Learning from i.i.d. data under model miss-specification

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Abstract

This paper introduces a new approach to learning from i.i.d. data under model miss-specification. This approach casts the problem of learning as minimizing the expected code-length of a Bayesian mixture code. To solve this problem, we build on PAC-Bayes bounds, information theory and a new family of second-order Jensen bounds. The key insight of this paper is that the use of the standard (first-order) Jensen bounds in learning is suboptimal when our model class is miss-specified (i.e. it does not contain the data generating distribution). As a consequence of this insight, this work provides strong theoretical arguments explaining why the Bayesian posterior is not optimal for making predictions that generalize under model miss-specification because the Bayesian posterior is directly related to the use of first-order Jensen bounds. We then argue for the use of second-order Jensen bounds, which leads to new families of learning algorithms. In this work, we introduce novel variational and ensemble learning methods based on the minimization of a novel family of second-order PAC-Bayes bounds over the expected code-length of a Bayesian mixture code. Using this new framework, we also provide novel hypotheses of why parameters in a flat minimum generalize better than parameters in a sharp minimum.

1 Introduction

The learning problem in machine learning is how to design machines to find patterns in a finite data sample that generalize, i.e. that applies to unseen data samples. In this work, we argue that learning approaches based on empirical risk minimization [Vapnik 1992] or Bayesian learning [Murphy 2012] are not optimal strategies to solve this generalization problem under model miss-specification and i.i.d. data. For the shake of simplicity, our analysis is focused on the use the log-loss and unsupervised settings, but also applies to general loss functions and supervised settings.

We assume we have a finite training data set of i.i.d. samples, \( D = \{x_1, \ldots, x_n\} \), where \( x \in \mathcal{X} \subseteq \mathbb{R}^K \). The samples in \( D \) are generated from some unknown data
generative distribution denoted $\nu(x)$. We also assume we have a parametric probability distribution over $\mathcal{X}$ denoted by $p(x; \theta)$, parametrized by some parameter vector $\theta \in \Theta \subseteq \mathbb{R}^M$. We denote $\mathcal{P} = \{p(x; \theta) : \theta \in \Theta\}$ the family of all possible distributions $p(x; \theta)$ parametrized by some $\theta \in \Theta$. Learning under model miss-specification means that $\nu \not\in \mathcal{P}$.

In empirical risk minimization (ERM) and under the log-loss, the learning problem can be interpreted as finding the parameter $\theta^*$ which defines the probabilistic model $p(x; \theta^*)$ which is closest to $\nu(x)$ in terms of Kullback-Leibler (KL) distance,

$$
\theta^* = \arg\min_{\theta} KL(\nu(x), p(x; \theta))
$$

which can be shown to be equivalent to minimize the so-called expected risk,

$$
\theta^* = \arg\min_{\theta} \mathbb{E}_{\nu(x)} \left[ \ln \frac{1}{p(x; \theta)} \right]
$$

As we do not have access to the data generative distribution, we have to minimize a proxy objective based on the data sample $D$, which is known as the empirical risk,

$$
\theta_{ERM} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ln \frac{1}{p(x_i; \theta)}
$$

Usually, a regularization term is also included to improve the quality of the solution. This approach has an information-theory interpretation based on the construction of optimal two-part codes for compressing the training data $D$ (Grunwald & Grunwald, 2007). The statistical consistency of this approach, i.e. how close are $p(x; \theta^*)$ and $p(x; \theta_{ERM})$, have been extensively studied by the machine learning community usually under i.i.d. data assumptions (Vapnik, 1992; Nagarajan & Kolter, 2019).

In this work, we approach the learning problem in a Bayesian way because we consider distributions over the parameters instead of single point estimates. Let us start introducing the so-called predictive posterior distribution,

$$
p(x) = \int p(x; \theta) \rho(\theta) d\theta = \mathbb{E}_{\rho(\theta)} [p(x; \theta)]
$$

where $\rho(\theta)$ is a probability distribution over $\Theta$ defining this predictive posterior.

