User-friendly introduction to PAC-Bayes bounds

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Abstract

Aggregated predictors are obtained by making a set of basic predictors vote according to some weights, that is, to some probability distribution.

Randomized predictors are obtained by sampling in a set of basic predictors, according to some prescribed probability distribution.

Thus, aggregated and randomized predictors have in common that they are not defined by a minimization problem, but by a probability distribution on the set of predictors. In statistical learning theory, there is a set of tools designed to understand the generalization ability of such procedures: PAC-Bayesian or PAC-Bayes bounds.

Since the original PAC-Bayes bounds [179, 134], these tools have been considerably improved in many directions (we will for example describe a simplified version of the localization technique of [41, 43] that was missed by the community, and later rediscovered as “mutual information bounds”). Very recently, PAC-Bayes bounds received a considerable attention: for example there was workshop on PAC-Bayes at NIPS 2017, (Almost) 50 Shades of Bayesian Learning: PAC-Bayesian trends and insights, organized by B. Guedj, F. Bach and P. Germain. One of the reasons of this recent success is the successful application of these bounds to neural networks [70].

An elementary introduction to PAC-Bayes theory is still missing. This is an attempt to provide such an introduction.

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1 Introduction

In a supervised learning problem, such as classification or regression, we are given a data
set, and we 1) fix a set of predictors and 2) find a good predictor in this set.

For example, when doing linear regression, you 1) chose to consider only linear predictors
and 2) use the least-square method to chose your linear predictor.

PAC-Bayes bounds will allow us to define and study “randomized” or “aggregated” pre-
dictors. By this, we mean that we will replace 2) by 2’) define weights on the predictors
and make them vote according to these weights or by 2”) draw a predictor according to some
prescribed probability distribution.

1.1 Machine learning and PAC bounds

1.1.1 Machine learning: notations

We will assume that the reader is already familiar with the setting of supervised learning
and the corresponding definitions. We briefly remind the notations involved here:
• an object set $\mathcal{X}$: photos, texts, $\mathbb{R}^d$ (equipped with a $\sigma$-algebra $\mathcal{S}_x$).

• a label set $\mathcal{Y}$, usually a finite set for classification problem or the set of real numbers for regression problems (equipped with a $\sigma$-algebra $\mathcal{S}_y$).

• a probability distribution $P$ on $(\mathcal{X} \times \mathcal{Y}, \mathcal{S}_x \otimes \mathcal{S}_y)$, which is not known.

• the data, or observations: $(X_1, Y_1), \ldots, (X_n, Y_n)$. From now, and until the end of Section 4, we assume that $(X_1, Y_1), \ldots, (X_n, Y_n)$ are i.i.d from $P$.

• a predictor is a measurable function $f : \mathcal{X} \rightarrow \mathcal{Y}$.

• we fix a set of predictors indexed by a parameter set $\Theta$ (equipped with a $\sigma$-algebra $\mathcal{T}$):

$$\{f_\theta, \theta \in \Theta\}.$$  

In regression, the basic example is $f_\theta(x) = \theta^T x$ for $\mathcal{X} = \Theta = \mathbb{R}^d$. The analogous for classification is:

$$f_\theta(x) = \begin{cases} 1 & \text{if } \theta^T x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

More sophisticated predictors: the set of all neural networks with a fixed architecture, $\theta$ being the weights of the network.

• a loss function, that is, a measurable function $\ell : \mathcal{Y}^2 \rightarrow [0, +\infty)$ with $\ell(y, y) = 0$. In a classification problem, a very common loss function is:

$$\ell(y', y) = \begin{cases} 1 & \text{if } y' \neq y \\ 0 & \text{if } y' = y \end{cases}.$$  

We will refer to it as the 0-1 loss function, and will use the following shorter notation: $\ell(y', y) = 1(y' \neq y)$. However, it is often more convenient to consider convex loss functions. For example, in binary classification: $\ell(y', y) = \max(1 - yy', 0)$ (the hinge loss). In regression problems, the most popular examples are $\ell(y', y) = (y' - y)^2$ the quadratic loss, or $\ell(y', y) = |y' - y|$ the absolute loss. Note that the original PAC-Bayes bounds in [134] were stated in the special case of the 0-1 loss, and this is also the case of most bounds published since then. However, PAC-Bayes bounds for regression with the quadratic loss were proven in [12], and in many works since then (they will be mentioned later). From now, and until the end of Section 4, we assume that $0 \leq \ell \leq C$. This might be either because we are using the 0-1 loss, or the quadratic loss but in a setting where $f_\theta(x)$ and $y$ are bounded.

• the generalization error of a predictor, or generalization risk, or simply risk:

$$R(f) = \mathbb{E}_{(X, Y) \sim P}[\ell(f(X), Y)].$$

For short, as we will only consider predictors in $\{f_\theta, \theta \in \Theta\}$ we will write

$$R(\theta) := R(f_\theta).$$

This function is not accessible because it depends on the unknown $P$. 


• for short, we put $\ell_i(\theta) := \ell(f_\theta(X_i), Y_i) \geq 0$.

• the empirical risk:

$$r(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell_i(\theta)$$

satisfies

$$\mathbb{E}_{(X_1,Y_1),\ldots,(X_n,Y_n)}[r(\theta)] = R(\theta).$$

Note that the notation for the last expectation is cumbersome. From now, we will write $\mathcal{S} = [(X_1,Y_1),\ldots,(X_n,Y_n)]$ and $\mathbb{E}_\mathcal{S}$ (for “expectation with respect to the sample”) instead of $\mathbb{E}_{(X_1,Y_1),\ldots,(X_n,Y_n)}$. In the same way, we will write $\mathbb{P}_\mathcal{S}$.

• an estimator is a function

$$\hat{\theta} : \bigcup_{n=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^n \to \Theta.$$ 

That is, to each possible dataset, with any possible size, it associates a parameter. (It must be such that the restriction of $\hat{\theta}$ to each $(\mathcal{X} \times \mathcal{Y})^n$ is measurable). For short, we write $\hat{\theta}$ instead of $\hat{\theta}((X_1,Y_1),\ldots,(X_n,Y_n))$. The most famous example is the Empirical Risk Minimizer, or ERM:

$$\hat{\theta}_{\text{ERM}} = \arg\min_{\theta \in \Theta} r(\theta)$$

(with a convention in case of a tie).

### 1.1.2 PAC bounds

Of course, our objective is to minimize $R$, not $r$. So the ERM strategy is motivated by the hope that these two functions are not so different, so that the minimizer of $r$ almost minimizes $R$. In what remains of this section, we will check to what extent this is true. By doing so, we will introduce some tools that will be useful when we will come to PAC-Bayes bounds.

The first of these tools is a classical result that will be useful in all this tutorial.

**Lemma 1.1 (Hoeffding’s inequality)** Let $U_1,\ldots,U_n$ be independent random variables taking values in an interval $[a,b]$. Then, for any $t > 0$,

$$\mathbb{E} \left[ e^{t \sum_{i=1}^{n} [U_i - \mathbb{E}(U_i)]} \right] \leq e^{\frac{nt^2(b-a)^2}{8}}.$$ 

The proof can be found for example in Chapter 2 of [37], which is a highly recommended reading, but it is so classical that you can as well find it on Wikipedia.

Fix $\theta \in \Theta$ and apply Hoeffding’s inequality with $U_i = \mathbb{E}[\ell_i(\theta)] - \ell_i(\theta)$ to get:

$$\mathbb{E}_\mathcal{S} \left[ e^{tn[R(\theta) - r(\theta)]} \right] \leq e^{\frac{nt^2}{8}}.$$ (1.1)
Now, for any $s > 0$,
\[
\mathbb{P}_S(R(\theta) - r(\theta) > s) = \mathbb{P}_S\left(e^{n[R(\theta) - r(\theta)]} > e^{nts}\right) \\
\leq \mathbb{E}_S\left(e^{n[R(\theta) - r(\theta)]}\right) e^{-nts} \quad \text{by Markov’s inequality,} \\
\leq e^{\frac{nt^2C^2}{8} - nts} \quad \text{by (1.1).}
\]
In other words,
\[
\mathbb{P}_S(R(\theta) > r(\theta) + s) \leq e^{\frac{nt^2C^2}{8} - nts}.
\]
We can make this bound as tight as possible, by optimizing our choice for $t$. Indeed, note that $nt^2C^2/8 - nts$ is minimized for $t = 4s/C^2$, which leads to
\[
\mathbb{P}_S(R(\theta) > r(\theta) + s) \leq e^{-\frac{2ns^2}{C^2}}. \quad (1.2)
\]
This means that, for a given $\theta$, the risk $R(\theta)$ cannot be much larger than the corresponding empirical risk $r(\theta)$. The order of this “much larger” can be better understood by introducing
\[
\varepsilon = e^{-\frac{2ns^2}{C^2}}
\]
and substituting $\varepsilon$ to $s$ in (1.2), which gives:
\[
\mathbb{P}_S\left(R(\theta) > r(\theta) + C\sqrt{\frac{\log \frac{1}{\varepsilon}}{2n}}\right) \leq \varepsilon. \quad (1.3)
\]
We see that $R(\theta)$ will usually not exceed $r(\theta)$ by more than a term in $1/\sqrt{n}$. This is not enough, though, to justify the use of the ERM. Indeed, (1.3) is only true for the $\theta$ that was fixed above, and we cannot apply it to $\hat{\theta}_\text{ERM}$ that is a function of the data. In order to study $R(\hat{\theta}_\text{ERM})$, we can use
\[
R(\hat{\theta}_\text{ERM}) - r(\hat{\theta}_\text{ERM}) \leq \sup_{\theta \in \Theta} [R(\theta) - r(\theta)] \quad (1.4)
\]
so we need a version of (1.3) that would hold uniformly on $\Theta$.

Let us now assume, until the end of Subsection 1.1, that the set $\Theta$ is finite, that is, $\text{card}(\Theta) = M < +\infty$. Then:
\[
\mathbb{P}_S(\sup_{\theta \in \Theta}[R(\theta) - r(\theta)] > s) = \mathbb{P}_S\left(\bigcup_{\theta \in \Theta} \{[R(\theta) - r(\theta)] > s\}\right) \\
\leq \sum_{\theta \in \Theta} \mathbb{P}_S(R(\theta) > r(\theta) + s) \\
\leq Me^{-\frac{2ns^2}{C^2}} \quad (1.5)
\]
thanks to (1.2). This time, put
\[ \varepsilon = Me^{-\frac{2n^2}{c^2}}, \]
plug into (1.5), this gives:
\[ \mathbb{P}_S \left( \sup_{\theta \in \Theta} |R(\theta) - r(\theta)| > C \sqrt{\frac{\log M}{2n}} \right) \leq \varepsilon. \]
Let us state this conclusion as a theorem (focusing on the complementary event).

**Theorem 1.2** Assume that \( \text{card}(\Theta) = M < +\infty. \) For any \( \varepsilon \in (0, 1), \)
\[ \mathbb{P}_S \left( \forall \theta \in \Theta, \ R(\theta) \leq r(\theta) + C \sqrt{\frac{\log M}{2n}} \right) \geq 1 - \varepsilon. \]
This result indeed motivates the introduction of \( \hat{\theta}_{\text{ERM}}. \) Indeed, using (1.4), with probability at least \( 1 - \varepsilon \) we have
\[ R(\hat{\theta}_{\text{ERM}}) \leq r(\hat{\theta}_{\text{ERM}}) + C \sqrt{\frac{\log M}{2n}} \]
\[ = \inf_{\theta \in \Theta} r(\theta) + C \sqrt{\frac{\log M}{2n}} \]
so the ERM satisfies:
\[ \mathbb{P}_S \left( R(\hat{\theta}_{\text{ERM}}) \leq \inf_{\theta \in \Theta} r(\theta) + C \sqrt{\frac{\log M}{2n}} \right) \geq 1 - \varepsilon. \]
Such a bound is usually called a PAC bound, that is, *Probably Approximately Correct* bound. The reason for this terminology, introduced by Valiant in [192], is as follows: Valiant was considering the case where there is a \( \theta_0 \in \Theta \) such that \( Y_i = f_{\theta_0}(X_i) \) holds almost surely. This means that \( R(\theta_0) = 0 \) and \( r(\theta_0) = 0, \) and so
\[ \mathbb{P}_S \left( R(\hat{\theta}_{\text{ERM}}) \leq C \sqrt{\frac{\log M}{2n}} \right) \geq 1 - \varepsilon, \]
which means that with large Probability, \( R(\hat{\theta}_{\text{ERM}}) \) is Approximately equal to the Correct value, that is, 0. Note that, however, this is only correct if \( \log(M)/n \) is small, that is, if \( M \) is not larger than \( \exp(n) \). This \( \log(M) \) in the bound is the price to pay to learn which of \( M \) predictors is the best.
Remark 1.1 The proof of Theorem 1.2 used, in addition to Hoeffding’s inequality, two tricks that we will reuse many times in this tutorial:

- given a random variable $U$ and $s \in \mathbb{R}$, for any $t > 0$,
  \[
  P(U > s) = P(e^{tU} > e^{ts}) \leq \frac{E(e^{tU})}{e^{ts}}
  \]
  thanks to Markov inequality. The combo “exponential + Markov inequality” is known as Chernoff bound. Chernoff bound is of course very useful together with exponential inequalities like Hoeffding’s inequality.

- given a finite number of random variables $U_1, \ldots, U_M$,
  \[
  P\left(\sup_{1 \leq i \leq M} U_i > s\right) = P\left(\bigcup_{1 \leq i \leq M} \{U_i > s\}\right) \leq \sum_{i=1}^{M} P(U_i > s).
  \]
  This argument is called the union-bound argument.

The next step in the study of the ERM would be to go beyond finite sets $\Theta$. The union bound argument has to be modified in this case, and things become a little more complicated. We will therefore stop here the study of the ERM: it is not our objective anyway.

If the reader is interested by the study of the ERM in general: Vapnik and Chervonenkis developed the theoretical tools for this study in 1969/1970, this is for example developed by Vapnik in [194]. The book [67] is a beautiful and very pedagogical introduction to machine learning theory, and Chapters 11 and 12 in particular are dedicated to Vapnik and Chervonenkis theory.

### 1.2 What are PAC-Bayes bounds?

I am now in better position to explain what are PAC-Bayes bounds. A simple way to phrase things: PAC-Bayes bounds are generalization of the union bound argument, that will allow to deal with any parameter set $\Theta$: finite or infinite, continuous... However, a byproduct of this technique is that we will have to change the notion of estimator.

**Definition 1.1** Let $\mathcal{P}(\Theta)$ be the set of all probability distributions on $(\Theta, \mathcal{T})$. A data-dependent probability measure is a function:

\[
\hat{\rho} : \bigcup_{n=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^n \rightarrow \mathcal{P}(\Theta)
\]
with a suitable measurability condition. We will write \( \hat{\rho} \) instead of \( \hat{\rho}((X_1, Y_1), \ldots, (X_n, Y_n)) \) for short.

In practice, when you have a data-dependent probability measure, and you want to build a predictor, you can:

- draw a random parameter \( \tilde{\theta} \sim \hat{\rho} \), we will call this procedure “randomized estimator”.
- use it to average predictors, that is, define a new predictor:
  \[
  f_{\hat{\rho}}(\cdot) = E_{\theta \sim \hat{\rho}}[f_\theta(\cdot)]
  \]
  called the aggregated predictor with weights \( \hat{\rho} \).

So, with PAC-Bayes bounds, we will extend the union bound argument to infinite, uncountable sets \( \Theta \), but we will obtain bounds on various risks related to data-dependent probability measures, that is:

- the risk of a randomized estimator, \( R(\tilde{\theta}) \),
- or the average risk of randomized estimators, \( E_{\theta \sim \hat{\rho}}[R(\theta)] \),
- or the risk of the aggregated estimator, \( R(f_{\hat{\rho}}) \).

You will of course ask the question: if \( \Theta \) is infinite, what will become the \( \log(M) \) term in Theorem 1.2 that came from the union bound? In general, this term will be replaced by the Kullback-Leibler divergence between \( \hat{\rho} \) and a fixed \( \pi \) on \( \Theta \).

**Definition 1.2** Given two probability measures \( \mu \) and \( \nu \) in \( \mathcal{P}(\Theta) \), the Kullback-Leibler (or simply KL) divergence between \( \mu \) and \( \nu \) is

\[
KL(\mu \| \nu) = \int \log \left( \frac{d\mu}{d\nu}(\theta) \right) \mu(d\theta) \in [0, +\infty]
\]

if \( \mu \) has a density \( \frac{d\mu}{d\nu} \) with respect to \( \nu \), and \( KL(\mu \| \nu) = +\infty \) otherwise.

**Example 1.1** For example, if \( \Theta \) is finite,

\[
KL(\mu \| \nu) = \sum_{\theta \in \Theta} \log \left( \frac{\mu(\theta)}{\nu(\theta)} \right) \mu(\theta).
\]

---

1. I don’t want to scare the reader with measurability conditions, as I will not check them in this tutorial anyway. Here, the exact condition to ensure that what follows is well defined is that for any \( A \in \mathcal{T} \), the function

\[
((x_1, y_1), \ldots, (x_n, y_n)) \mapsto [\hat{\rho}((x_1, y_1), \ldots, (x_n, y_n))](A)
\]

is measurable. That is, \( \hat{\rho} \) is a regular conditional probability.

2. See the title of van Erven’s tutorial: “PAC-Bayes mini-tutorial: a continuous union bound”. Note, however, that it is argued by Catoni in that PAC-Bayes bounds are actually more than that, we will come back to this in Section 4.
The following result is well known. You can prove it using Jensen’s inequality, or use Wikipedia again.

**Proposition 1.3** For any probability measures $\mu$ and $\nu$, $KL(\mu\|\nu) \geq 0$ with equality if and only if $\mu = \nu$.

### 1.3 Why this tutorial?

Since the “PAC analysis of a Bayesian estimator” by Shawe-Taylor and Williamson [179] and the first PAC-Bayes bounds proven by McAllester [134] [135], many new PAC-Bayes bounds appeared (we will see that many of them can be derived from Seeger’s bound [173]). These bounds were used in various contexts, to solve a wide range of problems. This led to hundreds of (beautiful!) papers. The consequence of this is that it’s quite difficult to be aware of all the existing work on PAC-Bayes bound.

As a reviewer for ICML or NeurIPS, I had very often to reject papers because these papers were re-proving already known results. Or, because these papers proposed bounds that were weaker than existing ones. In particular, it seems that many powerful techniques in Catoni’s book [43] are still ignored by the community (some are already introduced in earlier works [41] [42]).

On the other hand, it’s not always easy to get into PAC-Bayes bounds. I realize that most papers already assume some basic knowledge on these bounds, and that a monograph like [43] is quite technical to begin with. When a MSc or PhD student asks me for an easy-to-follow introduction on PAC-Bayes, I am never sure what to answer, and usually end up improvising such an introduction for one or two hours, with a piece of chalk and a blackboard. So it came to me recently that it might be useful to write a beginner-friendly tutorial, that I could send instead!

Note that there are already short tutorials on PAC-Bayes bounds, by McAllester and van Erven: [137] [193], the introductory slides by Fleuret are also very nice [73]. They are very good, and I recommend the reader to check them. However, they are focused on empirical bounds only. There are also surveys on PAC-Bayes bounds, such as Section 5 in [55] or [89]. These papers are very useful to navigate in the ocean of publications on PAC-Bayes bounds, and they helped me a lot when I was writing this document. Finally, in order to highlight the main ideas, I will not necessarily try to present the bounds with the tightest possible constants. In particular, many oracle bounds and localized bounds in Section 4 were introduced in [41] [43] with better constants. Thus I strongly recommend to read [43] after this tutorial, and the more recent papers mentioned below.

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3I might have done such mistakes myself, and I apologize if it is the case.

4I must confess that I started a first version of this document after two introductory talks at A. Tsybakov’s statistics seminar at ENSAE in September-October 2008. Then I got other things to do and I forgot about it. I taught online learning and PAC-Bayes bounds at ENSAE between 2014 and 2019, which made me think again about it. When I joined Emni Khan’s group in 2019, I started to think again about such a document, to share it with the members of the group who were willing to learn about PAC-Bayes. Of course the contents of the document had to be different, because of the enormous amount of very exciting papers that were published in the meantime. I finally started again from scratch in early 2021.
1.4 Two types of PAC bounds, organization of these notes

It is important to make a distinction between two types of PAC bounds.

Theorem 1.2 is usually referred to as an empirical bound. It means that, for any \( \theta \), \( R(\theta) \) is upper bounded by an empirical quantity, that is, by something that we can compute when we observe the data. This allows to define the ERM as the minimizer of this bound. It also provides a numerical certificate of the generalization error of the ERM. You will really end up with something like

\[
P_S \left( R(\hat{\theta}_{\text{ERM}}) \leq 0.12 \right) \geq 0.99.
\]

However, a numerical certificate on the generalization error does not tell you one thing. Can this 0.12 be improved using a larger sample size? Or is it the best that can be done with our set of predictors? The right tools to answer these questions are oracle PAC bounds. In these bounds, you have a control of the form

\[
P_S \left( R(\hat{\theta}_{\text{ERM}}) \leq \inf_{\theta \in \Theta} R(\theta) + r_n(\varepsilon) \right) \geq 1 - \varepsilon,
\]

where the remainder \( r_n(\varepsilon) \to 0 \) as fast as possible when \( n \to \infty \). Of course, the upper bound on \( R(\hat{\theta}_{\text{ERM}}) \) cannot be computed because we don’t know the function \( R \), so it doesn’t lead to a numerical certificate. Still, these bounds are very interesting, because they tell you how close you can expect \( R(\hat{\theta}_{\text{ERM}}) \) to be of the smallest possible value of \( R \).

In the same way, there are empirical PAC-Bayes bounds, and oracle PAC-Bayes bounds. The very first PAC-Bayes bounds by McAllester \[134, 135\] were empirical bounds. Later, Catoni \[11, 42, 43\] proved the first oracle PAC-Bayes bounds.

