p$ and the dictionary $D = (\varphi_m)_{m=1,\ldots,M}$.

2: **Output:** Dantzig density estimate $\widehat{f}^{AD} = f_{\widehat{\boldsymbol{\lambda}}^D}$.

3: **Init:** Set $\gamma = 1.01$.

4: Compute $\widehat{\beta}_m = \frac{1}{n}\sum_{i=1}^N \varphi_m(\boldsymbol{X}_i)$.

5: Compute $\widehat{\sigma}_m^2 = \frac{1}{n(n-1)}\sum_{i=2}^n \sum_{j=1}^{i-1}(\varphi_m(\boldsymbol{X}_i) - \varphi_m(\boldsymbol{X}_j))^2$.

6: Compute $\tilde{\sigma}_m^2$.

$$\tilde{\sigma}_m^2 = \widehat{\sigma}_m^2 + 2\|\varphi_m\|_\infty \sqrt{\frac{2\widehat{\sigma}_m^2 \gamma \log M}{n}} + \frac{8\|\varphi_m\|_\infty^2 \gamma \log M}{n}. \tag{3.20}$$

7: Compute $\eta_{\gamma,m}$

$$\eta_{\gamma,m} = \sqrt{\frac{2\tilde{\sigma}_m^2 \gamma \log M}{n}} + \frac{2\|\varphi_m\|_\infty \gamma \log M}{3n}.$$

8: Compute the coefficients $\widehat{\boldsymbol{\lambda}}^{D,\gamma}$ of the Dantzig estimate, $\widehat{\boldsymbol{\lambda}}^{D,\gamma} = \arg\min_{\boldsymbol{\lambda}\in\mathbb{R}^M} \|\boldsymbol{\lambda}\|_1$ such that $\boldsymbol{\lambda}$ satisfies the Dantzig constraint

$$\forall m \in \{1, \ldots, m\}, \quad |(\boldsymbol{G\lambda})_m - \widehat{\beta}_m| \leq \eta_{\gamma,m}. \tag{3.21}$$

9: Compute the mixture density $f_{\widehat{\boldsymbol{\lambda}}^D} = \sum_{m=1}^M \widehat{\lambda}_m^D \varphi_m$.

Figure 3.3: Adaptive Dantzig density estimation procedure

3.3.3 Kernel density estimation

The kernel density estimator (KDE) is a well established non-parametric way of estimating the probability density function of a random variable. We will recall in this section some material about KDE.
Let $X_1, \dots, X_n$ be i.i.d. random variables drawn from an unknown probability density f with respect to the Lebesgue measure on $\mathbb{R}$. The kernel density estimator $\widehat{f}_h$ is given by

$$\widehat{f}_h(x) \triangleq \frac{1}{nh} \sum_{i=1}^{n} K\Big(\frac{X_i - x}{h}\Big) \tag{3.22}$$

where $K : \mathbb{R} \to \mathbb{R}$ and $\int K(u)du = 1$ is called a kernel and h is the bandwidth. We used Gaussian kernel and three methods to select the bandwidth: Cross Validation, Scott's rule of thumb which is the default method in Scipy [Jones et al., 2001–] and the Sheather and Jones bandwidth selection procedure [Sheather and Jones, 1991].

Methods based on minimizing the AMISE

The most natural way to derive an estimator of the bandwidth would be to minimize the Mean Integrated Squared Error (MISE)

$$\mathrm{MISE}(h) := \mathbb{E}\Big[\int (\widehat{f}_h(x) - f(x))^2 dx\Big]. \tag{3.23}$$

Unfortunately, we can not rely on this quantity since f is unavailable. However, we can derive the first two terms of the asymptotic expansion of the MISE (AMISE). When $n \to \infty$ and $h = h(n) \to 0$, and under regularity assumptions on f and K, we have

$$\mathrm{AMISE}(h) = \frac{1}{nh} R(K) + \frac{h^4 \sigma_K^4}{4} R(f''), \tag{3.24}$$

where for an appropriate function g,

$$R(g) = \int g^2(x)dx \qquad \text{and} \qquad \sigma_g^2 = \int x^2 g(x)dx.$$

The reader can refer to the appendix of [Tsybakov, 2009] for a proof of this expansion. Setting the derivative w.r.t. h of the right hand side of eq. (3.24) to 0, we see that a suitable estimate of the bandwidth would be the solution of

$$h = \left(\frac{R(K)}{\sigma_K^4 R(f'')}\right)^{1/5} n^{-1/5}. \tag{3.25}$$

However, this cannot be done directly since we do not know $R(f'')$. In the special case where we consider that the kernels are Gaussian and the target density to be estimated is also a Gaussian with density $\phi_{(0,\sigma^2)}$, we have $R(\phi''_{(0,\sigma^2)}(x)) = 3/(8\sqrt{\pi}\sigma^5)$ and we can derive the Scott's rule of thumb in univariate case [Scott, 2015]

$$\widehat{h} = (4/3)^{1/5}\sigma n^{-1/5} \approx 1.06\widehat{\sigma} n^{-1/5}. \tag{3.26}$$

Without this assumption on the target density, we have to look deeper into the study of $R(f'')$. Several estimators of this quantity has been developed to circumvent this issue [Hall and Marron, 1987, Jones and Sheather, 1991, Sheather and Jones, 1991]. We will focus on a popular method from [Sheather and Jones, 1991]. The authors constructed a kernel density estimator of $R(f'')$

$$\widehat{S}(\widehat{\alpha}_2(h)) = \frac{1}{n(n-1)}(\widehat{\alpha}_2(h))^{-5} \sum_{i=1}^{n}\sum_{j=1}^{n} \Phi^{(4)}\Big(\frac{X_i - X_j}{\widehat{\alpha}_2(h)}\Big), \tag{3.27}$$

where $\Phi^{(i)}$ is the i^{th} derivative of the standard normal density. Note that $\widehat{\alpha}_2(h)$ depends on h. An estimator of $\widehat{\alpha}_2(h)$ can be built with specific properties on the diagonal elements of eq. (3.27)

$$\widehat{\alpha}_2(h) = 1.357\big(\widehat{S}(a)/\widehat{T}(b)\big)^{1/7} h^{5/7}, \tag{3.28}$$

with

$$\widehat{T}(b) = -\frac{1}{n(n-1)} b^{-7} \sum_{i=1}^{n}\sum_{j=1}^{n} \Phi^{(6)}\Big(\frac{X_i - X_j}{b}\Big), \tag{3.29}$$

and

$$a = 0.920\widehat{\lambda}n^{-1/7}, \quad b = 0.912\widehat{\lambda}n^{-1/9}, \tag{3.30}$$

where $\widehat{\lambda}$ is the sample interquartile range. We will not go into the details of these expressions but it is worth mentioning that $\widehat{T}(b)$ is a kernel density estimator of $R(f''')$. Therefore combining eq. (3.27), eq. (3.28) and eq. (3.29), we can solve eq. (3.25) over h via a Newton-Raphson procedure. The algorithm is given in Figure 3.4.

1: **Input:** A sample $\boldsymbol{X}_1, \dots, \boldsymbol{X}_n \in \mathbb{R}$.

2: **Output:** A bandwidth estimator $\widehat{h}$.

3: **Init:** Set $a = 0.920\widehat{\lambda}n^{-1/7}$ and $b = 0.912\widehat{\lambda}n^{-1/9}$.

4: Compute

$$\widehat{T}(b) = -\frac{1}{n(n-1)}b^{-7}\sum_{i=1}^{n}\sum_{j=1}^{n}\Phi^{(6)}\Big(\frac{X_i - X_j}{b}\Big). \tag{3.31}$$

5: Compute

$$\widehat{S}(a) = \frac{1}{n(n-1)}a^{-5}\sum_{i=1}^{n}\sum_{j=1}^{n}\Phi^{(4)}\Big(\frac{X_i - X_j}{a}\Big) \tag{3.32}$$

6: Define the function $\widehat{\alpha}_2(h) = 1.357\big(\widehat{S}(a)/\widehat{T}(b)\big)^{1/7}h^{5/7}$.

7: Solve over h

$$h - \left(\frac{R(K)}{\sigma_K^4\widehat{S}(\widehat{\alpha}_2(h))}\right)^{1/5} = 0. \tag{3.33}$$

Figure 3.4: Sheather and Jones bandwidth selection method.

Behavior of KDE in high dimension

It is well known that the kernel density estimator performs badly in the high dimensional setting, [Stone, 1980] proved that the kernel density estimator of a p times continuously differentiable density in dimension d converges at most at the rate $n^{-p/(2p+d)}$. Therefore, for a given target error, the size of the sample must increase exponentially as the dimension increases. For a study of kernel density estimators in the high dimensional setting, see Chapter 7 of [Scott, 2015].

3.4 Experimental Evaluation

In order to carry out an experimental evaluation, we constructed a set of target densities with different shapes and recorded the performances of the estimators. We considered different density dictionaries. Finally we assessed the performance through the Kullback-Leibler divergence and the L_2 distance. All the experiments reported in this section were conducted in the univariate case.

3.4.1 Dictionaries considered

We did experiments with the following two dictionaries containing various types of densities.

1. The first dictionary, denoted by D_{GL}, is composed of Gaussian and Laplace densities. The Gaussian densities have their means in the set $\{0, 0.2, 0.4, 0.6, 0.8, 1\}$ and their variances in $\{0.001, 0.01, 0.1, 1\}$. The Laplace densities have their means in $\{0, 0.2, 0.4, 0.6, 0.8, 1\}$ and their scales in $\{0.05, 0.1, 0.2, 0.5, 1\}$. Therefore, the dictionary D_{GL} has 54 elements. The plots of these functions are depicted in Figure 3.5.

2. The second dictionary, denoted by D_{GLU}, is obtained by enriching the first dictionary D_{GL} by the set of 10 uniform densities on the intervals $(i, i+0.1)$, $i \in \{0, 0.1, \ldots, 0.9\}$. This dictionary D_{GLU} has 64 elements.

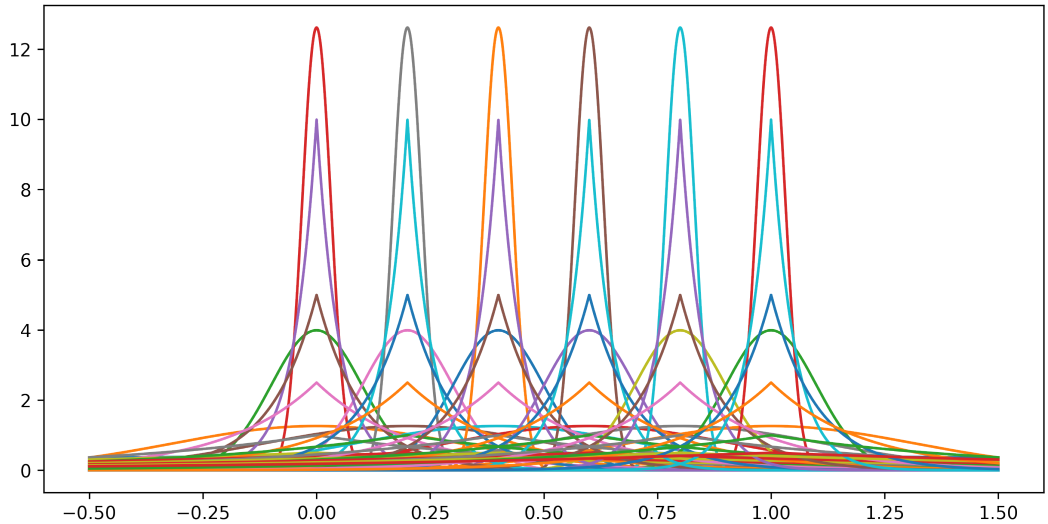


Figure 3.5: D_{GL}, set of Gaussian and Laplace densities.