The learning problem we study here is to find the probability distribution $\rho(\theta)$ which defines the predictive posterior distribution $p(x)$ which is closest to $\nu(x)$ in terms of Kullback-Leibler (KL) distance,

$$
\rho^* = \arg\min_{\rho} KL(\nu(x), \mathbb{E}_{\rho(\theta)} [p(x; \theta)])
$$

We will see later that this problem is equivalent to find the probability distribution $\rho(\theta)$ which defines a Bayesian mixture code (Grunwald & Grunwald, 2007) with the smallest code-length, in expectation, for the data samples generated from $\nu(x)$. As we do not have access to the data generative distribution, we employ PAC-Bayes bounds (McAllester, 1999) to bound this expected code-length using our finite data sample.
The learning problem then reduces to find the probability distribution $\rho(\theta)$ which minimizes this PAC-Bayes bound over the generalization performance of the Bayesian mixture code.

We show in this work that, under perfect model specification, the Bayesian posterior is an optimal choice because it minimizes a (first-order) PAC-Bayes bound over this expected code-length. However, we also show that, under model miss-specification, this (first-order) PAC-Bayes bound is suboptimal and, in consequence, the Bayesian posterior is suboptimal too for defining predictive posterior distributions that generalize. We then argue for the use of second-order PAC-Bayes bounds to design more optimal learning algorithms.

After this theoretical analysis, we introduce two new families of learning algorithms which are based on the minimization of these second-order PAC-Bayes bounds. The first one is a variational learning algorithm quite close to standard approaches (Blei et al., 2017) but with a modified evidence lower bound functional. And the second one is a simple ensemble learning algorithm (Dietterich, 2000) which can be seen as a particle-based variational inference method and which allows to jointly learn the whole ensemble of models using a simple gradient-based optimization method. This ensemble approach introduces a novel diversity term (Kuncheva & Whitaker, 2003) and provides a clear explanation about why ensembles need diversity to generalize better. Some experiments on toy data samples illustrate these learning algorithms. The code to reproduce these experiments can be found in the following public repository https://github.com/PGM-Lab/PAC2BAYES.

The insights of this work may help to explain why the use of Bayesian approaches do not consistently provide significant performance gains wrt maximum a posteriori (MAP) or (regularized) empirical risk minimization (ERM) estimates in large data samples regimes. We argue that in these large data sample regimes the Bayesian posterior tends to collapse around a single parameter, so the use of MAP/ERM estimates supposes a good approximation of this highly-peaked posterior and, in consequence, they provide similar prediction performance without the complexity of having to employ approximate Bayesian machinery. However, when we consider this new learning framework, we argue that the use of the so-called PAC^2-Bayesian posterior may provide significant improvements in the prediction performance.

We finally exploit the insights obtained in this work to provide novel hypotheses of why parameters in a flat minimum generalize better than parameters in a sharp minimum.

2 Background

2.1 Bayesian Learning

The solution to the learning problem under Bayesian settings (Bernardo & Smith, 2009) is the Bayesian posterior, which is computed by the Bayes’ rule,

$$ p(\theta|D) = \frac{\pi(\theta) \prod_{i=1}^{n} p(x_i|\theta)}{\int \pi(\theta) \prod_{i=1}^{n} p(x_i|\theta) d\theta} $$

3
where $\pi(\theta)$ is known as the prior distribution.

