Kullback-Leibler aggregation
and misspecified generalized linear models

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Abstract

In a regression setup with deterministic design, we study the pure aggregation problem and introduce a natural extension from Gaussian to distributions in the exponential family. While this extension bears strong connections with generalized linear models, it does not require identifiability of the parameter or even that the model on the systematic component is true. It is shown that this problem can be solved by constrained and/or penalized likelihood maximization and we derive sharp oracle inequalities that hold both in expectation and with high probability. A new proof technique that exploits the structure of the loss function is employed. It yields error bounds that are accurate already for small sample sizes. Finally all the bounds are proved to be optimal in minimax sense.

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Short title: Kullback-Leibler aggregation.

1 Introduction

The last decade has witnessed a growing interest in the general problem of aggregation, which turned out to be a flexible way to capture many statistical learning setups. Originally introduced in the regression framework by Nemirovski (2000) and Juditsky and Nemirovski (2000) as an extension of the problem of model selection, aggregation became a mature statistical field with the papers of Tsybakov (2003) and Yang (2004) where optimal rates of aggregation were derived. Subsequent applications to density estimation (Rigollet and Tsybakov, 2007) and classification (Belomestny and Spokoiny, 2007) constitute other illustrations of the generality and versatility of aggregation methods. In the pure aggregation setup, it is assumed that a collection of functions is given and the goal is to find a linear combination of these functions that exhibits a small risk.

The general problem of aggregation can be described as follows. Consider a finite family \( \mathcal{H} \) (hereafter called dictionary) of candidates for a certain statistical task. Assume also that the dictionary \( \mathcal{H} \) belongs to a certain linear space so that linear combinations of functions in \( \mathcal{H} \)
remain plausible candidates. For example, such candidates can be estimators constructed from a hold-out sample or simply basis functions or any system of function with good approximation properties. Indeed, the theory of aggregation is developed under minimal conditions on the dictionary $\mathcal{H}$. Building on original results regarding model selection for density estimation (Yang, 2000) and regression (Catoni, 2004), Nemirovski (2000) identified two new types of aggregation: convex aggregation, where the goal is to mimic the best convex combination of candidates in $\mathcal{H}$ and linear aggregation where the goal is to mimic the best linear combination of candidates in $\mathcal{H}$.

One salient feature of aggregation as opposed to standard statistical modeling, is that it does not rely on an underlying model. Indeed, the goal is not to estimate the parameters of an underlying ‘true’ model but rather to construct an estimator that mimics the performance of the best model in a given class, whether this model is true or not. From a statistical analysis standpoint, this difference is significant since performance cannot be measured in terms of parameters: there is no true parameter. Rather, a stochastic optimization point of view is adopted in aggregation. If $C$ denotes a class of linear combinations of functions in $\mathcal{H}$ and $R(\cdot)$ denotes a convex risk function, the goal pursued in aggregation is to construct an aggregate estimator $\hat{h}$, measurable with respect to the data at hand and such that

$$\mathbb{E} R(\hat{h}) \leq C \min_{f \in C} R(f) + \epsilon,$$

where $\epsilon$ is a small term that characterizes the performance of the given aggregate $\hat{h}$. As illustrated below, the remainder term $\epsilon$ is an explicit function of $M$ and $n$ that shows the interplay between these two fundamental parameters. Such oracle inequalities with optimal remainder term $\epsilon$ were originally derived by Yang (2000) and Catoni (2004) for model selection in the problems of density estimation and Gaussian regression respectively. They method that they used, called progressive mixture was later extended to more general stochastic optimization problems in Juditsky et al. (2008). However, only bounds in expectation have been derived for this estimator and it is argued in Audibert (2007) that this estimator cannot achieve optimal remainder terms with high probability. One contribution of this paper (Theorem 4.2) is to develop a new estimator that enjoys this desirable property.

When the model is misspecified, the minimum risk satisfies $\min_{f \in C} R(f) > 0$, and it is therefore important to obtain a leading constant $C = 1$. Many oracle inequalities with leading constant term $C > 1$ can be found in the literature for related problems. Oracle inequalities in Yang (2004) also exhibits a constant $C > 1$ but in that paper, the class $C = C_n$ actually depends on the sample size $n$ so that $\min_{f \in C_n} R(f)$ goes to 0 as $n$ goes to infinity under additional regularity assumptions. In this paper, we focus on the pure aggregation setup as defined by Nemirovski (2000) and Tsybakov (2003) where the class $C$ is fixed and remains very general. As a result, oracle inequalities considered here only have leading constant $C = 1$. Because they hold for finite $M$ and $n$, such oracle inequalities are truly finite sample results.

Recall that the setup of Tsybakov (2003) is the following. The observations consist of $n$ i.i.d copies of the random couple $(X, Y)$ where $X$ has known marginal distribution and $Y = f(X) + \xi$, where $\xi$ is a centered random variable with bounded variance and that is independent of $X$. Furthermore, in the case of convex aggregation, it is assumed that $\xi$ has a normal distribution $\mathcal{N}(0, \sigma^2)$. 

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We consider an extension of aggregation for Gaussian regression that encompasses distributions for responses in a one-parameter exponential family, with particular focus on the family of Bernoulli distributions in order to cover binary classification. A natural measure of risk in this problem is related to the Kullback-Leibler divergence between the distribution of the actual observations and that of observations generated from a given model. In a way, this extension is close to generalized linear models (see, e.g., McCullagh and Nelder, 1989), which are optimally solved by maximum likelihood estimation (see, e.g., Fahrmeir and Kaufmann, 1985). However, in the present aggregation framework, it is not assumed that there is one true model but we prove that maximum likelihood estimators still perform almost as well as the optimal solution of a suitable stochastic optimization problem. This generalized framework encompasses logistic regression as a particular case.

Throughout the paper, for any $x \in \mathbb{R}^M$, let $x_j$ denote its $j$-th coordinate. In other words, any vector $x \in \mathbb{R}^M$ can be written $x = (x_1, \ldots, x_M)$. Similarly an $n \times M$ matrix $H$ has coordinates $H_{i,j}, 1 \leq i \leq n, 1 \leq j \leq M$. The derivative of a function $b: \mathbb{R} \rightarrow \mathbb{R}$ is denoted by $b'$. Finally for any real valued function $f$, we denote by $\|f\|_{\infty} = \sup_x |f(x)| \in [0, \infty]$, its sup norm.

The paper is organized as follows. In Section 2, we recall a few important results about generalized linear models and some of their extensions. Then, in Section 3, we define the problem of Kullback-Leibler aggregation, which is the counterpart of generalized linear models but in a aggregation framework where the model may be misspecified. In particular, we exhibit a natural measure of performance that suggests the use of constrained likelihood maximization to solve it. Exact oracle inequalities, both in expectation and with high probability are gathered in Section 4 and their optimality for finite $M$ and $n$ is assessed in Section 5. These oracle inequalities for the case of large $M$ are illustrated on a logistic regression problem, similar to the problem of training a boosting algorithm, in Section 6. Finally, Section 7 contains the proofs of the main results together with useful properties on the concentration and the moments of sums of random variables with distribution in an exponential family.

## 2 Generalized linear regression

### 2.1 Setup and notation

Let $Y \in \mathcal{Y} \subset \mathbb{R}$ be a random variables and let $\hat{\mathcal{Y}}$ denote the convex hull of $\mathcal{Y}$. Let $\mathcal{X}$ be an abstract space and define the regression function $f: \mathcal{X} \rightarrow \hat{\mathcal{Y}}$ of $Y$ onto $X$ by $f(x) = \mathbb{E}[Y|X=x]$. The function $f$ is unknown and we observe a sample $(x_1, Y_1), \ldots, (x_n, Y_n)$ where the $x_i \in \mathcal{X}, i = 1, \ldots, n$ are deterministic and the $Y_i \in \mathcal{Y}, i = 1, \ldots, n$ are independent random variables such that $\mathbb{E}[Y_i|x_i] = f(x_i)$.

Consider the equivalence relation $\sim$ on the space of functions $f: \mathcal{X} \rightarrow \mathbb{R}$ that is defined such that $f \sim g$ if and only if $f(x_i) = g(x_i)$ for all $i = 1, \ldots, n$. Denote by $Q_{1:n}$ the quotient space associated to this equivalence relation and define the norm $\| \cdot \|$ by

$$\|f\|^2 = \frac{1}{n} \sum_{i=1}^{n} f^2(x_i), \quad f \in Q_{1:n}.$$ 

Note that $\| \cdot \|$ is a norm on the quotient space but only a seminorm on the whole space of functions $f: \mathcal{X} \rightarrow \mathbb{R}$. In what follows, it will be useful to define the inner product associated
to $\| \cdot \|$ by
\[
\langle f, g \rangle = \frac{1}{n} \sum_{i=1}^{n} f(x_i)g(x_i).
\]
Using this inner product, we can also denote the average of a function $f$ by
\[
\frac{1}{n} \sum_{i=1}^{n} f(x_i) = \langle f, 1 \rangle,
\]
where $1(\cdot)$ is the function in $Q_{1:n}$ that is identically equal to 1.

### 2.2 Generalized linear models

Recall that a random variable $Y \in \mathbb{R}$ has distribution in a (one-parameter) canonical exponential family if it admits a density with respect to a reference measure on $\mathbb{R}$ given by
\[
p(y; \theta) = \exp \left\{ y\theta - b(\theta) a + c(y) \right\}.
\]
(2.1)
The parameter $\theta \in \Theta \subset \mathbb{R}$ is called canonical parameter and $a > 0, b(\cdot)$ and $c(\cdot)$ are given. In the rest of this paper, we only consider functions $b(\cdot)$ that are twice continuously differentiable. When the reference measure is the Lebesgue measure on $\mathbb{R}$, exponential families encompass Gaussian or Gamma distributions. Discrete distributions that admit such a density with respect to the counting measure on the set of integers $\mathbb{Z}$ include Poisson and Bernoulli. A detailed treatment of exponential families of distributions together with examples can be found in Barndorff-Nielsen (1978); Brown (1986); McCullagh and Nelder (1989) and in Lehmann and Casella (1998). Several examples are also treated in Section 6 of the present paper. It can be easily shown that if $Y$ admits a density given by (2.1), then
\[
\mathbb{E}[Y] = b'(\theta),
\]
\[
\text{var}[Y] = ab''(\theta).
\]
(2.2)

We assume hereafter that distribution of $Y$ is not degenerate so that (2.2) ensures that $b$ is strictly convex and $b'$ is a bijection onto its image space.

Generalized linear models constitute a rich and versatile collection of models to estimate the function $f$, that allow $Y$ to have a variety of distributions. Such models assume that the conditional distribution of the observation $Y_i$ belongs to a given exponential family with expectation $E[Y_i] = f(x_i), i = 1, \ldots, n$. The dependency in $x$ is modeled by a systematic component $\eta : \mathcal{X} \to \mathbb{R}$ such that $g \circ f(x) = \eta(x)$ where $g : \bar{Y} \to \mathbb{R}$ is a link function. The choice of the link function is part of the modeling process but typically results from the following considerations. From (2.2), we have
\[
g \circ b'(\theta) = \eta \iff \theta = h(\eta),
\]
where $h = (g \circ b')^{-1}$. In the rest of the paper, we only consider the so-called canonical link function defined by $g = (b')^{-1}$ so that $h$ is the identity map and therefore the canonical parameter
\( \theta \) itself is modeled by the systematic component \( \eta \). Note that the technique employed in our proofs does not apply to other link functions in a straightforward way.

The strongest assumption on which the model relies is on the systematic component \( \eta \). In generalized linear models, it is assumed that \( \mathcal{X} \subset \mathbb{R}^d \) and that \( \eta \) is a linear function of \( x \), i.e., \( \eta(x) = \beta^\top x \), where \( \beta \in \mathbb{R}^d \) is a parameter to be estimated. Other forms for \( \eta \) have been considered in related models such as generalized additive models (Hastie and Tibshirani, 1990) and extended additive models (Friedman et al., 2000), which do not require that \( \mathcal{X} \subset \mathbb{R}^d \). Let \( \mathcal{H} = \{f_1, \ldots, f_M\} \) be a dictionary of functions \( f_j : \mathcal{X} \to \mathbb{R} \) and for any \( \lambda \in \mathbb{R}^M \), define the linear combination

\[
 f_\lambda = \sum_{j=1}^{M} \lambda_j f_j. 
\]

An extended additive model assumes that \( \eta \) is one of such linear combinations, namely that there exists \( \lambda \in \mathbb{R}^M \) such that for any \( x \in \mathcal{X} \):

\[
 \eta(x) = f_\lambda(x) = \sum_{j=1}^{M} \lambda_j f_j(x). 
\]

Extended additive models can be embedded in the more general problem of aggregation, which does not assume that the data is generated from one particular model but tries to mimic the model that is the closest to the true distribution of the data. In the next section, we recall the problem of aggregation as originally defined by Nemirovski (2000) for Gaussian regression and extend it along the same lines as extended additive models to distributions in the exponential family.

## 3 Kullback-Leibler aggregation

### 3.1 The problem of aggregation

Aggregation for the regression problem was introduced by Nemirovski (2000) and further developed by Tsybakov (2003) where the author considers a regression problem with random design that has known distribution. We now recall the main ideas of aggregation applied to the regression problem, with emphasis on its difference with the linear regression model and what the new challenges for this problem are.

In the framework of the previous section, consider a finite dictionary \( \mathcal{H} = \{f_1, \ldots, f_M\} \) such that \( \|f_j\| \) is finite and for any \( \lambda \in \mathbb{R}^M \), recall that \( f_\lambda \) denotes the linear combination of \( f_j \)'s defined in (2.3). Consider the following regression model with additive noise: we observe \( n \) independent random couples \((x_i, Y_i), i = 1, \ldots, n\) such that

\[
 Y_i = f(x_i) + \varepsilon_i, 
\]

where \( \varepsilon_i, i = 1, \ldots, n \), are some noise random variables. The goal of aggregation is to solve the following optimization problem

\[
 \min_{\lambda \in \Lambda} \|f_\lambda - f\|^2, 
\]
where \( \Lambda \) is a given subset of \( \mathbb{R}^M \) and \( f \) is unknown. Previous papers on aggregation in the regression problem have focused on three choices for the set \( \Lambda \) corresponding to the three different problems of aggregation originally introduced by Nemirovski (2000): \( \Lambda \) is the whole space \( \mathbb{R}^M \) (linear aggregation), \( \Lambda \) is the flat simplex of \( \mathbb{R}^M \) (convex aggregation) and \( \Lambda \) is the finite set formed by the \( M \) vectors in the canonical basis of \( \mathbb{R}^M \) (model selection aggregation) (see Bunea et al., 2007; Nemirovski, 2000; Juditsky and Nemirovski, 2000; Tsybakov, 2003; Yang, 2004, and subsection 3.2 below). In practice, the regression function \( f \) is unknown and it is impossible to perfectly solve (3.5). Our goal is therefore to recover an approximate solution of this problem in the following sense. We wish to construct an estimator \( \hat{\lambda}_n \) such that
\[
\| f_{\hat{\lambda}_n} - f \|^2 - \min_{\lambda \in \Lambda} \| f_\lambda - f \|^2,
\]
is as small as possible. An inequality that provides an upper bound on the (random) quantity in (3.6) in a certain probabilistic sense is called oracle inequality.