In some sense, empirical PAC-Bayes bounds are more useful in practice, and oracle PAC-Bayes bounds are theoretical objects. But this might be an oversimplification. I will show that empirical bounds are tools used to prove some oracle bounds, so they are also useful in theory. On the other hand, when we design a data-dependent probability measure, we don’t know if it will lead to large or small empirical bounds. A preliminary study of its theoretical properties through an oracle bound is the best way to ensure that it is efficient, and so that it has a chance to lead to small empirical bounds.

In Section 2 we will study an example of empirical PAC-Bayes bound, essentially taken from a preprint by Catoni \[11\]. We will prove it together, play with it, modify it in many ways. In Section 3 I provide various empirical PAC-Bayes bounds, and explain the race to tighter bounds. This led to bounds that are tight enough to provide good generalization bounds for deep learning, we will discuss this based on Dziugaite and Roy’s paper \[70\] and a more recent work by Pérez-Ortiz, Rivasplata, Shawe-Taylor, and Szepesvári \[156\].

In Section 4 we will turn to oracle PAC-Bayes bounds. I will explain how to derive these bounds from empirical bounds, and apply them to some classical set of predictors. We will examine the assumptions leading to fast rates in these inequalities.

Section 5 will be devoted to the various attempts to extend PAC-Bayes bounds beyond the setting introduced in this introduction, that is: bounded loss, and i.i.d observations. Finally, in Section 6 I will discuss briefly the connection between PAC-Bayes bounds and many
other approaches in machine learning and statistics, including the recent Mutual Information bounds (MI).

2 First step in the PAC-Bayes world

As mentioned above, there are many PAC-Bayes bounds. I will start in this section by a bound which is essentially due to Catoni in the preprint [41] (the same technique was used in the monograph [43] but with some modifications). Why this choice?

Well, any choice is partly arbitrary: I did my PhD thesis [1] with Olivier Catoni and thus I know his works well. So it’s convenient for me. But, also, in a first time, I don’t want here to provide the best bound. I want to show how PAC-Bayes bounds work, how to use them, and explain the different variants (bounds on randomized estimators, bounds on aggregated estimators, etc.). It appears that Catoni’s technique is extremely convenient to prove almost all the various type of bounds with a unique proof. Later, in Section 3, I will present alternative empirical PAC-Bayes bounds, this will allow you to compare them, and find the pros and the cons of each.

2.1 A simple PAC-Bayes bound

2.1.1 Catoni’s bound [41]

From now, and until the end of these notes, let us fix a probability measure \( \pi \in \mathcal{P}(\Theta) \). The measure \( \pi \) will be called the prior, because of a connection with Bayesian statistics that will be discussed in Section 6.

Theorem 2.1 For any \( \lambda > 0 \), for any \( \varepsilon \in (0, 1) \),

\[
P_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon}}{\lambda} \right) \geq 1 - \varepsilon.
\]

Let us prove Theorem 2.1. The proof requires a lemma that will be extremely useful in all these notes. This lemma has been known since Kullback [111] in the case of a finite \( \Theta \), but the general case is due to Donsker and Varadhan [68].

Lemma 2.2 (Donsker and Varadhan’s variational formula) For any measurable, bounded function \( h : \Theta \to \mathbb{R} \) we have:

\[
\log \mathbb{E}_{\theta \sim \pi} \left[ e^{h(\theta)} \right] = \sup_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho}[h(\theta)] - KL(\rho \| \pi) \right].
\]

Moreover, the supremum with respect to \( \rho \) in the right-hand side is reached for the Gibbs measure \( \pi_h \) defined by its density with respect to \( \pi \)

\[
\frac{d\pi_h}{d\pi}(\theta) = \frac{e^{h(\theta)}}{\mathbb{E}_{\theta \sim \pi}[e^{h(\theta)}]}, \quad (2.1)
\]
Proof of Lemma 2.2. Using the definition, just check that for any \( \rho \in \mathcal{P}(\Theta) \),

\[
KL(\rho \| \pi_h) = -\mathbb{E}_{\theta \sim \rho}[h(\theta)] + KL(\rho \| \pi) + \log \mathbb{E}_{\theta \sim \pi}[e^{h(\theta)}].
\]

Thanks to Proposition 1.3, the left hand side is nonnegative, and equal to 0 only when \( \rho = \pi_h \). \( \square \)

Proof of Theorem 2.1. The beginning of the proof follows closely the study of the ERM and the proof of Theorem 1.2. Fix \( \theta \in \Theta \) and apply Hoeffding’s inequality with \( U_i = \mathbb{E}[\ell_i(\theta)] - \ell_i(\theta) \): for any \( t > 0 \),

\[
\mathbb{E}[e^{tn[R(\theta) - r(\theta)]}] \leq e^{\frac{nt^2C^2}{8}}.
\]

We put \( t = \lambda/n \), which gives:

\[
\mathbb{E}[e^{\lambda[R(\theta) - r(\theta)]}] \leq e^{\frac{\lambda^2C^2}{8n}}.
\]

This is where the proof diverges from the proof of Theorem 1.2. We will now integrate this bound with respect to \( \pi \):

\[
\mathbb{E}_{\theta \sim \pi} \mathbb{E}[e^{\lambda[R(\theta) - r(\theta)]}] \leq e^{\frac{\lambda^2C^2}{8n}}.
\]

Thanks to Fubini, we can exchange the integration with respect to \( \theta \) and the one with respect to the sample:

\[
\mathbb{E}[e^{\lambda[R(\theta) - r(\theta)]}] \leq e^{\frac{\lambda^2C^2}{8n}}.
\]

(2.2)

and we apply Donsker and Varadhan’s variational formula (Lemma 2.2) to get:

\[
\mathbb{E}[e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho}[R(\theta) - r(\theta)] - KL(\rho \| \pi)] \leq e^{\frac{\lambda^2C^2}{8n}}.
\]

Rearranging terms:

\[
\mathbb{E}[e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho}[R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2C^2}{8n}}] \leq 1.
\]

(2.3)

The end of the proof uses Chernoff bound. Fix \( s > 0 \),

\[
\mathbb{P}_S \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho}[R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2C^2}{8n} > s \right] \leq \mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho}[R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2C^2}{8n}} \right] e^{-s} \leq e^{-s}.
\]

Solve \( e^{-s} = \varepsilon \), that is, put \( s = \log(1/\varepsilon) \) to get

\[
\mathbb{P}_S \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho}[R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2C^2}{8n} > \log \frac{1}{\varepsilon} \right] \leq \varepsilon.
\]

Rearranging terms give:

\[
\mathbb{P}_S \left[ \exists \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] > \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon}}{\lambda} \right] \leq \varepsilon.
\]

Take the complement to end the proof. \( \square \)
2.1.2 Exact minimization of the bound

We remind that the bound in Theorem 1.2,

\[
\mathbb{P}_S \left( \forall \theta \in \Theta, R(\theta) \leq r(\theta) + C\sqrt{\frac{\log \frac{M}{\varepsilon}}{2n}} \right) \geq 1 - \varepsilon,
\]

motivated the introduction of \( \hat{\theta}_{\text{ERM}} \), the minimizer of \( r \).

Exactly in the same way, the bound in Theorem 2.1,

\[
\mathbb{P}_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi)}{\lambda} + \log \frac{1}{\varepsilon} \right) \geq 1 - \varepsilon,
\]

motivates the study of a data-dependent probability measure \( \hat{\rho}_\lambda \) that would be defined as:

\[
\hat{\rho}_\lambda = \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{KL(\rho\|\pi)}{\lambda} \right\}.
\]

But does such a minimizer exist? It turns out that the answer is yes, thanks to Donsker and Varadhan’s variational formula again! Indeed, to minimize:

\[
\mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{KL(\rho\|\pi)}{\lambda}
\]

is equivalent to maximize

\[-\lambda \mathbb{E}_{\theta \sim \rho}[r(\theta)] - KL(\rho\|\pi)\]

which is exactly what the variational inequality does, with \( h(\theta) = -\lambda r(\theta) \). We know that the minimum is reached for \( \rho = \pi_{-\lambda r} \) as defined in (2.1). Let us summarize this in following definition and corollary.

**Definition 2.1** In the whole tutorial we will let \( \hat{\rho}_\lambda \) denote “the Gibbs posterior” given by \( \hat{\rho}_\lambda = \pi_{-\lambda r} \), that is:

\[
\hat{\rho}_\lambda(\mathrm{d}\theta) = \frac{e^{-\lambda r(\theta)}\pi(\mathrm{d}\theta)}{\mathbb{E}_{\theta \sim \pi}[e^{-\lambda r(\theta)}]}.
\]

(2.4)

**Corollary 2.3** The Gibbs posterior is the minimizer of the right-hand side of Theorem 2.1:

\[
\hat{\rho}_\lambda = \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{KL(\rho\|\pi)}{\lambda} \right\}.
\]

As a consequence, for any \( \lambda > 0 \), for any \( \varepsilon \in (0,1) \),

\[
\mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi) + \log \frac{1}{\varepsilon}}{\lambda} \right] \right) \geq 1 - \varepsilon.
\]
2.1.3 Some examples, and non-exact minimization of the bound

When you see something like:
\[ E_{\theta \sim \hat{\rho}} \left[ R(\theta) \right] \leq \inf_{\rho \in P(\Theta)} \left[ E_{\theta \sim \rho} \left[ r(\theta) \right] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\pi(\theta)}}{\lambda} \right] \]

I’m not sure you immediately see what is the order of magnitude of the bound. I don’t. In general, when you apply such a general bound to a set of predictors, I think it is quite important to make the bound more explicit. Let us process a few examples (I advise you to do the calculations on your own in these examples, and in other examples).

**Example 2.1 (Finite case)** Let us start with the special case where \( \Theta \) is a finite set, that is, \( \text{card}(\Theta) = M < +\infty \). We begin with the application of Corollary 2.3. In this case, the Gibbs posterior \( \hat{\rho}_\lambda \) of (2.4) is a probability on the finite set \( \Theta \) given by
\[ \hat{\rho}_\lambda(\theta) = \frac{e^{-\lambda r(\theta)\pi(\theta)}}{\sum_{\theta' \in \Theta} e^{-\lambda r(\theta')\pi(\theta')}}. \]

and we have, with probability at least \( 1 - \varepsilon \):
\[ E_{\theta \sim \hat{\rho}_\lambda} \left[ R(\theta) \right] \leq \inf_{\theta \in \Theta} \left[ r(\theta) + \frac{\lambda C^2}{8n} + \frac{KL(\delta_\theta \| \pi) + \log \frac{1}{\pi(\theta)}}{\lambda} \right]. \]  

As the bound holds for all \( \rho \in P(\Theta) \), it holds in particular for all \( \rho \) in the set of Dirac masses \( \{ \delta_\theta, \theta \in \Theta \} \). Obviously:
\[ E_{\theta \sim \delta_\theta} \left[ r(\theta) \right] = r(\theta) \]

and
\[ KL(\delta_\theta \| \pi) = \sum_{\theta \in \Theta} \log \left( \frac{\delta_\theta(\theta)}{\pi(\theta)} \right) \delta_\theta(\theta) = \log \frac{1}{\pi(\theta)}. \]

the previous bound implies
\[ \mathbb{P}_S \left( E_{\theta \sim \hat{\rho}_\lambda} \left[ R(\theta) \right] \leq \inf_{\theta \in \Theta} \left[ r(\theta) + \frac{\lambda C^2}{8n} + \frac{\log \frac{1}{\pi(\theta)}}{\lambda} \right] \right) \geq 1 - \varepsilon, \]  

with \( \log(1/0) = +\infty \). This gives us an intuition on the role of the measure \( \pi \): the bound will be tighter for \( \theta \)'s such that \( \pi(\theta) \) is large. However, \( \pi \) cannot be large everywhere: it is a probability distribution, so it must satisfy
\[ \sum_{\theta \in \Theta} \pi(\theta) = 1. \]

The larger the set \( \Theta \), the more this total sum of 1 will be spread, which will lead to large values of \( \log(1/\pi(\theta)) \).
If $\pi$ is the uniform probability, then $\log(1/\pi(\theta)) = \log(M)$, and the bound becomes:

$$
P_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\theta \in \Theta} r(\theta) + \frac{\lambda C^2}{8n} + \frac{\log \frac{M}{\epsilon}}{\lambda} \right) \geq 1 - \epsilon.
$$

The choice $\lambda = \sqrt{\frac{8n}{(C^2 \log(M/\epsilon))}}$ actually minimizes the right-hand side, this gives:

$$
P_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\theta \in \Theta} r(\theta) + C \sqrt{\frac{\log M}{2n}} \right) \geq 1 - \epsilon. \quad (2.7)
$$

That is, the Gibbs posterior $\hat{\rho}_\lambda$ satisfies the same bound as the ERM in Theorem 1.2. Note that the optimization with respect to $\lambda$ is a little more problematic when $\pi$ is not uniform, because the optimal $\lambda$ would depend on the data, which is not allowed. We will come back to the choice of $\lambda$ in the general case soon.

Let us also consider the statement of Theorem 2.1 in this case. With probability at least $1 - \epsilon$, we have:

$$
\forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \hat{\rho}}[r(\theta)] + \frac{\lambda C^2}{8n} + KL(\rho||\pi) + \frac{\log \frac{1}{\epsilon}}{\lambda}.
$$

Let us apply this bound to any $\rho$ in the set of Dirac masses $\rho \in \{\delta_{\theta}, \theta \in \Theta\}$. This gives:

$$
\forall \theta \in \Theta, R(\theta) \leq r(\theta) + \frac{\lambda C^2}{8n} + \frac{\log \frac{1}{\pi(\theta)} + \log \frac{1}{\epsilon}}{\lambda}
$$

and, when $\pi$ is uniform:

$$
\forall \theta \in \Theta, R(\theta) \leq r(\theta) + \frac{\lambda C^2}{8n} + \frac{\log \frac{M}{\epsilon}}{\lambda}
$$

As this bound holds for any $\theta$, it holds in particular for the ERM, which gives:

$$
R(\hat{\theta}_{\text{ERM}}) \leq \inf_{\theta \in \Theta} r(\theta) + \frac{\lambda C^2}{8n} + \frac{\log \frac{M}{\epsilon}}{\lambda}
$$

and, once again with the choice $\lambda = \sqrt{\frac{8n}{(C^2 \log(M/\epsilon))}}$, we recover exactly the result of Theorem 1.2:

$$
R(\hat{\theta}_{\text{ERM}}) \leq \inf_{\theta \in \Theta} r(\theta) + C \sqrt{\frac{\log M}{2n}}.
$$

The previous example leads to important remarks:

- PAC-Bayes bounds can be used to prove generalization bounds for Gibbs posteriors, but sometimes they can also be used to study more classical estimators, like the ERM. Many of the recent papers by Catoni with co-authors study robust non-Bayesian estimators thanks to sophisticated PAC-Bayes bounds [15].
the choice of $\lambda$ has a different status when you study the Gibbs posterior $\hat{\rho}_\lambda$ and the ERM. Indeed, in the bound on the ERM, $\lambda$ is chosen to minimize the bound, but the estimation procedure is not affected by $\lambda$. The bound for the Gibbs posterior is also minimized with respect to $\lambda$, but $\hat{\rho}_\lambda$ depends on $\lambda$. So, if you make a mistake when choosing $\lambda$, this will have bad consequences not only on the bound, but also on the practical performances of the method. This means also that if the bound is not tight, it is likely that the $\lambda$ obtained by minimizing the bound will not lead to good performances in practice. (As you will see soon, we present in Section 3 bounds that do not depend on a parameter like $\lambda$).

**Example 2.2 (Lipschitz loss and Gaussian priors)** Let us switch to the continuous case, so that we can derive from PAC-Bayes bounds some results that we wouldn’t be able to derive from a union bounds argument. We consider the case where $\Theta = \mathbb{R}^d$, the function $\theta \mapsto \ell(f_\theta(x), y)$ is $L$-Lipschitz for any $x$ and $y$, and the prior $\pi$ is a centered Gaussian: $\pi = \mathcal{N}(0, \sigma^2 I_d)$ where $I_d$ is the $d \times d$ identity matrix.

Let us, as in the previous example, study first the Gibbs posterior, by an application of Corollary 2.3. With probability at least $1 - \varepsilon$,

$$
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\rho \in \Pi(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi) + \log \frac{1}{\varepsilon}}{\lambda} \right].
$$

Once again, the right-hand side is an infimum over all possible probability distributions $\rho$, but it is easier to restrict to Gaussian distributions here. So:

$$
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\rho = \mathcal{N}(m, s^2 I_d)} \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi) + \log \frac{1}{\varepsilon}}{\lambda} \right]. \quad (2.8)
$$

Indeed, it is well known that, for $\rho = \mathcal{N}(m, s^2 I_d)$ and $\pi = \mathcal{N}(0, \sigma^2 I_d)$,

$$
KL(\rho\|\pi) = \frac{\|m\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{s^2}{\sigma^2} + \log \frac{\sigma^2}{s^2} - 1 \right].
$$

Moreover, the risk $r$ inherits the Lipschitz property of the loss, that is, for any $(\theta, \vartheta) \in \Theta^2$, $r(\theta) \leq r(\vartheta) + L\|\theta - \vartheta\|$. So, for $\rho = \mathcal{N}(m, s^2 I_d)$,

$$
\mathbb{E}_{\theta \sim \rho}[r(\theta)] \leq r(m) + L\mathbb{E}_{\theta \sim \rho}[\|\theta - m\|] \leq r(m) + L\sqrt{\mathbb{E}_{\theta \sim \rho}[\|\theta - m\|^2]} \text{ by Jensen’s inequality} = r(m) + Ls\sqrt{d}.
$$

Plugging this into (2.8) gives:

$$
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{m \in \mathbb{R}^d, s > 0} \left[ r(m) + Ls\sqrt{d} + \frac{\lambda C^2}{8n} + \frac{\|m\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{s^2}{\sigma^2} + \log \frac{\sigma^2}{s^2} - 1 \right] + \log \frac{1}{\varepsilon} \right].
$$
It is possible to minimize the bound completely in $s$, but for now, we will just consider the choice $s = \sigma / \sqrt{n}$, which gives:

\[
\mathbb{E}_{\theta \sim \tilde{\rho}_\lambda}[R(\theta)] \leq \inf_{m \in \mathbb{R}^d} \left[ r(m) + L\sigma \sqrt{\frac{d}{n}} + \frac{\lambda C^2}{8n} + \frac{\|m\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{1}{n} - 1 + \log(n) \right] + \log \frac{1}{\varepsilon} \right] \]

It is not possible to optimize the bound with respect to $\lambda$ as the optimal value would depend on $m$, however, a way to understand the bound (by making it worse!) is to restrict the infimum on $m$ to $\|m\| \leq B$ for some $B > 0$. Then we have:

\[
\mathbb{E}_{\theta \sim \tilde{\rho}_\lambda}[R(\theta)] \leq \inf_{m: \|m\| \leq B} \left[ r(m) + L\sigma \sqrt{\frac{d}{n}} + \frac{\lambda C^2}{8n} + \frac{\|B\|^2}{2\sigma^2} + \frac{d}{2} \log(n) + \log \frac{1}{\varepsilon} \right].
\]

In this case, we see that the optimal $\lambda$ is

\[
\lambda = \frac{1}{C} \sqrt{8n \left( \frac{\|B\|^2}{2\sigma^2} + \frac{d}{2} \log(n) + \log \frac{1}{\varepsilon} \right)}
\]

which gives:

\[
\mathbb{E}_{\theta \sim \tilde{\rho}_\lambda}[R(\theta)] \leq \inf_{m: \|m\| \leq B} \left[ r(m) + L\sigma \sqrt{\frac{d}{n}} + C \sqrt{\frac{\|B\|^2}{2\sigma^2} + \frac{d}{2} \log(n) + \log \frac{1}{\varepsilon}} \right].
\]

Note that our choice of $\lambda$ might look a bit weird, as it depends on the confidence level $\varepsilon$. This can be avoided by taking:

\[
\lambda = \frac{1}{C} \sqrt{8n \left( \frac{\|B\|^2}{2\sigma^2} + \frac{d}{2} \log(n) \right)}
\]

instead (check what bound you obtain by doing so!).