A table of the dictionary D_{GL} (and D_{GLU} with the uniform densities) can be found in Figure 3.17.

3.4.2 Densities considered

We considered 5 target densities corresponding to 5 different scenarios. The 1^{st} and 2^{nd} will asses the performance of our method on uniform based densities, the 3^{rd} and 4^{th} on dictionary based density. The last one is a complex density made from elements which are not in the dictionary that we will consider.

1. f_{unif}: A uniform density on $[0, 1]$.

2. f_{rect}: A mixture of uniform densities on subintervals. This density is called "Rectangular":

$$f_{\text{rect}} = \frac{10}{7}\mathbf{1}_{[0,1/5]} + \frac{5}{7}\mathbf{1}_{[1/5,2/5]} + \frac{10}{7}\mathbf{1}_{[2/5,3/5]} + \frac{10}{7}\mathbf{1}_{[4/5,1]}. \tag{3.34}$$

3. f_{gauss}: A mixture of 5 Gaussian densities taken from the dictionary D_{GL} equally centered in $[0, 1]$ with same variance:

$$f_{\text{gauss}} = \sum_{k=1}^{5} 0.2 f_k \quad \text{with} \quad f_k = \varphi_{(k/5, 0.001)}. \tag{3.35}$$

4. $f_{\text{gauss-lapl}}$: A mixture of 5 Gaussian and Laplace densities taken from the dictionary D_{GL} with different variances and scales:

$$\begin{aligned} f_{\text{gauss-lapl}} = 0.2\big(& \varphi_{(0,10^{-2})} + \varphi_{(0.2,10^{-3})} + \varphi_{(0.6,10^{-3})} \\ & + \text{Lapl}_{(0.4,0.2)} + \text{Lapl}_{(0.8,0.1)} \big). \end{aligned} \tag{3.36}$$

5. f_{ext}: A mixture of Gaussian and Laplace densities taken from another dictionary D_{out}:

$$f_{\text{ext}} = \sum_{k=1}^{7} \frac{1}{7} f_k \quad \text{with} \quad f_k \in D_{out}. \tag{3.37}$$

These target densities are plotted in Figure 3.6.

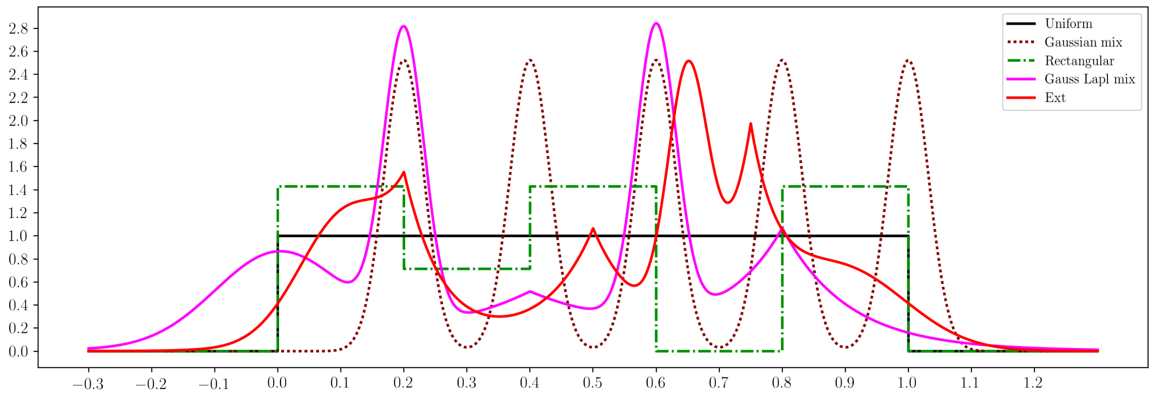


Figure 3.6: Five target densities considered.

3.4.3 Discussion of the results

In the numerical experiments reported in this section, the dictionaries used for the Adaptive Dantzig and the Maximum likelihood density estimators are D_{GL} and D_{GLU}. Note that the AD is the direct competitor of the MLE as both methods rely on a dictionary. However, in order to get a broader insight of what is going on, we also compared these dictionary based methods with other commonly used density estimators such as the EM algorithm on Gaussian mixtures with a model selection performed by the BIC criterion and Kernel Density Estimators (KDE). In the plots, KDE refers to the kernel density estimate with Scott's rule as chosen by default in the Python library Scipy, KDE-SJ refers to the KDE with the Sheather-Jones bandwidth selector and KDE CV refers to the KDE with bandwidth selected via cross-validation. The two latter were implemented by ourselves.

For each scenario of the target density, f_{unif}, f_{rect}, f_{gauss}, $f_{\text{gauss-lapl}}$, f_{ext} and for each sample size N with $N \in \{100, 500, 1000\}$, we ran 200 simulations. The boxplots of the errors are plotted in Figure 3.7-Figure 3.19. The running times of different arguments are depicted in Figure 3.20. A rapid observation is that the performance of the MLE is good both in Kullback-Leibler and L_2 losses, and it outperforms in all considered scenarios the AD estimator. This is true both in terms of statistical accuracy and computational complexity. The comparison with the other estimation methods is more subtle, and requires a closer look to the results.

Mis-specification bias

Obviously, the densities f_{unif}, f_{rect} and f_{ext} were not built with elements in the dictionary D_{GL}. In other terms, they do not lie in the convex hull of the dictionary D_{GL}. Furthermore, they can be hardly approximated by convex combinations of functions from D_{GL}. Therefore, it is clear that whatever the dictionary based approach we use, it will have a significant bias due to the "model mis-specification".

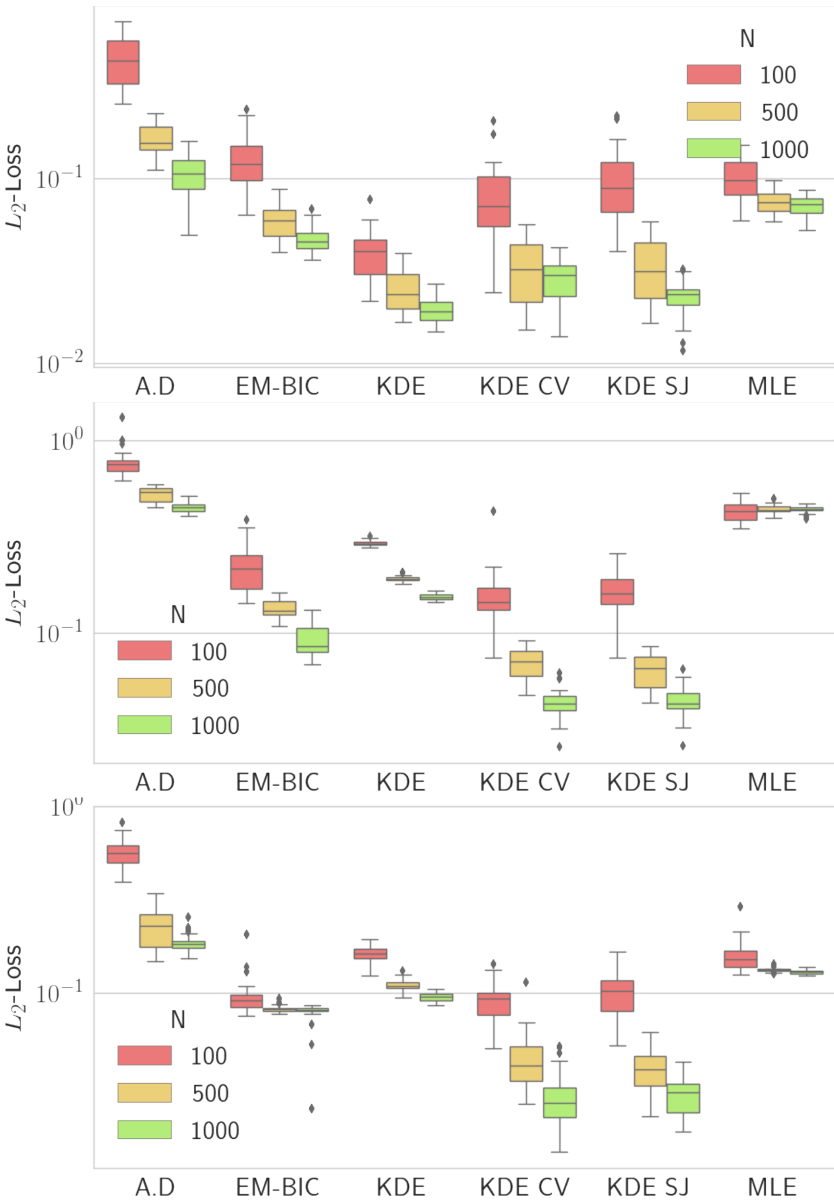


Figure 3.7: Results with f_{unif} (upper panel), f_{rect} (middle panel) and f_{ext} (lower panel) in $L2$ loss with D_{GL}.

Since the cardinality of the dictionary is chosen independently of the sample size n, this bias term is constant across different values of n. This is exactly what we observe in Figure 3.7. Such methods as the EM-BIC or various versions of KDE have an L_2 error that decreases significantly when the sample size increases, whereas the AD and, especially, the MLE show only a slight improvement of the error. This is a strong indication of the fact that the bias of the methods AD and MLE substantially dominates the bias, when the true density is chosen from the set $\{f_{\text{unif}}, f_{\text{rect}}, f_{\text{ext}}\}$. Thus, the apparently poor behavior of the MLE as compared to the EM-BIC and the KDE is not a surprise and, more importantly, it is not caused by the method of estimation itself but rather by the inappropriate choice of the dictionary.

Note that in all the experiments, the conclusions drawn from the error bars corresponding to the L_2-error can be drawn from the error bars corresponding to the KL-error.

Assessing estimation error

While for the three densities discussed in the foregoing paragraph the bias was largely dominating the variance, the situation is reversed for the densities f_{gauss} and $f_{\text{gauss-lapl}}$. Both of them belong to the convex hull of the dictionary D_{GL}, which implies that the mis-specification bias vanishes. Therefore, the error is mostly dominated by the estimation variance. This explains why for these two densities the MLE has the smallest error, both in L_2 and KL loss (see Figure 3.9 and Figure 3.10). Interestingly, the second best is EM-BIC, which performs better than the AD. Note that the default KDE in Scipy [Jones et al., 2001–] with Scott's rule presents poor results in these scenarios. This observation should come to mind of the practitioner when applying kernel density estimators with default package setting.