Notice that this is not a linear model since we do not assume that the function \( f \) is of the form \( f_\lambda \) for some \( \lambda \in \mathbb{R}^M \). Rather, the bias term \( \min_{\lambda \in \Lambda} \| f_\lambda - f \|^2 \) may not vanish and the goal is to mimic the linear combination with the smallest bias.

The notion of Kullback-Leibler aggregation defined in the next subsection broadens the scope of the above problem of aggregation to encompass other conditional distributions for \( Y \) given \( X \).

### 3.2 Kullback-Leibler aggregation

Recall that the ubiquitous squared norm \( \| \cdot \|^2 \) as a measure of performance for regression problems takes its roots in the Gaussian regression model. The Kullback-Leibler divergence between two probability distributions \( P \) and \( Q \) is defined by
\[
\mathcal{K}(P||Q) = \begin{cases} 
\int \log \left( \frac{dP}{dQ} \right) dP & \text{if } P \ll Q, \\
\infty & \text{otherwise.}
\end{cases}
\]
Denote by \( P_f \) the joint distribution of the observations \( Y_i, i = 1, \ldots, n \) under (3.4). If the noise random variables \( \varepsilon_i \) in (3.4) are i.i.d \( \mathcal{N}(0, \sigma^2) \) random variables, then
\[
\mathcal{K}(P_f||P_g) = \frac{n}{2\sigma^2} \| f - g \|^2,
\]
In order to allow an easier comparison between the results of this paper and the literature, consider a normalized Kullback-Leibler divergence defined by \( \bar{\mathcal{K}}(P_f||P_g) = \mathcal{K}(P_f||P_g)/n \). In the Gaussian regression setup, the quantity of interest in (3.6) can be written
\[
\mathbb{E}\mathcal{K}(P_f||P_{\hat{\lambda}_n}) - \min_{\lambda \in \Lambda} \mathcal{K}(P_f||P_\lambda),
\]
up to a multiplicative constant term equal to \( 2\sigma^2 \). Nevertheless, the quantity in (3.7) is meaningful for other distributions in the exponential family.

Consider \( n \) independent observations \( (x_i, Y_i), i = 1, \ldots, n \) from the regression model (3.4) and assume that the distribution of \( Y_i \) has density given by
\[
p(y; \theta_i) = \exp \left\{ \frac{y\theta_i - b(\theta_i)}{a} + c(y) \right\},
\]
(3.8)
where $\theta_i = (b')^{-1} \circ f(x_i)$.

Given a subset $\Lambda$ of $\mathbb{R}^M$, the goal of Kullback-Leibler aggregation (in short KL-aggregation) is to construct an estimator $\hat{\lambda}_n$ such that the excess-KL defined by

$$EKL(f_{\hat{\lambda}_n}, \Lambda, \mathcal{H}) = \bar{K}(P_f \parallel P_{b' \circ f_{\hat{\lambda}_n}}) - \inf_{\lambda \in \Lambda} \bar{K}(P_f \parallel P_{b' \circ f_{\lambda}}),$$

is as small as possible.

Whereas KL-aggregation is a purely finite sample problem, it bears connections with the asymptotic theory of model misspecification as defined in White (1982), following LeCam (1953) and Akaike (1973). White (1982) proves that if the regression function $f$ is not of the form $f = b' \circ f_{\lambda}$ for some $\lambda$ in the set of parameters $\Lambda$, then under some identifiability and regularity conditions, the maximum likelihood estimator converges to $\lambda^*$ defined by

$$\lambda^* = \arg\min_{\lambda \in \Lambda} \bar{K}(P_f \parallel P_{b' \circ f_{\lambda}}).$$

Since we plan to solve KL-aggregation with the maximum likelihood estimator, upper bounds on the excess-KL can be interpreted as finite sample versions of those original results.

Note that assuming that $Y_i$ admits a density of the form (3.8) with known cumulant function $b(\cdot)$ is a strong assumption unless $Y_i$ has Bernoulli distribution, in which case identification of this distribution is trivial from the context of the statistical experiment. We emphasize here that model misspecification pertains only to the systematic component.

**Remark 3.1** Bounds on the excess-KL can also be interpreted in terms of density estimation with the Kullback-Leibler divergence as a measure of performance. Indeed, the function $p(y; f_{\lambda}(x))$ is a natural candidate to estimate the conditional density of $Y$ given $X = x$, where $p(\cdot; \cdot)$ is given by (2.1).

We will consider the three choices for $\Lambda$ that are now standard and correspond to the three standard problems of aggregation originally introduced by Nemirovski (2000). Following the work of Tsybakov (2003) we provide upper bounds in the form of oracle inequalities together with minimax lower bounds to assess the optimality of said upper bounds. As we will see in the following sections, optimal rates are essentially the same for the problem of KL-aggregation as for the Gaussian regression model studied in Tsybakov (2003).

**Model selection aggregation.** The goal is mimic the best $f_j$ in the dictionary $\mathcal{H}$. Therefore, we can choose $\Lambda$ to be the finite set $\mathcal{V} = \{e_1, \ldots, e_M\}$ formed by the $M$ vectors in the canonical basis of $\mathbb{R}^M$. The optimal rate of model selection aggregation in the Gaussian case is $(\log M)/n$.

**Linear aggregation.** The goal is mimic the best linear combination of the $f_j$’s in the dictionary $\mathcal{H}$. Therefore, we can choose $\Lambda$ to be whole space $\mathbb{R}^M$. The optimal rate of linear aggregation in the Gaussian case is $M/n$.

**Convex aggregation.** The goal is mimic the best convex combination of the $f_j$’s in the dictionary $\mathcal{H}$. Therefore, we can choose $\Lambda$ to be the rescaled flat simplex of $\mathbb{R}^M$ denoted
by $\Lambda^+_1(R)$ and defined by

$$
\Lambda^+_1(R) = \left\{ \lambda \in \mathbb{R}^M : \lambda_j \geq 0, j = 1, \ldots, M, \sum_{j=1}^M \lambda_j = R \right\},
$$

where $R > 0$. In the sequel, upper bounds are stated for any subset of the $\ell_1$ ball of $\mathbb{R}^M$ with radius $R > 0$ denoted by $\Lambda_1(R)$ and defined by

$$
\Lambda_1(R) = \left\{ \lambda \in \mathbb{R}^M : \sum_{j=1}^M |\lambda_j| \leq R \right\}. \quad (3.10)
$$

While this set is more massive than $\Lambda^+_1(R)$, it results in bounds that are deteriorated by only a factor 2. The optimal rate of convex aggregation in the Gaussian case is $(M/n) \wedge \sqrt{\log(1 + M/\sqrt{n})}/n$.

Note that we use hereafter a looser definition of linear aggregation where $\Lambda$ is not restricted to be the whole space $\mathbb{R}^M$ but can also be any closed convex subset of $\mathbb{R}^M$ such as an $\ell_\infty$ ball of $\mathbb{R}^M$. In this sense, convex aggregation can be viewed as a special case of linear aggregation.

## 4 Main results

Let $Z = \{(x_1, Y_1), \ldots, (x_n, Y_n)\}$ be $n$ independent observations such that for each $i$, the density of $Y_i$ is of the form $p(y_i; \theta_i)$ as defined in (2.1) where $\theta_i = (b')^{-1} \circ f(x_i)$. Then, we can write for any $\lambda \in \mathbb{R}^M$,

$$
\mathcal{K}(P_f\|P_{b' \circ f, \lambda}) = -\frac{n}{a} \left( \langle f, f_\lambda \rangle - \langle b \circ f_\lambda, \mathbb{I} \rangle \right) - \sum_{i=1}^n \mathbb{E}[c(Y_i)] + \text{Ent}(P_f), \quad (4.1)
$$

where $\text{Ent}(P_f)$ denotes the entropy of $P_f$ and is defined by

$$
\text{Ent}(P_f) = \sum_{i=1}^n \mathbb{E} \left[ \log \left( p(Y_i; (b')^{-1} \circ f(x_i)) \right) \right].
$$

Note the term $- \sum_{i=1}^n \mathbb{E}[c(Y_i)] + \text{Ent}(P_f)$ does not depend on $\lambda$.

Recall that the log-likelihood of an estimator $\hat{\theta} = (\hat{\theta}_1, \ldots, \hat{\theta}_n) \in \mathbb{R}^n$ based on these observations is defined by

$$
\sum_{i=1}^n \log \left[ p(Y_i; \hat{\theta}_i) \right] = \sum_{i=1}^n \left\{ \frac{Y_i \hat{\theta}_i - b(\hat{\theta}_i)}{a} + c(Y_i) \right\}.
$$

Therefore, for estimators of the form $\hat{\theta}_i = f_\lambda(x_i)$, we are interested in maximizing the function

$$
\ell_n(\lambda) = \sum_{i=1}^n \left\{ Y_i f_\lambda(x_i) - \langle b \circ f_\lambda, \mathbb{I} \rangle \right\}. \quad (4.2)
$$
over a certain set $\Lambda$ that depends on the problem at hand.

We now give a series of bounds for the problem of KL-aggregation. All proofs are gathered in Section 7 and rely on the following conditions, which can be easily checked given the cumulant function $b$.

**Condition 1** The set of admissible parameters is $\Theta = \mathbb{R}$ and there exists a positive constant $B^2$ such that
\[ \sup_{\theta \in \Theta} b''(\theta) \leq B^2, \]

**Condition 2** We say that the couple $(\mathcal{H}, \Lambda)$ satisfies condition 2 if there exists a positive constant $\kappa^2$ such that
\[ b''(f_\lambda(x)) \geq \kappa^2, \]
uniformly for all $x \in \mathcal{X}$ and all $\lambda \in \Lambda$.

Conditions 1 and 2 are discussed in the light of several examples in section 6. Condition 1 is used only to ensure that the distributions of $Y_i$ have uniformly bounded variances and sub-Gaussian tails whereas condition 2 is a strong convexity condition that depends not only on the cumulant function $b$ but also on the aggregation problem at hand that is characterized by the couple $(\mathcal{H}, \Lambda)$.

### 4.1 Model selection aggregation

Recall that the goal of model selection aggregation is to mimic a function $f_j$ such that $K(\mathbb{P}_f \parallel \mathbb{P}_{f_j}) \leq K(\mathbb{P}_f \parallel \mathbb{P}_{f_k}), k \neq j$. A natural candidate would be the function in the dictionary that maximizes the function $\ell_n$ defined in (4.2) either over the finite set $\mathcal{V} = \{e_1, \ldots, e_M\}$ formed by the $M$ vectors in the canonical basis of $\mathbb{R}^M$ or over the convex hull of $\mathcal{V}$ which is given by $\Lambda_+^+(1)$. However, it has been established (see, e.g., Juditsky et al., 2008; Lecué, 2007b; Lecué and Mendelson, 2009) that such a choice yields suboptimal rates of convergence in general. As a consequence we resort to a more sophisticated example obtained by penalized log-likelihood minimization.

Let $\beta > 0$, be a tuning parameter to be chosen large enough and define $\hat{\lambda} \in \Lambda_+^+(1)$ to be the unique vector that solves the following convex optimization problem:
\[
\hat{\lambda} = \arg\max_{\lambda \in \Lambda_+^+(1)} \left\{ \sum_{j=1}^{M} \lambda_j \ell_n(e_j) + \ell_n(\lambda) + \beta H(\lambda) \right\},
\] (4.3)

where
\[
H(\lambda) = -\sum_{j=1}^{M} \lambda_j \log(\lambda_j),
\]
denotes the entropy of the vector $\lambda \in \Lambda_+^+(1)$ when regarded as a probability distribution on the finite set $\mathcal{V}$. We propose to solve model selection aggregation using the convex combination $f_{\hat{\lambda}}$. 

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Before giving bounds on the excess-KL of $f^\lambda$, we comment on the main difference between $\tilde{\lambda}$ and the following commonly used vector of weights $\tilde{\lambda} \in \Lambda^+_1(1)$ defined by:

$$\tilde{\lambda}_j = \frac{e^{\ell_n(e_j)/\beta}}{\sum_{k=1}^M e^{\ell_n(e_k)/\beta}}, \quad j = 1, \ldots, M.$$  \hspace{1cm} (4.4)

It can be shown (see, e.g., Dupuis and Ellis, 1997, Proposition 1.4.2) that $\tilde{\lambda}$ is the unique solution of the following optimization problem

$$\max_{\lambda \in \Lambda^+_1(1)} \left\{ \sum_{j=1}^M \lambda_j \ell_n(e_j) + \beta H(\lambda) \right\}.$$

The use of exponential weights to perform optimal model selection aggregation goes back to Catoni (2004) and Yang (2000) with the progressive mixture rule. Like its generalization proposed in Juditsky et al. (2008), it requires an additional and somewhat counterintuitive averaging step but the optimal rates of model selection that these estimators yield contributed to the general belief that this extra step was necessary. Recently, Audibert (2007) argued that such estimators yield suboptimal rates with high probability even though they behave optimally in expectation.

The estimator $\hat{\lambda}$ that we use here does not take the form of exponential weights and although both criteria are penalized by the entropy, they are quite different. In particular, in the proof of the following theorems, a key ingredient is the fact that the function $f^\lambda \mapsto \sum_{j=1}^M \lambda_j \ell_n(e_j) + \ell_n(\lambda)$ is strongly concave.