Finally, as in the previous example, we can also start from the statement of Theorem 2.1 with probability at least $1 - \varepsilon$,

\[
\forall \rho \in \mathcal{P} (\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon} \lambda}{\lambda},
\]

and restrict here $\rho$ to the set of Gaussian distributions $\mathcal{N}(m, s^2 I_d)$. This leads to the definition of a new data-dependent probability measure, $\tilde{\rho}_\lambda = \mathcal{N}(\tilde{m}, \tilde{s}^2 I_d)$ where

\[
(\tilde{m}, \tilde{s}) = \arg \min_{m \in \mathbb{R}^d, s > 0} \mathbb{E}_{\theta \sim \mathcal{N}(m, s^2 I_d)}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{\|m\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{e^2}{s^2} + \log \frac{s^2}{e^2} - 1 \right] + \log \frac{1}{\varepsilon} \lambda.
\]
While the Gibbs posterior \( \hat{\rho}_\lambda \) can be quite a complicated object, one simply has to solve this minimization problem to get \( \hat{\rho}_\lambda \). The probability \( \tilde{\rho}_\lambda \) is actually a special case of what is called a variational approximation of \( \hat{\rho}_\lambda \). Variational approximations are very popular in statistics and machine learning, and were indeed analyzed through PAC-Bayes bounds [8, 204]. We will come back to this in Section 6. For now, following the same computations, and using the same choice of \( \lambda \) as for \( \hat{\rho}_\lambda \), we obtain the same bound:

\[
\mathbb{E}_{\theta \sim \tilde{\rho}_\lambda}[R(\theta)] \leq \inf_{m : \|m\| \leq B} r(m) + L \sigma \sqrt{\frac{d}{n}} + C \sqrt{\frac{\|H\|^2}{2\sigma^2} + \frac{d}{2} \log(n) + \log \frac{1}{\varepsilon}}.
\]

**Example 2.3 (Model aggregation, model selection)** In the case where we have many sets of predictors, say \( \Theta_1, \ldots, \Theta_M \), equipped with priors \( \pi_1, \ldots, \pi_M \) respectively, it is possible to define a prior on \( \Theta = \bigcup_{j=1}^M \Theta_j \). For the sake of simplicity, assume that the \( \Theta_j \)'s are disjoint, and let \( p = (p(1), \ldots, p(M)) \) be a probability distribution on \( \{1, \ldots, M\} \). We simply put:

\[
\pi = \sum_{j=1}^M p(j) \pi_j.
\]

The minimization of the bound in Theorem 2.1 leads to the Gibbs posterior \( \hat{\rho}_\lambda \) that will put mass on all the \( \Theta_j \) in general, so this is a model aggregation procedure in the spirit of [135]. On the other hand, we can also restrict the minimization in the PAC-Bayes bound to distributions that would charge only one of the models, that is, to \( \rho \in \mathcal{P}(\Theta_1) \cup \cdots \cup \mathcal{P}(\Theta_M) \). Theorem 2.1 becomes:

\[
P_S \left( \forall j \in \{1, \ldots, M\}, \forall \rho \in \mathcal{P}(\Theta_j), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \right.
\]

\[
\leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi_j) + \log \frac{1}{p(j)}}{\lambda} \geq 1 - \varepsilon,
\]

that is

\[
P_S \left( \forall j \in \{1, \ldots, M\}, \forall \rho \in \mathcal{P}(\Theta_j), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \right.
\]

\[
\leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi_j) + \log \frac{1}{\rho(j)} + \log \frac{1}{\varepsilon}}{\lambda} \geq 1 - \varepsilon.
\]

Thus, we can propose the following procedure:

- first, we build the Gibbs posterior for each model \( j \),

\[
\hat{\rho}_\lambda^{(j)}(d\theta) = \frac{e^{-\lambda r(\theta) \pi_j(d\theta)}}{\int_{\Theta_j} e^{-\lambda r(\theta) \pi_j(d\theta)}},
\]
• then, model selection:

\[
\hat{j} = \text{argmin}_{1 \leq j \leq M} \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_j} [r(\theta)] + \frac{KL(\hat{\rho}_j \| \pi_j) + \log \frac{1}{p(\hat{j})}}{\lambda} \right\}.
\]

The obtained \(\hat{j}\) satisfies:

\[
\mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_j} [R(\theta)] \leq \min_{1 \leq j \leq M} \inf_{\rho \in \mathcal{P}(\Theta_j)} \left\{ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{KL(\rho \| \pi_j) + \log \frac{1}{p(\rho)} + \log \frac{1}{\epsilon}}{\lambda} \right\} \right) \geq 1 - \epsilon.
\]

2.1.4 The choice of \(\lambda\)

As discussed earlier, it is in general not possible to optimize the right-hand side of the PAC-Bayes equality with respect to \(\lambda\). For example, in 2.5, the optimal value of \(\lambda\) could depend on \(\rho\), which is not allowed by Theorem 2.1. In the previous examples, we have seen that in some situations, if one is lucky enough, the optimal \(\lambda\) actually does not depend on \(\rho\), but we still need a procedure for the general case.

A natural idea is to propose a finite grid \(\Lambda \subset (0, +\infty)\) and to minimize over this grid, which can be justified by a union bound argument.

**Theorem 2.4** Let \(\Lambda \subset (0, +\infty)\) be a finite set. For any \(\epsilon \in (0, 1)\),

\[
\mathbb{P}_S \left( \forall \rho \in \mathcal{P}(\Theta), \forall \lambda \in \Lambda, \mathbb{E}_{\theta \sim \rho} [R(\theta)] \leq \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{\text{card}(\Lambda)}{\epsilon}}{\lambda} \right) \geq 1 - \epsilon.
\]

**Proof.** Fix \(\lambda \in \Lambda\), and then follow the proof of Theorem 2.1 until (2.3):

\[
\mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n}} \right] \leq 1.
\]

Sum over \(\lambda \in \Lambda\) to get:

\[
\sum_{\lambda \in \Lambda} \mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n}} \right] \leq \text{card}(\Lambda)
\]

and so

\[
\mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta), \lambda \in \Lambda} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n}} \right] \leq \text{card}(\Lambda).
\]

The end of the proof is as for Theorem 2.1, we start with Chernoff bound. Fix \(s > 0\),

\[
\mathbb{P}_S \left[ \sup_{\rho \in \mathcal{P}(\Theta), \lambda \in \Lambda} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} > s \right]
\]
\[ \leq \mathbb{E}_\mathcal{S} \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta), \lambda \in \Lambda} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} \right] e^{-s} \leq \text{card}(\Lambda) e^{-s}. \]

Solve \( \text{card}(\Lambda) e^{-s} = \varepsilon \), that is, put \( s = \log(\text{card}(\Lambda) / \varepsilon) \) to get

\[ \mathbb{P}_\mathcal{S} \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} > \log \frac{\text{card}(\Lambda)}{\varepsilon} \right] \leq \varepsilon. \]

Rearranging terms gives:

\[ \mathbb{P}_\mathcal{S} \left[ \exists \rho \in \mathcal{P}(\Theta), \exists \lambda \in \Lambda, \mathbb{E}_{\theta \sim \rho} [R(\theta)] > \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \text{card}(\Lambda)}{\lambda} \right] \leq \varepsilon. \]

Take the complement to get the statement of the theorem. □

This leads to the following procedure. First, we remind that, for a fixed \( \lambda \), the minimizer of the bound is \( \hat{\rho}_\lambda = \pi - \lambda r \).

Then, we put:

\[ \hat{\rho} = \hat{\rho}_\lambda \text{ where} \]

\[ \hat{\lambda} = \arg \min_{\lambda \in \Lambda} \left\{ \mathbb{E}_{\theta \sim \pi - \lambda r} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\pi - \lambda r \| \pi) + \log \text{card}(\Lambda)}{\lambda} \right\}. \quad (2.9) \]

We have immediately the following result.

**Corollary 2.5** Define \( \hat{\rho} \) as in (2.9), for any \( \varepsilon \in (0, 1) \) we have

\[ \mathbb{P}_\mathcal{S} \left( \mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta), \lambda \in \Lambda} \left[ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \text{card}(\Lambda)}{\lambda} \right] \right) \geq 1 - \varepsilon. \]

We could for example propose an arithmetic grid \( \Lambda = \{1, 2, \ldots, n\} \). The bound in Corollary 2.5 becomes:

\[ \mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta), \lambda \in \Lambda} \left[ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{\varepsilon}{\lambda}}{\lambda} \right]. \]

It is also possible to transform the optimization on a discrete grid by an optimization on a continuous grid. Indeed, for any \( \lambda \in [1, n] \), we simply apply the bound to the integer part of \( \lambda, \lfloor \lambda \rfloor \), and remark that we can upper bound \( \lfloor \lambda \rfloor \leq \lambda \) and \( 1 / \lfloor \lambda \rfloor \leq 1 / (\lambda - 1) \). So the bound becomes:

\[ \mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta), \lambda \in [1, n]} \left[ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{\varepsilon}{\lambda}}{\lambda - 1} \right]. \]

The arithmetic grid is not the best choice, though: the \( \log(n) \) term can be improved. In order to optimize hyperparameters in PAC-Bayes bounds, Langford and Caruana [113] used
a geometric grid $\Lambda = \{e^k, k \in \mathbb{N}\} \cap [1, n]$, the same choice was used later by Catoni \[41, 43\].

Using such a bound in Corollary 2.5 we get

$$
\mathbb{E}_{\theta \sim \hat{\rho}}[R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{\log n}{\lambda/\varepsilon}}{\lambda/\varepsilon} \right].
$$

We conclude this discussion on the choice of $\lambda$ by mentioning that there are other PAC-Bayes bounds, for example McAllester’s bound \[135\], where there is no parameter $\lambda$ to optimize. We will study these bounds in Section 3.

2.2 PAC-Bayes bound on aggregation of predictors

In the introduction, right after Definition 1.1, I promised that PAC-Bayes bound would allow to control

- the risk of randomized predictors,
- the expected risk of randomized predictors,
- the risk of averaged predictors.

But so far, we only focused on the expected risk of randomized predictors (the second bullet point). In this subsection, we provide some bounds on averaged predictors, and in the next one, we will focus on the risk of randomized predictors.

We start by a very simple remark. When the loss function $u \mapsto \ell(u, y)$ is convex for any $y$, then the risk $R(\theta) = R(f_{\theta})$ is a convex function of $f_{\theta}$. Thus, Jensen’s inequality ensures:

$$
\mathbb{E}_{\theta \sim \rho}[R(f_{\theta})] \geq R(\mathbb{E}_{\theta \sim \rho}[f_{\theta}]).
$$

Plugging this into Corollary 2.3 gives immediately the following result.

**Corollary 2.6** Assume that $\forall y \in \mathcal{Y}$, $u \mapsto \ell(u, y)$ is convex. Define

$$
\hat{f}_{\hat{\rho}, \lambda}(\cdot) = \mathbb{E}_{\theta \sim \hat{\rho}, \lambda}[f_{\theta}(\cdot)]
$$

For any $\lambda > 0$, for any $\varepsilon \in (0, 1)$,

$$
\mathbb{P}_S \left( R(\hat{f}_{\hat{\rho}, \lambda}) \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\lambda/\varepsilon}}{\lambda/\varepsilon} \right] \right) \geq 1 - \varepsilon.
$$

That is, in the case of a convex loss function, like the quadratic loss or the hinge loss, PAC-Bayes bounds also provide bounds on the risk of aggregated predictors.

It is also possible to study $R(\mathbb{E}_{\theta \sim \rho}[f_{\theta}]) - \mathbb{E}_{\theta \sim \rho}[R(f_{\theta})]$ under other assumptions. For example, we can use the Lipschitz property as in Example 2.2. In the case of the quadratic loss, we have $R(\mathbb{E}_{\theta \sim \rho}[f_{\theta}]) - \mathbb{E}_{\theta \sim \rho}[R(f_{\theta})] = \mathbb{E}_{X} \left[ \text{Var}_{\theta \sim \rho}(f_{\theta}(X)) \right]$, this fact was used by Audibert to provide tight bounds on $R(\mathbb{E}_{\theta \sim \rho}[f_{\theta}])$, see page 22 in \[15\]. A similar idea was rediscovered later in classification to upper bound $R(\mathbb{E}_{\theta \sim \rho}[f_{\theta}]) - \mathbb{E}_{\theta \sim \rho}[R(f_{\theta})]$ by a variance term in \[81, 132\].
2.3 PAC-Bayes bound on a single draw from the posterior

**Theorem 2.7** For any $\lambda > 0$, for any $\varepsilon \in (0, 1)$, for any data-dependent probability measure $\tilde{\rho}$,

$$
\mathbb{P}_{S} \mathbb{P}_{\tilde{\theta} \sim \tilde{\rho}} \left( R(\tilde{\theta}) \leq r(\tilde{\theta}) + \frac{\lambda C^2}{8n} + \frac{\log \frac{d\pi}{d\tilde{\rho}}(\tilde{\theta}) + \log \frac{1}{\varepsilon}}{\lambda} \right) \geq 1 - \varepsilon.
$$

This bound simply says that if you draw $\tilde{\theta}$ from, for example, the Gibbs posterior $\hat{\rho}_\lambda$ (defined in (2.4)), you have the bound on $R(\tilde{\theta})$ that holds with large probability simultaneously on the drawing of the sample and of $\tilde{\theta}$.

**Proof.** Once again, we follow the proof of Theorem 2.1 until (2.2):

$$
\mathbb{E}_{\tilde{\rho}} \mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}} \left[ e^{\lambda[R(\theta)-r(\theta)]]} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}.
$$

Now, for any nonnegative function $h$,

$$
\mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}}[h(\theta)] = \int h(\theta)\pi(d\theta)
$$

$$
\geq \int \left\{ \frac{d\tilde{\rho}}{d\pi}(\theta) > 0 \right\} h(\theta)\pi(d\theta)
$$

$$
= \int \left\{ \frac{d\tilde{\rho}}{d\pi}(\theta) > 0 \right\} h(\theta)\frac{d\pi}{d\tilde{\rho}}(\theta)\tilde{\rho}(d\theta)
$$

$$
= \mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}} \left[ h(\theta)e^{-\log \frac{d\tilde{\rho}}{d\pi}(\theta)} \right]
$$

and in particular:

$$
\mathbb{E}_{S} \mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}} \left[ e^{\lambda[R(\theta)-r(\theta)]-\log \frac{d\tilde{\rho}}{d\pi}(\theta)} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}.
$$

I could go through the proof until the end, but I think that you now guess that it’s essentially Chernoff bound + rearrangement of the terms. □

2.4 Bound in expectation

We end this section by one more variant of the initial PAC-Bayes bound in Theorem 2.1, a bound in expectation with respect to the sample.

**Theorem 2.8** For any $\lambda > 0$, for any data-dependent probability measure $\tilde{\rho}$,

$$
\mathbb{E}_{S} \mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}}[R(\theta)] \leq \mathbb{E}_{S} \mathbb{E}_{\tilde{\theta} \sim \tilde{\rho}} \left[ r(\theta) + \frac{\lambda C^2}{8n} + \frac{KL(\tilde{\rho}\|\pi)}{\lambda} \right].
$$

In particular, for $\tilde{\rho} = \hat{\rho}_\lambda$ the Gibbs posterior,

$$
\mathbb{E}_{S} \mathbb{E}_{\tilde{\theta} \sim \hat{\rho}_\lambda}[R(\theta)] \leq \mathbb{E}_{S} \left[ \inf_{\rho \in \mathcal{P}(\theta)} \mathbb{E}_{\tilde{\theta} \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho\|\pi)}{\lambda} \right].
$$
These bounds in expectation are very convenient tools from a pedagogical point of view. Indeed, in Section 4 we will study oracle PAC-Bayes inequalities. While it is possible to derive oracle PAC-Bayes bounds both in expectation and with large probability, the one in expectation are much simpler to derive, and much shorter. Thus, I will mostly provide PAC-Bayes oracle bounds in expectation in Section 4, and refer the reader to [41, 43] for the corresponding bounds in probability.

Note that as the bound does not hold with large probability, as the previous bounds, it is no longer a PAC bound in the proper sense: Probably Approximately Correct. Once, I was attending a talk by Tsybakov where he presented some result from his paper with Dalalyan [64] that can also be interpreted as a “PAC-Bayes bound in expectation”, and he suggested the more appropriate EAC-Bayes acronym: Expectedly Approximately Correct (their paper is briefly discussed in Subsection 6.4 below). I don’t think this term was often reused since then. I also found recently in [85] the acronym MAC-Bayes: Mean Approximately Correct. In order to avoid any confusion I will stick to “PAC-Bayes bound in expectation”, but I like EAC and MAC! Early examples of PAC-Bayes bounds in expectation can be found in [1, 43, 107, 64].

Proof. Once again, the beginning of the proof is the same as for Theorem 2.1 until (2.3):

\[ E_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n}} \right] \leq 1. \]

This time, use Jensen’s inequality to send the expectation with respect to the sample inside the exponential function:

\[ e^{E_S \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} \right]} \leq 1, \]

that is,

\[ E_S \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} \right] \leq 0. \]

In particular,

\[ E_S \left[ \lambda \mathbb{E}_{\theta \sim \rho} [R(\theta) - r(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} \right] \leq 0. \]

Rearrange terms. \( \square \)

### 2.5 Applications of empirical PAC-Bayes bounds

The original PAC-Bayes bounds were stated for classification [134] and it became soon clear that many results could be extended to any bounded loss, thus covering for example bounded regression (we discuss in Section 5 how to get rid of the boundedness assumption). Thus, some papers are written in no specific setting, with a generic loss, that can cover classification, regression, or density estimation (this is the case, among others, of Chapter 1 of my PhD thesis [1] and the corresponding paper [2] where I studied a generalization of Catoni’s results of [43] to unbounded losses).
However, some empirical PAC-Bayes bounds were also developed or applied to specific models, sometimes taking advantage of some specificities of the model. We mention for example:

- ranking/scoring [160],
- density estimation [96],
- multiple testing [35] is tackled with related techniques,
- deep learning. Even though deep networks are trained for classification or regression, the application of PAC-Bayes bounds to deep learning is not straightforward. We discuss this in Section 3 based on [70] and more recent references.
- unsupervised learning, including clustering [177, 13], representation learning [149, 148], variational autoencoders [54].

Note that this list is non-exhaustive, and that many more applications are presented in Section 4 (more precisely, in Subsection 4.3).

3 Tight and non-vacuous PAC-Bayes bounds

3.1 Why is there a race to the tighter PAC-Bayes bound?

Let us start with a numerical application of the PAC-Bayes bounds we met in Section 2. First, assume we are in the classification setting with the 0-1 loss, so that $C = 1$. We are given a small set of classifiers, say $M = 100$, and that on the test set with size $n = 1000$, the best of these classifiers has an empirical risk $r_n = 0.26$. Let us use the bound in (2.7), that I remind here:

$$\mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq \inf_{\theta \in \Theta} r(\theta) + C \sqrt{\frac{\log M}{2n}} \right) \geq 1 - \varepsilon.$$ 

With $\varepsilon = 0.05$ this bound is:

$$\mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq 0.26 + 1. \sqrt{\frac{\log 100}{2 \times 1000}} \right) \geq 0.95.$$ 

So the classification risk using the Gibbs posterior is smaller than 0.322 with probability at least 95%.

Let us now switch to a more problematic example. We consider a very simple binary neural network, given by the following formula, for $x \in \mathbb{R}^d$, and where $\varphi$ is a nonlinear activation function (e.g. $\varphi(x) = \max(x, 0)$):

$$f_w(x) = 1 \left[ \sum_{i=1}^{M} w_i^{(2)} \varphi \left( \sum_{j=1}^{d} w_{j,i}^{(1)} x_j \right) \geq 0 \right]$$
and the weights $w^{(1)}_{j,i}$ and $w^{(2)}_i$ are all in $\{-1,+1\}$ for $1 \leq j \leq d$ and $1 \leq i \leq M$. Define $	heta = (w^{(1)}_{1,1}, w^{(1)}_{1,2}, \ldots, w^{(1)}_{d,M}, w^{(2)}_1, \ldots, w^{(2)}_M)$. Note that the set of all possible such networks has cardinality $2^{M(d+1)}$. Consider inputs that are $100 \times 100$ greyscale images, that is, $x \in [0,1]^d$ with $d = 10,000$, and a sample size $n = 10,000$. With neural networks, it is often the case that a perfect classification of the training sample is possible, that is, there is a $\theta$ such that $r(\theta) = 0$.

Even for a moderate number of units such as $M = 100$, this leads to the PAC-Bayes bound (with $\varepsilon = 0.05$):

$$
P_S \left( \mathbb{E}_{\theta \sim \rho_\lambda} [R(\theta)] \leq 1 - \sqrt{\frac{\log \frac{21,000 \cdot 100}{0.05} \cdot 2 \times 10,000}{13.58}} \right) \geq 0.95.
$$

So the classification risk using the Gibbs posterior is smaller than 13.58 with probability at least 95%. Which is not informative at all, because we already know that the classification risk is smaller than 1. Such a bound is usually referred to as a vacuous bound, because it does not bring any information at all. You can try to improve the bound by increasing the dataset. But you can check that even $n = 1,000,000$ still leads to a vacuous bound with this network.

Various opinions on these vacuous bounds are possible:

- “theory is useless. I don’t know why I would care about generalization guarantees, neural networks work in practice.” This opinion is lazy: it’s just a good excuse not to have to think about generalization guarantees. I will assume that since you are reading this tutorial, this is not your opinion.

- “vacuous bounds are certainly better than no bounds at all!” This opinion is cynical, it can be rephrased as “better have a theory that doesn’t work than no theory at all: at least we can claim we have a theory, and some people might even believe us”. But the theory just says nothing.

- “let’s get back to work, and improve the bounds”. Since the publication of the first PAC-Bayes bounds already mentioned [179, 134, 135], many variants were proven. One can try to test which one is the best in a given setting, try to improve the priors, try to refine the bound in many ways... In 2017, Dziugaite and Roy [70] obtained non-vacuous (even though not really tight yet) PAC-Bayes bounds for practical neural networks (since then, tighter bounds were obtained by these authors and by others). This is a remarkable achievement, and this also made PAC-Bayes theory immediately more popular than it was ever before.

Let’s begin this section with a review of some popular PAC-Bayes bounds: Subsection 3.2. We will then explain which bound, and which improvements led to tight generalization bounds for deep learning 3.3. In particular, we will focus on a very important approach to improve the bounds: data-dependent priors.
3.2 A few PAC-Bayes bounds

Note that the original works on PAC-Bayes focused only on classification with the 0-1 loss. So, for the whole Subsection 3.2 we assume that $\ell$ is the 0-1 loss function. Remember it means that $R$ and $r$ take value in $[0, 1]$ (so $C = 1$ in this subsection).

3.2.1 McAllester’s bound [134] and Maurer’s improved bound [133]

As the original paper by McAllester [134] focused on finite or denumerable sets $\Theta$, let us start with the first bound for a general $\Theta$, in [135].

Theorem 3.1 (Theorem 1 in [135]) For any $\varepsilon > 0$,

$$
\mathbb{P}_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \sqrt{KL(\rho\|\pi) + \log \frac{1}{\varepsilon} + \frac{5}{2} \log(n) + \frac{8}{n^2}} \right] \geq 1 - \varepsilon.
$$

Compared to Theorem 2.1, note that there is no parameter $\lambda$ here to optimize. On the other hand, one can no longer use 2.2 to minimize the right-hand side. A way to solve this problem is to make the parameter $\lambda$ appear artificially using the inequality $\sqrt{ab} \leq a\lambda/2 + b/(2\lambda)$ for any $\lambda > 0$:

$$
\mathbb{P}_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \right.
\leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \inf_{\lambda > 0} \left\{ \frac{\lambda}{4n - 2} + \frac{KL(\rho\|\pi) + \log \frac{2}{\varepsilon} + \frac{1}{2} \log(n)}{2\lambda} \right\} \geq 1 - \varepsilon. \tag{3.1}
$$

On the other hand, the prize to pay for an optimization with respect to $\lambda$ in Theorem 2.4 was a $\log(n)$ term, that is already in Maurer’s bound, for an arithmetic grid, and a $\log \log(n)$ term when using a geometric grid. So, asymptotically in $n$, Theorem 2.4 with a geometric grid will always lead to better results than Theorem 3.1. On the other hand, the constants in Theorem 3.1 are smaller, so the bound can be better for small sample sizes (a point that should not be neglected for tight certificates in practice!).