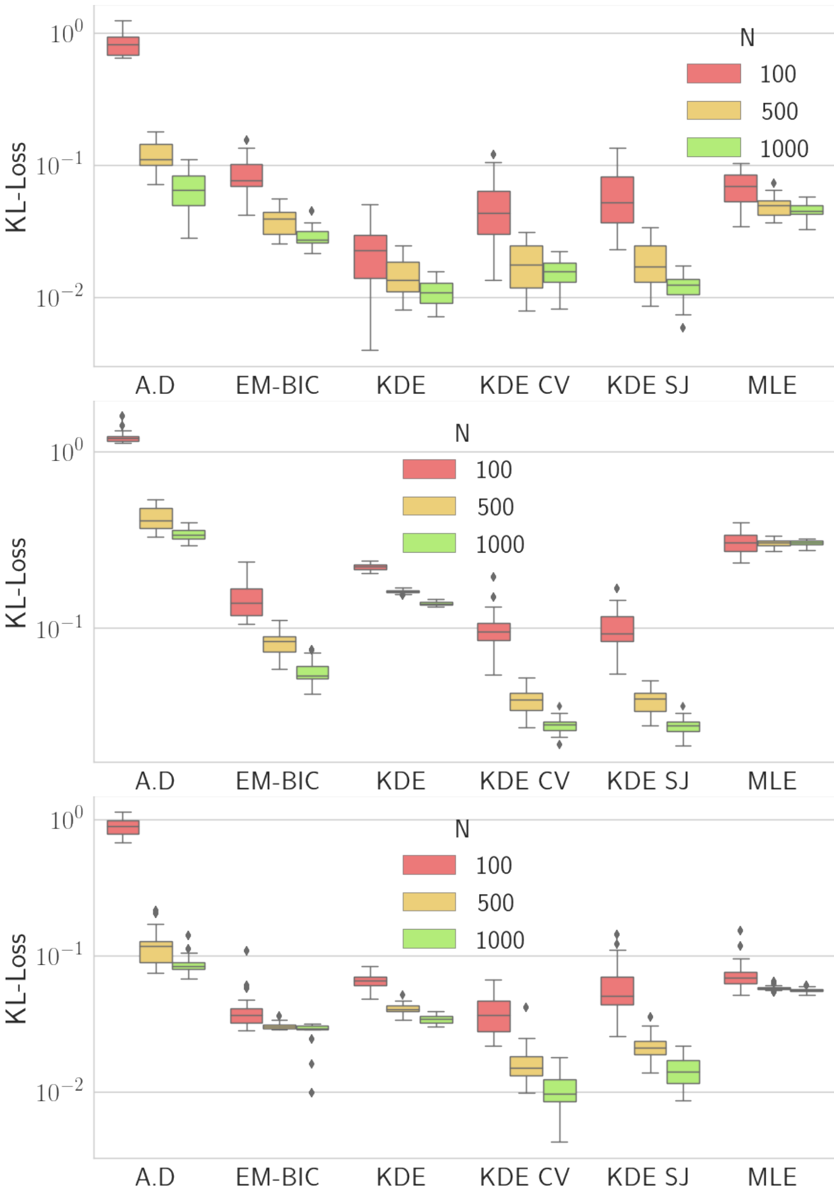


Figure 3.8: Results with f_{unif} (upper panel), f_{rect} (middle panel) and f_{ext} (lower panel) in KL loss with D_{GL}.

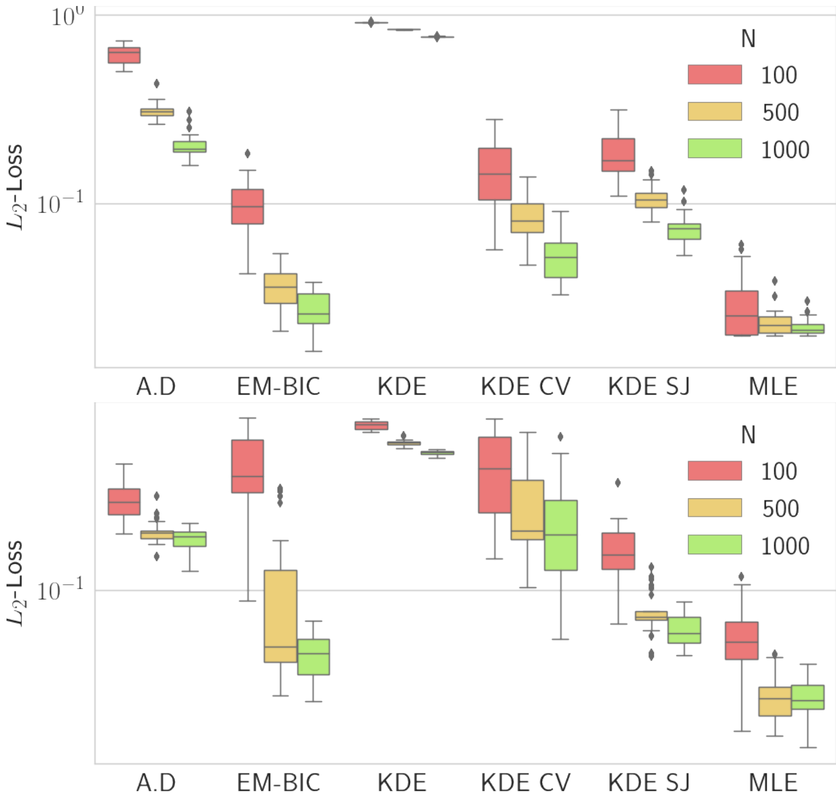


Figure 3.9: Results with f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel) in L_2 loss with D_{GL}.

One can also remark that the error of the MLE when estimating f_{gauss} is smaller than the one of estimating $f_{\text{gauss-lapl}}$. This is perfectly in line with the theory developed in previous chapter, telling that the variance term is proportional to the sparsity index. In these examples, the sparsity index of $f_{\text{gauss-lapl}}$ is larger than that of f_{gauss}.

Impact of the choice of the dictionary

The discussion of the foregoing paragraphs demonstrates the importance of the choice of the dictionary. The purpose of the additional experiments conducted with the same target densities but with a larger dictionary, D_{GLU}, is

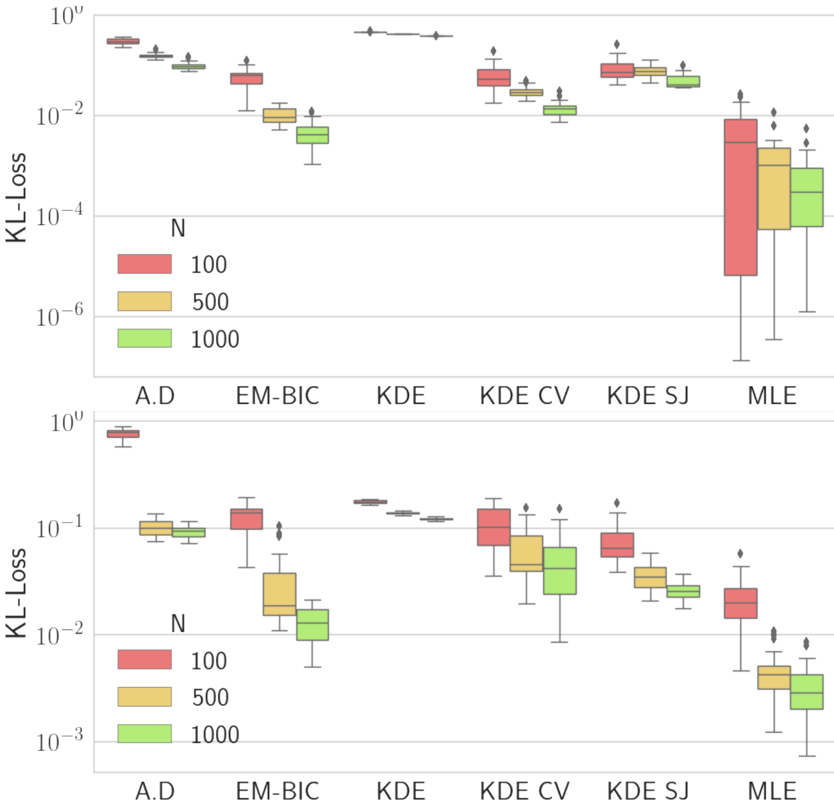


Figure 3.10: Results with f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel) in KL loss with D_{GL}.

to further illustrate this importance and to show that the size of the dictionary does not significantly impact the quality of estimation[1].

The inclusion of 10 uniform densities on $(0, 0.1), \ldots, (0.9, 1)$ to the dictionary D_{GL} removes the mis-specification bias in the case of a uniform and rectangular densities, and reduces it in the case of f_{ext}. The results are plotted in Figure 3.11 and Figure 3.18. We can see that the MLE becomes generally the best estimator when the density is uniform or rectangular. It is still slightly worse than the KDE with data-driven bandwidths for estimating f_{ext}. Finally, the results for the densities f_{gauss} and $f_{\text{gauss-lapl}}$ plotted on Figure 3.12 and Figure 3.19 confirm that adding new elements to the dictionary (even if they are "useless") do not deteriorate the quality of estimation. The ℓ_1-constraint allow us to avoid the overfitting.

Comparison of weights estimated by AD and MLE

A closer look on the estimated weights by AD and MLE gives us knowledge on the behavior of these estimators. We considered the full dictionary D_{GLU} and we provided a table of the indexes of components of this dictionary in Figure 3.17. We plotted the estimated weights of the true components of f_{gauss} and $f_{\text{gauss-lapl}}$ in Figure 3.13 and Figure 3.15. The MLE estimates correctly the real weights of f_{gauss} and most of the weights of $f_{\text{gauss-lapl}}$. We recall the reader that those weights were set to 0.2. However, AD did not succeed to estimate correctly these weights. It turns out that AD gave importance on components that overlap the true densities of the mixture as shown in Figure 3.14 with the uniform components. Both AD and MLE provide sparse estimators, this can be seen by looking at components not used in the dictionary (see Figure 3.16). As a matter of fact, the estimated weight vector

[1]It certainly does impact the running time

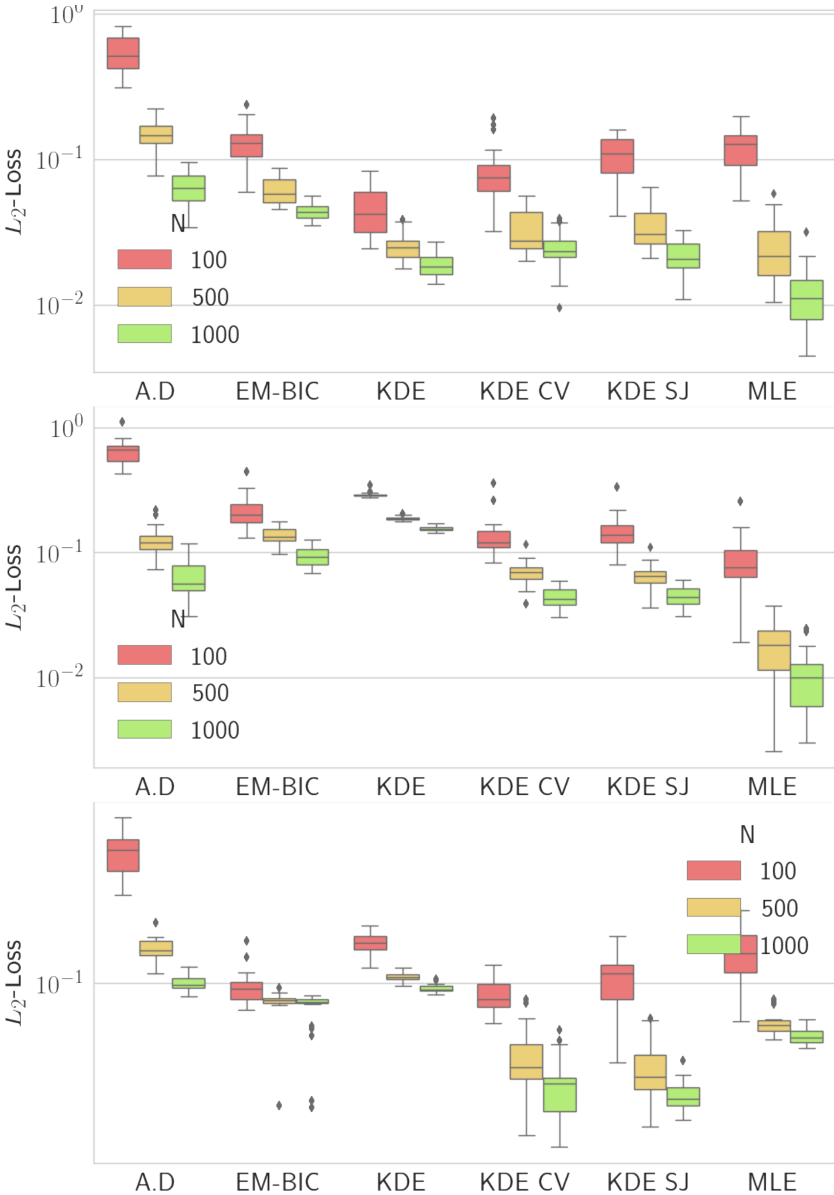


Figure 3.11: Results with f_{unif} (upper panel), f_{rect} (middle panel) and f_{ext} (lower panel) in L_2 loss with D_{GLU}.