**Theorem 4.1** Assume that condition 1 holds and that $(\mathcal{H}, \Lambda^+_1(1))$ satisfies condition 2. Recall that $\mathcal{V} = \{e_1, \ldots, e_M\}$ is the finite set formed by the $M$ vectors in the canonical basis of $\mathbb{R}^M$. Then, the aggregate $f^\lambda$ with $\lambda$ defined in (4.3) and $\beta \geq 8B^2a/\kappa^2$ satisfies

$$\mathbb{E}\left[\mathcal{E}_{KL}(f^\lambda, \mathcal{V}, \mathcal{H})\right] \leq \frac{\beta \log M}{a \cdot n}. \hspace{1cm} (4.5)$$

A similar result for $f^\tilde{\lambda}$ where $\tilde{\lambda}$ is given in (4.4) was obtained by Dalalyan and Tsybakov (2007) for a different class of regression problem with deterministic design under the squared loss. For random design, Juditsky et al. (2008) obtained essentially the same results for the mirror averaging algorithm. Also for random design, Lecué and Mendelson (2009) proposed a different estimator to solve this problem and give for the first time a bound with high probability with the optimal remainder term. Such a result was claimed by Audibert (2007) for a different estimator but comes without proof. Despite this recent effervescence, no bounds that hold with high probability have been derived for the deterministic design case considered here and the estimator proposed by Lecué and Mendelson (2009) is based on a sample splitting argument that does not extend to deterministic design. The next theorem aims at giving such an inequality for the aggregate $f^\lambda$. 

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Theorem 4.2 Assume that condition 1 holds and that \((\mathcal{H}, \Lambda^+_1(1))\) satisfies condition 2. Recall that \(\mathcal{V} = \{e_1, \ldots, e_M\}\) is the finite set formed by the M vectors in the canonical basis of \(\mathbb{R}^M\). Then, for any \(\delta > 0\), with probability \(1 - \delta\), the aggregate \(\hat{f}_\lambda\) with \(\hat{\lambda}\) defined in (4.3) and \(\beta \geq 8B^2a/\kappa^2\) satisfies
\[
\mathcal{E}_{\text{KL}}(\hat{f}_{\lambda_n}, \mathcal{V}, \mathcal{H}) \leq \frac{\beta \log(M/\delta)}{a},
\] (4.6)

The proofs of both theorems are gathered in subsection 7.2.

4.2 Linear aggregation

Let \(\Lambda \subset \mathbb{R}^M\) be a closed convex set or \(\mathbb{R}^M\) itself. The maximum likelihood aggregate over \(\Lambda \subset \mathbb{R}^M\) is uniquely defined as a function in the quotient space \(Q_{1:n}\) by the linear combination \(\hat{f}_{\lambda_n}\) with coefficients given by
\[
\hat{\lambda}_n \in \arg\max_{\lambda \in \Lambda} \ell_n(\lambda).
\] (4.7)

Note that both \(\hat{\lambda}_n\) and \(\lambda^* \in \arg\min_{\lambda \in \Lambda} \mathcal{K}(P_{f^*} || P_{f_{\lambda^*}})\) exist as soon as \(\Lambda\) is a closed convex set (see Ekeland and Téman, 1999, Chapter II, Proposition 1.2). Likewise, from the same proposition, we find that if \(\Lambda = \mathbb{R}^M\), condition 2 entails that both \(\hat{\lambda}_n\) and \(\lambda^*\) exist. Indeed, under condition 2, the function \(b\) is convex coercive and thus both functionals \(f_{\lambda} \mapsto -\sum_{i=1}^{n} \{Y_i f_{\lambda}(x_i) - \langle b \circ f_{\lambda}, 1\rangle\}\) and \(f_{\lambda} \mapsto -\langle f, f_{\lambda} \rangle + \langle b \circ f_{\lambda}, 1\rangle\) are convex and coercive. Thus, the aggregates \(f_{\lambda^*}\) and \(f_{\lambda_n}\) are uniquely defined as functions in the quotient space \(Q_{1:n}\), even though \(\lambda^*\) and \(\lambda_n\) may not be unique.

If the observations \(Z\) were actually drawn from an exponential family with canonical parameter \(\theta_i^*\), we could apply the asymptotic theory of maximum likelihood estimation to obtain consistency results. The goal here is not only to derive bounds on the quantity in (3.7) without assuming that the model holds but also to have precise finite sample bounds that explicitly depend on the sample size \(n\) and the size \(M\) of the dictionary.

We first extend the original results of Nemirovski (2000) and Tsybakov (2003) by providing bounds on the expected excess-KL, \(\mathbb{E}[\mathcal{E}_{\text{KL}}(\hat{f}_{\lambda_n}, \Lambda, \mathcal{H})]\) where \(\Lambda\) is either a closed convex set or \(\Lambda = \mathbb{R}^M\), which corresponds to the problem of linear aggregation.

Theorem 4.3 Let \(\Lambda\) be a closed convex subset of \(\mathbb{R}^M\) or \(\mathbb{R}^M\) itself, such that \((\mathcal{H}, \Lambda)\) satisfies condition 2. If the marginal variances satisfy \(\mathbb{E}[Y_i - f(x_i)]^2 \leq \sigma^2\) for any \(i = 1, \ldots, n\), then the maximum likelihood aggregate \(\hat{f}_{\lambda_n}\) over \(\Lambda\) satisfies
\[
\mathbb{E}[\mathcal{E}_{\text{KL}}(\hat{f}_{\lambda_n}, \Lambda, \mathcal{H})] \leq \frac{2\sigma^2 D}{a\kappa^2 n},
\]
\[
\mathbb{E}\|\hat{f}_{\lambda_n} - f_{\lambda^*}\|^2 \leq \frac{4\sigma^2 D}{\kappa^4 n},
\] (4.8)
where $D \leq M$ is the dimension of the linear span of $\mathcal{H}$ and

$$\lambda^* \in \arg\min_{\lambda \in \Lambda} K(P_f \| P_{\lambda^*}).$$

Vectors $\lambda^* \in \arg\min_{\lambda \in \Lambda} K(P_f \| P_{\lambda^*})$ are oracles since they cannot be computed without the knowledge of $P_f$. The oracle distribution $P_{\lambda^*}$ corresponds to the distribution of the form $P_{\lambda^*}$, $\lambda \in \Lambda$ that is the closest to the true distribution $P_f$ in terms of Kullback-Leibler divergence. Introducing this oracle allows us to assess the performance of the maximum likelihood aggregate, without assuming that $P_f$ is of the form $P_{\lambda^*}$ for some $\lambda \in \Lambda$. Notice also that from (2.2), the bounded variance condition $\mathbb{E}[Y_i - f(x_i)]^2 \leq \sigma^2$ is a direct consequence of condition 1 with $\sigma^2 = aB^2$.

Theorem 4.3 is valid in expectation. In other words it characterizes the rates of KL-aggregation attained by the maximum likelihood aggregate in average with respect to the realizations of the sample $Z$. The following theorem shows that these bounds are not only valid in expectation but also with high probability.

Theorem 4.4 Let $\Lambda$ be a closed convex subset of $\mathbb{R}^M$ or $\mathbb{R}^M$ itself and such that $(\mathcal{H}, \Lambda)$ satisfies condition 2. Moreover let condition 1 hold and let $D$ be the dimension of the linear span of the dictionary $\mathcal{H} = \{f_1, \ldots, f_M\}$. Then, for any $\delta > 0$, with probability $1 - \delta$, the maximum likelihood aggregate $f_{\lambda_n}$ over $\Lambda$ satisfies

$$\mathcal{E}_{KL}(f_{\lambda_n}, \Lambda, \mathcal{H}) \leq \frac{8B^2 D}{\kappa^2} \frac{\log \left( \frac{4}{\delta} \right)}{n},$$

$$\|f_{\lambda_n} - f_{\lambda^*}\| \leq \frac{16aB^2 D}{\kappa^4} \frac{\log \left( \frac{4}{\delta} \right)}{n},$$

where $\lambda^* \in \arg\min_{\lambda \in \Lambda} K(P_f \| P_{\lambda^*})$.

We see that the price to pay to obtain bounds with high probability is essentially the same as for the bounds in expectation up to an extra multiplicative term of order $\log(1/\delta)$.

4.3 Convex aggregation

In this subsection, we fix $R > 0$ and assume that $\Lambda \subset \Lambda_1(R)$ is a closed convex set where $\Lambda_1(R)$ is the $\ell_1$ ball of $\mathbb{R}^M$ with radius $R$ defined in (3.10). Note that both a maximum likelihood estimator $\hat{\lambda}_n$ and an oracle $\lambda^* \in \arg\min_{\lambda \in \Lambda} K(P_f \| P_{\lambda^*})$ exist as soon as $\Lambda$ is a closed convex set (see Ekeland and Témam, 1999, Chapter II, Proposition 1.2).

Recall that if $(\mathcal{H}, \Lambda)$ satisfies condition 2, Theorems 4.3 and 4.4 also hold. The following theorems ensure a better rate for the maximum likelihood aggregate $f_{\lambda_n}$ over $\Lambda_1(R)$ when $D$ and thus $M$, becomes much larger than $n$. It extends the problem of convex aggregation defined by Nemirovski (2000), Juditsky and Nemirovski (2000) and Tsybakov (2003) to case where the conditional distribution of the response variables is not restricted to be Gaussian.

Theorem 4.5 Fix $R > 0$ and let $\Lambda$ be any closed convex subset of the ball $\Lambda_1(R)$ defined in (3.10). Let condition 1 hold and assume that the dictionary $\mathcal{H}$ consists of functions satisfying
\( \| f_j \| \leq 1 \), for any \( j = 1, \ldots, M \). Then, the maximum likelihood aggregate \( f_{\lambda_n} \) over \( \Lambda \) satisfies

\[
\mathbb{E} \left[ \mathcal{E}_{KL}(f_{\lambda_n}, \Lambda, \mathcal{H}) \right] \leq 4eRB \sqrt{\frac{\pi}{a}} \sqrt{\frac{\log M}{n}}. \tag{4.10}
\]

Moreover, if \((\mathcal{H}, \Lambda)\) satisfies condition 2, then

\[
\mathbb{E} \| f_{\lambda_n} - f_{\lambda^*} \|^2 \leq \frac{8eRB}{\kappa^2} \sqrt{\pi a} \sqrt{\frac{\log M}{n}},
\]

where \( \lambda^* \in \arg\min_{\lambda \in \Lambda} \mathcal{K}(P_f \| P_{b' \circ f_{\lambda}}) \).

The bounds of Theorem 4.5 also have a counterpart with high probability as shown in the next theorem.

**Theorem 4.6** Fix \( R > 0 \) and let \( \Lambda \) be any closed convex subset of the ball \( \Lambda_1(R) \) defined in (3.10). Fix \( M \geq 3 \), let condition 1 hold and assume that the dictionary \( \mathcal{H} \) consists of functions satisfying \( \| f_j \| \leq 1 \), for any \( j = 1, \ldots, M \). Then, for any \( \delta > 0 \), with probability \( 1 - \delta \), the maximum likelihood aggregate \( f_{\lambda_n} \) over \( \Lambda \) satisfies

\[
\mathbb{E} \left[ \mathcal{E}_{KL}(f_{\lambda_n}, \Lambda, \mathcal{H}) \right] \leq 8RB \sqrt{\frac{\pi e}{a}} \sqrt{\frac{\log M}{n}} \sqrt{\log(2/\delta)}. \tag{4.11}
\]

Moreover, if \((\mathcal{H}, \Lambda)\) satisfies condition 2, then on the same event of probability \( 1 - \delta \), it holds

\[
\| f_{\lambda_n} - f_{\lambda^*} \|^2 \leq \frac{16RB}{\kappa^2} \sqrt{\pi e a} \sqrt{\frac{\log M}{n}} \sqrt{\log(2/\delta)}, \tag{4.12}
\]

where \( \lambda^* \in \arg\min_{\lambda \in \Lambda} \mathcal{K}(P_f \| P_{b' \circ f_{\lambda}}) \).

This explicit logarithmic dependence in the dimension \( M \) illustrates the benefit of the \( \ell_1 \) constraint for high dimensional problems. Raskutti et al. (2009) have obtained essentially the same result as Theorem 4.6 for the special case of Gaussian linear regression. While their proof technique yields significantly larger constants, they also cover the case of aggregation over \( \ell_q \) balls for \( q < 1 \) explicitly. However, their result is limited to the linear regression model where the regression function \( f \) is of the form \( f = f_{\lambda^*} \) for some \( \lambda^* \in \Lambda_1(R) \).

Most of the bounds for convex aggregation that have appeared in the literature hold for the expected excess-KL. While many papers provide bounds with high probability (see, e.g. Koltchinskii, 2008; Mitchell and van de Geer, 2009, and references therein), they typically do not hold for the excess-KL itself but for a quantity related to

\[
\bar{\mathcal{K}}(P_f \| P_{b' \circ f_{\lambda_n}}) - C \min_{\lambda \in \Lambda} \bar{\mathcal{K}}(P_f \| P_{b' \circ f_{\lambda}}),
\]

where \( C > 1 \) is a constant. When the quantity \( \min_{\lambda \in \Lambda} \bar{\mathcal{K}}(P_f \| P_{b' \circ f_{\lambda}}) \) is not small enough, such bounds can become inaccurate. A notable exception is Nemirovski et al. (2008, Proposition 2.2) where the authors derive a result similar to Theorem 4.6 under a different but similar set of assumptions. Most importantly, their bounds do not hold for the maximum likelihood estimator but for the output of a recursive stochastic optimization algorithm.
4.4 Discussion

As mentioned before, it is worth noticing that the technique employed in proving the bounds in expectation of the previous subsection yield bounds with high probability at almost no extra cost. More precisely, our proofs do not employ the usual techniques to bound the suprema of empirical process.

While the original motivation for aggregation, as put forward by Nemirovski (2000) is to aggregate estimators constructed from a hold-out sample, mainly to obtain adaptive estimators (see Yang, 2004; Lecué, 2007a; Rigollet and Tsybakov, 2007), it is now standard to present results in the pure aggregation framework where the goal is to aggregate deterministic functions as in Tsybakov (2003) and the section above. Maximum likelihood aggregation can yield adaptive estimators in nonparametric estimation by aggregating projection estimators constructed from a preliminary sample. In addition, the new results of Theorem 4.6 potentially yield much stronger results than usual adaptation results that are in expectation. Also, such results can be applied not only to regression but also to binary classification as detailed in Section 6.

We finally mention the question of persistence posed by Greenshtein and Ritov (2004) and further studied by Greenshtein (2006) and Bartlett et al. (2009). In these papers, the goal is to find performance bounds that explicitly depend on $n$, $M$ and the radius $R$ of the $\ell_1$ ball $\Lambda_1(R)$. More precisely, allowing $M$ and $R$ to depend on $n$, persistence asks the question of which regime gives remainder terms that converge to 0. While we do not pursue directly this question, we obtain such bounds for deterministic design and show that the constrained maximum likelihood estimator on a closed convex subset of the $\ell_1$ ball is persistent as long as $R = R(n) = o \left( \sqrt{n / \log(M)} \right)$. The original result of Greenshtein and Ritov (2004) in this sense allows only $R = o \left( \left[ n / \log(M) \right]^{1/4} \right)$ but when the design is random with unknown distribution. The use of deterministic design in the present paper, makes the prediction task much easier. Indeed, a significant amount of work to prove persistence has been made toward describing general conditions on the distribution of the design to ensure persistence at a rate $R = o \left( \sqrt{n / \log(M)} \right)$, as in Greenshtetein (2006) and Bartlett et al. (2009).