It is possible to minimize the right-hand side in (3.1) with respect to $\rho$, and this will lead to a Gibbs posterior: $\hat{\rho} = \pi_{-2\lambda r}$. It is also possible to minimize it with respect to $\lambda$, but the minimization in $\lambda$ when $\rho$ itself depends on $\lambda$ is a bit more tricky. We want to mention on this problem the more recent paper [188]. The authors proved a bound that is easier to minimize simultaneously in $\lambda$ and $\rho$.

3.2.2 Catoni’s bound (another one) [43]

Theorem 2.1 was based on Catoni’s preprint [41]. Catoni’s monograph [43] provide many other bounds.
Theorem 3.2 (Theorem 1.2.6 of [43]) Define, for $a > 0$, the function of $p \in (0, 1)$

$$\Phi_\alpha(p) = \frac{- \log \left(1 - p [1 - e^{-a}] \right)}{a}.$$

Then, for any $\lambda > 0$, for any $\epsilon > 0$,

$$\mathbb{P}_S \left\{ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \Phi_\alpha^{-1}(\lambda) \left[ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + KL(\rho \| \pi) + \log \frac{1}{\lambda} \frac{1}{2}\epsilon \right] \right\} \geq 1 - \epsilon. \quad (3.2)$$

Actually, we have

$$\Phi_\alpha^{-1}(q) = \frac{1 - e^{-aq}}{1 - e^{-a}},$$

and inequalities on the exponential function lead to the following consequence of Theorem 3.2

$$\mathbb{P}_S \left\{ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \frac{\lambda}{n} \mathbb{E}_{\theta \sim \rho}[r(\theta)] + KL(\rho \| \pi) + \log \frac{1}{\lambda} \frac{1}{2}\epsilon \right\} \geq 1 - \epsilon. \quad (3.3)$$

3.2.3 Seeger’s bound [173] and Maurer’s bound [133]

Let us now propose a completely different bound. This bound is very central in the PAC-Bayesian theory: we will see that many other bounds can be derived from this one. A first version was proven by Seeger and Langford [114, 173] and is often referred to as Seeger’s bound. The bound was slightly improved by Maurer [133], so we will here provide Maurer’s version of Seeger’s bound.

Let $B_p$ denote the probability distribution of a Bernoulli random variable $V$ with parameter $p$, that is, $\mathbb{P}(V = 1) = p = 1 - \mathbb{P}(V = 0)$. Then we have:

$$KL(B_p \| B_q) = p \log \frac{p}{q} + (1 - p) \log \frac{1 - p}{1 - q} =: kl(p|q),$$

which can be used as a metric on $[0, 1]$.

Theorem 3.3 (Theorem 5 in [133]) For any $\epsilon > 0$,

$$\mathbb{P}_S \left\{ \forall \rho \in \mathcal{P}(\Theta), kl(\mathbb{E}_{\theta \sim \rho}[r(\theta)] \| \mathbb{E}_{\theta \sim \rho}[R(\theta)]) \leq \frac{KL(\rho \| \pi) + \log 2\sqrt{\pi}}{n} \right\} \geq 1 - \epsilon.$$

Under this form, the bound is not very explicit, so we will derive a few of its consequences. Following Seeger [173], we define:

$$kl^{-1}(q | b) = \sup\{p \in [0, 1] : kl(p|q) \leq b\}.$$
Then the bound becomes:

\[
P_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq kl^{-1} \left( \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{KL(\rho \| \pi) + \log \frac{2\sqrt{n}}{\varepsilon}}{n} \right) \right] \geq 1 - \varepsilon.
\]

So we can deduce more explicit bounds from Seeger’s bound simply by providing explicit bounds on the function \(kl^{-1}\). In Section 3 in [156], it is mentioned that Theorem 3.1 can be recovered in such a way, with improved constants, using Pinsker’s inequality \(kl(p|q) \geq 2(p - q)^2\). We will now see other consequences of Seeger’s bound.

### 3.2.4 Tolstikhin and Seldin’s bound [189]

A better upper bound of \(kl\) is used by Tolstikhin and Seldin [189]:

\[ kl^{-1}(q|b) \leq q + \sqrt{2qb} + 2b. \]

Plugging this in Seeger’s inequality leads to Tolstikhin and Seldin’s bound [189].

**Theorem 3.4 ((3) in [189])** For any \(\varepsilon > 0\),

\[
P_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \sqrt{2\mathbb{E}_{\theta \sim \rho}[r(\theta)] \frac{KL(\rho \| \pi) + \log \frac{2\sqrt{n}}{\varepsilon}}{2n} + 2 \frac{KL(\rho \| \pi) + \log \frac{2\sqrt{n}}{\varepsilon}}{2n}} \right] \geq 1 - \varepsilon.
\]

Note the amazing thing with this bound: while its dependence with respect to \(n\) is in general \(1/\sqrt{n}\), as all the PAC-Bayes bounds seen so far, the dependence drops to \(1/n\) if \(\mathbb{E}_{\theta \sim \rho}[r(\theta)] = 0\). This was actually not a surprise, because a similar phenomenon is known for the ERM [194].

More generally, we will see in Section 4 a general assumption that characterizes the best possible learning rate in classification problems. And as a special case, the noiseless case indeed leads to rates in \(1/n\). One more word about Theorem 3.4 the authors acknowledge that the majoration of \(kl^{-1}\) they use was actually suggested by McAllester [136]. They also prove a completely new bound, the so-called PAC-Bayes-Empirical-Bernstein inequality, that even improve on Theorem 3.4 but we will not provide it here. Let us summarize the important take home message from Theorem 3.4:

- in general, empirical PAC-Bayes bounds are in \(1/\sqrt{n}\),

- in the noiseless case \(\mathbb{E}_{\theta \sim \rho}[r(\theta)] = 0\), it is possible to have a bound in \(1/n\), on the condition that one uses the right PAC-Bayes inequality, for example Theorem 3.4, Theorem 3.3, or the PAC-Bayes-Empirical-Bernstein inequality.

This is very important for the application of these bounds to neural networks, as deep networks usually allow to classify the training data perfectly.
3.2.5 Thieman, Igel, Wintenberger and Seldin’s bound

According to [156], it can also be recovered as a consequence of Seeger’s bound, using
\[ \sqrt{ab} \leq \frac{\lambda a}{2} + \frac{b}{2\lambda}. \]

It appears to be extremely tight and convenient in practice (see Subsection 3.3 below).

**Theorem 3.5** For any \( \varepsilon > 0 \), for any \( \lambda \in (0, 2) \),
\[
P_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \frac{\mathbb{E}_{\theta \sim \rho}[r(\theta)]}{1 - \frac{\lambda}{2}} + \frac{KL(\rho\|\pi) + \log \frac{2\sqrt{n}}{\varepsilon}}{n\lambda \left(1 - \frac{\lambda}{2}\right)} \right] \geq 1 - \varepsilon.
\]

Here again, we observe the \( 1/n \) regime when \( \mathbb{E}_{\theta \sim \rho}[r(\theta)] = 0 \) (for example for \( \lambda = 1 \)).

3.2.6 A bound by Germain, Lacasse, Laviolette and Marchand [82]

Let us conclude this discussion by a nice generalization of Theorem 3.3 by Germain, Lacasse, Laviolette and Marchand [82].

**Theorem 3.6 (Theorem 2.1 in [82])** Let \( \mathcal{D} : [0, 1]^2 \to \mathbb{R} \) be any convex function. For any \( \varepsilon > 0 \),
\[
P_S \left[ \forall \rho \in \mathcal{P}(\Theta), \mathcal{D}(\mathbb{E}_{\theta \sim \rho}[r(\theta)], \mathbb{E}_{\theta \sim \rho}[R(\theta)]) \leq \frac{KL(\rho\|\pi) + \log \frac{e^{\mathcal{D}(r(\theta), R(\theta))}}{n}}{n \varepsilon} \right] \geq 1 - \varepsilon.
\]

As discussed by the authors, \( \mathcal{D}(p, q) = kl(p\|q) \) leads to Theorem 3.3, and \( \mathcal{D}(p, q) = -\log[1 - p(1 - e^{-C})] - Cq \) leads to Catoni’s bound given in Theorem 3.2 above. This leads to a natural question: is there a function \( \mathcal{D} \) that will lead to a strict improvement of Theorem 3.3? The question is investigated in [74]. Overall, it seems that no function \( \mathcal{D} \) will lead to a bound that will be smaller, in expectation, than Theorem 3.3 up to the \( \log(2\sqrt{n}) \) term.

Theorem 3.6 has another important advantage that will be discussed in Section 5.

More bounds are known, but it’s not possible to mention all, so I apologize if I didn’t cite a bound you like, or your bound. Some other variants will be discussed later, in Section 6, in particular: bounds for unbounded losses \( \ell \), bounds for non i.i.d data, and also some bounds where the KL divergence \( KL(\rho\|\pi) \) is replaced by another divergence.

3.3 Tight generalization error bounds for deep learning

3.3.1 A milestone: non vacuous generalization error bounds for deep networks by Dziugaite and Roy [70]

PAC-Bayes bounds were applied to (shallow) neural networks as early as in 2002 by Langford and Caruana [113]. We also applied them with O. Wintenberger to prove that shallow networks can consistently predict time series [10]. McAllester proposed an application of
PAC-Bayes bounds to dropout, a tool used for training neural networks, in his tutorial [137]. But none of these techniques seemed to lead to tight bounds for deep networks... until 2017, when Dziugaite and Roy [70] obtained the first non-vacuous generalization error bounds for deep networks on the MNIST dataset based on Theorem 3.3 (Seeger’s bound). Since then, there was a regain of interest in PAC-Bayes bounds to obtain the tightest possible certificates.

At first sight, [70] is an application of Seeger’s bound to a deep neural network, but many important ideas and refinements were used to lead to a non vacuous bound (according to the authors, some of them being original, some of them based on ideas from earlier works like [113]). Let us describe here briefly these ingredients, the reader should of course read the paper for more details and insightful explanations:

- the posterior is constrained to be Gaussian (similar to the above “non-exact minimization of the bound” in Subsection 2.1.3): \( \rho_{w,s^2} = \mathcal{N}(w,s^2I_d) \). Thus, the PAC-Bayes bound only has to be minimized with respect to the parameter \((w,s^2)\), which allows to use an optimization algorithm to minimize the bound (the authors mention that fitting Gaussian distributions to neural networks was already proposed in [97] based on the MDL principle, which will be discussed in Section 6).

- the choice of an adequate upper bound on \( \text{kl}^{-1} \) in Seeger’s bound in order to make the bound easier to minimize.

- Seeger’s bound holds for the 0 – 1 loss, but Dziugaite and Roy upper bounded the empirical risk by a convex, Lipschitz upper bound in order to make the bound easier to minimize (note that this is a standard approach in classification):

\[
E_{\theta \sim \rho}[r(\theta)] = E_{\theta \sim \rho} \left[ \frac{1}{n} \sum_{i=1}^{n} 1(f_\theta(X_i) \neq Y_i) \right] \leq E_{\theta \sim \rho} \left[ \frac{1}{n} \sum_{i=1}^{n} \log \frac{1 + e^{-Y_i f_\theta(X_i)}}{\log 2} \right].
\]

- the use of the Stochastic Gradient Algorithm (SGD) to minimize the bound (up to our knowledge, the first use of SGD to minimize a PAC-Bayes bound was [82] for linear classification). Of course, this is standard in deep learning, but there is a crucial observation that SGD tends to converge to flat minima. This is very important, because around a flat minima \( w^* \), we have \( r(w) \simeq r(w^*) \) and thus \( E_{\theta \sim \rho_{w,s^2}}[r(\theta)] \simeq r(\theta^*) \) even for quite large values of \( s^2 \). On the other hand, for a sharp minimum \( w^* \), \( E_{\theta \sim \rho_{w,s^2}}[r(\theta)] \simeq r(\theta^*) \) only for very small values of \( s^2 \) which tends to make the PAC-Bayes bound larger (see Example 2.2 above).

- finally, the authors used a data dependent prior: \( \mathcal{N}(w_0,\sigma^2I) \), where \( \sigma^2 \) is chosen to minimize the bound (this is justified in theory thanks via a union bound argument as in Subsection 2.1.4 above). The mean \( w_0 \) is not optimized, but the authors point out that the choice \( w_0 = 0 \) is not good and they actually draw \( w_0 \) randomly, as is usually done in non-Bayesian approaches to initialize SGD.
On the MNIST data set, the authors obtain empirical bounds between 0.16 and 0.22, thus, non vacuous. The classification performance of their posterior is actually around 0.03, so they conclude that there is still room for improvement. Indeed, since then, a wide range of papers, from very theoretical to very computational, studied PAC-Bayes bounds for deep networks [125, 147, 208, 118, 195, 112, 190, 31, 75, 156, 185, 157, 57, 104, 181]. We discuss recent results from [156] below, but first, we want to discuss in detail one of the most important ingredients above: the data-dependent prior.

### 3.3.2 Bounds with data-dependent priors

To use data in order to improve the prior is actually an old idea: we found such approaches in [173, 41, 42, 206, 43, 154, 120, 70, 71, 69]. Note that the original PAC-Bayes bounds do not allow to take a data-dependent prior. Thus, some additional work is required to make this possible (e.g., the union bound on $\sigma^2$ in [70] discussed above). Note that the very first occurrence of this idea is due to Seeger in [173]. Seeger proposed to split the sample in two parts. The first part is used to define $\Theta$ and the prior $\pi$, and the PAC-Bayes bound is applied on the second part of the sample (that is, conditionally on the first part). Seeger used this technique to study the generalization of Gaussian processes. Later Catoni used it [41] to prove generalization error bounds on compression schemes. We will here describe in detail two other approaches: first, Catoni’s “localization” technique, because it will also be important in Sections 4 and 6, and then a recent bound from [71].

First, let us discuss the intuition leading to Catoni’s method. We discussed in Section 2, just after (2.6), that the bound is tighter for parameters $\theta$ for which $\pi(\theta)$ is large, and less tight for parameters $\theta$ for which $\pi(\theta)$ is small: in the finite case, we remind that the Kullback-Leibler divergence led to a term in $\log(1/\pi(\theta))$ in the bound. Based on this idea, we might want to construct a prior $\pi$ that gives a large weight to the relevant parameters, that is, to parameters such that $R(\theta)$ is small. This exactly corresponds to $\pi - \beta R$ for some $\beta > 0$, where $\pi - \beta R$ is given by

$$
\frac{d\pi - \beta R}{d\pi}(\theta) = \frac{e^{-\beta R(\theta)}}{E_{\theta \sim \pi}[e^{-\beta R(\theta)}]}.
$$

This choice is not data-dependent, and thus allowed by theory. But in practice, it cannot be used, because $R(\theta) = E_{(X,Y) \sim P}[\ell(f_\theta(X), Y)]$ is of course unknown (still, we use the prior $\pi - \beta R$ in Section 4 below, in theoretical bounds that are not meant to be evaluated on the data). For empirical bounds, Catoni proved that $KL(\rho, \pi - \beta R)$ can be upper bounded, with large probability, by $KL(\rho, \pi - \xi r)$ for $\xi = \beta/(\lambda + g(\lambda/n)\lambda^2/n)$, plus some additional terms ($g$ being Bernstein’s function, that will be defined in Section 4). Plugging this result into Theorem 2.1, he obtains the following “localized bound” (Lemma 6.2 in [41]):

$$
P_S \left( \forall \rho, E_{\theta \sim \rho}[R(\theta)] \leq \frac{(1 - \xi)E_{\theta \sim \rho}[r(\theta)] + KL(\rho \| \pi - \xi r) + (1 + \xi) \log \frac{2}{\varepsilon}}{(1 - \xi)\lambda + (1 + \xi) g \left( \frac{\lambda}{n} \right) \frac{\lambda^2}{n}} \right) \geq 1 - \varepsilon
$$

which means that we are allowed to use $\pi - \xi r$, that is data-dependent, as a prior! This bound is a little scary at first, because it depends on many parameters. We will provide simpler
localized bounds in Section 4 in order to explain their benefits (in particular, it allows to remove some log(n) terms in the rates of convergences). For now, simply accept that the bound is usually tighter than Theorem 2.1, but in practice, we have to calibrate both λ and β, which makes it a little more difficult to use. Thus, I am not aware of any application of this technique to neural networks, but we will show in Section 4 that, used on PAC-Bayes oracle inequalities, it leads to an improvement of the order of the bound. I would advise the reader to read [41] or [43] to learn many consequences of this localization technique, see also the paper by Tong Zhang [206].

Dziugaite and Roy proved in [71] that any data-dependent prior can actually be used in Seeger’s bound, under a differential privacy condition, at the cost of a small modification of the bound.

**Theorem 3.7 (Theorem 4.2 in [71])** Assume we have a function Π that maps any sample s = ((x_1, y_1),..., (x_n, y_n)) into a prior π = Π(S). Remind that the data is S = ((X_1, Y_1),..., (X_n, Y_n)) and define, for any i ∈ {1,...,n}, S_i ′ a copy of S where (X_i, Y_i) is replaced by (X'_i, Y'_i) ∼ P independent from S. Assume that Π is such that, for any i ∈ {1,...,n}, for any B, \[ P_S(Π(S) ∈ B) ≤ e^η P_{S_i ′}(Π(S_i ′) ∈ B) \]

(we say that Π is η-differentially private). Then, for any ε > 0,

\[ P_S\left( ∀ρ, kl(\mathbb{E}_{θ∼ρ}[R(θ)] | \mathbb{E}_{θ∼ρ}[r(θ)]) ≤ \frac{KL(ρ||Π(S)) + \log \frac{4√n}{ε}}{n} + \frac{η^2}{2} + η\sqrt{\frac{\log \frac{4}{ε}}{2n}} \right) ≥ 1 - ε. \]

For more on PAC-Bayes and differential privacy, see [152, 22].

### 3.3.3 Comparison of the bounds and tight certificates for neural networks [156]

Recently, Pérez-Ortiz, Rivasplata, Shawe-Taylor and Szepesvári [156] trained neural networks in the spirit of [70] on the MNIST and CIFAR-10 datasets. They use the PAC-Bayes with backprop algorithm from [167]. They obtain state of the art test errors (0.02 on MNIST), and improve the generalization bounds of [70] (0.0279 on MNIST, a very tight bound!). The paper is very interesting even beyond neural networks, as the authors compare numerically many of the PAC-Bayes bounds listed above. Note that consistently on the experiments, the bound from [188] is the tightest bound (Theorem 3.5 above). We do not list here all the nice tricks used by the authors to obtain tighter bounds, but we strongly recommend the reader who wants to work on this topic to read this paper in detail. An important point to note that is, in order to avoid to check that a given data-dependent prior is η-differentially private, they tune the priors through a simple sample-splitting, very much in the spirit of [173]: the prior is built on a first part of the sample, and the PAC-Bayes bound is evaluated (and minimized) on the second part of the sample.

For another comparison of the bounds, in the small-data regime, see [74].
4 PAC-Bayes oracle inequalities and fast rates

As explained in Subsection 1.4 above, empirical PAC-Bayes bounds are very useful as they provide a numerical certificate for randomized estimators or aggregated predictors. But we also mention another type of PAC-Bayes bounds: oracle PAC-Bayes bounds. In this section, we provide examples of PAC-Bayes oracle bounds. Interestingly, the first PAC-Bayes oracle inequality we state below is actually derived from empirical PAC-Bayes inequality.

4.1 From empirical inequalities to oracle inequalities

As for empirical bounds, we can prove oracle bounds in expectation, and in probability. We will first present a simple version of each. Later, we will focus on bounds in expectation for the sake of simplicity: these bounds are much shorter to prove. But all the results we will prove in expectation have counterparts in probability, that the reader can find in [41, 43] for example.

4.1.1 Bound in expectation

We start by a reminder of (the second claim of) Theorem 2.8: for any \( \lambda > 0 \),

\[
\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \mathbb{E}_{\mathcal{S}} \left[ \inf_{\rho \in \mathcal{P}(\theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho||\pi)}{\lambda} \right\} \right],
\]

where we remind that \( \hat{\rho}_\lambda \) is the Gibbs posterior (defined in (2.4)). From there, we have the following:

\[
\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \mathbb{E}_{\mathcal{S}} \left[ \inf_{\rho \in \mathcal{P}(\theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho||\pi)}{\lambda} \right\} \right] \\
\leq \inf_{\rho \in \mathcal{P}(\theta)} \mathbb{E}_{\mathcal{S}} \left\{ \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho||\pi)}{\lambda} \right\} \\
= \inf_{\rho \in \mathcal{P}(\theta)} \left[ \mathbb{E}_{\theta \sim \rho} \{ \mathbb{E}_{S}[r(\theta)] \} + \frac{\lambda C^2}{8n} + \frac{KL(\rho||\pi)}{\lambda} \right]
\]

where we used Fubini theorem in the last equality. But, by definition, \( \mathbb{E}_{S}[r(\theta)] = R(\theta) \). Thus, we obtain the following theorem.

**Theorem 4.1** For any \( \lambda > 0 \),

\[
\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[R(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho||\pi)}{\lambda} \right\}.
\]
Example 4.1 (Finite case, continued) In the context of Example 2.1, that is, card(Θ) = M < +∞, with λ = \sqrt{8n/(C^2 \log(M))} and π uniform on Θ we obtain the bound:

\[ E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq \inf_{\theta \in \Theta} R(\theta) + \frac{C \sqrt{\log(M)}}{2n}. \]

Note that this time, we don’t have a numerical certificate on \( E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \). But on the other hand, we know that our predictions are the best theoretically possible, up to at most \( C \sqrt{\log(M)/2n} \) (such an information is not provided by an empirical PAC-Bayes inequality).

A natural question after Example 4.1 is: is it possible to improve the rate 1/\( \sqrt{n} \)? Is it possible to ensure that our predictions are the best possible up to a smaller term? The answer is “no” in the worst case, but “yes” quite often. These faster rates will be the object of the following subsections. But first, as promised, we provide an oracle PAC-Bayes bound in probability.