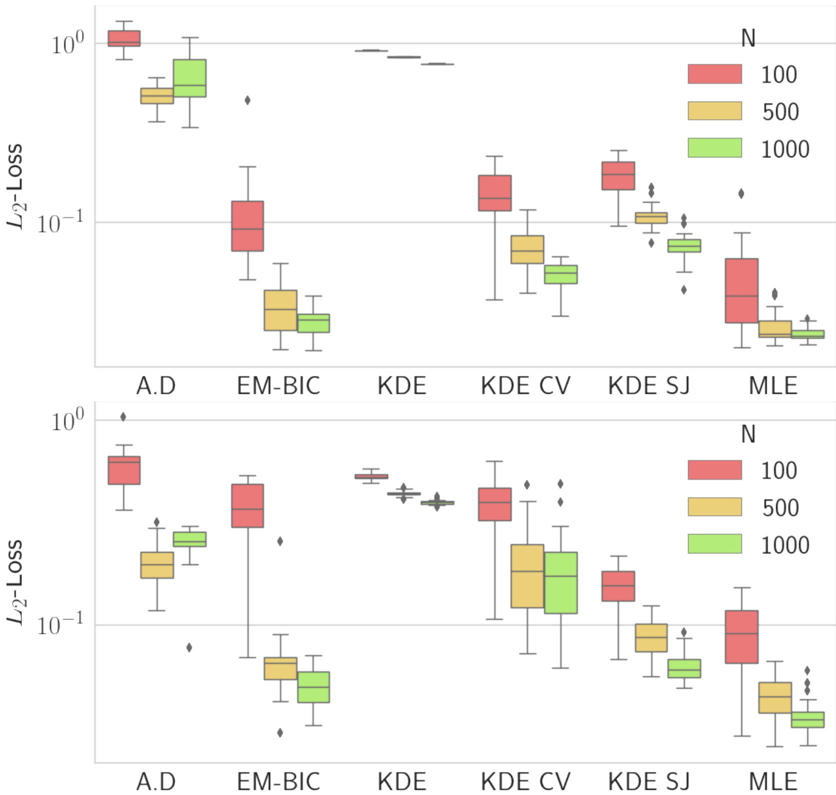


Figure 3.12: Results with f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel) in $L2$ loss with D_{GLU}.

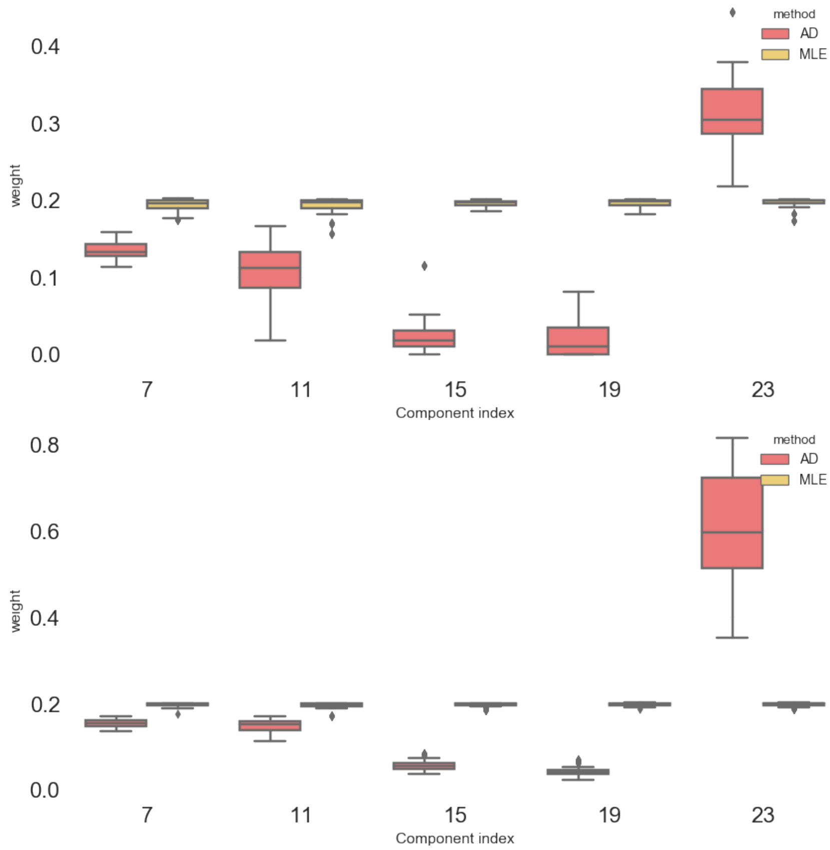


Figure 3.13: Estimated weights of the components of f_{gauss}, with $N = 500$ (upper panel) and $N = 1000$ (lower panel).

by AD is more sparse that MLE, but AD is more prone to be influenced by overlapping densities.

Concluding remarks

To conclude, the performance of the MLE method in these simulations is promising to achieve a good mixture density estimate. In addition, the computational efficiency of the MLE displayed in Figure 3.20 makes it highly attractive for performing density estimation. Our algorithm was coded in Python with some elements accelerated with the Just-In-Time (JIT) com-

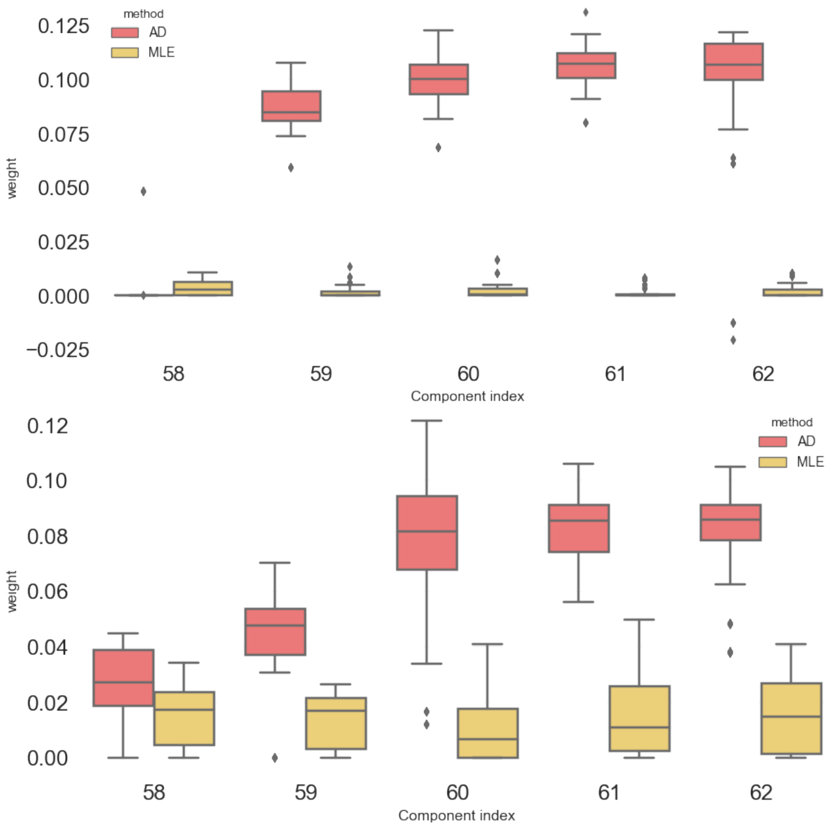


Figure 3.14: Estimated weights of uniform components of the dictionary for f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel) with $N = 1000$.

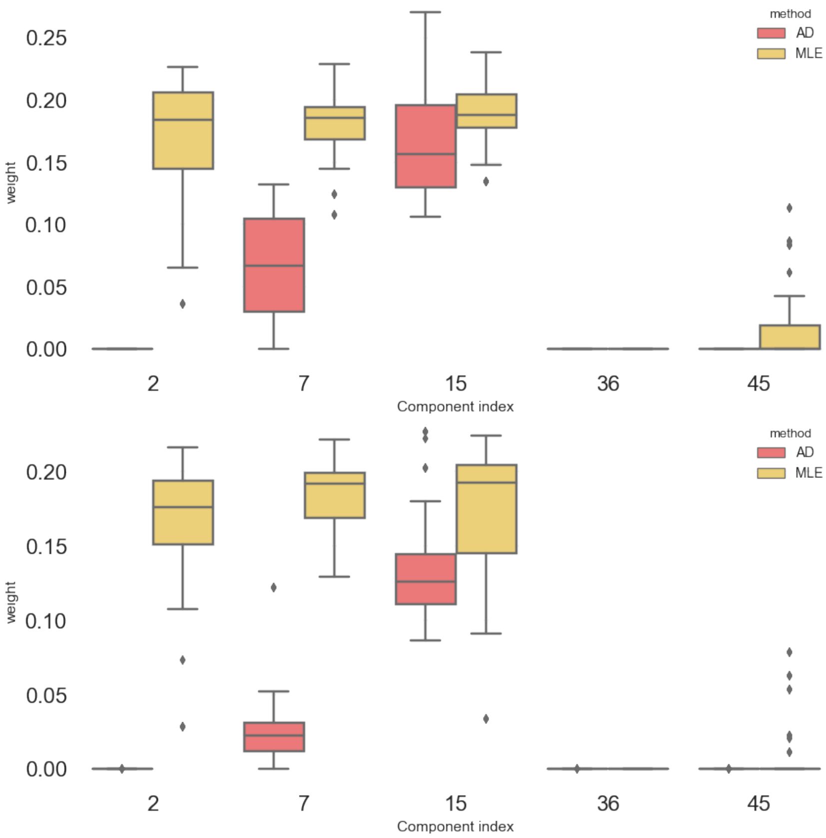


Figure 3.15: Estimated weights of the components of $f_{\text{gauss-lapl}}$, with $N = 500$ (upper panel) and $N = 1000$ (lower panel).