5 Optimal rates of aggregation

In Section 4, we have derived upper bounds for the excess-risk both in expectation and with high probability under appropriate conditions. The bounds in expectation can be summarized as follows. For each $\Lambda \in \{V, \Lambda_1(1), \mathbb{R}^M \}$, there exits an estimator $T_n$ such that

$$\mathbb{E} [\epsilon_{KL}(T_n, \Lambda, \mathcal{H})] \leq C \Delta_{n,M}(\Lambda),$$
where \( C > 0 \) and

\[
\Delta_{n,M}(\Lambda) = \begin{cases} 
\frac{D}{n} \land \frac{\log M}{n}, & \text{if } \Lambda = \mathcal{V} \quad \text{(model selection aggregation)}, \\
\frac{D}{n}, & \text{if } \Lambda \subseteq \mathbb{R}^M \quad \text{(linear aggregation)}, \\
\frac{D}{n} \land \sqrt{\frac{\log M}{n}}, & \text{if } \Lambda = \Lambda_1(1) \quad \text{(convex aggregation)},
\end{cases}
\tag{5.13}
\]

where \( D \leq M \land n \) is the dimension of the linear span of the dictionary \( \mathcal{H} \) and \( \Lambda \subseteq \mathbb{R}^M \) means the \( \Lambda \) is either a closed convex subset of \( \mathbb{R}^M \) or \( \mathbb{R}^M \) itself. Note that for model selection aggregation, the estimator that achieves this rate is given by

\[
T_n = f_{\hat{\lambda}_n} \mathbb{I}(D \geq \log M) + f_{\hat{\lambda}_n} \mathbb{I}(D \leq \log M),
\]

where \( \hat{\lambda}_n \) is defined in \((4.4)\), \( f_{\hat{\lambda}_n} \) is the maximum likelihood aggregate over \( \Lambda_1(1) \) and \( \mathbb{I}(\cdot) \) denotes the indicator function. In the rest of the paper, we call \( \hat{\lambda}_n \) the rank of \( \mathcal{H} \). Clearly, the lower bound for linear aggregation does not hold for any closed convex subset of \( \mathbb{R}^M \) since \( \{0\} \) is such a set and clearly \( \Delta_{n,M}(\{0\}) \equiv 0 \). We will prove the lower bound on the \( \ell_\infty \) box defined by

\[
\Lambda_\infty(1) = \left\{ x \in \mathbb{R}^M : \max_{1 \leq j \leq M} |x_j| \leq 1 \right\}.
\]

For linear and model selection aggregation, these rates are known to be optimal in the Gaussian case where the design is random but with known distribution (Tsybakov, 2003) and where the design is deterministic (Rigollet and Tsybakov, 2010). For convex aggregation, it has been established by Tsybakov (2003) (see also Rigollet and Tsybakov, 2010) that the optimal rate of convergence for Gaussian regression is of order \( \sqrt{\log(1 + eM/\sqrt{n})/n} \), which is equivalent to the upper bounds obtained in Theorems 4.5–4.6 of the present paper when \( M \gg \sqrt{n} \) but is smaller in general. To obtain better rates, one may resort to more complicated, combinatorial procedures such as the ones derived in the papers cited above but the full description of this idea goes beyond the scope of this paper.

In this section, we prove that these rates are minimax optimal under weaker conditions that are also satisfied by the Bernoulli distribution. The notion of optimality for aggregation employed here is the one introduced by Tsybakov (2003). Before stating the main result of this section, we need to introduce the following definition. Fix \( \kappa^2 > 0 \) and let \( \Gamma(\kappa^2) \) be the level set of the function \( \Gamma'' \) defined by

\[
\Gamma(\kappa^2) = \{ \theta \in \mathbb{R} : b''(\theta) \geq \kappa^2 \}.
\tag{5.14}
\]

In the Gaussian case, it is clear from Table 1 that \( \Gamma(\kappa^2) = \mathbb{R} \) for any \( \kappa^2 \leq 1 \). For the cumulant function of the bernoulli distribution, when \( \kappa^2 < 1/4 \), \( \Gamma(\kappa^2) \) is a compact symmetric interval given by

\[
\left[ 2 \log \left( \frac{1 - \sqrt{1 - 4\kappa^2}}{2\kappa} \right), 2 \log \left( \frac{1 + \sqrt{1 - 4\kappa^2}}{2\kappa} \right) \right].
\]
Furthermore, we have $\Gamma(1/4) = \{0\}$ and $\Gamma(\kappa^2) = \emptyset$, for $\kappa^2 > 1/4$. In the next theorem, we assume that for a given $\kappa^2 > 0$, $\Gamma(\kappa^2)$ is convex. This is clearly the case when the cumulant functions $b$ is such that $b''$ is quasi-concave, i.e., satisfies for any $\theta, \theta' \in \mathbb{R}, u \in [0, 1]$,

$$b''(u\theta + (1-u)\theta') \geq \min\{b''(\theta), b''(\theta')\}.$$  

This assumption is satisfied for the Gaussian and Bernoulli distributions.

Let $\bar{D}$ denote the class of dictionaries $\mathcal{H} = \{f_1, \ldots, f_M\}$ such that $\|f_j\| \vee \|f_j\|_{\infty} \leq 1, j = 1, \ldots, M$. Moreover, for any convex set $\Lambda \subseteq \mathbb{R}^M$, denote by $I(\Lambda)$ the interval $[-H_{\infty}, H_{\infty}]$, where

$$H_{\infty} = H_{\infty}(\Lambda) = \sup_{\mathcal{H} \in \bar{D}} \sup_{\lambda \in \Lambda} \sup_{x \in \mathcal{X}} |f_\lambda(x)| \in [0, \infty].$$  

(5.15)

For example, we have

$$I(\Lambda) = \begin{cases} [-1, 1] & \text{if } \Lambda = \mathcal{V} \quad \text{(model selection aggregation)}, \\ \mathbb{R} & \text{if } \Lambda = \mathbb{R}^M \quad \text{(linear aggregation)}, \\ [-R, R] & \text{if } \Lambda = \Lambda_1(R) \quad \text{(convex aggregation)}. \end{cases}$$

For properly state the minimax lower bounds, we use the notation

$$\mathcal{E}_{KL}(T_n, \Lambda, \mathcal{H}) = \mathcal{E}_{KL}(T_n, \Lambda, f, \mathcal{H}),$$

that makes the dependence in the regression function $f$ explicit. Finally, we denote by $E_f$ the expectation with respect to the distribution $P_f$.

**Theorem 5.1** Fix $M \geq 2, n \geq 1, D \geq 1, \kappa^2 > 0$, and assume that condition 1 holds. Moreover, assume that $\Gamma(\kappa^2)$ is convex and that for a given set $\Lambda \subseteq \mathbb{R}^M$, we have $I(\Lambda) \subset \Gamma(\kappa^2)$. Then, there exists a dictionary $\mathcal{H} \in \bar{D}$, with rank less than $D$, and positive constants $c^*, \delta$ such that

$$\inf_{T_n \to \Gamma(\kappa^2)} \sup_{\Lambda \in \Lambda} P_{b \circ f_\lambda} \left[ \mathcal{E}_{KL}(T_n, \Lambda, b' \circ f_\lambda, \mathcal{H}) > c^* \kappa^2 2a \Delta^*_{n,M}(\Lambda) \right] \geq \delta,$$  

(5.16)

and

$$\inf_{T_n \to \Gamma(\kappa^2)} \sup_{\Lambda \in \Lambda} E_{b \circ f_\lambda} \left[ \mathcal{E}_{KL}(T_n, \Lambda, b' \circ f_\lambda, \mathcal{H}) \right] \geq \delta c^* \kappa^2 2a \Delta^*_{n,M}(\Lambda),$$  

(5.17)

where the infimum is taken over all estimators that take values in $\Gamma(\kappa^2)$ and where

$$\Delta^*_{n,M}(\Lambda) = \begin{cases} \frac{D}{n} \land \log M \\ \frac{D}{n} \\ \frac{D}{n} \land \sqrt{\frac{\log(1 + eM/\sqrt{n})}{n}} \end{cases} \quad \text{if } \Lambda = \mathcal{V} \quad \text{(model selection aggregation)},$$

(5.18)
This theorem essentially covers the Gaussian and the Bernoulli case for which condition 1 is satisfied. Lower bounds for aggregation in the Gaussian case have already been proved in Rigollet and Tsybakov (2010, Section 6) in a weaker sense. Indeed, we enforce here that $\mathcal{H} \subseteq \mathcal{D}$ and has rank bounded by $D$ whereas Rigollet and Tsybakov (2010) use unbounded dictionaries with rank that may exceed $D$ by a logarithmic multiplicative factor.

Note that the lower bound concerns only estimators of the regression function that are of the form $b' \circ T_n$. Nevertheless, these are the only estimators that make sense since (2.2) implies that $f$ takes values in the range of $b'$. In addition, observe that from (5.17), the least favorable regression functions are of the form $f = b' \circ f_\lambda, \lambda \in \Lambda$ as it is usually the case in aggregation (see, e.g., Tsybakov, 2003).

A consequence of Theorem 5.1 is that the rates of convergence obtained in Section 4, both in expectation and with high probability, cannot be improved without further assumptions except for the logarithmic term of convex aggregation.

The proof of Theorem 5.1 is postponed to subsection 7.4.

6 Examples

6.1 Examples of exponential families

This subsection is a reminder of the versatility of exponential families of distributions and its goal is to illustrate conditions 1 and 2 on some examples. Most of the material can be found for example in McCullagh and Nelder (1989). The form of the density described in (2.1) is usually referred to as natural form. More generally, an exponential family of univariate distributions is defined as a family of distributions with density

$$p(y; \theta) = \exp \left\{ \frac{T(y)\theta - b(\theta)}{a} + c(y) \right\},$$

where $T(Y)$ is a given sufficient statistic. Here, only the case where $T(\cdot)$ is the identity function is studied but we now recall that it already encompasses many different distributions. Table 1 gives examples of distributions that have such a density. For distributions with several parameters, it is assumed that all parameters but $\theta$ are known. For the Normal and Gamma distributions, the reference measure is the Lebesgue measure whereas for the Bernoulli, Negative Binomial and Poisson distributions, the reference measure is the counting measure on $\mathbb{Z}$. For all these distributions, the cumulant function $b(\cdot)$ is twice continuously differentiable.

Observe first that only the Normal and Bernoulli distributions satisfy condition 1. Indeed, all other distributions in the table do not have sub-Gaussian tails and therefore, we cannot use Lemma 7.1 to control the deviations and moments of the sum of independent random variables. Therefore, only Theorem 4.3 applies to the remaining distributions even though direct computation of the moments can yield results of the same type as Theorems 4.5-4.6 but with bounds that are larger by orders of magnitude.

Another important message of Table 1 is that the constant $\kappa^2$ can depend on the constant $H_\infty$ defined in (5.15). Consequently the $L_2$ distance $\|f_\hat{\lambda}_n - f_\lambda^*\|$ is affected by the constant $\kappa^2$ and thus by $H_\infty$. However, the constant $B^2$ does not depend on $H_\infty$. Therefore, the bounds on the excess-KL presented in Theorems 4.5 and 4.6 hold without extra assumption of the
Table 1: Exponential families of distributions and constants in conditions 1 and 2 where $H_\infty$ is defined in (5.15). (Source: McCullagh and Nelder, 1989)

dictionary. For the Normal distribution, $\kappa^2 = B^2 = 1$ regardless of the value $H_\infty$, which makes it a particular case.

6.2 Bounds for logistic regression with a large dictionary

Let us now focus on the Bernoulli distribution. Recall that in the setup of binary classification (see, e.g., Boucheron et al., 2005, for a survey on this topic), we observe a collection of independent random couples $(x_1, Y_1), \ldots, (x_n, Y_n)$ such that $Y_i \in \{0, 1\}$ has Bernoulli distribution with parameter $f(x_i)$, $i = 1, \ldots, n$. As shown in the survey by Boucheron et al. (2005), there exists a tremendous amount of work in this topic and we will focus on the so-called boosting type algorithms. A dictionary of base classifiers $\mathcal{H} = \{f_1, \ldots, f_M\}$, i.e., functions taking values in $[-1, 1]$, is given and training a boosting algorithm consists in combining them in such a way that $f_\lambda(x_i)$ predicts $f(x_i)$ well.

This part of the paper is mostly inspired by Friedman et al. (2000) who propose a statistical view of boosting. Specifically, they offer an interpretation of the original AdaBoost algorithm introduced in Freund and Schapire (1996) as a sequential optimization procedure that fits an extended additive model for a particular choice of the loss function. Then they propose to directly maximize the Bernoulli log-likelihood using quasi-Newton optimization and derive a new algorithm called LogitBoost. Even though, we do not detail how maximization of the likelihood is performed, LogitBoost aims at solving the same problem as the one studied here. One difference here is that while extended additive models assume that there exists $\lambda \in \Lambda \subset \mathbb{R}^M$ such that the regression function is of the form $f = (b')^{-1} \circ f_\lambda$, maximum likelihood aggregation does not. The paper of Friedman et al. (2000) focuses on the optimization side of the problem and does not contain finite sample results. A recent attempt to compensate for a lack of statistical analysis can be found in Mease and Wyner (2008) and the many discussions that it produced. We propose to contribute to this discussion by illustrating some statistical aspects of LogitBoost.
based on the rates derived in Section 4 and in particular, how its performance depends on the size of the dictionary.