4.1.2 Bound in probability

As we derived the oracle inequality in expectation of Theorem 4.1 from the empirical inequality in expectation of Theorem 2.8, we will now use the empirical inequality in probability from Theorem 2.1 to prove the following oracle inequality in probability. Note, however, that the proof is slightly more complicated, and that this leads to different (and worse) constants within the bound.

**Theorem 4.2** For any \( \lambda > 0 \), for any \( \varepsilon \in (0, 1) \),

\[ \mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [R(\theta)] + \frac{\lambda C^2}{4n} + \frac{2 KL(\rho || \pi) + \log \frac{2}{\varepsilon}}{\lambda} \right\} \right) \geq 1 - \varepsilon. \]

**Proof:** first, apply Theorem 2.1 to \( \rho = \hat{\rho}_\lambda \), as was done to obtain Corollary 2.3. This gives:

\[ \mathbb{P}_S \left( \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho || \pi) + \log \frac{1}{\lambda}}{\lambda} \right] \right) \geq 1 - \varepsilon. \] (4.1)

We will now prove the reverse inequality, that is:

\[ \mathbb{P}_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho} [r(\theta)] \leq \mathbb{E}_{\theta \sim \rho} [R(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho || \pi) + \log \frac{1}{\lambda}}{\lambda} \right) \geq 1 - \varepsilon. \] (4.2)

Note that the proof of (4.2) is exactly similar to the proof of Theorem 2.1 except that we replace \( U_i \) by \( -U_i \). So, the reader who is comfortable enough with this kind of proof can skip this part, or prove (4.2) as an exercise. Still, we provide a complete proof for the sake of completeness. Fix \( \theta \in \Theta \) and apply Hoeffding’s inequality with \( U_i = \ell_i(\theta) - \mathbb{E}[\ell_i(\theta)] \), and \( t = \lambda/n \):

\[ \mathbb{E}_S \left[ e^{\lambda [r(\theta) - R(\theta)]} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}. \]
Integrate this bound with respect to $\pi$:

$$\mathbb{E}_{\theta \sim \pi} \mathbb{E}_S \left[ e^{\lambda [r(\theta) - R(\theta)]} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}.$$

Apply Fubini:

$$\mathbb{E}_S \mathbb{E}_{\theta \sim \pi} \left[ e^{\lambda [r(\theta) - R(\theta)]} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}$$

and then Donsker and Varadhan’s variational formula (Lemma 2.2):

$$\mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [r(\theta) - R(\theta)] - KL(\rho \| \pi)} \right] \leq e^{\frac{\lambda^2 C^2}{8n}}.$$

Rearranging terms:

$$\mathbb{E}_S \left[ e^{\sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [r(\theta) - R(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n}} \right] \leq 1.$$

Chernoff bound gives:

$$\mathbb{P}_S \left[ \sup_{\rho \in \mathcal{P}(\Theta)} \lambda \mathbb{E}_{\theta \sim \rho} [r(\theta) - R(\theta)] - KL(\rho \| \pi) - \frac{\lambda^2 C^2}{8n} > \log \frac{1}{\varepsilon} \right] \leq \varepsilon.$$

Rearranging terms:

$$\mathbb{P}_S \left[ \exists \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho} [r(\theta)] > \mathbb{E}_{\theta \sim \rho} [R(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon}}{\lambda} \right] \leq \varepsilon.$$

Take the complement to get (4.2).

Consider now 4.1 and 4.1. A union bound gives:

$$\mathbb{P}_S \left( \bigcup_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{\lambda C^2}{8n} + \frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon}}{\lambda} \right\} \right) \geq 1 - 2\varepsilon \quad (4.3)$$

Plug the upper bound on $\mathbb{E}_{\theta \sim \rho} [r(\theta)]$ from the second line into the first line to get:

$$\mathbb{P}_S \left( \mathbb{E}_{\theta \sim \rho} [R(\theta)] \leq \inf_{\rho \in \mathcal{P}(\Theta)} \mathbb{E}_{\theta \sim \rho} [r(\theta)] + 2\frac{\lambda C^2}{8n} + 2\frac{KL(\rho \| \pi) + \log \frac{1}{\varepsilon}}{\lambda} \right) \geq 1 - 2\varepsilon \quad (4.4)$$

Just replace $\varepsilon$ by $\varepsilon/2$ to get the statement of the theorem. □

### 4.2 Bernstein assumption and fast rates

As mentioned above, the rate $1/\sqrt{n}$ that we have obtained in almost PAC-Bayes bounds seen so far is not always the tightest possible. Actually, this can be seen in Tolstikhin and Seldin’s bound (Theorem 3.4): in this bound, it is clear that if there is a $\rho$ such that $\mathbb{E}_{\theta \sim \rho} [r(\theta)] = 0$, then the bound becomes in $1/n$.

It appears that rates in $1/n$ are possible in a more general setting, under an assumption often referred to as Bernstein assumption. This is well known for (“non Bayesian”) PAC bounds [25], but it seems to me that this fact seems to be ignored by some papers on PAC-Bayes.
Definition 4.1  From now, we will let $\theta^*$ denote a minimizer of $R$ when it exists:

$$R(\theta^*) = \min_{\theta \in \Theta} R(\theta).$$

When such a $\theta^*$ exists, and when there is a constant $K$ such that, for any $\theta \in \Theta$,

$$\mathbb{E}_S \{[\ell_i(\theta) - \ell_i(\theta^*)]^2\} \leq K[R(\theta) - R(\theta^*)]$$

we say that Bernstein assumption is satisfied with constant $K$.

PAC-Bayes oracle bounds based using explicitly Bernstein’s assumption can be found in [41, 206, 43]. Before we state such a bound, let us explore situations where this assumption is satisfied.

Example 4.2 (Classification without noise) Consider classification with the $0 − 1$ loss: $\ell_i(\theta) = 1(Y_i \neq f_\theta(X_i))$. If the optimal classifier does not make any mistake, that is, if $R(\theta^*) = 0$, we have necessarily $\ell_i(\theta^*) = 0$ almost surely. We refer to this situation as “classification without noise”. In this case, we have obviously:

$$\mathbb{E}_S \{[\ell_i(\theta) - \ell_i(\theta^*)]^2\} = \mathbb{E}_S \{[1(Y_i \neq f_\theta(X_i)) - 0]^2\} = \mathbb{E}_S \{1(Y_i \neq f_\theta(X_i))\} = R(\theta) = 1.$$

so Bernstein assumption is satisfied with constant $K = 1$. Actually, this can be extended beyond the $0 − 1$ loss: for any loss $\ell$ with values in $[0, C]$, if $R(\theta^*) = 0$, then Bernstein assumption is satisfied with constant $K = C$.

Example 4.3 (Mammen and Tsybakov margin assumption) More generally, still in classification with the $0 − 1$ loss, consider the function $\eta(x) = \mathbb{E}_S(Y_i|X_i = x)$. Mammen and Tsybakov [131] proved that, if $|\eta(X_i) - 1/2| \geq \tau$ almost surely for some $\tau > 0$, then Bernstein assumption holds for some $K$ that depends on $\tau$. The case $\tau = 1/2$ leads back to the previous example (noiseless classification), but $0 < \tau < 1/2$ is a more general assumption.

Example 4.4 (Lipschitz and strongly convex loss function) Assume that $\Theta$ is convex. Let $\rho_i$ be a function $\Theta^2 \to \mathbb{R}_+$ and assume that $\ell_i$ is satisfies:

$$\forall \theta \in \Theta, \frac{\ell_i(\theta) + \ell_i(\theta^*)}{2} - \ell_i\left(\frac{\theta + \theta^*}{2}\right) \geq \frac{1}{8\alpha}\rho_i^2(\theta, \theta^*) \tag{4.5}$$

and

$$\forall \theta \in \Theta, |\ell_i(\theta) - \ell_i(\theta^*)| \leq L\rho_i(\theta, \theta^*). \tag{4.6}$$
In the special case where \( \rho(\theta, \theta') \) is a metric on \( \Theta \), (4.5) will be satisfied if the loss is \( \alpha \)-strongly convex in \( \theta \), and (4.6) will be satisfied if the loss is \( L \)-Lipschitz in \( \theta \) with respect to \( \rho_i \). Note that \( \rho_i \) may depend implicitly of \( (X_i, Y_i) \) (as does \( \ell_i(\theta) \)).

Bartlett, Jordan and McAuliffe [22] proved that, under these assumptions, Bernstein assumption is satisfied with constant \( K = 4L^2\alpha \). The proof is so luminous than I cannot resist giving it:

\[
\mathbb{E}_S \{ [\ell_i(\theta) - \ell_i(\theta^*)]^2 \} \leq L^2 \mathbb{E}_S \{ \rho_i(\theta, \theta^*)^2 \} \quad \text{by (4.6)}
\leq 8L^2 \alpha \mathbb{E}_S \left\{ \frac{\ell_i(\theta) + \ell_i(\theta^*)}{2} - \ell_i \left( \frac{\theta + \theta^*}{2} \right) \right\} \quad \text{by (4.5)}
\leq 8L^2 \alpha \left[ \frac{R(\theta) + R(\theta^*)}{2} - R \left( \frac{\theta + \theta^*}{2} \right) \right]
\]

where in the last equation, we used \( R(\theta^*) \leq R \left( \frac{\theta + \theta^*}{2} \right) \). Thus:

\[
\mathbb{E}_S \{ [\ell_i(\theta) - \ell_i(\theta^*)]^2 \} \leq 4L^2 \alpha [R(\theta) - R(\theta^*)]
\]

and thus Bernstein assumption is satisfied with constant \( K = 4L^2\alpha \).

**Theorem 4.3** Assume Bernstein assumption is satisfied with some constant \( K > 0 \). Take \( \lambda = n / \max(2K, C) \), we have:

\[
\mathbb{E}_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta) - R(\theta^*)] \leq 2 \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [R(\theta)] - R(\theta^*) + \frac{\max(2K, C)KL(\rho\|\pi)}{n} \right\}.
\]

We postpone the applications to Subsection 4.3 but we just want to explain now how the bound is used in general: we only have to find a \( \rho \) such that \( \mathbb{E}_{\theta \sim \rho} [R(\theta)] \approx R(\theta^*) \) to obtain:

\[
\mathbb{E}_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq R(\theta^*) + \frac{2\max(2K, C)KL(\rho\|\pi)}{n},
\]

hence the rate in \( 1/n \). We will provide more accurate statements in Subsection 4.3.

**Remark 4.1** There is a more general version of Bernstein condition: where there are constants \( K > 0 \) and \( \kappa \in [1, +\infty) \) such that, for any \( \theta \in \Theta \),

\[
\mathbb{E}_S \{ [\ell_i(\theta) - \ell_i(\theta^*)]^2 \} \leq K [R(\theta) - R(\theta^*)]^\frac{1}{\kappa}
\]

we say that Bernstein assumption is satisfied with constants \( (K, \kappa) \). We will not study the general case here, but we mention that, in the case of classification, this can also be interpreted in terms of margin [131]. Under such an assumption, some oracle PAC-Bayes inequalities for classification are proven in [133] that leads to rates in \( 1/n^{\kappa/(2\kappa - 1)} \). These results were extended to general losses in [2]. These rates are known to be optimal in the minimax sense [110]. Finally, for recent results and a comparison of all the type of conditions leading to fast rates in learning theory (including situations with unbounded losses), see [88].
Remark 4.2 All the PAC-Bayes inequalities seen before Section 4 were empirical. They lead to rates in $1/\sqrt{n}$, except in the noiseless case $R(\theta^*) = 0$ where we obtained the rate $1/n$. In this section, we built:

- an oracle inequality with rates $1/\sqrt{n}$. Note that an empirical inequality was part of the proof.
- an oracle inequality with rate $1/n$. It is important to note that the proof we will propose does not involve any empirical inequality. Similarly, the proofs in [43, 2] for the rates in $1/n^{\kappa/(2\kappa-1)}$ do not involve empirical inequalities. (The reader might remark that (4.8) in the proof below is almost an empirical inequality, but the term $r(\theta^*)$ is not empirical as it depends on the unknown $\theta^*$).

It is thus natural to ask: are there empirical inequalities leading to rates in $1/n$ or $1/n^{\kappa/(2\kappa-1)}$ beyond the noiseless case? The answer is “yes” for “non-Bayesian” PAC bounds [20], based on Rademacher complexity: there are empirical bounds on $R(\hat{\theta}_{\text{ERM}}) - R(\theta^*)$. In the PAC-Bayesian case, it is a little more complicated (unless one uses the bound to control the risk of a non-Bayesian estimator such as the ERM). This is discussed in [85].

Before stating the proof of Theorem 4.3, we remind a very classical result. For a proof, see Theorem 5.2.1 in [42], or [138].

Lemma 4.4 (Bernstein’s inequality) Let $g$ denote the Bernstein function defined by $g(0) = 1$ and, for $x \neq 0$,

$$g(x) = \frac{e^x - 1 - x}{x^2}.$$ 

Let $U_1, \ldots, U_n$ be i.i.d random variables such that $\mathbb{E}(U_i)$ is well defined and $U_i - \mathbb{E}(U_i) \leq C$ almost surely for some $C \in \mathbb{R}$. Then

$$\mathbb{E}\left(e^{t \sum_{i=1}^n [U_i - \mathbb{E}(U_i)]}\right) \leq e^{\theta(Ct)n^2 \text{Var}(U_i)}.$$ 

Proof of Theorem 4.3: We follow the general proof scheme for PAC-Bayes bounds, with some important differences. First, Hoeffding’s inequality will be replaced by Bernstein’s inequality. But another very important point is to use the inequality on the “relative losses” $\ell_i(\theta^*) - \ell_i(\theta)$ instead of the loss $\ell_i(\theta)$ (for this reason, these bounds are sometimes called “relative bounds”). This is to ensure that we can use Bernstein condition. So, let us fix $\theta \in \Theta$ and apply Lemma 4.4 to $U_i = \ell_i(\theta^*) - \ell_i(\theta)$. Note that $\mathbb{E}(U_i) = R(\theta^*) - R(\theta)$, thus we obtain:

$$\mathbb{E}\mathcal{S}\left(e^{tn[R(\theta) - R(\theta^*) - r(\theta) + r(\theta^*])}\right) \leq e^{\theta(Ct)n^2 \text{Var}_S(U_i)}.$$ 

Put $\lambda = tn$ and note that

$$\text{Var}_S(U_i) \leq \mathbb{E}_S(U_i^2) = \mathbb{E}_S\left\{[\ell_i(\theta^*) - \ell_i(\theta)]^2\right\}$$

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\[ \leq K [R(\theta) - R(\theta^*)] \]

thanks to Bernstein condition. Thus:

\[ \mathbb{E}_\mathcal{S} \left( e^{\lambda [R(\theta) - R(\theta^*) - r(\theta) + r(\theta^*)]} \right) \leq e^{\lambda^{\frac{\lambda^2 C}{n} K [R(\theta) - R(\theta^*)]}}. \]

Rearranging terms:

\[ \mathbb{E}_\mathcal{S} \left( e^{\lambda \left[ 1 - N g \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} \right] [R(\theta) - R(\theta^*)] - r(\theta) + r(\theta^*)} \right) \leq 1. \] (4.7)

The next steps are now routine: we integrate \( \theta \) with respect to \( \pi \) and apply Fubini and Donsker and Varadhan’s variational formula to get:

\[ \mathbb{E}_\mathcal{S} \left( e^{\lambda \sup_{\rho \in \mathcal{P}(\Theta)} \left\{ [1 - N g \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n}] [R(\theta) - R(\theta^*)] - r(\theta) + r(\theta^*) \right\} - KL(\rho || \pi) \right) \leq 1. \]

In particular for \( \rho = \hat{\rho}_\lambda \) the Gibbs posterior of \( \Theta \), we have, using Jensen and rearranging terms:

\[ \left[ 1 - K g \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} \right] \left\{ \mathbb{E}_\mathcal{S}\mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \right\} \leq \mathbb{E}_\mathcal{S} \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [r(\theta)] - r(\theta^*) + \frac{KL(\hat{\rho}_\lambda || \pi)}{\lambda} \right\}. \]

From now we assume that \( \lambda \) is such that \( \left[ 1 - K g \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} \right] > 0 \), thus

\[ \mathbb{E}_\mathcal{S} \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \leq \frac{\mathbb{E}_\mathcal{S} \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} \left[ r(\theta) \right] - r(\theta^*) + \frac{KL(\hat{\rho}_\lambda || \pi)}{\lambda} \right\}}{1 - K g \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n}}. \]

In particular, take \( \lambda = n / \max(2K, C) \). We can check that: \( \lambda \leq n/(2K) \Rightarrow K\lambda/n \leq 1/2 \) and \( \lambda \leq n/C \Rightarrow g(\lambda C/n) \leq g(1) \leq 1 \), so

\[ Kg \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} \leq \frac{1}{2} \]

and thus

\[ \mathbb{E}_\mathcal{S} \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \leq 2 \mathbb{E}_\mathcal{S} \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} \left[ r(\theta) \right] - r(\theta^*) + \frac{KL(\hat{\rho}_\lambda || \pi)}{\lambda} \right\}. \] (4.8)

Finally, note that \( \hat{\rho}_\lambda \) minimizes the quantity in the expectation in the right-hand side, this can be rewritten:

\[ \mathbb{E}_\mathcal{S} \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \leq 2 \mathbb{E}_\mathcal{S} \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [r(\theta)] - r(\theta^*) + \frac{\max(2K, C) K L(\rho || \pi)}{n} \right\} \]

\[ \leq 2 \inf_{\rho \in \mathcal{P}(\Theta)} \mathbb{E}_\mathcal{S} \left\{ \mathbb{E}_{\theta \sim \rho} [r(\theta)] - r(\theta^*) + \frac{\max(2K, C) K L(\rho || \pi)}{n} \right\} \]

\[ = 2 \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [R(\theta)] - R(\theta^*) + \frac{\max(2K, C) K L(\rho || \pi)}{n} \right\}. \] □
4.3 Applications of Theorem 4.3

Example 4.5 (Finite set of predictors) We come back to the setting of Example 2.1: \( \text{card}(\Theta) = M \) and \( \pi \) is the uniform distribution over \( \Theta \). Assuming Bernstein condition holds with constant \( K \), we apply Theorem 4.3 and, as was done in Example 2.1, we restrict the supremum to \( \rho \in \{ \delta_\theta, \theta \in \Theta \} \). This gives, for \( \lambda = n/\max(2K, C) \),

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) 
\leq 2 \inf_{\theta \in \Theta} \left\{ R(\theta) - R(\theta^*) + \frac{\max(2K, C) \log(M)}{n} \right\}.
\]

In particular, for \( \theta = \theta^* \), this becomes:

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + \frac{2 \max(2K, C) \log(M)}{n}.
\]

Note that the rate \( \sqrt{\log(M)/n} \) from Example 2.1 becomes \( \log(M)/n \) under Bernstein assumption.

Example 4.6 (Lipschitz loss and Gaussian priors) We now tackle the setting of Example 2.2 under Bernstein assumption with constant \( K \). Let us remind that \( \Theta = \mathbb{R}^d \), \( \theta \mapsto \ell(f_\theta(x), y) \) is \( L \)-Lipschitz for any \( (x, y) \), and \( \pi = N(0, \sigma^2 I_d) \). We apply Theorem 4.3, for \( \lambda = n/\max(2K, C) \):

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + 2 \inf_{m \in \mathbb{R}^d, s > 0} \left[ R(\theta) - R(\theta^*) + \frac{\max(2K, C) KL(\rho||\pi)}{n} \right].
\]

Following the same derivations as in Example 2.2, with \( m = \theta^* \),

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + 2 \inf_{s > 0} \left[ Ls \sqrt{d} + \frac{\max(2K, C) \left\{ \frac{\|\theta^*\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{\sigma^2}{s^2} + \log \frac{\sigma^2}{s^2} - 1 \right] \right\}}{n} \right].
\]

Here again, we would seek for the exact optimizer in \( s \), but for example \( s = \sqrt{d/n} \) we obtain:

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + 2 \left[ \frac{Ld}{n} + \frac{\max(2K, C) \left\{ \frac{\|\theta^*\|^2}{2\sigma^2} + \frac{d}{2} \left[ \frac{\sigma^2}{n\sigma^2} + \log \frac{\sigma^2 n^2}{d} \right] \right\}}{n} \right]
\]

that is

\[
E_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + \frac{2d}{n} \left[ \frac{\max(2K, C)}{2} \log \left( \frac{\sigma^2 n^2}{d} \right) + L + \frac{d}{2n\sigma^2} \right] + \frac{\max(2K, C) \|\theta^*\|^2}{n\sigma^2}
\]

\[
= R(\theta^*) + O \left( \frac{d \log(n)}{n} \right).
\]
Example 4.7 (Lipschitz loss and Uniform priors) We propose a variant of the previous example, with a different prior. We still assume Bernstein assumption with constant $K$, $\theta \mapsto \ell(f_\theta(x), y)$ is $L$-Lipschitz for any $(x, y)$, and this time $\Theta = \{\theta \in \mathbb{R}^d : \|\theta\| \leq B\}$ and $\pi$ is uniform on $\Theta$. We apply Theorem 4.3 with $\lambda = n/\max(2K,C)$ and restrict the infimum to $\rho = U(\theta_0, s)$ the uniform distribution on $\{\theta : \|\theta - \theta_0\| \leq s\} = B(\theta_0, s)$. We obtain:

$$\mathbb{E}_S\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + 2 \inf_{\rho = U(\theta_0, s) \in \mathbb{R}^d, s > 0} \left[R(\theta) - R(\theta^*) + \frac{\max(2K,C)KL(\rho\|\pi)}{n}\right].$$

For any $s > 0$, there exists $\theta_0 \in \Theta$ such that $\theta^* \in B(\theta_0, s) \subset \Theta$ and we have:

$$\mathbb{E}_{\theta \sim U(\theta_0, s)}[R(\theta) - R(\theta^*)] \leq Ls,$$

so

$$\mathbb{E}_S\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + 2 \inf_{s > 0} \left[Ls + \frac{\max(2K,C)d\log\left(\frac{B}{s}\right)}{n}\right].$$

The minimum of the right-hand side is exactly reached for $s = \frac{\max(2K,C)d}{Ln}$ and we obtain, for $n$ large enough (in order to ensure that $s \leq B$):

$$\mathbb{E}_S\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] \leq R(\theta^*) + \frac{2\max(2K,C)d\log\left(\frac{eBLn}{\max(2K,C)}\right)}{n}.$$
• matrix regression \[183, 3, 62, 61\].