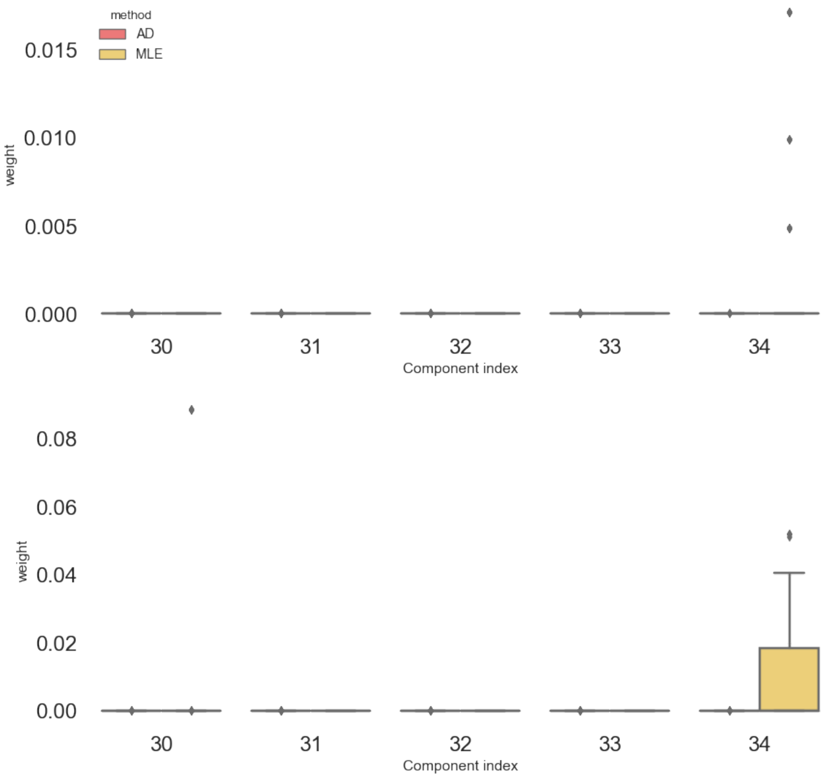


Figure 3.16: Estimated weights of non-used components of the dictionary for f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel), with $N = 1000$.

0	Normal(0 , 1)	22	Normal(1 , 0.01)	44	Laplace(0.8 , 0.05)
1	Normal(0 , 0.1)	23	Normal(1 , 0.001)	45	Laplace(0.8 , 0.1)
2	Normal(0 , 0.01)	24	Laplace(0 , 0.05)	46	Laplace(0.8 , 0.2)
3	Normal(0 , 0.001)	25	Laplace(0 , 0.1)	47	Laplace(0.8 , 0.5)
4	Normal(0.2 , 1)	26	Laplace(0 , 0.2)	48	Laplace(0.8 , 1)
5	Normal(0.2 , 0.1)	27	Laplace(0 , 0.5)	49	Laplace(1 , 0.05)
6	Normal(0.2 , 0.01)	28	Laplace(0 , 1)	50	Laplace(1 , 0.1)
7	Normal(0.2 , 0.001)	29	Laplace(0.2 , 0.05)	51	Laplace(1 , 0.2)
8	Normal(0.4 , 1)	30	Laplace(0.2 , 0.1)	52	Laplace(1 , 0.5)
9	Normal(0.4 , 0.1)	31	Laplace(0.2 , 0.2)	53	Laplace(1 , 1)
10	Normal(0.4 , 0.01)	32	Laplace(0.2 , 0.5)	54	Uniform(0.0 , 0.1)
11	Normal(0.4 , 0.001)	33	Laplace(0.2 , 1)	55	Uniform(0.1 , 0.2)
12	Normal(0.6 , 1)	34	Laplace(0.4 , 0.05)	56	Uniform(0.2 , 0.3)
13	Normal(0.6 , 0.1)	35	Laplace(0.4 , 0.1)	57	Uniform(0.3 , 0.4)
14	Normal(0.6 , 0.01)	36	Laplace(0.4 , 0.2)	58	Uniform(0.4 , 0.5)
15	Normal(0.6 , 0.001)	37	Laplace(0.4 , 0.5)	59	Uniform(0.5 , 0.6)
16	Normal(0.8 , 1)	38	Laplace(0.4 , 1)	60	Uniform(0.6 , 0.7)
17	Normal(0.8 , 0.1)	39	Laplace(0.6 , 0.05)	61	Uniform(0.7 , 0.8)
18	Normal(0.8 , 0.01)	40	Laplace(0.6 , 0.1)	62	Uniform(0.8 , 0.9)
19	Normal(0.8 , 0.001)	41	Laplace(0.6 , 0.2)	63	Uniform(0.9 , 1.0)
20	Normal(1 , 1)	42	Laplace(0.6 , 0.5)		
21	Normal(1 , 0.1)	43	Laplace(0.6 , 1)		

Figure 3.17: Indexes of components of the dictionary D_{GL} and D_{GLU}

piler Numba [Lam et al., 2015]. Compared to compiled optimized versions of KDE and EM from Scipy and Scikit-Learn[Pedregosa et al., 2011], we are confident that the computation time of our algorithm can be further decreased. Another important point is in the case of high dimensional data, KDE and EM+BIC methods are known to present poor performance. Our method needs the computation of the matrix $(f_j(X_i))_{(i,j)\in[N]\times[K]}$ which might consume a lot of memory. Some techniques such as a Mini-batch approach can help. Furthermore, at the light of the results in the uniform and rectangular case, the choice of the dictionary is a cornerstone in density estimation. The size of the dictionary should be chosen by considering both statistical arguments and computational limitations.

3.5 A method for constructing the dictionary of densities

In this section, we propose a data-driven method to construct a dictionary of densities for the KL-aggregation algorithm. We compare mixture densities estimated by this dictionary generation method and the KL-aggregation algorithm with the Kernel density estimator with the bandwidth selected via cross-validation and the Expectation-Maximization algorithm with the BIC criterion in different dimensional settings. We show experimentally that the KL-aggregation algorithm with a dictionary provided by this method offers good performance at an attractive computation cost.

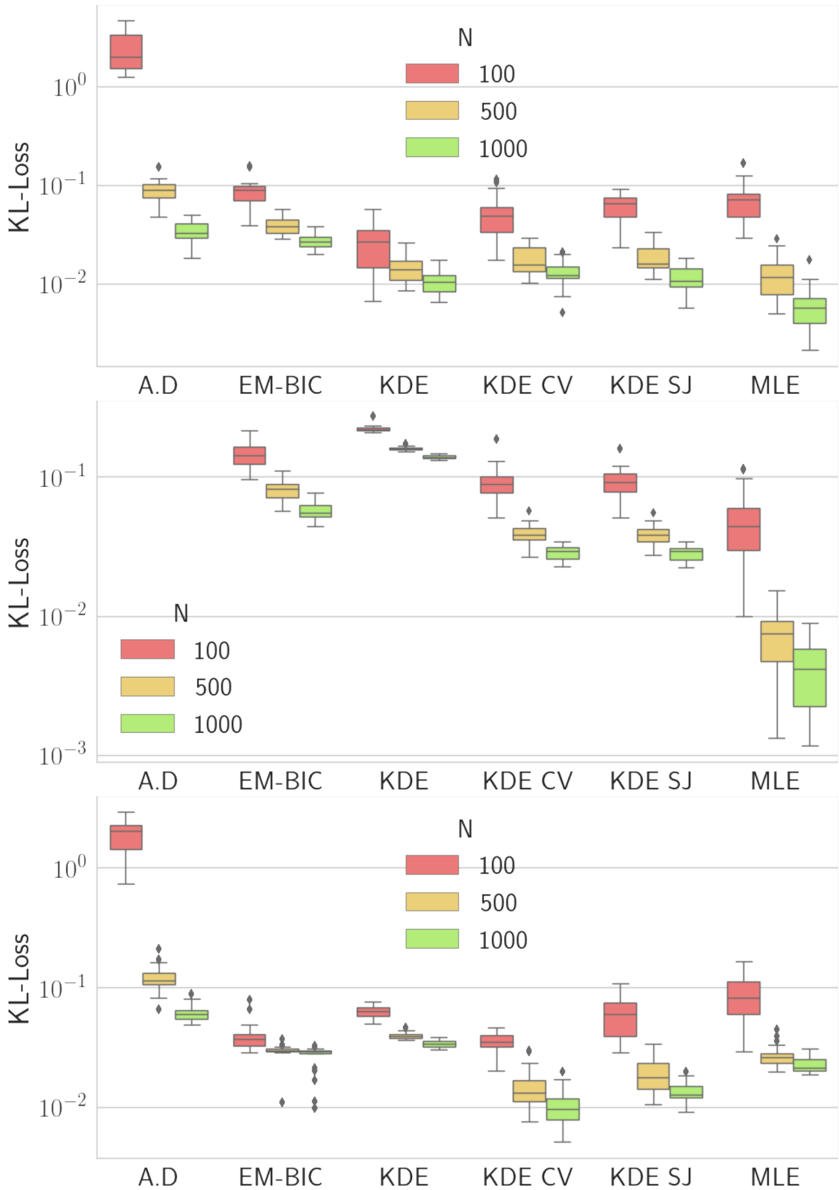


Figure 3.18: Results with f_{unif} (upper panel), f_{rect} (middle panel) and f_{ext} (lower panel) in KL loss with D_{GLU}.

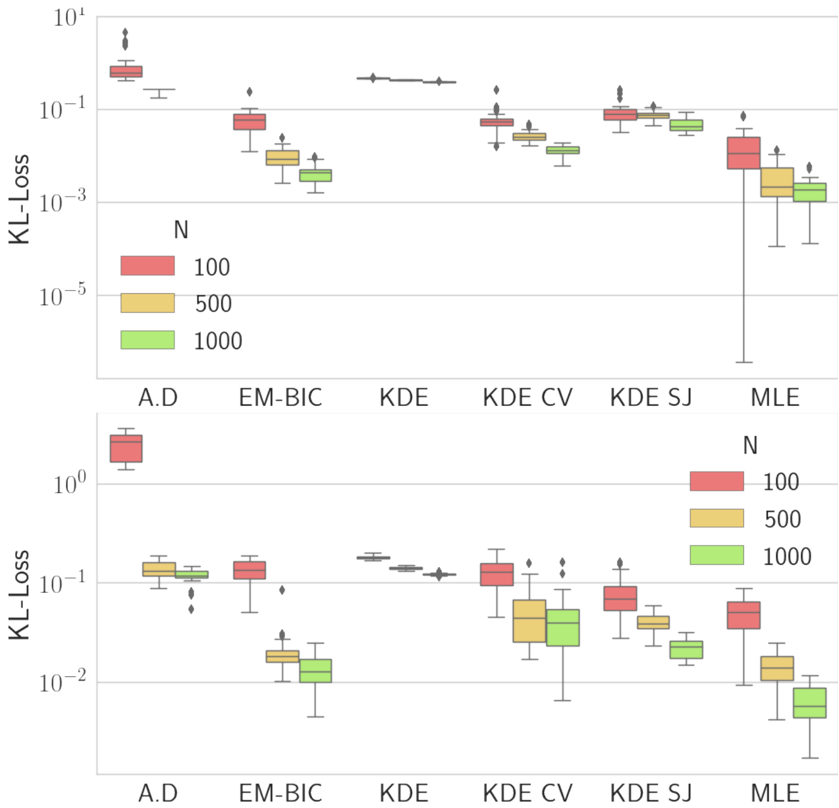


Figure 3.19: Results with f_{gauss} (upper panel) and $f_{\text{gauss-lapl}}$ (lower panel) in KL loss with D_{GLU}.