Given a convex subset $\Lambda \subset \mathbb{R}^M$ and a convex function $\varphi : \mathbb{R} \rightarrow \mathbb{R}$, training a boosting algorithm and more generally a large margin classifier, consists in minimizing the risk function defined by

$$R_\varphi(f_\lambda) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[\varphi(-\tilde{Y}_i f_\lambda(x_i))]$$

over $\lambda \in \Lambda$, where $\tilde{Y}_i = 2Y_i - 1 \in \{-1, 1\}$. It is usually required that $\varphi$ be monotonically non decreasing on $\mathbb{R}$ and satisfy $\varphi(0) = 1$. Typical choices for $\varphi(\cdot)$ are $\exp(\cdot)$ or the hinge loss $\max(\cdot - 1, 0)$. It is not hard to show that minimizing the Kullback-Leibler divergence $\mathcal{K}(P_f \parallel P_{\psi(f_\lambda)})$, is equivalent to choosing

$$\varphi(x) = \frac{\log (1 + e^x)}{\log 2},$$

up to the normalizing constant $\log 2$ that appears to ensure that $\varphi(0) = 1$. For the choice of $\varphi$ defined in (6.19), we have

$$R_\varphi(f_\lambda) - \min_{\lambda \in \Lambda} R_\varphi(f_\lambda) = \frac{1}{\log 2} \mathcal{E}_{\text{KL}}(f_\lambda, \Lambda, \mathcal{H}).$$

In boosting algorithms, the size of the dictionary $M$ is much larger than the sample size $n$ so that the results of Theorems 4.3–4.4 are useless and it is necessary to constrain $\lambda$ to be in a ball $\Lambda_1(R)$ so that $H_\infty = R$. Given that for the Bernoulli distribution, we have $a = 1, B^2 = 1/4$, the constants in the main theorems can be explicitly computed and in fact, they remain low. We can therefore apply Theorems 4.5–4.6 to obtain the following corollary that gives oracle inequalities for the $\varphi$-risk $R_\varphi$, both in expectation and with high probability. We focus on the case where $M$ is (much) larger than $\sqrt{n}$ as it is usually the case in boosting.

**Corollary 6.1** Consider the boosting problem with a given dictionary of base classifiers and let $\varphi$ be the convex function defined in (6.19). Then, the maximum likelihood aggregate $f_{\Lambda_1}$ over $\Lambda_1(R)$ defined in (4.7) satisfies

$$\mathbb{E}[R_\varphi(f_{\Lambda_1})] \leq \min_{\lambda \in \Lambda_1(R)} R_\varphi(f_\lambda) + \frac{2eR\sqrt{\pi}}{\log 2} \sqrt{\frac{\log M}{n}}.$$ 

Moreover, for any $\delta > 0$, with probability $1 - \delta$, it holds

$$R_\varphi(f_{\Lambda_1}) \leq \min_{\lambda \in \Lambda_1(R)} R_\varphi(f_\lambda) + \frac{4R\sqrt{\pi e}}{\log 2} \sqrt{\frac{\log M}{n}} \sqrt{\frac{\log(2/\delta)}}.$$ 

One striking feature of the bounds in this corollary is the simplicity of the constants. Similar results can be obtained using standard techniques to control suprema of empirical processes as in Massart (2007) and Koltchinskii (2008) for example, but such general techniques are bound to yield larger constants.
7 Proof of the main results

In this section, we prove the main theorems. We begin by recalling some properties of exponential families of distributions. While similar results can be found in the literature, the results presented below are tailored to our needs. In particular, the constants in the upper bounds are explicit and kept as small as possible. In this section, for any \( \omega \in \ell_2(\mathbb{R}) \), denote by \( |\omega|_2 \) its \( \ell_2 \)-norm defined by

\[
|\omega|_2 = \sqrt{\sum_j \omega_j^2}.
\]

7.1 Some useful results on canonical exponential families

Let \( Y \in \mathbb{R} \) be a random variable with distribution in a canonical exponential family that admits a density with respect to a reference measure on \( \mathbb{R} \) given by

\[
p(y; \theta) = \exp \left\{ \frac{y\theta - b(\theta)}{a} + c(y) \right\}, \quad \theta \in \mathbb{R}.
\]

(7.1)

The cumulant function \( b(\cdot) \) not only contains information about the first two moments but all the moments of \( Y \) through the moment generating function (MGF). Indeed, it can be easily shown (see, e.g., Lehmann and Casella, 1998, Theorem 5.10) that the MGF of \( Y \) is given by

\[
\mathbb{E}[e^{tY}] = e^{b(\theta + at) - b(\theta)}.
\]

(7.2)

Using the MGF we can derive the Chernoff-type bounds presented in the following lemma.

**Lemma 7.1** Let \( \omega = (\omega_1, \ldots, \omega_n) \in \mathbb{R}^n \) be a vector of deterministic weights. Let \( Y_1, \ldots, Y_n \) be independent random variables such that \( Y_i \) has density \( p(\cdot; \theta_i) \) defined in (7.1), \( \theta_i \in \mathbb{R}, i = 1, \ldots, n \) and define the weighted sum \( S_n^\omega = \sum_{i=1}^n \omega_i Y_i \). Assume that the second derivative of \( b \) is uniformly bounded:

\[
\sup_{\theta \in \mathbb{R}} b''(\theta) \leq B^2.
\]

(7.3)

Then the following inequalities hold,

\[
\mathbb{E}[\exp(s|S_n^\omega - \mathbb{E}(S_n^\omega)|)] \leq \exp \left( \frac{s^2 B^2 a |\omega|_2^2}{2} \right),
\]

(7.4)

\[
\mathbb{P}[|S_n^\omega - \mathbb{E}(S_n^\omega)| > t] \leq 2 \exp \left( -\frac{t^2}{2aB^2 |\omega|_2^2} \right),
\]

(7.5)

and for any \( r \geq 0 \), we have

\[
\mathbb{E}|S_n^\omega - \mathbb{E}(S_n^\omega)|^r \leq C_r |\omega|_2^r,
\]

(7.6)

where \( C_r = r(2aB^2)^{r/2}\Gamma(r/2) \) and \( \Gamma(\cdot) \) denotes the Gamma function. Moreover, for any \( r \geq 1 \), the following simpler bound holds

\[
(\mathbb{E}|S_n^\omega - \mathbb{E}(S_n^\omega)|^r)^{1/r} \leq 2B \sqrt{\pi ar} |\omega|_2.
\]

(7.7)
Proof. Using respectively (7.2), (2.2) and (7.3), we get

\[ \mathbb{E}[\exp(s(S_n^\omega - \mathbb{E}(S_n^\omega)))] = \exp \left( \frac{1}{a} \sum_{i=1}^{n} [b(\theta_i + as\omega_i) - b(\theta_i) - a \epsilon_i b'(\theta_i)] \right) \leq \exp \left( \frac{s^2 B a |\omega|^2}{2} \right), \]

The same inequality holds with \( s \) replaced by \(-s \) so (7.4) holds.

We now turn to the proof of (7.5). From the Markov inequality, for any \( s > 0 \), we have

\[ \mathbb{P}[S_n^\omega - \mathbb{E}(S_n^\omega) > t] \leq e^{-st} \mathbb{E}[\exp(s(S_n^\omega - \mathbb{E}(S_n^\omega)))]. \]

Together with (7.4), this inequality yields

\[ \mathbb{P}[S_n^\omega - \mathbb{E}(S_n^\omega) > t] \leq \inf_{s > 0} e^{\frac{s^2 B a |\omega|^2}{2} - st} = e^{-\frac{t^2}{2aB^2|\omega|^2}}. \]

The same reasoning using \( s < 0 \) instead of \( s > 0 \) yields (7.5).

Finally, observe that

\[ \mathbb{E}|S_n^\omega - \mathbb{E}(S_n^\omega)|^r = \int_0^\infty \mathbb{P}(|S_n^\omega - \mathbb{E}(S_n^\omega)| > t^{1/r}) dt \leq 2 \int_0^\infty \exp \left( -\frac{t^{2/r}}{2aB^2|\omega|^2} \right) dt, \]

where we used (7.5) in the last inequality. Using a change of variable, it is not hard to see that this bound yields (7.6). To prove (7.7), we use the following upper bound on the Gamma function based on Stirling’s approximation

\[ \Gamma(z) \leq \sqrt{2\pi} \left( \frac{z}{e} \right)^z e^{\frac{1}{12z}}, \quad z \geq 1. \]

It yields for any \( r \geq 1 \)

\[ C_r^{1/r} = r^{1/r} B \sqrt{2a [\Gamma(r/2)]^{1/r}} \leq B \sqrt{2a \pi} e^{\frac{3}{2e} \cdot \frac{1}{3}} \leq 2B \sqrt{\pi a r}, \]

where, in the first inequality, we used the fact that for any \( r > 0 \), \( r^{1/r} \leq e^{1/e} \).

For the Gaussian distribution \( \mathcal{N}(\theta, \sigma^2) \), recall that \( a = \sigma^2 \) and \( B^2 = 1 \) and (7.5) yields the usual tail bound for the sum of independent Gaussian random variables. For the Bernoulli distribution, we have \( a = 1 \) and \( B^2 = 1/4 \), which yields Hoeffding’s inequality (see, e.g., Massart, 2007, Proposition 2.7).

7.2 Proof of Theorems 4.1 and 4.2

According to (4.1), minimizing \( \lambda \mapsto \mathcal{K}(P_f \| P_{b^\lambda}) \) is equivalent to maximizing \( \lambda \mapsto L(\lambda) \) where

\[ L(\lambda) = \langle f, f_\lambda \rangle - \langle b \circ f_\lambda, \mathbb{I} \rangle. \quad (7.8) \]
Note that for any \( \Lambda \subset \mathbb{R}^M \), the set of optimal solutions \( \Lambda^* \) satisfies
\[
\Lambda^* = \arg\min_{\lambda \in \Lambda} K(P_f\|P_{b \circ f_\lambda}) = \arg\max_{\lambda \in \Lambda} L(\lambda).
\]
Moreover, for any \( \lambda \in \Lambda, \lambda^* \in \Lambda^* \), we have
\[
L(\lambda^*) - L(\lambda) = a\mathcal{E}_{KL}(f_\lambda, \Lambda, \mathcal{H}). \tag{7.9}
\]
For any fixed \( \lambda \in \Lambda_1^+ (1) \), define the following quantities:
\[
S_n(\lambda) = \sum_{j=1}^{M} \lambda_j \ell_n(e_j) + \ell_n(\lambda) = \sum_{i=1}^{n} \left\{ 2Y_i f_\lambda(x_i) - b \circ f_\lambda(x_i) - \sum_{j=1}^{M} \lambda_j b \circ f_j(x_i) \right\},
\]
\[
S(\lambda)n \sum_{j=1}^{M} \lambda_j L(e_j) + nL(\lambda) = \sum_{i=1}^{n} \left\{ 2f(x_i) f_\lambda(x_i) - b \circ f_\lambda(x_i) - \sum_{j=1}^{M} \lambda_j b \circ f_j(x_i) \right\}.
\]
and observe that \( S(\lambda) = \mathbb{E}[S_n(\lambda)] \) and that for any \( \lambda \in \Lambda_1^+ (1) \),
\[
S_n(\lambda) - S(\lambda) = 2 \sum_{i=1}^{n} (Y_i - f(x_i)) f_\lambda(x_i).
\]
By definition of \( \hat{\lambda} \), we have for any \( \lambda \in \Lambda_1^+ (1) \) that
\[
S(\hat{\lambda}) \geq S(\lambda) - \Delta_n(\lambda) + \beta H(\lambda) - \beta \log M, \tag{7.10}
\]
where
\[
\Delta_n(\lambda) = 2 \sum_{i=1}^{n} (Y_i - f(x_i)) f_{\hat{\lambda} - \lambda}(x_i) + \beta H(\hat{\lambda}) - \beta \log M.
\]
The following lemma is useful to control the term \( \Delta_n(\lambda) \) both in expectation and with high probability.

**Lemma 7.2** Under condition 1, for any \( \lambda \in \Lambda_1^+ (1) \) we have
\[
\mathbb{E} \left[ \exp \left( \frac{\Delta_n(\lambda)}{\beta} - \frac{2B^2an}{\beta^2} \sum_{j=1}^{M} \hat{\lambda}_j \|f_j - f_\lambda\|^2 \right) \right] \leq 1.
\]
Proof. Using Jensen’s inequality, we get

\[
\mathbb{E} \left[ \exp \left( \frac{\Delta_n(\lambda)}{\beta} - \frac{2B_2a n}{\beta^2} \sum_{j=1}^M \lambda_j \| f_j - f_\lambda \|^2 \right) \right]
\]

\[= \mathbb{E} \left[ \exp \left( \frac{2}{\beta} \sum_{i=1}^n (Y_i - f(x_i)) f_\lambda(x_i) - \sum_{j=1}^M \lambda_j \log(M \lambda_j) - \frac{2B_2a n}{\beta^2} \sum_{j=1}^M \lambda_j \| f_j - f_\lambda \|^2 \right) \right]
\]

\[\leq \mathbb{E} \left[ \sum_{j=1}^M \hat{\lambda}_j \exp \left( \frac{2}{\beta} \sum_{i=1}^n (Y_i - f(x_i))(f_j(x_i) - f_\lambda(x_i)) - \log(M \hat{\lambda}_j) - \frac{2B_2a n}{\beta^2} \| f_j - f_\lambda \|^2 \right) \right]
\]

\[= \frac{1}{M} \sum_{j=1}^M \mathbb{E} \left[ \exp \left( \frac{2}{\beta} \sum_{i=1}^n (Y_i - f(x_i))(f_j(x_i) - f_\lambda(x_i)) - \frac{2B_2a n}{\beta^2} \| f_j - f_\lambda \|^2 \right) \right]
\]

Now, from (7.4), which holds under condition 1, we have for any \( s > 0 \) and any \( \lambda, \lambda' \in \Lambda^+_1(1) \) that

\[\mathbb{E} \left[ \exp \left( \frac{2}{\beta} \sum_{i=1}^n (Y_i - f(x_i)) (f_\lambda(x_i) - f_\lambda'(x_i)) \right) \right] \leq \exp \left( \frac{2B_2a n}{\beta^2} \| f_\lambda - f_\lambda' \|^2 \right),\]

and the result of the lemma follows from the previous two displays. \( \blacksquare \)

Take any \( \hat{\lambda} \in \text{argmax}_{\lambda \in \Lambda^+_1(1)} S(\lambda) \) and observe that condition 2 together with a second order Taylor expansion of the function \( S(\cdot) \) around \( \hat{\lambda} \) gives for any \( \lambda \in \Lambda^+_1(1) \)

\[S(\lambda) \leq S(\hat{\lambda}) + [\nabla_\lambda S(\hat{\lambda})]^\top (\lambda - \hat{\lambda}) - \frac{n\kappa^2}{2} \| f_\lambda - f_\hat{\lambda} \|^2,
\]

where \( \nabla_\lambda S(\hat{\lambda}) \) denotes the gradient of \( \lambda \mapsto S(\lambda) \) at \( \hat{\lambda} \). Since \( \hat{\lambda} \) is a maximizer of \( \lambda \mapsto S(\lambda) \) over the set \( \Lambda^+_1(1) \) to which \( \lambda \) also belongs, we find that \( \nabla_\lambda S(\hat{\lambda})^\top (\lambda - \hat{\lambda}) \leq 0 \) so that

\[S(\hat{\lambda}) - S(\lambda) \geq \frac{n\kappa^2}{2} \| f_\lambda - f_\hat{\lambda} \|^2.
\]

Together with (7.10), the previous display yields

\[\frac{n\kappa^2}{2} \| f_\lambda - f_\hat{\lambda} \|^2 \leq S(\hat{\lambda}) - S(\lambda) \leq \Delta_n(\hat{\lambda}) + \beta \log M,
\]

where we used the fact that \( H(\hat{\lambda}) \geq 0 \).