• matrix completion: continuous case \[129, 127, 128\] and binary case \[58\]; more generally
tensor completion in \[184\] is tackled with related techniques.

• quantum tomography \[130\].

• deep learning \[51\].

• unsupervised learning: estimation of the Gram matrix for PCA \[45, 207\] and kernel-
PCA \[84, 91\],

• ...

4.4 Dimension and rate of convergence

Let us recap the examples of Sections 2 and 4 seen so far. In each case, we were able to prove a result of the form:

\[
\mathbb{E}_S \mathbb{E}_{\theta \sim \rho} \left[ R(\theta) \right] \leq R(\theta^*) + \text{rate}_n(\pi) \quad \text{where} \quad \text{rate}_n(\pi) \xrightarrow{n \to \infty} 0
\]

for an adequate choice of \( \lambda > 0 \). The way \( \text{rate}_n(\pi) \) depends on \( \Theta \) characterizes the difficulty of learning predictors in \( \Theta \) when using the prior \( \pi \): it is similar to other approaches in learning theory, where the learning rate depends on the “complexity of \( \Theta \)”. More precisely (we remind that all the results seen so far are for a bounded loss function):

• when \( \Theta \) is finite and \( \pi \) is uniform, \( \text{rate}_n(\pi) \) is in \( \sqrt{\log(M)/n} \) in general, and in \( \log(M)/n \) under Bernstein condition.

• when \( \Theta = \mathbb{R}^d \) and \( \pi = \mathcal{N}(0, \sigma^2 I_d) \), \( \text{rate}_n(\pi) \) is in \( \sqrt{\|	heta^*\|^2 + d \log(n)/n} \) in general, and in \( [\|	heta^*\|^2 + d \log(n)]/n \) under Bernstein condition.

• left as an exercise (idea from \[64\]): when \( \Theta = \mathbb{R}^d \) and \( \pi \) is a multivariate Student, \( \text{rate}_n(\pi) \) is in \( \sqrt{\log(\|	heta^*\| + d \log(n))}/n \) in general, and in \( [\log(\|	heta^*\| + d \log(n))] /n \) under Bernstein condition.

• when \( \Theta \) is a compact subset of \( \mathbb{R}^d \) and \( \pi \) is uniform, \( \text{rate}_n(\pi) \) is in \( \sqrt{d \log(n)/n} \) in general, and in \( d \log(n)/n \) under Bernstein condition.

The calculations leading to these results are in Examples \[2.2, 4.6\] and \[4.7\]. A closer look at these examples reveals a common strategy: we assumed conditions ensuring that it is possible to write

\[
\inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} \left[ R(\theta) - R(\theta^*) \right] + \frac{KL(\rho\|\pi)}{\beta} \right] \leq \frac{d}{\beta} \log \left( \frac{\beta}{c} \right) \quad (4.9)
\]

for some constants \( c \) and \( d \) (\( d \) being actually the dimension of the model). Then, we can plug this inequality into Theorem \[4.4\] or when Bernstein assumption is satisfied, into Theorem \[4.3\].
to obtain a rate of convergence. Let us now turn this into a formal statement under Bernstein assumption (the case without Bernstein assumption is left as an exercise to the reader).

**Theorem 4.5** Assume that there are constants \( \beta_0, c_\pi, d_\pi \) such that, for any \( \beta \geq \beta_0 \),

\[
\beta \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [R(\theta) - R(\theta^*)] + \frac{KL(\rho\|\pi)}{\beta} \right] \leq d_\pi \log \left( \frac{\beta}{c_\pi} \right). \tag{4.10}
\]

Under Bernstein condition with constant \( K > 0 \), with \( \lambda = n/\max(2K,C) \), we have as soon as \( \lambda \geq \beta_0 \),

\[
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq R(\theta^*) + \frac{2d_\pi \max(2K,C) \log \left( \frac{n}{c_\pi \max(2K,C)} \right)}{n}.
\]

The proof is direct, by plugging (4.10) into Theorem 4.3 with \( \lambda = \beta \).

We will end this subsection by connecting the assumption in (4.10) to other classical assumptions in Bayesian statistics and machine learning. A first direct remark, based on Lemma 2.2, is that (4.10) is equivalent to

\[
f(\beta) := -\log \mathbb{E}_{\theta \sim \pi} \left\{ e^{-\beta [R(\theta) - R(\theta^*)]} \right\} \leq d_\pi \log \left( \frac{\beta}{c_\pi} \right).
\]

If the inequality was actually an inequality, we would have \( f'(\beta) = d_\pi / \beta \), that is, \( \beta f'(\beta) = d_\pi \). It is direct to check that \( f'(\beta) = \mathbb{E}_{\theta \sim \pi} [R(\theta) - R(\theta^*)] \) (we do it for example in the following proof). This motivated the following definition (Catoni [43]).

**Definition 4.2** We say that Catoni’s dimension assumption is satisfied for dimension \( d_\pi > 0 \) if

\[
\sup_{\beta \geq 0} \beta \mathbb{E}_{\theta \sim \pi} [R(\theta) - R(\theta^*)] = d_\pi.
\]

**Lemma 4.6** Under Catoni’s dimension assumption with dimension \( d_\pi \), for any \( \beta \geq \beta_0 = d_\pi/C \),

\[
-\log \mathbb{E}_{\theta \sim \pi} \left\{ e^{-\beta [R(\theta) - R(\theta^*)]} \right\} \leq d_\pi \log \left( \frac{eC\beta}{d_\pi} \right).
\]

In other words, if Catoni’s dimension assumption is satisfied, then the assumption of Theorem 4.3 given by (4.10) is satisfied with \( c_\pi = d_\pi/(eC) \).

**Proof:** Define

\[
f(\xi) = -\log \mathbb{E}_{\theta \sim \pi} e^{-\xi [R(\theta) - R(\theta^*)]}
\]

for any \( \xi \geq 0 \). First, note that

\[
f(0) = -\log \mathbb{E}_{\theta \sim \pi} e^0 = -\log(1) = 0.
\]

Moreover, we can check that \( f \) is differentiable and that

\[
f'(\xi) = \frac{\mathbb{E}_{\theta \sim \pi} \left\{ [R(\theta) - R(\theta^*)] e^{-\xi [R(\theta) - R(\theta^*)]} \right\}}{\mathbb{E}_{\theta \sim \pi} \left\{ e^{-\xi [R(\theta) - R(\theta^*)]} \right\}}.
\]
\[= \mathbb{E}_{\theta \sim \pi} [R(\theta) - R(\theta^*)] \leq \frac{d_\pi}{\xi} \]

where we used Definition 4.2 for the last inequality. But we also have the (simpler) inequality:

\[
f'(\xi) = \frac{\mathbb{E}_{\theta \sim \pi} \{ [R(\theta) - R(\theta^*)]e^{-\xi[R(\theta) - R(\theta^*)]} \}}{\mathbb{E}_{\theta \sim \pi} \{ e^{-\xi[R(\theta) - R(\theta^*)]} \}} \leq \frac{\mathbb{E}_{\theta \sim \pi} \{ Ce^{-\xi[R(\theta) - R(\theta^*)]} \}}{\mathbb{E}_{\theta \sim \pi} \{ e^{-\xi[R(\theta) - R(\theta^*)]} \}} = C.
\]

Combining both bounds, \(f'(\xi) \leq \min(C, d_\pi/\xi)\). Integrating for \(0 \leq \xi \leq \beta\) gives:

\[
f(\beta) = f(\beta) - f(0) = \int_0^\beta f'(\xi) d\xi \leq \int_0^{d_\pi} C d\xi + \int_0^\beta \frac{d_\pi}{\xi} d\xi = C \frac{d_\pi}{\beta} + d_\pi \log(\beta) - d_\pi \log \left( \frac{d_\pi}{C} \right) = d_\pi \log \left( \frac{eC\beta}{d_\pi} \right). \quad \Box
\]

Another classical condition is as follows.

**Definition 4.3** We say that the prior mass condition is satisfied with constants \(c\) and \(d_\pi\) if there is \(r_0 > 0\) such that, for any \(r \leq r_0\),

\[
\pi\{\theta \in \Theta : R(\theta) - R(\theta^*) \leq r\} \geq \left( \frac{r}{c} \right)^{d_\pi}.
\]

This type of condition is classical to analyze the asymptotics of Bayesian estimators in statistics [83].

**Lemma 4.7** Under the prior mass condition with constants \(c\) and \(d_\pi\), (4.10) is satisfied with \(c_\pi = d_\pi/(ec)\), for any \(\beta \geq \beta_0 = d_\pi/r_0\).

**Proof:** The proof mimics the strategy of Example 4.7, but in a more general setting. We define, for any \(r > 0\), \(\rho_r\) as the restriction of \(\pi\) to \(\{\theta \in \Theta : R(\theta) - R(\theta^*) \leq r\}\). Then,

\[
f(\beta) = \inf_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [R(\theta) - R(\theta^*)] + \frac{KL(\rho||\pi)}{\beta} \right]
\]

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\[ \leq \inf_{r > 0} \left[ \mathbb{E}_{\theta \sim \rho} [R(\theta) - R(\theta^*)] + \frac{KL(\rho_r \| \pi)}{\beta} \right] \]
\[ \leq \inf_{r > 0} \left[ r + \frac{\log \frac{1}{\pi(\{\theta \in \Theta : R(\theta) - R(\theta^*) \leq r \})}}{\beta} \right]. \]

We put \( r = d_\pi/\beta \). Note that as \( \beta \geq d_\pi/r_0 \), \( r \leq r_0 \) and thus
\[ f(\beta) \leq r + \frac{d_\pi \log \frac{c}{\beta}}{\beta} = \frac{d_\pi}{\beta} + \frac{d_\pi}{\beta} \log \left( \frac{c\beta}{d_\pi} \right) = \frac{d_\pi}{\beta} \log \left( \frac{e c \beta}{d_\pi} \right). \] □

### 4.5 Getting rid of the log terms: Catoni’s localization trick

We have seen in Subsection 3.3 Catoni’s idea to replace the prior by \( \pi - \beta R \) for some \( \beta > 0 \), where \( \pi - \beta R \) is given by Definition 4.2. This technique is called “localization” of the bound by Catoni. Used in empirical bounds, this trick can lead to tighter bound. We will study its effect on oracle bounds. Let us start by providing a counterpart of Theorem 4.3 using this trick (with \( \beta = \lambda/4 \)).

**Theorem 4.8** Assume that Bernstein condition holds for some \( K > 0 \), and take \( \lambda = n/\max(2K, C) \). Then
\[ \mathbb{E}_S \{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \} \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ 3\mathbb{E}_{\theta \sim \rho} [R(\theta) - R(\theta^*)] + \frac{4 \max(2K, C) KL(\rho \| \pi - \frac{\lambda}{4} R)}{n} \right\}. \]

Before we give the proof, we will show a striking consequence: the \( \log(n) \) terms in the last bullet point in the list of rates of convergence can be removed:

- when Catoni’s dimension \( d_\pi < \infty \), rate \( \mathcal{R}(\pi) \) is in \( \sqrt{d_\pi/n} \) in general, and in \( d_\pi/n \) under Bernstein condition, *if we use a localized bound.*

Indeed, take \( \rho = \pi - \frac{\lambda}{4} R = \pi - \{n/[4 \max(2K,C)]\} R \) in the right-hand side of Theorem 4.8
\[ \mathbb{E}_S \{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \} \leq 3\mathbb{E}_{\theta \sim \pi - \frac{\lambda}{4} R} [R(\theta) - R(\theta^*)] + \frac{0}{n}. \]

Using Definition 4.2 we obtain the following corollary.

**Corollary 4.9** Assume that Catoni’s dimension condition is satisfied with dimension \( d_\pi > 0 \). Assume that Bernstein condition holds for some \( K > 0 \), and take \( \lambda = n/\max(2K, C) \), then:
\[ \mathbb{E}_S \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] \leq R(\theta^*) + \frac{12d_\pi \max(2K, C)}{n}. \]

We can also briefly detail the consequence of the bound in the finite case.
Example 4.8 (The finite case) When \( \text{card}(\Theta) = M \) is finite and \( \pi \) is uniform on \( \Theta \), Theorem 4.8 applied to \( \rho = \delta_{\theta^*} \) gives:

\[
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \right\} \leq \frac{4 \max(2K, C) KL(\delta_{\theta^*} \parallel \pi - \frac{1}{n})}{n} = \frac{4 \max(2K, C) \log \sum_{\theta \in \Theta} e^{-\frac{1}{n}[R(\theta) - R(\theta^*)]}}{n} = \frac{4 \max(2K, C) \log \sum_{\theta \in \Theta} e^{-\frac{1}{\max(2K, C)}[R(\theta) - R(\theta^*)]}}{n}.
\]

(4.11)

Of course, we have:

\[
\sum_{\theta \in \Theta} e^{-\frac{1}{\max(2K, C)}[R(\theta) - R(\theta^*)]} \leq M
\]

and thus we recover the rate in \( \log(M)/n \):

\[
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \right\} \leq \frac{4 \max(2K, C) \log(M)}{n}.
\]

On the other hand, in some situations, we can do better from (4.11). Fix a threshold \( \tau > 0 \) and define \( m_\tau = \text{card}(\{\theta \in \Theta : R(\theta) - R(\theta^*) \leq \tau\}) \in \{1, \ldots, M\} \). Then we obtain the bound:

\[
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \hat{\rho}_\lambda} [R(\theta)] - R(\theta^*) \right\} \leq \frac{4 \max(2K, C) \log \left( m_\tau + e^{-\frac{m_\tau}{\max(2K, C)} (M - m_\tau)} \right)}{n}
\]

which will be much smaller for large \( n \).

Proof of Theorem 4.8: we follow the proof of Theorem 4.3 until (4.7) that we remind here:

\[
\mathbb{E}_S \left( e^{\lambda \left\{ [1-Kg(\frac{\lambda C}{n}) \frac{1}{n}][R(\theta) - R(\theta^*)] - r(\theta) + r(\theta^*) \right\}} \right) \leq 1.
\]

Now, we integrate this with respect to \( \pi_{-\beta R} \) for some \( \beta > 0 \) and use Fubini:

\[
\mathbb{E}_S \mathbb{E}_{\theta \sim \pi_{-\beta R}} \left( e^{\lambda \left\{ [1-Kg(\frac{\lambda C}{n}) \frac{1}{n}][R(\theta) - R(\theta^*)] - r(\theta) + r(\theta^*) \right\}} \right) \leq 1
\]

and Donsker and Varadhan’s formula:

\[
\mathbb{E}_S \left( e^{\sup_{\rho \in \mathcal{P}(\Theta)} \left\{ \lambda \mathbb{E}_{\theta \sim \rho} \left[ [1-Kg(\frac{\lambda C}{n}) \frac{1}{n}][R(\theta) - R(\theta^*)] - r(\theta) + r(\theta^*) \right] - KL(\rho \parallel \pi_{-\beta R}) \right\}} \right) \leq 1.
\]

At this point, we write explicitly

\[
KL(\rho \parallel \pi_{-\beta R}) = \mathbb{E}_{\theta \sim \rho} \left[ \log \left( \frac{d\rho}{d\pi_{-\beta R}}(\theta) \right) \right] = \mathbb{E}_{\theta \sim \rho} \left[ \log \left( \frac{d\rho}{d\pi}(\theta) \mathbb{E}_{\theta \sim \pi} \left[ e^{-\beta[R(\theta) - R(\theta^*)]} \right] \right) \right]
\]

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\[
KL = KL(\rho|\pi) + \beta E_{\theta \sim \rho}[R(\theta) - R(\theta^*)] + \log E_{\theta \sim \pi}[e^{-\beta[R(\theta) - R(\theta^*)]}]
\]

which, plugged in the last formula, gives:

\[
E_S \left( e^{\lambda \sup_{\rho \in P(\Theta)} \left\{ E_{\theta \sim \rho} \left\{ 1 - Kg \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} - \frac{\beta}{\lambda} \right\} \right\} - KL(\rho|\pi) - \log E_{\theta \sim \pi}[e^{-\beta[R(\theta) - R(\theta^*)]}] \right) \leq 1.
\]

We apply Jensen and rearrange terms to obtain, for any randomized estimator \( \hat{\rho} \),

\[
E_S \left\{ E_{\theta \sim \hat{\rho}}[R(\theta)] - R(\theta^*) \right\} \leq \frac{KL(\rho||\pi)}{\lambda} + \frac{KL(\rho||\pi - \beta R)}{\lambda} + \frac{\log E_{\theta \sim \pi}[e^{-\beta[R(\theta) - R(\theta^*)]}]}{\lambda}
\]

Here again, the r.h.s is minimized for \( \hat{\rho} = \hat{\rho}_\lambda \) the Gibbs posterior, and we obtain:

\[
E_S \left\{ E_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) \right\} \leq \frac{KL(\rho||\pi)}{\lambda} + \frac{KL(\rho||\pi - \beta R)}{\lambda} + \frac{\log E_{\theta \sim \pi}[e^{-\beta[R(\theta) - R(\theta^*)]}]}{\lambda}
\]

where we used again the formula on \( KL(\rho||\pi - \beta R) \) for the last step. So, for \( \beta \) and \( \lambda \) such that

\[
Kg \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} - \frac{\beta}{\lambda} < 1
\]

we have:

\[
E_S \left\{ E_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) \right\} \leq \frac{1 - \frac{\beta}{\lambda}}{1 - Kg \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} - \frac{\beta}{\lambda}} \frac{KL(\rho||\pi - \beta R)}{\lambda}
\]

For example, for \( \lambda = n / \max(2K, C) \) we have already seen that

\[
Kg \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} \leq \frac{1}{2}
\]

and taking \( \beta = \lambda/4 \) leads to

\[
E_S \left\{ E_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) \right\} \leq \frac{\frac{3}{4} E_{\theta \sim \rho}[R(\theta) - R(\theta^*)] \frac{\max(2K, C) KL(\rho||\pi - \frac{1}{4} R)}{n \left( \frac{\lambda C}{n} \right) \frac{\lambda}{n} - \frac{\beta}{\lambda}}}{1 - \frac{\beta}{\lambda}}
\]

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that is
\[
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \hat{p}_x} [R(\theta) - R(\theta^*)] \right\} \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ 3\mathbb{E}_{\theta \sim \rho} [R(\theta) - R(\theta^*)] + \frac{4\max(2K, C) KL (\rho \parallel \pi \| R)}{n} \right\}
\]
which ends the proof. □

We end up this section with the following comment page 15 in Catoni's book [43]: “some of the detractors of the PAC-Bayesian approach (which, as a newcomer, has sometimes received a suspicious greeting among statisticians) have argued that it cannot bring anything that elementary union bound arguments could not essentially provide. We do not share of course this derogatory opinion, and while we think that allowing for non atomic priors and posteriors is worthwhile, we also would like to stress that the upcoming local and relative bounds could hardly be obtained with the only help of union bounds”.

5 Beyond “bounded loss” and “i.i.d observations”

If you follow the proof of the PAC-Bayesian inequalities seen so far, you will see that the “bounded loss” and “i.i.d observations” assumptions are used only to apply Lemma 1.1 (Hoeffding’s inequality) or Lemma 4.4 (Bernstein’s inequality). In other words, in order to prove PAC-Bayes inequalities for unbounded losses or dependent observations, all we need is a result similar to Hoeffding or Bernstein’s inequalities (also called exponential moment inequalities) in this context.

In the past 15 years, many variants of PAC-Bayes bounds were developed for various applications based on this remark. In this section, we provide some pointers. In the end, some authors now prefer to assume directly that the data is such that it satisfies a given exponential inequality. One of the merits of Theorem 3.6 above (that is, Germain, Lacasse, Laviolette and Marchand’s bound [82]) is to make it very explicit: the exponential moment appears in the bound. Since [82], we used in our paper with James Ridgway and Nicolas Chopin [9] a similar approach: we defined a “Hoeffding assumption” and a “Bernstein assumption” that corresponds to data satisfying a Hoeffding type inequality, or a Bernstein type inequality + the usual Bernstein condition (Definition 4.1). A similar point of view is used in [166].

Remark 5.1 Note that it is possible to prove a PAC-Bayes inequality like Theorem 2.1 starting directly from (2.2), that is, assuming that an exponential moment inequality is satisfied in average under the prior π, which does not necessarily it has to hold for each θ. We will not develop this approach here, examples are detailed in [9, 92, 166].

5.1 “Almost” bounded losses (Sub-Gaussian and sub-gamma)

5.1.1 The sub-Gaussian case

Hoeffding’s inequality for \( n = 1 \) variable \( U_1 \) taking values in \([a, b]\) simply states that
\[
\mathbb{E} \left( e^{t[U_1 - \mathbb{E}(U_1)]} \right) \leq e^{\frac{t^2(b-a)^2}{8}}.
\]
Then that the general case is obtained by:

\[ E \left( e^{t \sum_{i=1}^{n} [U_i - E(U_i)]]} \right) = \prod_{i=1}^{n} E \left( e^{t [U_i - E(U_i)]} \right) \text{ (by independence)} \]

\[ \leq \prod_{i=1}^{n} e^{t^2 \frac{(b-a)^2}{8}} = e^{nt^2 \frac{(b-a)^2}{8}}. \]

Alternatively, if we simply assume that, for some \( C > 0 \),

\[ E \left( e^{t [U_i - E(U_i)]} \right) \leq e^{Ct^2} \] \hspace{1cm} (5.1)

for some constant \( C \), similar derivations lead to:

\[ E \left( e^{t \sum_{i=1}^{n} [U_i - E(U_i)]]} \right) \leq e^{nCt^2}, \]

on which we can build PAC-Bayes bounds. We can actually rephrase Hoeffding’s inequality by: “if \( U_1 \) takes values in \([a, b]\), then (5.1) is satisfied for \( C = (b-a)^2/8 \).