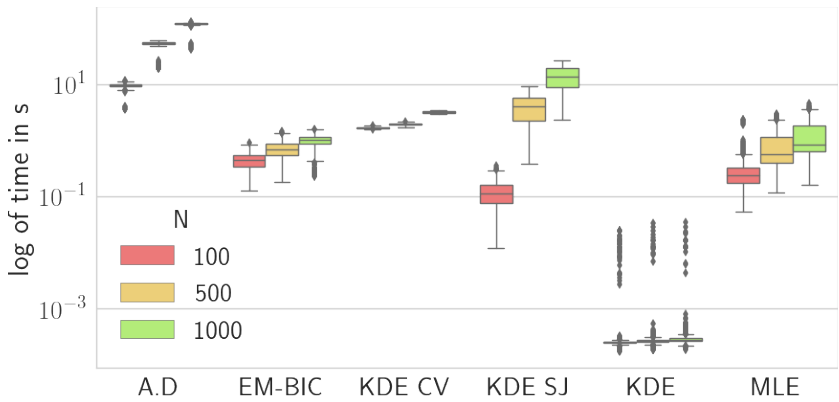


Figure 3.20: Computation times

3.5.1 Implementation of the dictionary generator

Given a sample $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n \in \mathbb{R}^p$, we construct the set of principal components C of the design matrix $\boldsymbol{X}$ by PCA. Then we build the set S of all subspaces spanned by two elements of C:

$$S = \{\text{span}(\boldsymbol{v}_i, \boldsymbol{v}_j),\, (\boldsymbol{v}_i, \boldsymbol{v}_j) \in C.\}. \tag{3.38}$$

On each subspace of S, we perform a clustering to find groups. For each group, we consider the points assigned to it in the original space and recover the empirical mean, the sample variance and construct a normal density with these parameters. A simple implementation would consider all principal components and thus $\frac{p(p-1)}{2}$ subspaces. On each of these subspace a clustering method such as K-means with an arbitrary large number of clusters K would be applied. The whole complexity would be $\mathcal{O}(p^2 n^{2K+1})$. To reduce the computational complexity of this procedure, especially in high dimension, we adopted three strategies:

1. Select the most informative components obtained via the PCA. One can use different techniques such as the Truncated SVD or the method proposed in [Gavish and Donoho, 2014] which circumvent the issue of not knowing rank($\boldsymbol{X}$). They considered the recovery of low-rank matrices from noisy data by hard thresholding of singular values by studying the asymptotic MSE. The AMSE-optimal choice of hard threshold would be for a n-by-p matrix with $n \neq p$, $\widehat{\tau}_* = \omega(\beta).y_{med}$, with $\beta = n/p$, y_{med} is the median singular value of $\boldsymbol{X}$ and $\omega(\beta)$ is described in [Gavish and Donoho, 2014]. An approximation of $\omega(\beta)$ is $\omega(\beta) \approx 0.56\beta^3 - 0.95\beta^2 + 1.82\beta + 1.43$.

2. Perform a model selection for each clustering which reduces the number

of densities added to the dictionary. The method chosen is EM with BIC.

3. We address the problem of density duplicates in the dictionary originating from the same subset of points. We saw in the previous section that overlapping densities can degrade the performance of our estimators. One would like to remove these similar densities by performing a two-sample test. The reduction of multivariate two-sample testing to a binary classification problem follows from Friedman in [Friedman, 2003]. To test whether two densities P and Q are equal, we draw two samples $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ and $\{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$ from P and Q respectively and construct the dataset

$$\mathcal{D} = \{(\boldsymbol{u}_i, l_i)\}_{i=1}^{n+m} \coloneqq \{(\mathbf{y}_i, -1)\}_{i=1}^{n} \cup \{(\mathbf{z}_i, 0)\}_{i=1}^{m}. \tag{3.39}$$

We shuffle $\mathcal{D}$ and keep a record of the original assignments for each sample in $\mathcal{D}$. Then, we split this dataset into two parts, $\mathcal{D}_{tr}$ for training a binary classifier and $\mathcal{D}_{te}$ for predicting the classification scores $\{s_i\}_{i=1}^{n+m}$. We consider the two sets S_+ and S_-, the first one contains the scores of the samples originating from $\{\mathbf{z}_i\}_{i=1}^{m}$ and S_- contains the scores of the samples originating from $\{\mathbf{y}_i\}_{i=1}^{n}$. We can view S_+ and S_- as two samples drawn from two probability distributions, $p_+(s)$ and $p_-(s)$, and apply a goodness-of-fit test such as the univariate Kolmogorov–Smirnov test, for testing the equality of these two densities. The resulting test statistic is the statistic for the multivariate two-sample test for the equality of the distributions P and Q.

The dictionary construction procedure is given in Figure 3.21

3.5.2 Experimental evaluation

We created a mixture of 6 components in dimension 5, see Figure 3.22, which mimics data that can be seen in real use cases. The simulation were run in dimension 3, 4 and 5 by selecting the corresponding first axis. We generated $N \in \{200, 500, 1000, 5000\}$ points and ran 200 simulations for each scenario (N, dimension). We used the dictionary generation procedure for the KL-aggregation algorithm with $K_{max} = 10$ on each subspaces and significance level $\alpha = 0.05$. The dataset has been split into two equal parts, one for the dictionary generation algorithm and the other for the KL-aggregation algorithm. We compared the L_2-loss and KL-loss of our method to EM-BIC ($K_{max} = 20$) and KDE-CV (The bandwidth h is selected via cross-validation in $[0.01, \ldots, 1]$ in an equal partition of 20 elements). The computation times were also recorded.

Note: imagerie ?

Results without the selection of principal components and the goodness-of-fit test for the dictionary generator algorithm.

We compared, first, the KL-algorithm with the dictionary generated by our procedure to KDE-CV and EM-BIC without the two computation optimization techniques discussed before (selection of principal components and the deletion of similar densities). The time given for MLE is the total computational time of the generation of the dictionary and the aggregation algorithm. In the three scenarios (dimension 3,4 and 5), our algorithm presents same performance as EM-BIC in L_2 and KL loss with a better result when $N = 5000$ (see Figures 3.23 to 3.25). Both methods outperforms KDE-CV in all scenarios. This indicates that the set of bandwidths explored for KDE-CV does not fit the data correctly. Increasing the size of this set would increase dramatically the computation times of KDE-CV. Despite the quadratic increase of the size of the dictionary with the dimension, our algorithm takes less time to compute than KDE-CV and slightly more than EM-BIC.

Results with the selection of principal components and the goodness-of-fit test for the dictionary generator algorithm.

Adding the two computation optimization techniques, our algorithm still performs better than KDE-CV and has similar performance than EM-BIC in L_2-loss (see Figures 3.26 to 3.28). Unfortunately our method shows a bigger error variance for the KL-loss, especially when $N = 5000$. This behavior is not expected and may be due to incorrect settings and subtleties in the implementation. Despite adding more "intelligence" in the construction of the dictionary, this procedures counterbalance the cost of adding too much densities to the KL-aggregation algorithm and therefore leads to smaller computational times independent of the size of the sample. Note that we implemented our methods in Python without Just-In-Time compilations and therefore suffers significant computation overhead compared to Numpy's implementation of EM-BIC and KDE-CV. We are confident that a proper optimized implementation would be significantly faster. This remark highlights the attractiveness of our methods when the size of the sample increases.

3.5.3 Concluding remarks

To conclude, the density dictionary generation method we developed is well suited for our KL-aggregation algorithm. Without the techniques that we implemented to lighten the density dictionary, our methods performs as well as EM-BIC in KL-loss and L_2-loss and slightly better with a large sample ($N = 5000$). With the selection of principal components and the tests of similarity of densities in the dictionary, we tried to solve the problem of computational complexity of our method as the dimension and the size of the sample increase. On this setting, our method shows computation times independent of the size of the sample. Unfortunately, our algorithm shows a large error variance when $N = 5000$ in KL-loss. We are confident that a fine tuning of the parameters of the selection of principal components method and of the tests of similarity of densities would solve this problem. Moreover, we observed in our simulations that the use of the selection of principal components technique and the tests of density similarities to lighten the density dictionary gives us an estimation of the number of real clusters in the data and can be seen as a parameter-free clustering method. From this perspective, our method can be related to a subspace clustering method.

Input: $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ with $\boldsymbol{X}_i \in \mathbb{R}^p$. And K_{max}, maximum number of clusters for EM-BIC, significance level α.

Output: A dictionary of densities $D = \{f_1, \ldots, f_M\}$.

1: Construct the set Ω of singular values of the design matrix $\boldsymbol{X} \in \mathbb{R}^{p\times n}$ which are greater than $\omega(\beta).y_{med}$ with y_{med} median of singular values, $\beta = p/n$ and $\omega(\beta) \approx 0.56\beta^3 - 0.95\beta^2 + 1.82\beta + 1.43$.

2: Construct the set of principal components $\bar{C}$ corresponding to the singular values in Ω.

for $\boldsymbol{v}_i, \boldsymbol{v}_j \in \bar{C}$ **do**

3: Run EM-BIC with maximum K_{max} clusters on the data projected to $\mathrm{span}(\boldsymbol{v}_i, \boldsymbol{v}_j)$, $\boldsymbol{X}_1^{(i,j)}, \ldots, \boldsymbol{X}_n^{(i,j)}$, and construct clusters of points $G_1, \ldots, G_K$.

4: For each cluster G_m, $m \in [K]$, compute the mean $\widehat{\boldsymbol{\mu}}_m$ and variance $\widehat{\boldsymbol{\Sigma}}_m$ of the points assigned to G_m in the original space $\mathbb{R}^P$.

5: Add to the dictionary D the Gaussian densities $\{\varphi_{(\widehat{\boldsymbol{\mu}}_m, \widehat{\boldsymbol{\sigma}}_m)}\}_{m\in[K]}$.

end for.

for $\widehat{f}_i, \widehat{f}_j \in D$ **do**

6: Draw two samples $\{\mathbf{y}_1, \ldots, \mathbf{y}_l\}, \{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$ from $\boldsymbol{Y} \sim \widehat{f}_i$ and $\boldsymbol{Z} \sim \widehat{f}_j$ and construct the dataset $\mathcal{D} = \{(\boldsymbol{u}_i, l_i)\}_{i=1}^{n+m} := \{(\mathbf{y}_i, -1)\}_{i=1}^{n} \cup \{(\mathbf{z}_i, 0)\}_{i=1}^{m}$.

7: Shuffle and split $\mathcal{D}$ into $\mathcal{D}_{tr}$ and $\mathcal{D}_{te}$.

8: Train a binary classifier on $\mathcal{D}_{tr}$ and get the classification scores $\{s_i\}$ on $\mathcal{D}_{te}$.

9: Separate $\{s_i\}$ into $\{s_i\}^+$, scores of points drawn from $\boldsymbol{Z}$ and $\{s_i\}^-$ for $\boldsymbol{Y}$.

10: Perform a two-samples Kolmogorov-Smirnov test on $\{s_i\}^+$ and $\{s_i\}^-$ and reject H_0 (The two multivariate samples are drawn from the same distribution) with significance level α.

11: **If** H_0 rejected, remove $\widehat{f}_j$ of D, **else**, keep $\widehat{f}_i$ and $\widehat{f}_j$.

end for.