Proof of Theorem 4.1.

Using the convexity inequality \( t \leq e^t - 1 \) for any \( t \in \mathbb{R} \), Lemma 7.2 yields

\[\mathbb{E} \left[ \Delta_n(\hat{\lambda}) \right] \leq \frac{2B_2a n}{\beta} \mathbb{E} \sum_{j=1}^M \hat{\lambda}_j \| f_j - f_\lambda \|^2 = \frac{2B_2a n}{\beta} \left( \mathbb{E} \sum_{j=1}^M \hat{\lambda}_j \| f_j - f_\lambda \|^2 + \mathbb{E} \| f_\hat{\lambda} - f_\lambda \|^2 \right)
\]
The previous display combined with (7.11) gives
\[ S(\hat{\lambda}) - \mathbb{E}[S(\hat{\lambda})] \leq \frac{2B^2a}{\beta} \mathbb{E} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2 + \frac{4B^2a}{\beta \kappa^2} \left[ S(\hat{\lambda}) - \mathbb{E}[S(\hat{\lambda})] \right] + \beta \log M. \]

It implies that for \( \beta \geq 8B^2a/\kappa^2 \)
\[ S(\bar{\lambda}) - \mathbb{E}[S(\hat{\lambda})] \leq \frac{4B^2a}{\beta} \mathbb{E} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2 + 2\beta \log M. \] (7.12)

Observe now that a second order Taylor expansion of the function \( L(\cdot) \) around \( \hat{\lambda} \), together with condition 2 gives for any \( \lambda \in \Lambda^+ \)
\[ L(\lambda) \leq L(\hat{\lambda}) + [\nabla_\lambda L(\hat{\lambda})]^T (\lambda - \hat{\lambda}) - \frac{\kappa^2}{2} \| f_{\lambda} - f_{\hat{\lambda}} \|^2. \]

Thus
\[ \sum_{j=1}^{M} \hat{\lambda}_j L(e_j) \leq L(\hat{\lambda}) - \frac{\kappa^2}{2} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2. \]

It follows that
\[ S(\hat{\lambda}) = n \sum_{j=1}^{M} \lambda_j L(e_j) + nL(\hat{\lambda}) \leq 2nL(\hat{\lambda}) - \frac{n\kappa^2}{2} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2. \]

Combined with (7.12), the above inequality yields
\[ S(\bar{\lambda}) - 2n\mathbb{E}[L(\hat{\lambda})] \leq \left( \frac{4B^2a}{\beta} - \frac{n\kappa^2}{2} \right) \mathbb{E} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2 + 2\beta \log M \leq 2\beta \log M, \]
for \( \beta \geq 8B^2a/\kappa^2 \).

Note that for any \( j = 1, \ldots, M \), \( S(\bar{\lambda}) \geq S(e_j) = 2nL(e_j) \) so that from (7.9), we get
\[ a\mathbb{E}[\mathcal{E}_{KL}(f_{\bar{\lambda}}, \mathcal{V}, \mathcal{H})] = \max_{1 \leq j \leq M} L(e_j) - \mathbb{E}[L(\hat{\lambda})] \leq \frac{\beta}{n} \log M. \]

**Proof of Theorem 4.2.** From the Markov inequality and Lemma 7.2 we get for any \( \lambda \in \Lambda^+ \) and any \( \delta > 0 \) that
\[ \mathbb{P} \left[ \Delta_n(\lambda) - \frac{2B^2a}{\beta} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2 > \beta \log(1/\delta) \right] \leq \delta. \]

Thus, the event \( A_\delta(\delta) \) on which
\[ \Delta_n(\lambda) \leq \frac{2B^2a}{\beta} \sum_{j=1}^{M} \hat{\lambda}_j \| f_j - f_{\hat{\lambda}} \|^2 + \beta \log(1/\delta) \]
has probability greater that \( 1 - \delta \). Theorem 4.2 follows by applying the same steps as in the proof of Theorem 4.1 but on the event \( A_\delta(\delta) \) instead of in expectation.
7.3 Proof of Theorems 4.3-4.6

The following lemma exploits the strong convexity property stated in condition 2.

**Lemma 7.3** Let $\phi_1, \ldots, \phi_D$ be an orthonormal basis of the linear span of the dictionary $\mathcal{H}$. Let $\Lambda$ be a closed convex subset of $\mathbb{R}^M$ or $\mathbb{R}^{M}$ itself and assume that $(\mathcal{H}, \Lambda)$ satisfies condition 2. Denote by $\lambda^*$ any maximizer of the function $\lambda \mapsto L(\lambda)$ over the set $\Lambda$. Then any maximum likelihood estimator $\hat{\lambda}_n$ satisfies

$$\frac{\kappa^2}{2} \|f_{\lambda_n} - f_{\lambda^*}\|^2 \leq L(\lambda^*) - L(\hat{\lambda}_n) \leq \frac{2}{\kappa^2} \sum_{j=1}^{D} \zeta_j^2,$$

(7.13)

where $\zeta_j = \frac{1}{n} \sum_{i=1}^{n} Y_i \phi_j(x_i) - \langle f, \phi_j \rangle, j = 1, \ldots, D$. Moreover, if $\Lambda \subset \Lambda(R), R > 0$ is a closed convex set, then $\hat{\lambda}_n$ satisfies

$$\frac{\kappa^2}{2} \|f_{\lambda_n} - f_{\lambda^*}\|^2 \leq L(\lambda^*) - L(\hat{\lambda}_n) \leq 2R \max_{1 \leq j \leq M} |\xi_j|$$

(7.14)

where $\xi_j = \frac{1}{n} \sum_{i=1}^{n} Y_i f_j(x_i) - \langle f, f_j \rangle, j = 1, \ldots, M$.

**Proof.** A second order Taylor expansion of the function $L(\cdot)$ around $\lambda^*$ gives for any $\lambda \in \Lambda$

$$L(\lambda) \leq L(\lambda^*) + \left[ \nabla_\lambda L(\lambda^*) \right]^\top (\lambda - \lambda^*) - \frac{\kappa^2}{2} \|f_\lambda - f_{\lambda^*}\|^2,$$

where we used condition 2 and where $\nabla_\lambda L(\lambda^*)$ denotes the gradient of $\lambda \mapsto L(\lambda)$ at $\lambda^*$. Since $\lambda^*$ is a maximizer of $\lambda \mapsto L(\lambda)$ over the set $\Lambda$ to which $\lambda$ also belongs, we find that $\nabla_\lambda L(\lambda^*)^\top (\lambda - \lambda^*) \leq 0$ so that

$$L(\lambda^*) - L(\lambda) \geq \frac{\kappa^2}{2} \|f_\lambda - f_{\lambda^*}\|^2,$$

(7.15)

for any $\lambda \in \Lambda$, which gives the left inequalities in (7.13) and (7.14).

Next, from the definition of $\hat{\lambda}_n$, we have

$$L(\hat{\lambda}_n) \geq L(\lambda^*) + T_n(\lambda^* - \hat{\lambda}_n),$$

(7.16)

where

$$T_n(\mu) = \frac{1}{n} \sum_{i=1}^{n} Y_i f_\mu(x_i) - \langle f, f_\mu \rangle, \mu \in \mathbb{R}^M.$$

Writing $f_\mu = \sum_{j=1}^{D} \nu_j \phi_j, \nu \in \mathbb{R}^D$, we find that

$$T_n(\mu) = \sum_{j=1}^{D} \nu_j \left( \frac{1}{n} \sum_{i=1}^{n} Y_i \phi_j(x_i) - \langle f, \phi_j \rangle \right) = \sum_{j=1}^{D} \nu_j \zeta_j,$$

and

Define the random variable

$$V_n = \sup_{\mu \in \mathbb{R}^M : \|f_\mu\| > 0} \frac{|T_n(\mu)|}{\|f_\mu\|}.$$
so that $V_n$ satisfies

$$V_n = \sup_{\nu \in \mathbb{R}^D} \left| \sum_{j=1}^D \nu_j \zeta_j \right| = \left( \sum_{j=1}^D \zeta_j^2 \right)^{1/2}.$$  

Since $T_n(\lambda^* - \hat{\lambda}_n) \geq -V_n \|f_{\lambda^* - \hat{\lambda}_n}\|$, it yields together with (7.16) that

$$L(\hat{\lambda}_n) \geq L(\lambda^*) - \|f_{\lambda^* - \hat{\lambda}_n}\| \left( \sum_{j=1}^D \zeta_j^2 \right)^{1/2}. \quad (7.17)$$

Combining (7.17) and (7.15) with $\lambda = \hat{\lambda}_n$, we get (7.13).

We now turn to the proof of (7.14). From (7.16), and the Hölder inequality, we have

$$L(\lambda^*) - L(\hat{\lambda}_n) \leq \left( \sum_{j=1}^M |\hat{\lambda}_{n,j} - \lambda_j^*| \right) \max_{1 \leq j \leq M} |\xi_j|,$$

$$\leq 2R \max_{1 \leq j \leq M} |\xi_j|.$$  

Combined with (7.15), this inequality yields (7.14).

In view of (7.9), to complete the proof of Theorems 4.3–4.6, it is sufficient to bound from above the quantities appearing on the right hand side of (7.13) and (7.14). This is done using results from subsection 7.1 and by observing that the random variables $\zeta_j$ and $\xi_j$ are of the form

$$\zeta_j = S_n^{(\zeta_j)} - \mathbb{E}(S_n^{(\zeta_j)}) = n \frac{\phi_j(x_i)}{n}, \quad |\zeta_j|_2 = 1, \quad \sigma^2 = \frac{1}{\sqrt{n}} \quad (7.18)$$

and

$$\xi_j = S_n^{(\xi_j)} - \mathbb{E}(S_n^{(\xi_j)}) = n \frac{f_j(x_i)}{n}, \quad |\xi_j|_2 \leq \frac{1}{\sqrt{n}} \quad (7.19)$$

where the last inequality is obtained under the assumption that $\max_{1 \leq j \leq M} \|f_j\|^2 \leq 1$.

**Proof of Theorem 4.3.** Since the random variables $Y_i, i = 1, \ldots, n$ are mutually independent, we have

$$\mathbb{E}[\zeta_j^2] = \text{var} \left( \frac{1}{n} \sum_{i=1}^n Y_i \phi_j(x_i) \right) = \frac{1}{n^2} \sum_{i=1}^n \text{var}(Y_i) \phi_j^2(x_i) \leq \frac{\sigma^2}{n^2} \sum_{i=1}^n \phi_j^2(x_i) = \frac{\sigma^2}{n}.$$  

Together with (7.9) and (7.13), this bound completes the proof of Theorem 4.3.

**Proof of Theorem 4.4**
For any $s, t > 0$, we have

\[
\mathbb{P}\left[ \sum_{j=1}^{D} \zeta_j^2 > t \right] = \mathbb{P}\left[ \frac{1}{D} \sum_{j=1}^{D} \zeta_j^2 > \frac{t}{D} \right] 
\leq e^{-\frac{st}{2D}} \mathbb{E}\left[ e^{\frac{s}{D} \sum_{j=1}^{D} \zeta_j^2} \right] \quad \text{(Markov’s inequality)}
\leq e^{-\frac{st}{2D}} \frac{1}{D} \sum_{j=1}^{D} \mathbb{E}\left[ e^{s \zeta_j^2} \right] \quad \text{(Jensen’s inequality)}
\leq e^{-\frac{st}{2D}} \frac{1}{D} \sum_{j=1}^{D} \sum_{p=0}^{\infty} \frac{s^p}{p!} \mathbb{E}\left[ \zeta_j^{2p} \right] \quad \text{(Fatou’s lemma)}. 
\]

But (7.6), which holds under condition 1, and (7.18) yield

\[
\mathbb{E}[\zeta_j^{2p}] \leq C_{2p} \omega(\zeta_j)^2 = \frac{C_{2p}}{n^p} = 2p! \left( \frac{2aB^2}{n} \right)^p .
\]

Therefore, the last two displays yield

\[
\mathbb{P}\left[ \sum_{j=1}^{D} \zeta_j^2 > t \right] \leq 2e^{-\frac{st}{2D}} \sum_{p=0}^{\infty} \left( \frac{2saB^2}{n} \right)^p .
\]

Finally, taking $s = n/(4aB^2)$ yields

\[
\mathbb{P}\left[ \sum_{j=1}^{D} \zeta_j^2 > t \right] \leq 4e^{-\frac{nt}{4aB^2D}} .
\]

Theorem 4.4 follows by taking $t = \frac{4aB^2D}{n} \log(4/\delta)$ in the previous display together with (7.9) and (7.13).

Proof of Theorem 4.5. Using successively Jensen’s inequality and (7.7), which holds under condition 1, we find that for any $r \geq 1$, it holds

\[
\mathbb{E}\left[ \max_{1 \leq j \leq M} |\xi_j| \right] \leq \mathbb{E}\left[ \sum_{j=1}^{M} |\xi_j|^r \right]^{1/r} \leq M^{1/r} \max_{1 \leq j \leq M} \left( \mathbb{E}[|\xi_j|^r] \right)^{1/r} \leq 2BM^{1/r} \sqrt{\frac{\pi ar}{n}} ,
\]

where we used (7.7) and (7.19) in the second inequality. Choosing now $r = \log M$, yields

\[
\mathbb{E}\left[ \max_{1 \leq j \leq M} |\xi_j| \right] \leq 2eB \sqrt{\frac{\pi a \log M}{n}} .
\]

Combined with (7.9) and (7.14) the previous inequality completes the proof of Theorem 4.5.