It appears that (5.1) is satisfied by some unbounded variables. For example, it is well known that, if \( U_i \sim N(m, \sigma^2) \) then

\[ E \left( e^{t [U_i - E(U_i)]} \right) = e^{\frac{t^2 \sigma^2}{2}}, \]

that is (5.1) with \( C = \sigma^2/2 \). Actually, it can be proven that a variables \( U_1 \) will satisfy (5.1) if and only if its tails \( P(|U_1| \geq t) \) converge to zero (when \( t \to \infty \)) as fast as the ones of a Gaussian variable, that is \( P(|U_1| \geq t) \leq \exp(-t^2/C') \) for some \( C' > 0 \) (see e.g. Chapter 1 in [48]). This is the reason beyond the following terminology.

**Definition 5.1** A random variable \( U \) such that

\[ E \left( e^{t [U - E(U)]} \right) \leq e^{Ct^2} \]

for some finite \( C \) is called a sub-Gaussian random variable (with constant \( C \)).

Based on this definition, we can state for example the following variant of Theorem 2.1 that will be valid for (some!) unbounded losses.

**Theorem 5.1** Assume that for any \( \theta \) the \( \ell_i(\theta) \) are independent and sub-Gaussian random variables with constant \( C \). Then for any \( \varepsilon \geq 0 \), for any \( \lambda > 0 \),

\[ P_S \left( \forall \rho \in \mathcal{P}(\Theta), E_{\theta \sim \rho}[R(\theta)] \leq E_{\theta \sim \rho}[r(\theta)] + \frac{\lambda C^2}{n} + \frac{KL(\rho||\pi) + \log \frac{1}{\varepsilon}}{\lambda} \right) \geq 1 - \varepsilon. \]

(We don’t provide the proof as all the ingredients were explained to the reader).

In the literature, PAC-Bayes bounds explicitely stated for sub-Gaussian losses can be found in [9].
5.1.2 The sub-gamma case

We will not provide details, but variables satisfying inequalities similar to Bernstein’s inequality are called sub-gamma random variables, sometimes sub-exponential random variables. A possible characterization is: \( P(|U_1| \geq t) \leq \exp(-t/C') \) for some \( C' > 0 \). Such variables include: gamma (and exponential) random variables, Gaussian variables and bounded variables.

Chapter 2 of [37] provides a very detailed and pedagogical overview of exponential moment inequalities for independent random variables, and in particular we refer the reader to their Section 2.4 for more details on sub-gamma variables (but I have to warn you, this book is so cool you will find difficult to stop at the end of Chapter 2 and will end up reading everything).

In the literature, PAC-Bayes bounds for sub-gamma random variables can be found as early as 2001: [42] (Chapter 5). These are these bounds that are used to prove minimax rates in various parametric and non-parametric problems in the aforementioned [4, 90, 129].

5.1.3 Remarks on exponential moments

Finally, exponential moments inequalities for random variables such that \( P(|U_1| \geq t) \leq \exp(-t^\alpha/C') \) where \( \alpha \geq 1 \) are studied in Chapter 1 in [48] (the set of such variables is called an Orlicz space).

Still, note that all these random variables are defined such that they satisfy more or less the same exponential inequalities than bounded variables. And indeed, for these variables, \( P(|U_1| \geq t) \) is very small when \( t \) is large — hence the title of this section: almost bounded variables. We will now discuss briefly how to go beyond this case.

5.2 Heavy-tailed losses

By heavy-tailed variables, we mean typically random variables \( U_1 \) such that \( P(|U_1| \geq t) \) is for example in \( t^{-\alpha} \) for some \( \alpha > 0 \).

5.2.1 The truncation approach

In my PhD thesis [1], I studied a truncation technique for general losses \( \ell_i(\theta) \). That is, write:

\[
\ell_i(\theta) = \ell_i(\theta)1(\ell_i(\theta) \leq s) + \ell_i(\theta)1(\ell_i(\theta) > s)
\]

for some \( s > 0 \). The first term is bounded by \( s \), so we can use exponential moments inequalities on it, while I used inequalities on the tails \( P(|\ell_i(\theta)| \geq s) \) to control the second term. For the sake of completeness I state one of the bounds obtained by this technique (with \( s = n/\lambda \)).

**Theorem 5.2 (Corollary 2.5 in [1])** Define

\[
\Delta_{n,\lambda}(\theta) = \mathbb{E}_{(X,Y) \sim P} \left\{ \max \left[ \ell(f_\theta(X), Y) - \frac{n}{\lambda}, 0 \right] \right\}
\]
and
\[
\tilde{r}_{\lambda,n}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \Psi_\lambda \left[ \min \left( \ell(f_\theta(X_i), Y_i), \frac{n}{\lambda} \right) \right],
\]
where
\[
\Psi_\alpha(u) := -\log(1 - u^\alpha) \quad \text{and thus} \quad \Psi_\alpha^{-1}(v) = \frac{1 - e^{-\alpha v}}{\alpha}.
\]
Then, for any \( \varepsilon > 0 \), for any \( \lambda > 0 \),
\[
P_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[\tilde{r}(\theta)] + \frac{KL(\rho\|\pi) + \log \frac{1}{\varepsilon}}{\lambda} + \mathbb{E}_{\theta \sim \rho}[\Delta_{n,\lambda}(\theta)] \right) \geq 1 - \varepsilon,
\]
Note that \( \tilde{r}_{\lambda,n}(\theta) \) is an approximation of \( r(\theta) \) when \( \lambda/n \) is small enough (usually \( \lambda \sim \sqrt{n} \) in this bound). The function \( \Psi_\alpha \) plays a role similar to the function \( \Phi_\alpha \) in Catoni’s bound (Theorem 3.2), and more explicit inequalities can be derived by upper-bounding \( \Psi_\alpha^{-1} \). Finally, \( \Delta_{n,\lambda}(\theta) \) corresponds to the tails of the loss function. Actually, for a bounded loss, we will have \( \Delta_{n,\lambda}(\theta) = 0 \) for \( n/\lambda \) large enough. In the sub-exponential setting, \( \Delta_{n,\lambda}(\theta) > 0 \) but will usually not be the dominant term in the right-hand side. However, in [1], I provide upper bounds on \( \Delta_{n,\lambda}(\theta) \) in \( O((\lambda/n)^{s-1}) \) where \( s \) is such that \( \mathbb{E}(\ell^s_i) < +\infty \), but this term is dominant in this case (and thus, it slows down the rate of convergence). This truncation argument is reused in [2] but only the oracle bounds are provided there.

5.2.2 Bounds based on moment inequalities

Based on techniques developed in [100, 29], [5] proved inequalities similar to PAC-Bayes bounds, that hold for heavy-tailed losses (they can also hold for non i.i.d losses, we will discuss this point later). Curiously, these bounds depend no longer on the Kullback-Leibler divergence, but on other divergences. An example of such an inequality is provided here and relies only on the assumption that the losses have a variance.

Theorem 5.3 (Corollary 1 in [3]) Assume that the \( \ell_i(\theta) \) are independent and such that \( \text{Var}(\ell_i(\theta)) \leq \kappa < \infty \). Then, for any \( \varepsilon > 0 \),
\[
P_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \sqrt{\frac{\kappa(1 + \chi^2(\rho\|\pi))}{n\varepsilon}} \right) \geq 1 - \varepsilon,
\]
where \( \chi^2(\rho\|\pi) \) is the chi-square divergence:
\[
\chi^2(\rho\|\pi) = \int \left[ \left( \frac{d\rho}{d\pi}(\theta) \right)^2 - 1 \right] \pi(d\theta) \quad \text{if} \quad \rho \ll \pi \quad \text{and} \quad \chi^2(\rho\|\pi) = +\infty \quad \text{otherwise}.
\]
Interestingly, the minimization of the bound with respect to $\rho$ leads to an explicit solution, see [5]. Note that the dependence of the rate in $\varepsilon$ is much worse than in Theorem 2.1. This was later dramatically improved by [151]. Still, as for the truncation approach described earlier, this approach leads to slow rates of convergence for heavy-tailed variables.

### 5.2.3 Bounds based on robust losses

In [44] Olivier Catoni proposed a robust loss function $\psi$ used to estimate the mean of heavy-tailed random variables (note that this is also based on ideas from an earlier paper [18]). As a result, [44] obtains, for the mean of heavy-tailed variables, confidence intervals very similar to the ones of estimators of the mean of a Gaussian. This loss function was used in conjunction with PAC-Bayes bounds in [45, 84] to study non-Bayesian estimators.

More recently, Holland [99] derives a full PAC-Bayesian theory for possibly heavy-tailed losses based on Catoni’s technique. The idea is as follows. Put

$$
\psi(u) = \begin{cases} 
-\frac{2\sqrt{2}}{3} & \text{if } u < -\sqrt{2}, \\
-\frac{u^3}{6} & \text{if } -\sqrt{2} \leq u \leq \sqrt{2}, \\
\frac{2\sqrt{2}}{3} & \text{otherwise}
\end{cases}
$$

and, for any $s > 0$,

$$
r_{\psi,s}(\theta) = \frac{s}{n} \sum_{i=1}^{n} \psi \left( \frac{\ell_i(\theta)}{s} \right).
$$

The idea is that, even when $\ell_i(\theta)$ is unbounded, the new version of the risk, $r_{\psi,s}(\theta)$, so the study of its deviations could be done through classical means. There is some additional work to connect $E_S[r_{\psi,s}(\theta)]$ to $R(\theta)$ for a well chosen $s$, and [99] obtains the following result.

**Theorem 5.4 (Theorem 9 in [99])** Let $\varepsilon > 0$. Assume that the $\ell_i(\theta)$ are independent and

- $\mathbb{E}(\ell_i(\theta)^2) \leq M_2 < +\infty$ and $\mathbb{E}(\ell_i(\theta)^3) \leq M_3 < +\infty$,
- for any $\theta \in \Theta$, $R(\theta) \leq \sqrt{nM_2/(4 \log(1/\varepsilon))},$
- $\varepsilon \leq e^{-1/9} \approx 0.89$, and put

$$
\pi_n^*(\Theta) = \frac{\mathbb{E}_{\theta \sim \pi} \left[ e^{\sqrt{n}[R(\theta) - r_{\psi,s}(\theta)]} \right]}{\mathbb{E}_{\theta \sim \pi} \left[ e^{R(\theta) - r_{\psi,s}(\theta)} \right]},
$$

then, for $s := nM_2/[2 \log(1/\varepsilon)]$,

$$
P_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r_{\psi,s}(\theta)] + \frac{KL(\rho||\pi) + M_2 + \log\left( \frac{sM_3}{\varepsilon^2} \right)}{\sqrt{n}} + \pi_n^*(\Theta) - 1 \right) \geq 1 - \varepsilon.
$$

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Note that, on the contrary to Theorem 5.3 above, the bound is very similar to the one in the bounded case (heavy-tailed variables do not lead to slower rates). In particular, we have a good dependence of the bound in $\varepsilon$, and the presence of $KL(\rho\|\pi)$ that is much smaller than $\chi^2(\rho\|\pi)$. The only notable difference is the restriction in the range of $\varepsilon$ (which is of no consequence in practice), and the term $\pi_n^*(\Theta)$. Unfortunately, as discussed in Remark 10 of [99], this term will deteriorate the rate of convergence when the $\ell_i(\theta)$ are not sub-Gaussian (to my knowledge, it is not known if it will lead to better or worse rates than the ones obtained through truncation).

5.3 Dependent observations

5.3.1 Inequalities for dependent variables

There are versions of Hoeffding and Bernstein’s inequalities for dependent random variables, under various assumptions on this dependence. This can be used in the case where the observations are actually a time series, or a random field.

For example, in our paper with O. Wintenberger [10] we learn auto-regressive predictors of the form $\hat{X}_t = f_\theta(X_{t-1}, \ldots, X_{t-k})$ for weakly dependent time series with a PAC-Bayes bound. The proof relies on Rio’s version of Hoeffding’s inequality [163]. In our paper, only slow rates in $1/\sqrt{n}$ are provided. Later, fast rates in $1/n$ were proven in another paper with O. Wintenberger and X. Li [3] for (less general) mixing time series thanks to Samson’s version of Bernstein’s inequality [172].

More exponential moment inequalities (and moment inequalities) for dependent variables can be found in the paper [199] and in the book dedicated to weak dependence [66]. Other time series models where PAC-Bayes bounds were used include martingales [176], Markov chains [21], continuous dynamical systems [93], LTI systems [72]...

5.3.2 A simple example

The weak-dependence conditions are quite general but they are also quite difficult to understand and the definitions are sometimes cumbersome. We only provide a much simpler example based on a more restrictive assumption, $\alpha$-mixing. This result comes from [5] and extends Theorem 5.3 to time series.

**Definition 5.2** Given two $\sigma$-algebras $\mathcal{F}$ and $\mathcal{G}$, we define

$$\alpha(\mathcal{F}, \mathcal{G}) = \sup \{\text{Cov}(U, V); 0 \leq U \leq 1, U \text{ is } \mathcal{F}\text{-measurable}, 0 \leq V \leq 1, V \text{ is } \mathcal{G}\text{-measurable}\}.$$ 

Note that if $\mathcal{F}$ and $\mathcal{G}$ are independent, $\alpha(\mathcal{F}, \mathcal{G}) = 0$.

**Definition 5.3** Given a time series $U = (U_t)_{t \in \mathbb{Z}}$ we define its $\alpha$-mixing coefficients by

$$\forall h \in \mathbb{Z}, \alpha_h(U) = \sup_{t \in \mathbb{N}} \alpha(\sigma(U_t), \sigma(U_{t+h})).$$
Theorem 5.5 (Corollary 2 in \[5\]) Let $X = (X_t)_{t \in \mathbb{Z}}$ be a real-valued stationary time series. Define, for $\theta = (\theta_1, \theta_2) \in \mathbb{R}^2$, $\ell_t(\theta) = (X_t - \theta_1 - \theta_2 X_{t-1})^2$ and $R(\theta) = \mathbb{E}_X[\ell_t(\theta)]$ (it does not depend on $t$ as the series is stationary). Define

$$r(\theta) = \sum_{t=1}^n \ell_t(\theta)$$

the empirical risk based on the observation of $(X_0, \ldots, X_n)$. Assume the prior $\pi$ is chosen such that

$$\int \|\theta\|^6 \pi(d\theta) \leq M_6 < +\infty$$

(for example a Gaussian prior). Assume that $X$ the $\alpha$-mixing coefficients of $X$ satisfy:

$$\sum_{t \in \mathbb{Z}} \left[ \alpha_t(X) \right]^{1/2} \leq A < +\infty.$$

Assume that $\mathbb{E}(X_i^6) \leq C < +\infty$. Define $\nu = 32C^{3/2}A(1 + 4M_6)$. Then, for any $\epsilon > 0$,

$$\mathbb{P}_S \left( \forall \rho \in \mathcal{P}(\Theta), \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[r(\theta)] + \sqrt{\frac{\nu (1 + \chi^2(\rho\|\pi))}{n\epsilon}} \right) \geq 1 - \epsilon.$$

5.4 Other non i.i.d settings

5.4.1 Non identically distributed observations

When the data is independent, but non-identically distributed, that is, $(X_i, Y_i) \sim P_i$, we can still introduce

$$r(\theta) = \frac{1}{n} \sum_{i=1}^n \ell_i(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(f_\theta(X_i), Y_i)$$

and

$$R(\theta) = \mathbb{E}[r(\theta)] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{(X_i, Y_i) \sim P_i}[\ell(f_\theta(X_i), Y_i)].$$

The proofs of most exponential inequalities still hold in this setting (for example, Hoeffding inequality when the losses are bounded). Based on this remark, the full book \[43\] is written for independent, but not necessarily identically distributed observations. Of course, if we actually have $P_i = P$ for any $i$, we recover the usual case $R(\theta) = \mathbb{E}_{(X,Y) \sim P}[\ell(f_\theta(X), Y)]$.

5.4.2 Shift in the distribution

A common problem in machine learning practice is the shift in distribution: one learns a classifier based on i.i.d observations $(X_i, Y_i) \sim P$. But in practice, the data to be predicted are drawn from another distribution $Q$, that is: $R(\theta) = \mathbb{E}_{(X,Y) \sim Q}[\ell(f_\theta(X), Y)] \neq \mathbb{E}_{(X,Y) \sim P}[\ell(f_\theta(X), Y)]$. There is still a lot of work to do to address this practical problem, but an interesting approach is proposed in \[80\]: the authors use a technique called domain adaptation to allow the use of PAC-Bayes bounds in this context.
5.4.3 Meta-learning

Meta-learning is a scenario when one solves many machine learning tasks simultaneously, and the objective is to improve this learning process for yet-to-come tasks. A popular formalization (but not the only one possible) is:

- each task \( t \in \{1, \ldots, T\} \) corresponds to a probability distribution \( P_t \). The \( P_t \)'s are i.i.d from some \( \mathcal{P} \).

- for each task \( t \), an i.i.d sample \( (X^t_1, Y^t_1), \ldots, (X^t_n, Y^t_n) \) is drawn from \( P_t \). Thus, we observe the empirical risk of task \( t \):

\[
\hat{r}_t(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_{\theta}(X^t_i), Y^t_i)
\]

and use PAC-Bayes bounds to learn a good \( \theta_t \) for this task.

- based on the data of tasks \( \{1, \ldots, T\} \), we want to improve the learning process for a yet non-observed task \( P_{T+1} \sim \mathcal{P} \).

This improvement differs from one application to the other, for example: learn a better parameter space \( \Theta_{T+1} \subset \Theta \), learn a better prior, learn better hyperparameters like \( \lambda \)... PAC-Bayes bounds for meta-learning were studied in [155, 12, 105, 169, 122, 140, 123, 74, 161, 164]. I believe PAC-Bayes bound are particularly convenient for meta-learning problems, and thus that this direction of research is very promising.

6 Related approaches in statistics and machine learning theory

In this section, we list some connections between PAC-Bayes theory and other approaches in statistics and machine learning. We will mostly provide references, and will use mathematics more heuristically than in the previous sections. Note that these connections are well-known and were discussed in the literature, see for example [20].

6.1 Bayesian inference in statistics

In Bayesian statistics, we are given a sample \( X_1, \ldots, X_n \) assumed to be i.i.d from some \( P_{\theta^*} \) in a model \( \{P_{\theta}, \theta \in \Theta\} \). A prior \( \pi \) is given on the parameter set \( \Theta \). When each \( P_{\theta} \) has a density \( p_{\theta} \) with respect to a given measure, the likelihood function is defined by

\[
\mathcal{L}(\theta; X_1, \ldots, X_n) := \prod_{i=1}^{n} p_{\theta}(X_i).
\]
According to the Bayesian paradigm, all the information on the parameter that can be inferred from the sample is in the posterior distribution

$$\pi(d\theta|X_1, \ldots, X_n) = \frac{\mathcal{L}(\theta; X_1, \ldots, X_n)\pi(d\theta)}{\int \mathcal{L}(\theta'; X_1, \ldots, X_n)\pi(d\theta')}.$$ 

A direct remark is that $\pi(d\theta|X_1, \ldots, X_n)$ can be seen as a Gibbs posterior. Indeed, as

$$\left[\prod_{i=1}^{n} p_\theta(X_i)\right]\pi(d\theta) = e^{\sum_{i=1}^{n} \log p_\theta(X_i)}\pi(d\theta)$$

we can define the loss $\ell_i(\theta) = -\log p_\theta(X_i)$ and the corresponding empirical risk is the negative log-likelihood:

$$r(\theta) = \frac{1}{n} \sum_{i=1}^{n} [\log p_\theta(X_i)],$$

and we have

$$\pi(\cdot|X_1, \ldots, X_n) = \pi_{-nr}$$

$$= \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} \left[ \frac{1}{n} \sum_{i=1}^{n} [\log p_\theta(X_i)] \right] + \frac{KL(\rho||\pi)}{n} \right\}. \quad (6.1)$$

This connection is for example discussed in \[15, 79\]. Note, however, that log-likelihoods are rarely bounded, which prevents to use the simplest PAC-Bayes bounds to study the consistency of $\pi(d\theta|X_1, \ldots, X_n)$.

### 6.1.1 Gibbs posteriors, generalized posteriors

Independently from the PAC-Bayes community, the Bayesian statistics community proposed to generalize the posterior, by replacing the log-likelihood by minus a risk function. Often, the resulting generalised posterior is called a Gibbs posterior. This is done for example in \[103, 186\] in order to estimate some parameters of the distributions of the data without having to model the whole distribution. Another instance of such generalized posteriors are fractional, or tempered posteriors, $\pi_{-\alpha r}$, where $r$ is the negative log-likelihood and $\alpha < 1$. Grünwald proved that in some contexts where the posterior $\pi(d\theta|X_1, \ldots, X_n)$ is not consistent, a tempered posterior for $\alpha$ small enough will be \[85\]. Gibbs posteriors are discussed in a decision theoretic framework by \[34\]. An asymptotic study of Gibbs posteriors, using different arguments than PAC-Bayes bounds (but related), can be found in \[187\] and some the references therein.