If a new observation $x'$ arrives we compute the posterior predictive distribution to make predictions about $x'$,

$$p(x'|D) = \int p(x'|\theta)p(\theta|D)d\theta$$

The main issue when applying Bayesian machine learning (Murphy, 2012) in real settings is the computation of the (multi-dimensional) integral of the Bayesian posterior. Usually, the computation of this integral is not tractable and we have to resort to approximate methods. Variational inference (VI) (Blei et al., 2017) is a popular method in Bayesian machine learning to compute an approximation of the Bayesian posterior. In standard VI settings, we choose a tractable family of probability distributions over $\Theta$, denoted by $Q$, and the learning problem consists on finding the probability distribution $q \in Q$ which is closest to the Bayesian posterior in terms of (inverse) KL distance,

$$\arg \min_{q \in Q} KL(q(\theta), p(\theta|D))$$

(2)

For solving the above minimization problem, we exploit the following equality,

$$\ln p(D) = \mathcal{L}(q) + KL(q(\theta), p(\theta|D)),$$

(3)

where $\ln p(D)$ is the marginal likelihood of the training data, and $\mathcal{L}(q)$ is defined as

$$\mathcal{L}(q) = \mathbb{E}_{q(\theta)}[\ln p(D|\theta)] - KL(q, \pi),$$

$\mathcal{L}(q)$ is known as the evidence lower bound (ELBO) function because it is a lower-bound of the marginal likelihood of the training data,

$$\ln p(D) \geq \mathcal{L}(q).$$

So, due to the equality of Equation (3), the minimization problem of Equation (2) is equivalent to the following maximization problem,

$$\arg \max_{q \in Q} \mathbb{E}_{q(\theta)}[\ln p(D|\theta)] - KL(q, \pi)$$

(4)

There is a myriad of powerful methods for solving this maximization problem for many different probabilistic models (see (Zhang et al., 2018) for a recent review).

The ELBO function $\mathcal{L}(q)$ also provides an insightful characterization of the Bayesian posterior,

**Lemma 1.** If the Bayesian posterior belongs to $Q$, i.e. $p(\theta|D) \in Q$, then the Bayesian posterior can be characterized as the maximum of the ELBO function,

$$p(\theta|D) = \arg \max_{q \in Q} \mathbb{E}_{q(\theta)}[\ln p(D|\theta)] - KL(q, \pi)$$

(5)

**Proof.** It follows by looking at the equality of Equation (3). As the lhs of the equality is constant, when maximizing $\mathcal{L}(q)$ we also minimize the $KL$ term. As this KL term is always positive or zero, we can deduce that the maximum of $\mathcal{L}(q)$ is attained for $p(\theta|D)$. □
2.2 PAC-Bayesian Analysis

The PAC-Bayes framework (McAllester, 1999) provides data-dependent generalization guarantees for Gibbs or randomized classifiers. Like in frequentist learning theories, the main assumption in the PAC-Bayes framework is that your training data sample \( D = \{ (x_1, y_1), \ldots, (x_n, y_n) \} \) is generated from some data generative distribution denoted by \( \nu(x, y) \). Thus, we assume that \( D \) is an i.i.d. sample of \( n \) observations, which we denote as \( D \sim \nu^n(x, y) \). Following a frequentist perspective, we consider a loss function \( \ell : \Omega \times \mathcal{X} \times \mathcal{Y} \to [0, 1] \). Then, we define the empirical loss on the sample \( D \), denoted \( \hat{L} (\theta, D) \), and the generalization loss for the hypothesis \( \theta \), denoted \( L(\theta) \), as

\[
\hat{L} (\theta, D) = \frac{1}{n} \sum_{i=1}^{n} \ell(\theta, x_i, y_i) \quad \quad L(\theta) = \mathbb{E}_{\nu(x,y)}[\ell(\theta, x, y)]
\]

The PAC-Bayesian theory provides probably approximate correct generalization bounds on the (unknown) expected loss \( \mathbb{E}_{\rho(\theta)}[L(\theta)] \) given the empirical estimate \( \mathbb{E}_{\rho(\theta)}[\hat{L}(\theta, D)] \) and some other parameters, which includes a prior \( \pi(\theta) \) over the hypothesis space \( \Theta \) independent of the training sample. The following result, due to (Catoni, 2007), states a standard PAC-Bayes bound,