Proof of Theorem 4.6
For any \( r \geq 1 \), \( s, t > 0 \), we have

\[
\mathbb{P} \left[ \max_{1 \leq j \leq M} |\xi_j| > t \right] \leq \mathbb{P} \left[ \left( \sum_{j=1}^{M} |\xi_j|^r \right)^{1/r} > t \right] = \mathbb{P} \left[ \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2/r} > \frac{t^2}{M^{2/r}} \right] \leq e^{-\frac{t^2}{M^{2/r} \mathbb{E} \left[ \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2/r} \right]}} \leq e^{-\frac{s^2}{M^{2/r} \sum_{j=1}^{M} |\xi_j|^r}} \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2p/r}, \tag{7.20}
\]

where we used the Markov inequality and a Taylor expansion coupled with Fatou’s lemma respectively. We now control the term \( \mathbb{E} \left[ \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2p/r} \right] \).

Assume first that \( p \leq r/2 \). Then, using respectively Jensen’s inequality, (7.19) and (7.7), we get

\[
\mathbb{E} \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2p/r} \leq \left( \frac{1}{M} \sum_{j=1}^{M} \mathbb{E}|\xi_j|^r \right)^{2p/r} \leq \left( 2B \sqrt{\pi ar} \omega(\xi_j) \right)^{2p} \leq \left( 2B \sqrt{\pi ar} \right)^{2p}.
\]

Next, if \( p > r/2 \), Jensen’s inequality yields

\[
\mathbb{E} \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2p/r} \leq \frac{1}{M} \sum_{j=1}^{M} \mathbb{E}|\xi_j|^{2p} \leq C_{2p} \left( \frac{2aB^2}{n} \right)^{p} = 2p! \left( \frac{2aB^2}{n} \right)^{p},
\]

where in the last inequality, we used (7.6) and (7.19).

Recalling that \( r \geq 1 \), the last two displays yield

\[
\sum_{p=0}^{\infty} \frac{s^p}{p!} \mathbb{E} \left( \frac{1}{M} \sum_{j=1}^{M} |\xi_j|^r \right)^{2p/r} \leq \sum_{0 \leq p \leq r/2} \frac{1}{p!} \left( \frac{4\pi saB^2r}{n} \right)^{p} + 2 \sum_{p > r/2} \left( \frac{2saB^2}{n} \right)^{p} \leq \sum_{p=0}^{\infty} \left( \frac{4\pi saB^2r}{n} \right)^{p}. \tag{7.21}
\]

Choosing now \( r = 2 \log M \) and \( s = n/(16\pi aB^2 \log M) \) yields together with (7.20) that

\[
\mathbb{P} \left[ \max_{1 \leq j \leq M} |\xi_j| > t \right] \leq 2e^{-\frac{nt^2}{16\pi aB^2 \log M}}. \tag{7.22}
\]

Together with (7.9) and (7.14), this bound completes the proof of Theorem 4.6 by taking \( t = 4B \sqrt{\pi a \log M \log(2/\delta)} \).
7.4 Proof of Theorem 5.1

Note first that (5.16) implies (5.17). Indeed, by the Markov inequality, we have for any $\mu > 0$

$$
\frac{1}{\mu} E_{\theta|g} [\mathcal{E}_{KL}(T_n, \Lambda, b' \circ f_\lambda, \mathcal{H})] \geq P_{\theta|T_n} [\mathcal{E}_{KL}(T_n, \Lambda, b' \circ f_\lambda, \mathcal{H}) > \mu].
$$

Besides, (5.16) follows if we prove

$$
\inf_{T_n \to \Gamma(\kappa^2)} \max_{g \in \mathcal{G}} P_{\theta|T_n} \left[ \tilde{K}(P_{\theta|g} \| P_{\theta|T_n}) \geq c_{\alpha} \frac{\kappa^2}{2a} \Delta^*_n \right] \geq \delta,
$$

where $\mathcal{G}$ is a finite family of functions such that $\mathcal{G} \subset \{f_\lambda : \lambda \in \Lambda\}$.

The rest of the proof consists in two steps. We first reduce the lower bound (7.23) to a lower bound on the squared prediction risk. In the second step, we use standard techniques to bound the squared prediction risk from below.

1. Fix an estimator $T_n$ that takes values in $\Gamma(\kappa^2)$ and recall that from (4.1), we have for any $g \in \mathcal{G}$

$$
\mathcal{K}(P_{\theta|g} \| P_{\theta|T_n}) = -\frac{n}{a} \langle g, T_n \rangle - \langle b \circ T_n, \mathbb{I} \rangle - \sum_{i=1}^n \mathbb{E}[c(Y_i)] + \text{Ent}(P_g).
$$

A second order Taylor expansion along the segment $\{\alpha g + (1-\alpha)T_n : \alpha \in [0,1]\} \subset \Gamma(\kappa^2)$ yields

$$
\tilde{K}(P_{\theta|g} \| P_{\theta|T_n}) \geq \frac{\kappa^2}{2a} \|g - T_n\|^2,
$$

where we used the fact that $\alpha = 1$ minimizes the function $\alpha \mapsto \mathcal{K}(P_{\theta|g} \| P_{\theta|T_n} + (1-\alpha)T_n)$ over $[0,1]$ and that the value at the minimum is zero. Therefore, in view of (7.23), it is sufficient to prove that

$$
\inf_{T_n} \max_{g \in \mathcal{G}} P_{\theta|T_n} \left\{ \|g - T_n\|^2 > c_{\alpha} \Delta^*_n \right\} \geq \delta,
$$

where the infimum is taken over all estimators.

2. The problem has now been reduced to proving a minimax lower bound for estimation in squared prediction risk and can be solved using standard arguments from Tsybakov (2009, Chapter 2), and in particular Theorem 2.5. This theorem requires upper bounds on the quantities $\mathcal{K}(P_{\theta|g} \| P_{\theta|T_n} )$, $g, h \in \mathcal{G}$, where $P_{\theta|g}$ denotes the joint distribution of the observations $(Y_1, \ldots, Y_n)$ with $\mathbb{E}[Y_i] = b' \circ g(x_i)$. Since the observations are independent, it holds

$$
\mathcal{K}(P_{\theta|g} \| P_{\theta|T_n} ) = \sum_{i=1}^n \mathcal{K}(P_{\theta|g} \| P_{\theta|T_n} ),
$$

where $P_{\theta|g}$ denotes the distribution of $Y_i$ with $\mathbb{E}[Y_i] = b' \circ g(x_i)$. Upper bounds on the Kullback-Leibler divergence can be obtained using condition 1. Indeed, for any $g, h \in Q_{1:n}$, a second order Taylor expansion yields

$$
\mathcal{K}(P_{\theta|g} \| P_{\theta|T_n} ) \leq \frac{B^2}{2a} \|g(x_i) - h(x_i)\|^2.
$$

(7.25)
We now review the conditions that we have already imposed on the family $G$ to achieve the reduction in $1_o$, together with those that are sufficient to apply Tsybakov’s theorem.

(A) $\mathcal{H} \in \bar{D}$ with rank less than $D$

(B) $G \subset \{f_\lambda : \lambda \in \Lambda\}$

(C) $\|g - h\|^2 \geq 2 e^* \Delta^*_{n,M}(\Lambda), \quad \forall \ g, h \in G$

(D) $K(P^n_{\theta|g}||P^n_{\theta|oh}) < \log(\text{card}(G))/8, \quad \forall \ g, h \in G$

If the four conditions above are satisfied, then Theorem 2.5 of Tsybakov (2009) implies that there exists $\delta > 0$ such that (7.24) and thus (7.23) holds.

The rest of the proof consists in carefully choosing the family $G$ and depends on the aggregation problem at hand. Several of the subsequent constructions are based on the following class of matrices. For any $1 \leq D \leq M \wedge n$, consider the random matrix $X$ of size $D \times M$ such that its elements $X_{i,j}, i = 1, \ldots, D, \ j = 1, \ldots, M$ are i.i.d. Rademacher random variables, i.e., random variables taking values 1 and $-1$ with probability $1/2$.

Assume $S$ is a positive integer that satisfies

$$\frac{S}{D} \log \left( 1 + \frac{eM}{S} \right) < C_0 , \quad (7.26)$$

for some positive constant $C_0 < 1/2$. Theorem 5.2 in Baraniuk et al. (2008) (see also subsection 5.2.1 in Rigollet and Tsybakov, 2010) entails that if (7.26) holds for $C_0$ small enough, then there exists a nonempty set $\mathcal{M}(D)$ of matrices obtained as realizations of the matrix $X$ that enjoy the following weak restricted isometry (wri) property: for any $X \in \mathcal{M}(D)$, there exists constants $\bar{\chi} \geq \bar{\chi} > 0$, such that for any $\lambda \in \mathbb{R}^M$ with at most $2S$ nonzero coordinates,

$$\bar{\chi}|\lambda|^2 \leq \frac{||X\lambda||^2}{D} \leq \bar{\chi}|\lambda|^2 , \quad (7.27)$$

when $S$ satisfies (7.26).

**Model selection aggregation.**

Recall that in this case $\Delta^*_{n,M}(\mathcal{V}) = (D \wedge \log M)/n$ and assume first that

$$D \geq \frac{2}{C_0} \log \left( 1 + \frac{eM}{2} \right) . \quad (7.28)$$

Take the dictionary $\mathcal{H} = \{f_1, \ldots, f_M\}$ to be such that for any $j = 1, \ldots, M$,

$$f_j(x_i) = \begin{cases} \tau \sqrt{\frac{D \wedge \log M}{D}} X_{i,j} & \text{if } i \leq D, \\ 0 & \text{otherwise,} \end{cases}$$

where $X \in \mathcal{M}(D)$ and $\tau \in (0,1)$ is to be chosen later. Clearly, this dictionary has rank less than $D$. We simply choose the family $G = \{f_1, \ldots, f_M\}$ and check conditions (A)–(D).

Conditions (A)–(B). Since $0 < \tau < 1$ and $D \leq n$, we have

$$||f_j||^2 = \tau^2 \frac{D \wedge \log M}{D} \leq \tau^2 \leq 1, \quad ||f_j||_\infty = \tau \sqrt{\frac{D \wedge \log M}{D}} \leq \tau \leq 1 , . \quad (30)$$
so that \((A)\) holds. Moreover, \((B)\) clearly holds.

Conditions \((C)\)–\((D)\). For any \(f_j, f_k \in \mathcal{G}, j \neq k\), the WRI condition \((7.27)\), which holds for \(S = 2\) under \((7.28)\) yields

\[
2\tau^2 \frac{D \log M}{n} \leq \|f_j - f_k\|^2 \leq 2\tau^2 \frac{D \log M}{n}.
\]

The left inequality implies that \((C)\) holds with \(c^* = \tau^2 \frac{D}{n}\). Finally, \((7.25)\) and the right inequality in the above display yield

\[
\mathcal{K}(P_{\theta \circ f_j}^{1:n} || P_{\theta \circ f_k}^{1:n}) = \sum_{i=1}^{D} \mathcal{K}(P_{\theta \circ f_j}^{i} || P_{\theta \circ f_k}^{i}) \leq \frac{B^2 n}{2a} \|f_j - f_k\|^2 \leq \frac{\tau^2 B^2}{a} \chi (D \log M).
\]

As a result, \((D)\) holds as long as \(\tau < \sqrt{a/(8B^2 \chi)}\).

Assume now that

\[
D < \frac{2}{C_0} \log \left(1 + \frac{eM}{2}\right).
\]  

(7.29)

Define \(D' \geq 1\) to be the largest integer such that \(D' \leq D\) and \(2^{D'} \leq M\). It is not hard to show that if \(M \geq 4\), equation \((7.29)\) yields

\[
D' \geq \frac{C_0 \log 2}{2 \log(1 + eM)} D = C_1 D.
\]

Besides, if \(M \leq 3\), we have \(D \leq 3\) and \(D' = 1\) so that \(D' \geq D/3 \geq C_1 D\). Consider the set of functions \(\phi_1, \ldots, \phi_{D'}\) such that \(\phi_j(x_i) = 1\), if and only if \(j = i, i = 1, \ldots, n\). For any \(\omega = (\omega_1, \ldots, \omega_{D'}) \in \{0,1\}^{D'}\) define the function \(\phi_\omega = \sum_{j=1}^{D'} \omega_j \phi_j\) and observe that for any \(\omega' \in \{0,1\}^{D'}\),

\[
\|\phi_\omega - \phi_{\omega'}\|^2 = \frac{1}{n} \rho(\omega, \omega'),
\]  

(7.30)

where \(\rho(\omega, \omega') = \sum_{i=1}^{D'} (\omega_j - \omega'_j)^2\) denotes the Hamming distance between \(\omega\) and \(\omega'\). Rigollet and Tsybakov (2010, Lemma 8.3) guarantees the existence of a subset \(\{\omega^{(1)}, \ldots, \omega^{(d)}\} \subset \{0,1\}^{D'}\) such that \(\log d > C_2 D'\) and for any \(1 \leq j < k \leq d\),

\[
\rho(\omega^{(j)}, \omega^{(k)}) \geq \frac{D'}{4},
\]  

(7.31)

where \(C_2\) is a numerical constant. From the definition of \(D'\), we have \(d \leq M\) and we choose the dictionary \(H\) to be composed of functions \(f_j = \tau \phi_{\omega^{(j)}}, j = 1, \ldots, d\), where \(0 < \tau < 1\) is to be chosen later and \(f_j \equiv 0\), \(j = d + 1, \ldots, M\). Clearly, this dictionary has rank less than \(D' \leq D\).

We simply choose the family \(\mathcal{G} = \{f_1, \ldots, f_d\}\) and check conditions \((A) – (D)\).

Conditions \((A)–(B)\). Since \(0 < \tau < 1\) and \(D' \leq D \leq n\), we have for any \(j = 1, \ldots, d\),

\[
\|f_j\|^2 = \frac{\tau^2}{n} \sum_{i=1}^{D'} \omega_i^{(j)} \leq \tau^2 \leq 1, \quad \|f_j\|_{\infty} = \tau \max_{1 \leq i \leq D'} \omega_i^{(j)} \leq \tau \leq 1,
\]

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so that (A) holds. Moreover, (B) also holds.

Conditions (C)–(D). For any \( f_j, f_k \in \mathcal{G}, j \neq k \), (7.30) and (7.31) yield
\[
\|f_j - f_k\|^2 = \frac{\tau^2}{n} \rho(\omega(j), \omega(k)) \geq \frac{\tau^2 D'}{4n} \geq \frac{\tau^2 C_1 D}{4n},
\]
which implies that (C) holds with \( c_* = \tau^2 C_1 / 8 \). Finally, (7.25) and (7.30) yield
\[
\mathcal{K}(P_{\nu / \sigma f_j} \| P_{\nu / \sigma f_k}) \leq \frac{B^2 n}{2a} \frac{\|f_j - f_k\|^2}{\rho(\omega(j), \omega(k))} \leq \frac{\tau^2 B^2 D'}{a}.
\]
To complete the proof of (D), it is enough to observe that \( D' < \frac{\log d}{c_2} \) and to choose \( \tau \leq \sqrt{C_3 a/(8B^2)} \).