### 6.1.2 Contraction of the posterior in Bayes nonparametrics

A very active field of research is the study of the contraction of the posterior in Bayesian statistics: the objective is to prove that $\pi(d\theta|X_1, \ldots, X_n)$ concentrates around the true parameter $\theta^*$ when $n \to \infty$. We refer the reader to \[170, 53\] on this topic, see also \[23\] on high-dimensional models specifically. Usually, such results require two assumptions:
a technical condition, the existence of tests to discriminate between members of the model \( \{P_\theta, \theta \in \Theta\} \),

and the prior mass condition, which states that enough mass is given by the prior to a neighborhood of \( \theta^* \). In other words, \( \pi(\{\theta : d(\theta, \theta^*) \leq \delta\}) \) does not converge too fast to 0 when \( \delta \to 0 \), for some distance or risk measure \( d \). For example, we can assume that there is a sequence \( r_n \to 0 \) when \( n \to \infty \) such that

\[
\pi(\{\theta : d(\theta, \theta^*) \leq r_n\}) \geq e^{-nr_n}.
\] (6.2)

Note that the prior mass condition can also be used in conjunction with PAC-Bayes bounds, to show that the bound is small. For example consider the PAC-Bayes inequality of Theorem 4.3: under a Bernstein condition with constant \( K \) and for a well chosen \( \lambda \),

\[
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) \leq 2 \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[R(\theta)] - R(\theta^*) + \frac{\max(2K, C) KL(\rho, \pi)}{n} \right\}.
\]

Assume that the prior mass condition holds with \( d(\theta, \theta^*) = R(\theta) - R(\theta^*) \) and take

\[
\rho(d\theta) = \frac{\pi(d\theta)1(\{d(\theta, \theta^*) \leq r_n\})}{\pi(\{\theta : d(\theta, \theta^*) \leq r_n\})}.
\]

We obviously have:

\[
\mathbb{E}_{\theta \sim \rho}[R(\theta)] - R(\theta^*) \leq r_n
\]

and direct a calculation gives

\[
KL(\rho \| \pi) = -\log \pi(\{\theta : d(\theta, \theta^*) \leq r_n\}) \leq nr_n
\]

so the bound becomes:

\[
\mathbb{E}_{\theta \sim \hat{\rho}_\lambda}[R(\theta)] - R(\theta^*) \leq 2[1 + \max(2K, C)]r_n \xrightarrow{n \to \infty} 0.
\]

Thanks to this connection, [30] proved the contraction of tempered posteriors using essentially only a prior mass condition, using a new PAC-Bayes bound.

### 6.1.3 Variational approximations

In many applications where the dimension of \( \Theta \) is large, sampling from \( \pi(d\theta|X_1, ..., X_n) \) becomes a very difficult task. In order to overcome this difficulty, a recent trend is to approximate this probability distribution by a tractable approximation. Formally, we would chose a set \( \mathcal{F} \) of probability distributions (for example, Gaussian distributions with diagonal covariance matrix) and define the following approximation of the posterior:

\[
\hat{\rho} = \arg\min_{\rho \in \mathcal{F}} KL(\rho \| \pi(\cdot|X_1, ..., X_n)).
\]
This is called a variational approximation in Bayesian statistics, we refer the reader to [30] for recent survey on the topic. Note that, by definition of $\pi(d\theta|X_1,\ldots,X_n)$ we also have

$$\hat{\rho} = \operatorname*{argmin}_{\rho \in F} \left\{ \mathbb{E}_{\theta \sim \rho} \left[ \frac{1}{n} \sum_{i=1}^{n} \left[ -\log p_\theta(X_i) \right] \right] + \frac{KL(\rho||\pi)}{n} \right\}$$

that is, a restricted version of (6.1).

This leads to two remarks:

- non-exact minimization of PAC-Bayes bounds, as in Subsubsection 2.1.3, can be interpreted as variational approximations of Gibbs posteriors. Note that this is also the case of the Gaussian approximation that was used for neural networks in [70]. This led to our paper [9], dedicated to the consistency of variational approximations of Gibbs posteriors proven via PAC-Bayes bounds, see also the results in [180].

- on the other hand, little was known at that time on the theoretical properties of variational approximations of the posterior in statistics. Using the fact that variational approximations of tempered posteriors are constrained minimizers of the PAC-Bayes bound of [30], we studied in [8] the consistency of such approximations. As a byproduct we have a generalization of the prior mass condition for variational inference (see (2.1) and (2.2) in [8]). These results were extended to the standard posterior $\pi(d\theta|X_1,\ldots,X_n)$ in [204, 205].

More theoretical studies on variational inference (using PAC-Bayes, or not) appeared at the same time or since: [52, 101, 132, 50, 158, 53, 21, 19, 150, 76].

The most general version of (6.1) we are aware of is:

$$\hat{\rho} = \operatorname*{argmin}_{\rho \in F} \left\{ \mathbb{E}_{\theta \sim \rho} [r(\theta)] + \frac{D(\rho||\pi)}{n} \right\} \quad (6.3)$$

where $D$ is any distance or divergence between probability distributions. Here, the Bayesian point of view is generalized in three directions:

1. the negative log-likelihood is replaced by a more general notion of risk $r(\theta)$, as in PAC-Bayes bounds and in Gibbs posteriors,

2. the minimization over $\mathcal{P}(\Theta)$ is replaced by the minimization over $\mathcal{F}$, in order to keep things tractable, as in variational inference,

3. finally, the $KL$ divergence is replaced by a general $D$. Note that this already happened in Theorem 5.3 above.

This triple generalization, and the optimization point of view on Bayesian statistics is strongly advocated in [110] (in particular reasons to replace $KL$ by $D$ are given in this paper that seem to me more relevant in practice than Theorem 5.3).

In this spirit, [168, 49] provided PAC-Bayes type bounds where $D$ is the Wasserstein distance.
Remark 6.1 Note that, when $D \neq KL$, (6.3) is no longer equivalent to
\[
\hat{\theta} = \arg\min_{\theta \in \mathcal{F}} D(\theta)\|\pi(\cdot|X_1,\ldots,X_n)).
\] (6.4)

The paper [110] discusses why (6.3) is a more natural generalization, and [78] shows that (6.4) leads to difficult minimization problems. Note however that there are also some theoretical results on (6.4) in [102].

6.2 Empirical risk minimization

We already pointed out in the introduction the link between empirical risk minimization (based on PAC bounds) and PAC-Bayes.

When the parameter space $\Theta$ is not finite as in Theorem 1.2 above, the $\log(M)$ term is replaced by a measure of the complexity of $\Theta$ called the Vapnik-Chervonenkis dimension (VC-dim). We simply mention that in Section 2 of [41], Catoni builds a well-chosen data dependent prior such that the VC-dim of $\Theta$ appears explicitly in the PAC-Bayes bound. There is a similar construction in Chapter 3 in [41]. However, in the paper [124], Livni and Moran "provide an example where the VC dimension is finite, yet the PAC-Bayes approach fails. Note however that this problem was solved recently by [85] thanks to "conditional PAC-Bayes bounds". This is discussed below together with Mutual Information bounds.

Similarly, generalization bounds for Support Vectors Machines are based on a quantity called the margin. This quantity can also appear in PAC-Bayes bounds [115, 95, 43, 32].

Audibert and Bousquet studied a PAC-Bayes version of the chaining argument [17]. See also versions based on Mutual Information bounds [14, 56].

Finally, [201] proved PAC-Bayes bounds using Rademacher complexity.

6.3 Online learning

6.3.1 Sequential prediction

Sequential classification focuses on the following problem. At each time step $t$,

- a new object $x_t$ is revealed,
- the forecaster must propose a prediction $\hat{y}_t$ of the label of $y_t$,
- the true label $y_t \in \{0,1\}$ is revealed and the forecaster incurs a loss $\ell(\hat{y}_t, y_t)$, and updates his/her knowledge.

Similarly, online regression and other online prediction problems are studied.

Prediction strategies are often evaluated through upper bounds on the regret $\mathcal{R}_{eg}(T)$ given by:
\[
\mathcal{R}_{eg}(T) := \sum_{t=1}^{T} \ell(\hat{y}_t, y_t) - \inf_{\theta} \ell(f_{\theta}(x_t), y_t)
\]
where \(\{f_\theta, \theta \in \Theta\}\) is a family of predictors as in Section 1 above. However, a striking point is that most regret bounds hold without any stochastic assumption on the data \((x_t, y_t)_{t=1,...,T}\): they are not assumed to be independent not to have any link whatsoever with any statistical model. On the other hand, assumptions on the function \(\theta \mapsto \ell(f_\theta(x_t), y_t)\) are unavoidable (depending on the strategies: boundedness, Lipschitz condition, convexity, strong convexity, etc.).

A popular strategy, strongly related to the PAC-Bayesian approach, is the exponentially weighted average (EWA) forecaster, also known as weighted majority algorithm or multiplicative update rule \([121, 196, 46, 109]\) (we also refer to \([27]\) on the halving algorithm that can be seen as an ancestor of this method). This strategy is defined as follows. First, let \(\rho_1 = \pi\) be a prior distribution on \(\Theta\), and fix a learning rate \(\eta > 0\). Then, at each time step \(t\):

- the prediction is given by
  \[
  \hat{y}_t = \mathbb{E}_{\theta \sim \rho_t}[f_\theta(x)],
  \]
- when \(y_t\) is revealed, we update
  \[
  \rho_{t+1}(d\theta) = \frac{e^{-\eta \ell(f_\theta(x), y_t)} \rho_t(d\theta)}{\int_\Theta e^{-\eta \ell(f_\theta(x), y_t)} \rho_t(d\theta)}.
  \]

We provide here a simple regret bound that can be found in \([47]\) (stated for a finite \(\Theta\) but the extension is direct). Note the formal analogy with PAC-Bayes bounds.

**Theorem 6.1** Assume that, for any \(t\), \(0 \leq \ell(f_\theta(x_t), y_t) \leq C\) (bounded loss assumption) and \(\theta \mapsto \ell(f_\theta(x_t), y_t)\) is a convex function. Then, for any \(T > 0\),

\[
\sum_{t=1}^T \ell(\hat{y}_t, y_t) \leq \inf_{\rho \in \mathcal{P}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho}[\ell(f_\theta(x_t), y_t)] + \frac{\eta C^2 T}{8} + \frac{KL(\rho\|\pi)}{\eta} \right\}.
\]

In particular, when \(\Theta\) is finite with \(\text{card}(\Theta) = M\) and \(\pi\) is uniform, the restriction of the infimum to Dirac masses leads to

\[
\sum_{t=1}^T \ell(\hat{y}_t, y_t) \leq \inf_{\theta \in \Theta} \ell(f_\theta(x_t), y_t) + \frac{\eta C^2 T}{8} + \frac{\log(M)}{\eta}
\]

and thus with \(\eta = \frac{2 C}{\sqrt{2 log(M) T}}\),

\[
\mathcal{R}eg(T) \leq C \sqrt{\frac{T \log(M)}{2}}.
\]

Choices of \(\eta\) that do not depend on the time horizon \(T\) are possible \([47]\). Smaller regret bounds, up to \(\log(T)\) or even constants, are known under stronger assumptions \([47, 16]\). We refer the reader to \([178, 153]\) for more up to date introductions to online learning.
While there is no stochastic assumption on the data in Theorem 6.1, it is possible to deduce inequalities in probability or in expectation from it under additional assumptions (for example, the assumption that the data is i.i.d.). This is described for example in Chapter 5 in [178], but does not always lead to optimal rates. A more up-to-date discussion on this topic with more general results can be found in [33].

Finally, note that many other strategies than EWA are studied: online gradient algorithm, follow-the-regularized-leader (FTRL), online mirror descent (OMD)... EWA is actually derived as a special case of FTRL and OMD in many references (e.g. [178]) but conversely, [98, 108] derive OMD and online gradient a EWA applied with various approximations (compare to Section 2 and the remark that on can use PAC-Bayes inequalities to provide generalization error bounds on non-Bayesian methods like the ERM).

6.3.2 Bandits and reinforcement learning (RL)

Other online problems received a considerable attention in the past few years. In bandits, the forecaster only receives feedback on the loss of his/her prediction, but not on the losses what he/she would have incurred under other predictions. We refer the reader to [39] for an introduction to bandits. Note that some strategies used for bandits are derived from EWA. Some authors derived strategies or regret bounds directly from PAC-Bayes bounds [174, 175]. Bandits themself are a subclass of a larger family of learning problems: reinforcement learning (RL). Some generalization bounds similar to PAC-Bayes for RL were derived in [197].

6.4 Aggregation of estimators in statistics

Given a set \( \mathcal{E} \) of statistical estimators, the aggregation problem consists in finding a new estimator, called the aggregate, that would perform as well as the best estimator in \( \mathcal{E} \), see [144] for a formal definition and variants of the problem. The optimal rates are derived in [191]. Many aggregates share a formal similarity with the EWA of online learning and with the Gibbs posterior of the PAC-Bayes approach, we refer the reader to [144, 106, 202, 139, 203, 125, 119, 116, 64, 40, 183, 65, 60, 63, 59, 62, 126, 61]. In some of these papers, the connection to PAC-Bayes bounds is explicit: Theorem 1 in [64] is referred to as a PAC-Bayes bound in the paper. It is actually an oracle PAC-Bayes bound in expectation. It leads to fast rates in the spirit of Theorem 4.3 but with different assumptions (in particular, the \( X_i \)'s are not random there).

6.5 Information theoretic approaches

A note on the terminology: a huge number of statistical and machine learning results mentioned above rely on tools from information theory (Tong Zhang’s beautiful paper [206] actually proves PAC-Bayesian bounds under the name “information theoretic bounds”, I hope it’s not the reason why it is often not cited by the PAC-Bayes community). My goal here is not to classify what is an information theoretic approach and what is not, I’m cer-
tainly not qualified for that. I simply want to point out the connection to two families of methods inspired directly from information theory.

6.5.1 Minimum description length

In Rissanen’s Minimum Description Length (MDL) principle, the idea is to penalize the empirical error of a classifier by its shortest description [165]. We refer the reader to [24, 87] for more recent presentations of this very fruitful approach. Note that given a prefix code on a finite alphabet Θ, it is possible to build a probability distribution $\pi(\theta) \simeq 2^{-L(\theta)}$ where $L(\theta)$ is the length of the code of $\theta$, so MDL provides a way to define priors in PAC-Bayes bounds, see Chapter 1 in Catoni’s lecture notes [42].

6.5.2 Mutual information bounds (MI)

Recently, some generalization error bounds appeared where the complexity is measured in terms of the mutual information between the sample and the estimator.

**Definition 6.1** Let $U$ and $V$ be two random variables with joint probability distribution $P_{U,V}$. Let $P_U$ and $P_V$ denote the marginal distribution of $U$ and $V$ respectively. The mutual information (MI) between $U$ and $V$ is defined as:

$$I(U,V) := KL(P_{U,V} \parallel P_U \otimes P_V).$$

In [171], Russo and Zou introduced generalization error bounds (in expectation) that depend on the mutual information between the predictors and the labels. In particular, when $\hat{f}$ is obtained by empirical risk minimization, they recover bounds depending of the VC-dimension of $\Theta$.

Russo and Zou’s result were improved and extended Raginsky, Rakhlin, Tsao, Wu and Xu [159, 200]. In particular, Subsection 4.3 [200] prove powerful MI inequalities, and then recovers from them a bound in expectation that is almost exactly Theorem 2.8 above. However, in the same way PAC-Bayes community not aware of Zhang’s “information theoretic bounds” [206], it seems that the authors of [200] are not aware of PAC-Bayes bounds. Recently, the connection between MI bounds and PAC-Bayes was pointed out in [22]. There, the authors provide a unified approach, and derive various bounds under different assumptions on the loss.

In their Theorem 2.3 in [143], Negrea, Haghifam, Dziugaite, Khisti and Roy write explicitly the connection between MI bounds and PAC-Bayes bounds. So we state here their result, or rather, a simplified version (by setting their parameter $m$ to 0).

**Theorem 6.2** (Theorem 2.3 in [143], with $m = 0$) Using the notations and assumptions of Section 4, assume that the losses $\ell_i(\theta)$ are sub-Gaussian with parameter $C$, then, for any data-dependent $\hat{\rho}$,

$$\mathbb{E}_S\left\{\mathbb{E}_{\theta \sim \hat{\rho}}[R(\theta)] - \mathbb{E}_{\theta \sim \hat{\rho}}[r(\theta)]\right\} \leq \sqrt{\frac{2C I(\theta, S)}{n}} \leq \sqrt{\frac{2C \mathbb{E}_S[KL(\hat{\rho} \parallel \pi)]}{n}}.$$
A few comments on this result:

- the first inequality is actually Theorem 1 of [200]. Note however that Theorem 2.3 in [143] contains more information, as setting their parameter $m \neq 0$ allows to get a data-dependent prior. The paper contains more new results, and a beautiful application to derive empirical bounds on the performance of stochastic gradient descent (SGD). On this topic, see also the recent [38, 198, 145].

- we can see here that the MI bound

$$
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \tilde{\rho}} [R(\theta)] - \mathbb{E}_{\theta \sim \hat{\rho}} [r(\theta)] \right\} \leq \sqrt{\frac{2C I(\theta, S)}{n}}
$$

(6.5)

is tighter than the the PAC-Bayes bound in expectation

$$
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \tilde{\rho}} [R(\theta)] - \mathbb{E}_{\theta \sim \hat{\rho}} [r(\theta)] \right\} \leq \sqrt{\frac{2C \mathbb{E}_S [KL(\tilde{\rho} \parallel \pi)]}{n}}.
$$

(6.6)

However, an MI bound cannot be used as is in practice. Indeed, $I(\theta, S)$ depends on the distribution of the sample $S$ that is unknown in practice. In order to use (6.5), one must upper bound $I(\theta, S)$ by a quantity that does not depend on the sample.

- in two discussions page 14 and page 51 in [43], Catoni discusses the optimization of PAC-Bayes bounds with respect to the prior. In order to explain the discussion done there, apply $\sqrt{ab} \leq a/(2\lambda) + b\lambda/2$ to (6.6) to get a “Catoni style” bound:

$$
\mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \tilde{\rho}} [R(\theta)] - \mathbb{E}_{\theta \sim \hat{\rho}} [r(\theta)] \right\} \leq \frac{C \lambda}{2n} + \frac{\mathbb{E}_S [KL(\tilde{\rho} \parallel \pi)]}{\lambda}
$$

and thus

$$
\mathbb{E}_S \mathbb{E}_{\theta \sim \tilde{\rho}} [R(\theta)] \leq \mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \tilde{\rho}} [r(\theta)] + \frac{C \lambda}{2n} + \frac{KL(\tilde{\rho} \parallel \pi)}{\lambda} \right\}
$$

(compare to Theorem 2.8 above). Let $\tilde{\rho}$ be any data-dependent measure that is absolutely continuous with respect to $\pi$ almost-surely, thus

$$
\frac{d\tilde{\rho}}{d\pi}(\theta)
$$

is well-defined. Catoni defines $\mathbb{E}_S (\tilde{\rho})$ the probability measure defined by

$$
\frac{d\mathbb{E}_S (\tilde{\rho})}{d\pi}(\theta) = \mathbb{E}_S \left( \frac{d\tilde{\rho}}{d\pi}(\theta) \right).
$$

Direct calculations show that $\mathbb{E}_S [KL(\tilde{\rho} \parallel \pi)] = \mathbb{E}_S [KL(\tilde{\rho} \parallel \mathbb{E}_S (\tilde{\rho}))] + KL(\mathbb{E}_S (\tilde{\rho}) \parallel \pi) = I(\theta, S) + KL(\mathbb{E}_S (\tilde{\rho}) \parallel \pi)$ and thus:

$$
\mathbb{E}_S \mathbb{E}_{\theta \sim \tilde{\rho}} [R(\theta)] \leq \mathbb{E}_S \left\{ \mathbb{E}_{\theta \sim \tilde{\rho}} [r(\theta)] \right\} + \frac{C \lambda}{2n} + \frac{I(\theta, S) + KL(\mathbb{E}_S (\tilde{\rho}) \parallel \pi)}{\lambda}.
$$
So the choice to replace \( \pi \) by \( E_{S}(\tilde{\rho}) \) gives the MI bound:

\[
E_{S}E_{\theta \sim \tilde{\rho}}[R(\theta)] \leq E_{S} \{E_{\theta \sim \tilde{\rho}}[r(\theta)]\} + \frac{C\lambda}{2n} + \frac{I(\theta, S)}{\lambda}.
\]

The choice \( \lambda = \sqrt{2nI(\theta, S)/C} \) leads to

\[
E_{S}E_{\theta \sim \tilde{\rho}}[R(\theta)] \leq E_{S} \{E_{\theta \sim \tilde{\rho}}[r(\theta)]\} + \sqrt{\frac{2C I(\theta, S)}{n}}.
\]

In other words, MI bounds can be seen as KL bounds optimized with respect to the prior. Of course, as we said above, MI bound cannot be computed in practice. Catoni proposes an interpretation of his localization technique as taking the prior \( \pi - \beta R \) to approximate \( E_{S}(\pi - \lambda r) \), and then to upper bound \( KL(\rho \| \pi - \beta R) \) via empirical bounds. As we have seen in Section 3, this leads to empirical bounds with data-dependent priors, and in Section 4, this leads to improved PAC-Bayes oracle bounds. All this is pointed out by Grünwald, Steinke and Zakynthinou \[85\]: “Catoni already mentions that the prior that minimizes a MAC-Bayesian bound is the prior that turns the KL term into the mutual information”.

Similarly to PAC-Bayesian bounds, MI bounds can be stated with other divergences than KL \[146\].

Thanks to MI bounds, it is also possible to provide an exact formula (not an upper bound) for the generalization error of the Gibbs posterior in terms of the symmetrized version of the KL bound \[11\].

From \[28, 142\], it is known that MI bounds can fail in some situations where the VC dimension is finite: thus, they suffer the same limitation as PAC-Bayes bounds proven in \[124\]. Recently, using ideas from the PAC-Bayes literature \[15, 13, 141\] and in the MI literature \[182, 94\], Grünwald, Steinke and Zakynthinou \[85\] unified MI bounds and PAC-Bayes bounds, as they developed “conditional” MI and PAC-Bayes bounds. These bounds are proven to be small for any set of classifiers with finite VC dimension. Thus, they don’t suffer the limitations of PAC-Bayes and MI bounds of \[28, 142, 124\]. To cite the results of \[85\] would go beyond the framework of this “easy introduction”, but one of the main point of this tutorial is to prepare the reader not familiar with PAC-Bayes bounds, Bernstein assumption etc. to read this paper.

### 7 Conclusion

We hope that the reader

- has a better view of what a PAC-Bayes bound is, and what can be done with such a bound,

- is at least a little convinced that these bounds are quite flexible, that they can be used in a wide range of contexts, and for different objectives in ML,
• wants to read many of the references listed above, that provide tighter bounds and clever applications.

I believe that PAC-Bayes bounds (and all the related approaches, including mutual information bounds, etc.) will play an important role in the study of deep learning (in the wake of \[\text{[70]}\]), in RL \[\text{[197]}\] and in meta-learning \[\text{[155, [12]}\ [169].

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