Figure 3.21: Procedure for generating a dictionary of densities

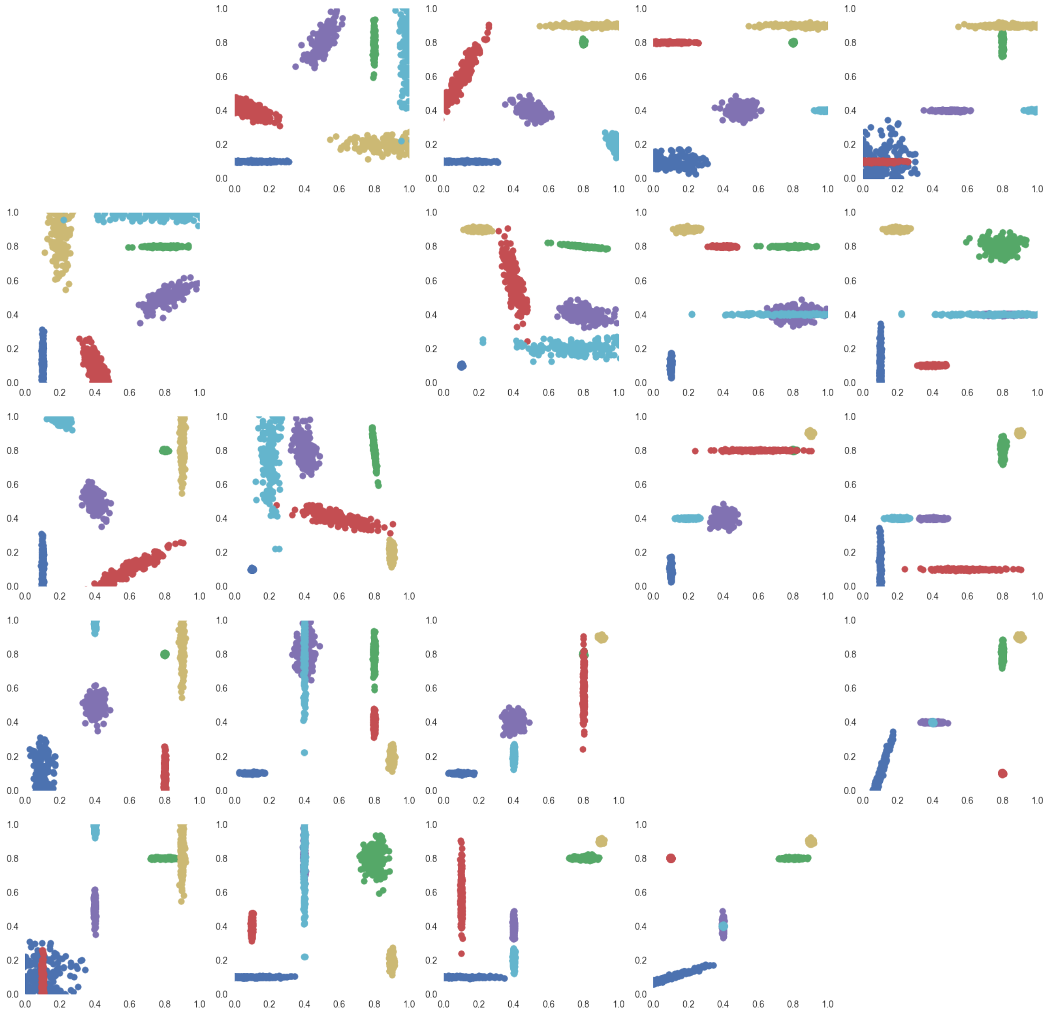


Figure 3.22: Simulated data for the dictionary generator algorithm and KL-aggregation

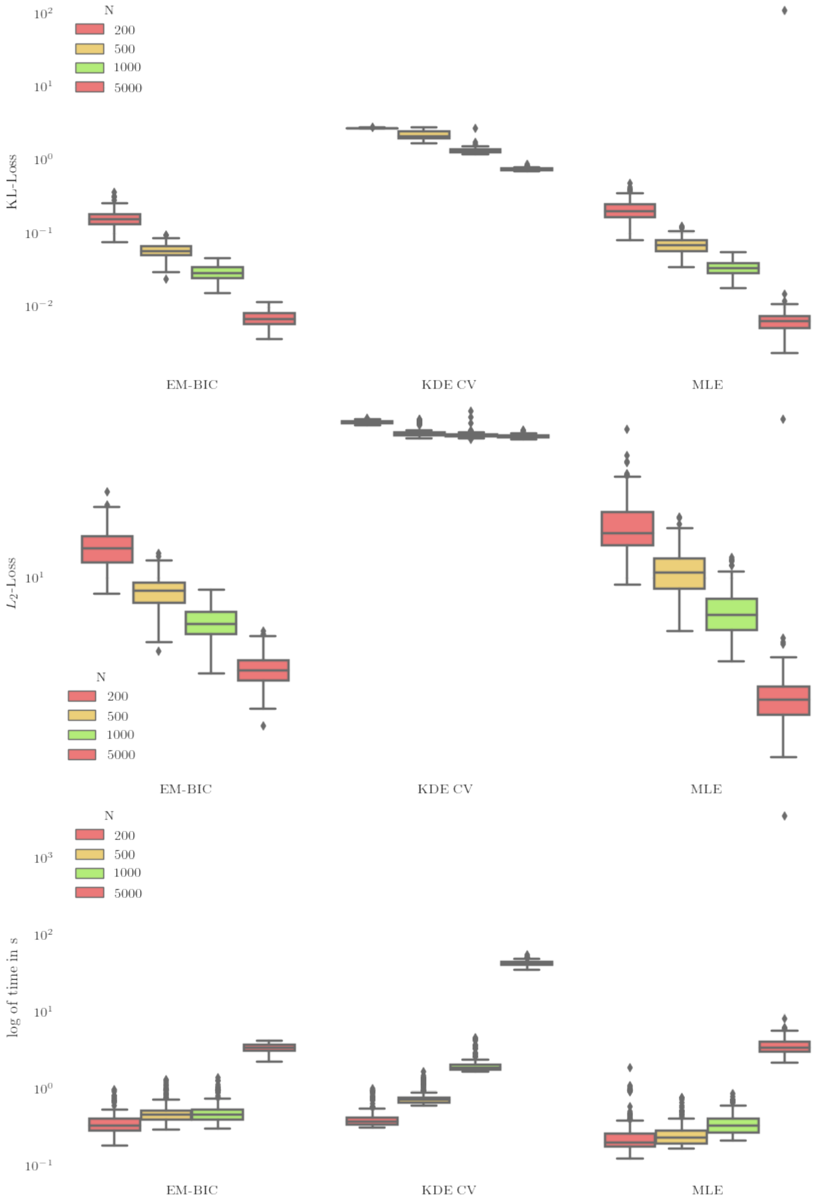


Figure 3.23: Results for dimension 3. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). Without dictionary generation optimizations.

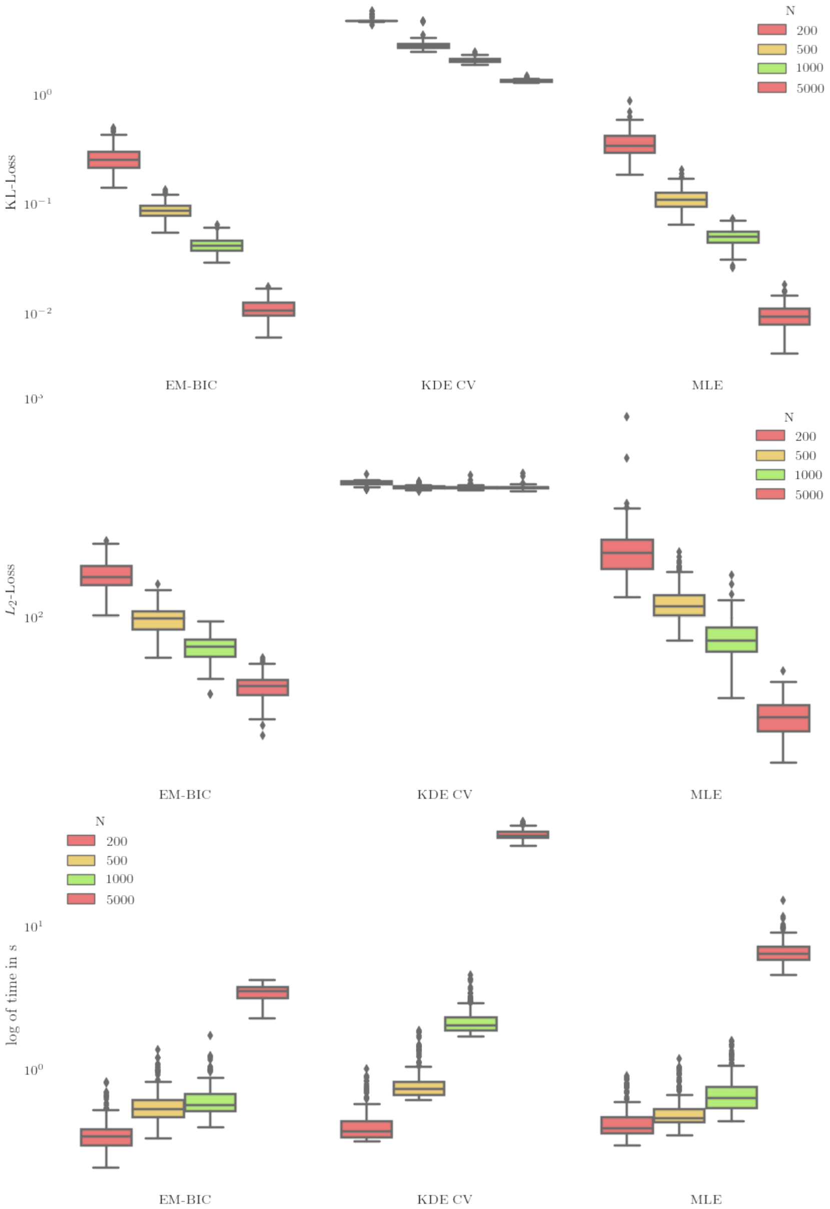


Figure 3.24: Results for dimension 4. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). Without dictionary generation optimizations.

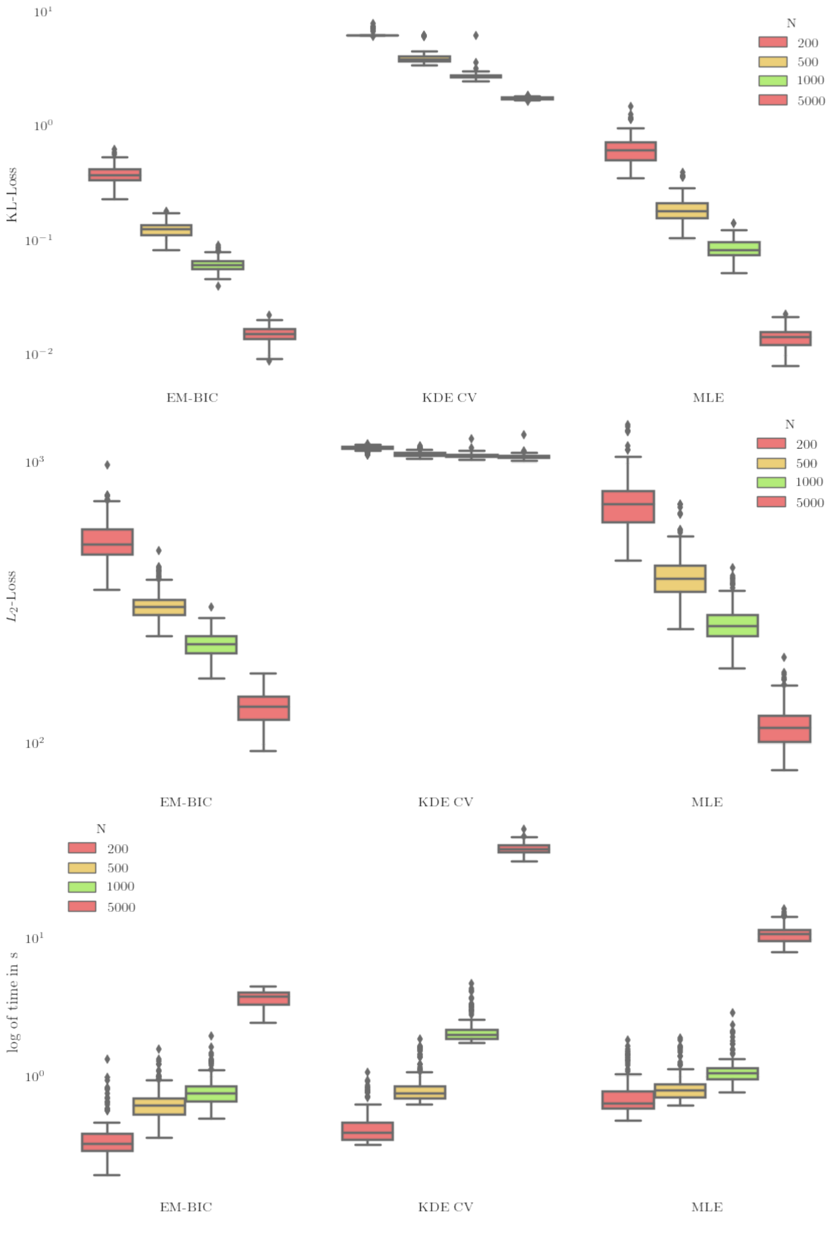


Figure 3.25: Results for dimension 5. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). Without dictionary generation optimizations.