**Linear aggregation.**

Recall that in this case \( \Delta^*_{n,M}(\Lambda) = D/n \). Recall that for any \( j = 1, \ldots, M, \phi_j(x_i) = 1 \) if and only if \( i = j, i = 1, \ldots, n \). Take the dictionary \( \mathcal{H} = \{f_1, \ldots, f_M\} \) where \( f_j = \tau \phi_j \) for some \( \tau \in (0, 1) \) to be chosen later if \( 1 \leq j \leq D \) and \( f_j \equiv 0 \) if \( j > D \). Clearly this dictionary has rank less than \( D \). Similarly to the case of model selection covered above, Rigollet and Tsybakov (2010, Lemma 8.3) guarantees the existence of a subset \( \{ \omega(1), \ldots, \omega(d) \} \subset \{0, 1\}^D \) such that \( \log d > C_3 D \) and for any \( 1 \leq j < k \leq d \),
\[
\rho(\omega(j), \omega(k)) \geq \frac{D}{4}. \tag{7.32}
\]
We choose \( \mathcal{G} = \{g_1, \ldots, g_d\} \), where \( g_j = \sum_{k=1}^D \omega_k^{(j)} f_k \). We now check conditions (A)–(D).

Conditions (A)–(B). We have for any \( j = 1, \ldots, d \),
\[
\|f_j\|^2 \leq \frac{7}{n} \leq 1, \quad \|f_j\|_\infty \leq \tau \leq 1,
\]
so that (A) holds. Moreover, since for any \( j \), \( \max_i |\omega_i^{(j)}| \leq 1 \), condition (B) also holds for any \( \Lambda \supset \Lambda_\infty(1) \).

Conditions (C)–(D). For any \( g_j, g_k \in \mathcal{G}, j \neq k \), (7.30) and (7.32) yield
\[
\|g_j - g_k\|^2 = \frac{\tau^2}{n} \rho(\omega(j), \omega(k)) \geq \frac{\tau^2 D}{4n},
\]
which implies that (C) holds with \( c_* = \tau^2 / 8 \). Finally, (7.25) and (7.30) yield
\[
\mathcal{K}(P_{\nu / \sigma g_j} \| P_{\nu / \sigma g_k}) \leq \frac{B^2 n}{2a} \|g_j - g_k\|^2 = \frac{\tau^2 B^2}{2a} \rho(\omega(j), \omega(k)) \leq \frac{\tau^2 B^2 D}{a}.
\]
To complete proof of (D), it is enough to observe that \( D < \frac{\log d}{c_3} \) and to choose \( \tau \leq \sqrt{C_3 a/(8B^2)} \).

**Convex aggregation.**

Recall that in this case
\[
\Delta^*_{n,M}(\Lambda_1(1)) = \frac{D}{n} \wedge \sqrt{\frac{\log(1 + \frac{e M}{\sqrt{n}})}{n}}.
\]
If (7.29) holds, then we choose \( \mathcal{G} \) to be the same family as in this second part of the proof for model selection. Indeed, conditions \((A)\)–\((D)\) have all been checked with \( \Lambda = \mathcal{V} \subset A_1(1) \). Hereafter, we assume that
\[
D \geq \frac{2}{C_0} \log \left( 1 + \frac{eM}{2} \right). \tag{7.33}
\]

We divide the rest of the proof into two cases: large \( D \) and small \( D \). For both cases, we take the same dictionary \( \mathcal{H} = \{ f_1, \ldots, f_M \} \) to be such that for any \( j = 1, \ldots, M \), \( i = 1, \ldots, n \), \( k = 1, \ldots D \),
\[
f_j(x_i) = \begin{cases} X_{k,j} & \text{if } i = k \mod D, \\ 0 & \text{otherwise}, \end{cases}
\]
where \( X \in \mathcal{M}(D) \). Note that the rank of \( \mathcal{H} \) is at most \( D \) and that \( \mathcal{H} \in \mathcal{D} \) since
\[
\|f_j\|_2^2 = \frac{|n/D|D}{n} \leq 1, \quad \|f_j\|_\infty = 1.
\]
where \( |n/D| \) denotes the integer part of \( n/D \). Therefore, \((A)\) holds.

For both cases, the choice of \( \mathcal{G} \) relies on the following property. For any \( \ell = 1, \ldots M \), let \( \Omega_\ell \) be the subset of \( \{0, 1\}^M \) defined by
\[
\Omega_\ell = \left\{ \omega \in \{0, 1\}^M : \sum_{j=1}^M \omega_j = \ell \right\}. \tag{7.34}
\]
Recall that according to Rigollet and Tsybakov (2010, Lemma 8.3), for any \( \ell \leq M/2 \), there exists a subset \( \{\omega^{(1)}, \ldots, \omega^{(d)}\} \subset \Omega_\ell \) such that \( \log d > C_4 \ell \log(1 + eM/\ell) \) and for any \( 1 \leq j < k \leq d \),
\[
\rho(\omega^{(j)}, \omega^{(k)}) \geq \frac{\ell}{4}.
\]

Assume first that \( D \) is large:
\[
D \geq \frac{3}{2C_0} \sqrt{n \log \left( 1 + \frac{eM}{\sqrt{n}} \right)}. \tag{7.35}
\]

Since \( D \leq M \), it implies that \( D \geq \nu \sqrt{n} \geq 2 \sqrt{n} \) where \( \nu \geq 2 \) is the solution of
\[
\nu = \frac{3}{(2C_0)} \sqrt{\log(1 + e\nu)}.
\]
Let \( m \) be the largest integer such that
\[
m \leq \sqrt{\frac{n}{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)}}, \tag{7.36}
\]
and observe that \( m \geq 1 \) if \( n \geq \log(1 + eM/\sqrt{n}) \). But \( n \geq D \) together with (7.33) imply that
\[
n \geq D \geq \frac{2}{C_0} \log \left( 1 + \frac{eM}{2} \right) \geq \frac{1}{C_0} \log \left( 1 + \frac{eM}{\sqrt{n}} \right).
\]
We conclude that \( m \geq 1 \) by observing that \( C_0 < 1/2 \). Furthermore, it clearly holds that \( m \leq \sqrt{n} \), which in turn implies that \( m \leq M/2 \) since \( M \geq D \geq 2\sqrt{n} \).

According to Rigollet and Tsybakov (2010, Lemma 8.3), there exists a subset \( \{\omega^{(1)}, \ldots, \omega^{(d)}\} \subset \Omega_m \) such that \( \log d > C_4 m \log(1 + eM/m) \) and for any \( 1 \leq j < k \leq d \),

\[
\rho(\omega^{(j)}, \omega^{(k)}) \geq \frac{m}{4}.
\]

We choose the family \( \mathcal{G} = \{g_1, \ldots, g_d\}, g_j = \frac{r}{m} f(\omega^{(j)}), j = 1, \ldots, d \), where \( r \in (0, 1) \) is to be chosen later and check conditions \((B)-(D)\).

**Condition (B).** Note that \( \mathcal{G} \subset \{f_\lambda : \lambda \in \Lambda_1(1)\} \) since \( \frac{r}{m} \sum_k \omega^{(j)}_k = \tau \leq 1 \) for any \( j = 1, \ldots, d \) and condition \((B)\) holds.

**Conditions \((C)-(D)\).** Note that from (7.36) and the monotonicity of the function \( x \mapsto x \log(1 + eM/x) \), we have

\[
\frac{m}{D} \log \left( 1 + \frac{eM}{m} \right) \leq \frac{1}{D} \sqrt{\frac{n}{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)}} \sqrt{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)} \leq \frac{3}{2D} \sqrt{n \log \left( 1 + \frac{eM}{\sqrt{n}} \right)} \leq C_0,
\]

where we used respectively the fact that \( \log(1 + ab) \leq \log(1 + a) + \log(b), a > 0, b \geq 1 \), and (7.35). The previous display implies that (7.26) holds with \( S = m \) and we can apply (7.27) to obtain that for any \( g_j, g_k \in \mathcal{G}, j \neq k \),

\[
\|g_j - g_k\|^2 = \frac{\tau^2}{m^2} \|f(\omega^{(j)}) - f(\omega^{(k)})\|^2 \geq \frac{\tau^2}{m^2} \frac{D|n/D|}{nm^2} \rho(\omega^{(j)}, \omega^{(k)}) \geq \frac{\tau^2 \sqrt{n}}{8m} \geq \frac{\tau^2 \sqrt{n}}{8} \frac{\log(1 + eM/n)}{n},
\]

where in the last inequality, we used (7.36). We have proved that \((C)\) holds with \( c_x = \tau^2 \sqrt{\chi}/16 \).

To prove \((D)\), note that (7.25) and (7.27) yield

\[
\mathcal{K}(P_{\theta \in \mathcal{G}j}^{1:n}, P_{\theta \in \mathcal{G}k}^{1:n}) \leq \frac{\tau^2 B^2 n}{2a} \|f(\omega^{(j)}) - f(\omega^{(k)})\|^2 \leq \frac{\tau^2 B^2 \sqrt{\chi}}{2a} \frac{D|n/D|}{m^2} \rho(\omega^{(j)}, \omega^{(k)}) \leq \frac{\tau^2 B^2 \sqrt{\chi}}{a} \frac{n}{m}.
\]

Since \( m \geq 1 \), the definition of \( m \) and the fact that \( m \leq \sqrt{n} \) yield

\[
\frac{n}{m} \leq 4m \log \left( 1 + \frac{eM}{m} \right) < \frac{4}{C_4} \log d.
\]

Choosing \( \tau \leq \sqrt{aC_4/(32B^2 \sqrt{\chi})} \) completes the proof of \((D)\).

We now turn to the case where \( D \) is small. More precisely, assume that

\[
D < \frac{3}{2C_0} \sqrt{n \log \left( 1 + \frac{eM}{\sqrt{n}} \right)}.
\]
Let $\ell$ be the largest integer such that
\[ \frac{\ell}{D} \log \left( 1 + \frac{eM}{\ell} \right) \leq C_0, \]
(7.38)
and let $q > 0$ be such that
\[ q^2 = \frac{\tau^2}{n} \log \left( 1 + \frac{eM}{\ell} \right), \]
(7.39)
where $\tau \in (0, 1/2)$ is to be chosen later. It is clear from (7.33) that $\ell \geq 2$. Furthermore, $\ell < M/2$ since $D \leq M$ and $C_0 < 1/2$ imply that $\ell = M/2$ violates (7.38). Let $\{\omega^{(1)}, \ldots, \omega^{(d)}\} \subset \Omega_\ell$ be the subset obtained from Rigollet and Tsybakov (2010, Lemma 8.3) such that $\log d > C_4 \log(1 + eM/\ell)$. We choose the family $G = \{g_1, \ldots, g_d\}$, $g_j = q f_{\omega^{(j)}}$, $j = 1, \ldots, d$ and check conditions (B)–(D).

Conditions (B). Note that
\[ q^2 \ell^2 = \frac{\tau^2 \ell}{n} \log \left( 1 + \frac{eM}{\ell} \right) \leq \frac{\tau^2 C_0 D}{n}, \]
(7.40)
where we used (7.38).

If $M \leq 4\sqrt{n}$, using the fact that $\ell \leq M/2$, we get
\[ q^2 \ell^2 \leq \frac{\tau^2 C_0 \ell D}{n} \leq \frac{\tau^2 C_0 M D}{2n} \leq \frac{\tau^2 C_0 M^2}{2n} \leq 4\tau^2 \leq 1, \]
since $\tau < 1/2$.

If $M > 4\sqrt{n}$ note first that (7.37) yields
\[ \frac{9n}{3C_0 D} \leq \frac{3}{2} \sqrt{\frac{n}{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)}}, \]
Thus, using the monotonicity of the function $x \mapsto x \log(1 + eM/x)$, we get
\[ \frac{9n/(4C_0 D)}{D} \log \left( 1 + \frac{eM}{9n/(4C_0 D)} \right) > \frac{3}{2D} \sqrt{\frac{n}{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)}} \log \left( 1 + \frac{2eM}{3\sqrt{n}} \sqrt{\log \left( 1 + \frac{eM}{\sqrt{n}} \right)} \right) \]
\[ > \frac{3}{2D} \sqrt{n \log \left( 1 + \frac{eM}{\sqrt{n}} \right)} \geq C_0, \]
where we used the assumption that $M > 4\sqrt{n}$ in the last but one inequality. As a result, $9n/(4C_0 D)$ violates (7.38) and $\ell \leq 9n/(4C_0 D)$. It yields
\[ q^2 \ell^2 \leq \frac{9\tau^2}{4} \leq \tau \leq 1, \]
35
since $\tau < 1/2 < 2/3$. Thus, in both cases $q^2\ell^2 \leq 1$, which implies that $\mathcal{G} \subset \{ f_\lambda : \lambda \in \Lambda_1(1) \}$ so that condition $(B)$ holds.

Conditions $(C)–(D)$. Note that $(7.26)$ holds with $S = \ell$ by $(7.38)$ and we can apply $(7.27)$ to obtain that for any $g_j, g_k \in \mathcal{G}$, $j \neq k$,

$$
\|g_j - g_k\|^2 = q^2\|f_{\omega(j)} - f_{\omega(k)}\|^2 \geq \frac{\tau^2\chi_D n D}{n} \log \left( 1 + \frac{eM}{\ell} \right) \rho(\omega(j), \omega(k)) \geq \frac{\tau^2\chi D}{8n} \ell \log \left( 1 + \frac{eM}{\ell} \right).
$$

From the definition of $\ell$, we have

$$
\ell \log \left( 1 + \frac{eM}{\ell} \right) \geq \frac{2\ell}{2} \log \left( 1 + \frac{eM}{2\ell} \right) > C_0 D.
$$

The last two displays complete the proof of $(C)$ with $c_\ast = \tau^2\chi C_0/32$. To prove $(D)$, note that $(7.25)$ and $(7.27)$ yield

$$
K(P_{b_{\omega g_j}}^{1:n}|P_{b_{\omega g_k}}^{1:n}) \leq \frac{q^2B^2\ell^2}{a} \|f_{\omega(j)} - f_{\omega(k)}\|^2 \leq \frac{\tau^2B^2\chi}{a} \ell \log \left( 1 + \frac{eM}{\ell} \right) \leq \frac{\tau^2B^2\chi}{aC_4} \log d.
$$

Choosing $\tau \leq \sqrt{aC_4/(8B^2\chi)}$ completes the proof of $(D)$.

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