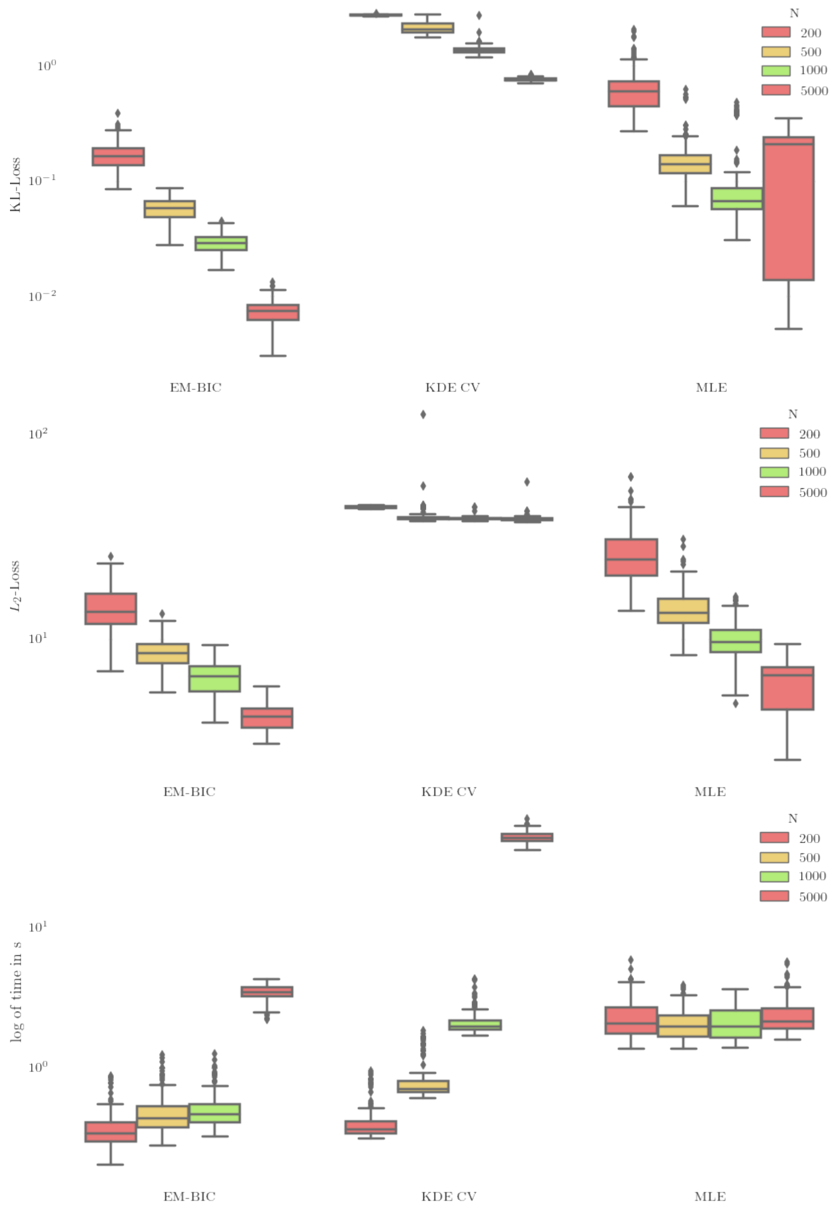


Figure 3.26: Results for dimension 3. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). With selection of principal components and deletion of similar densities.

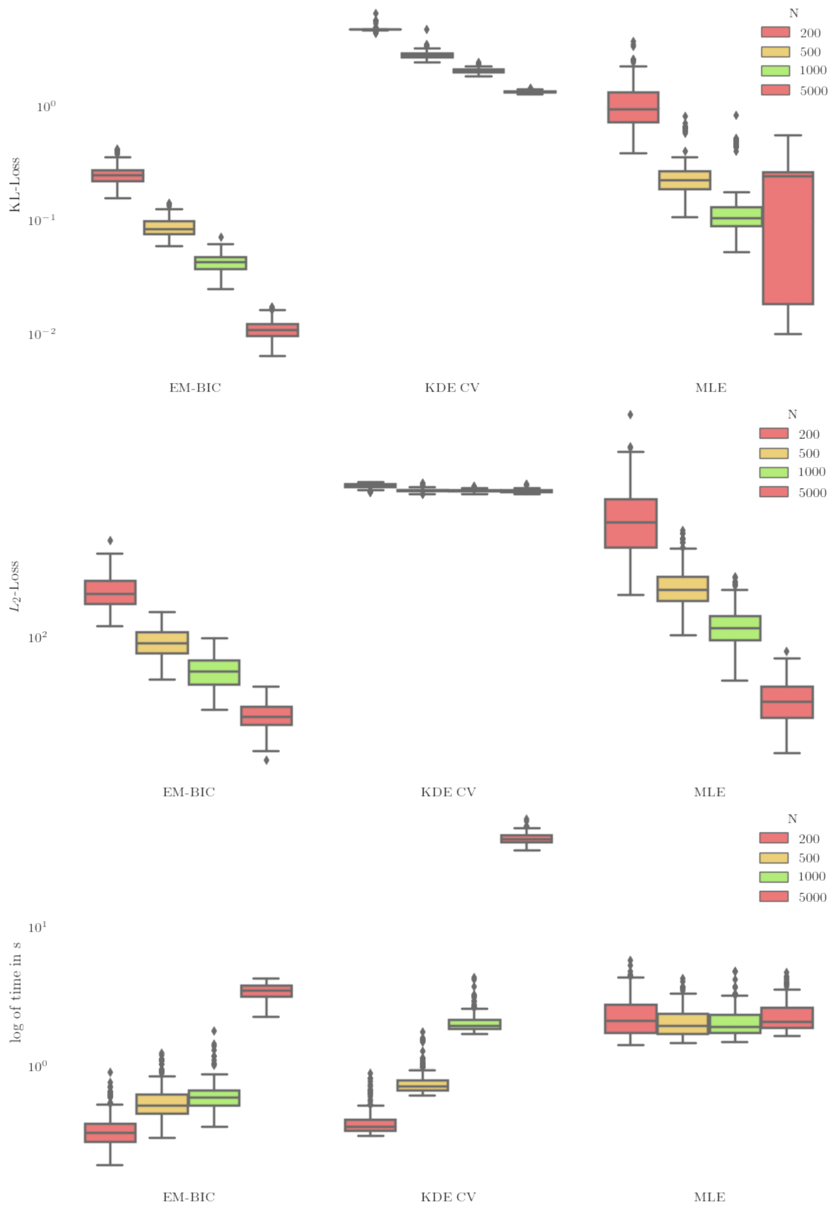


Figure 3.27: Results for dimension 4. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). With selection of principal components and deletion of similar densities.

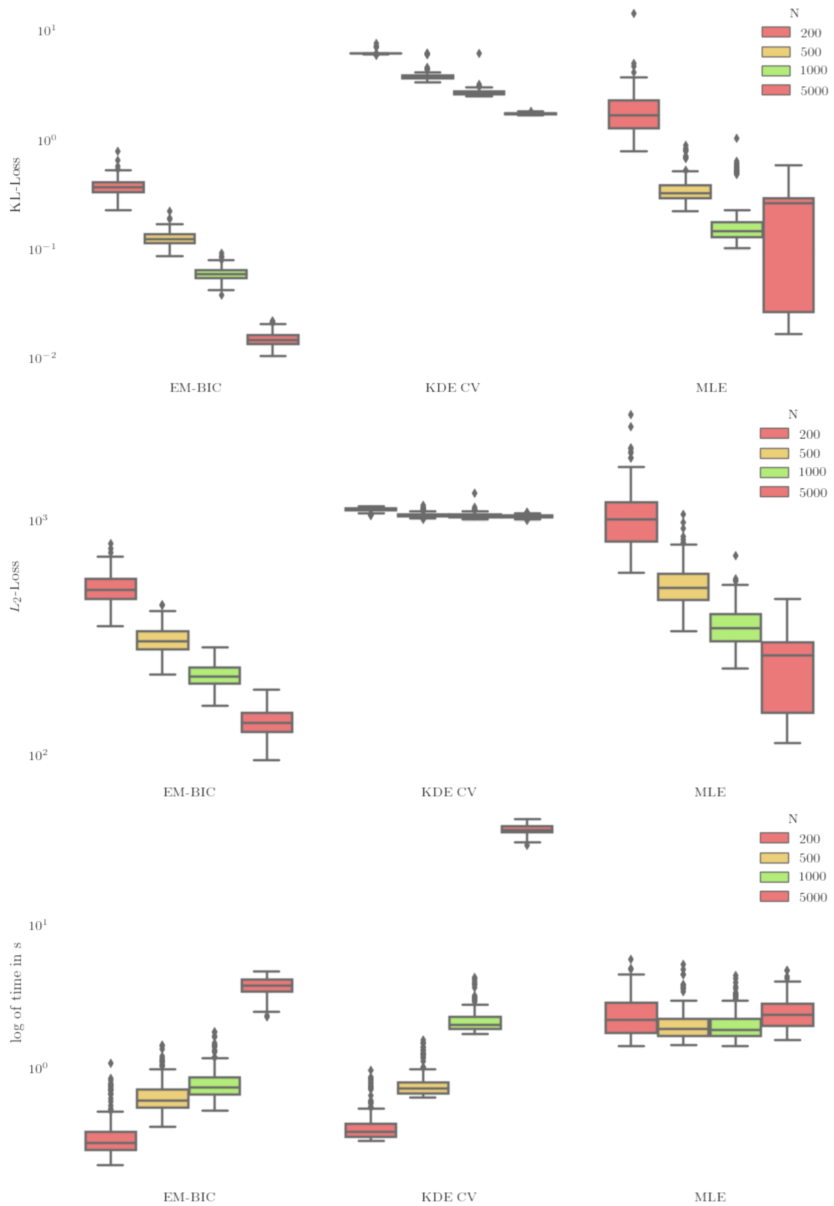


Figure 3.28: Results for dimension 5. KL-Loss (upper panel), L_2-Loss (middle panel) and computation time (lower panel). With selection of principal components and deletion of similar densities.

Chapter 4

Appendix and notes

4.1 Notes on "Model-Based Clustering of High-Dimensional Data: A review"

From Bouveyron and Brunet [2013]

> FA-based models choose the latent subspace(s) maximizing the projected variance whereas the Discriminative latent mixture (DLM) model chooses the latent subspace which maximizes the separation between the groups.

The DLM model assumes that Y is linked to a latent variable $X \in \mathbb{E}$ where $\mathbb{E} \subset \mathbb{R}^p$ through a linear relationship

$$Y = UX + \varepsilon \tag{4.1}$$

$\mathbb{E}$ is the most dicriminative subspace of dimension $d \leq K - 1$

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