**Theorem 1.** (Catoni, 2007, Theorem 1.2.6) For any prior distribution \( \pi \) over \( \Theta \) and for any \( \xi \in (0, 1) \) and \( C > 0 \), with probability at least 1 − \( \xi \) over draws of training data \( D \sim \nu^n(x, y) \), for all mixture distribution \( \rho \) over \( \Theta \),

\[
\mathbb{E}_{\rho(\theta)}[L(\theta)] \leq \frac{1}{1 - e^{-c}} \left( C \mathbb{E}_{\rho(\theta)}[\hat{L}(\theta, D)] + \frac{KL(\rho, \pi)}{n} + \frac{\ln \frac{1}{\xi}}{n} \right)
\]

The above result shows how an optimal \( \rho \) distribution should optimizes the trade-off between the empirical expected loss \( \mathbb{E}_{\rho(\theta)}[\hat{L}(\theta, D)] \) and the KL divergence between \( \rho \) and the prior \( \pi \). This last term acts as a regularizer avoiding that the distribution \( \rho \) collapses around a single parameter minimizing the empirical loss.

For the rest of the paper, unless otherwise stated, we will only work with the so-called log-loss, so we will use the notation introduced in this section to refer to the log-loss.

2.3 Minimum Description Length and Information Theory

The Minimum Description Length (MDL) principle (Grünwald & Grunwald, 2007) is a generic method for model selection which relates learning with data compression. MDL builds on the idea that any pattern in the data can be exploited for compressing the data. And that the more we are able to compress the data the more we learn about the data (Grünwald & Grunwald, 2007). So, among all the possible models, we should choose the one which best compresses the training data.

\footnote{We temporarily introduce \( y \) in this section to make the notation consistent with the focused of PAC-Bayesian theory on supervised classification.}

\footnote{Yang et al., 2019, Theorem 2.2) is equivalent and easier to read.}
Information theory (Shannon, 1948) provides the well-known one-to-one relationship between a probabilistic model \( p(x|\theta) \) and a coding scheme, because \( \ell(x, \theta) = \ln \frac{1}{p(x|\theta)} \) defines the maximum number of nats needed to optimally encode the observation \( x \) according to the code scheme defined by \( \theta \). So, according to MDL, we should select the hypothesis \( \theta \) that best compress the training data \( D \) with fewer nats. I.e. we should select the hypothesis \( \theta \) which minimizes \( L(D, \theta) = \sum_{i=1}^{n} \ln \frac{1}{p(x_i|\theta)} \), which is the number of nats needed to encode the training data set \( D \) according to hypothesis \( \theta \). Moreover, according to MDL, we must also consider the coding length of the hypothesis \( \theta \) (to prevent for overfitting), which can be done by defining a prior \( \pi(\theta) \) over the hypothesis space \( \Theta \), which defines the number of nats needed to encode \( \theta \). \( \pi(\theta) \) induces a penalty to account for the complexity of \( \Theta \). The optimal hypothesis according to this two-part coding scheme is the one that minimizes the following quantity,

\[
\min_{\theta \in \Theta} L(D, \theta) + \ln \frac{1}{\pi(\theta)}
\]

Bayesian mixture codes (Grunwald & Grunwald, 2007) are an alternative class of coding schemes. A Bayesian mixture code would assign the following code length to the training data set \( D \),

\[
\bar{L}(D, \pi) = -\ln \mathbb{E}_{\pi(\theta)} \left[ \prod_{i=1}^{n} p(x_i|\theta) \right] = -\ln p(D)
\]

where \( \pi(\theta) \) plays the role of the mixture distribution of the Bayesian code.

Bayesian codes control the complexity of the hypothesis space \( \Theta \) by taking expectation or, equivalently, marginalizing out over \( \pi(\theta) \). For finite hypothesis spaces, Bayesian mixture codes always provides better coding schemes than two-part coding schemes (Grunwald & Grunwald, 2007).

### 2.4 The Dirac-delta Function

The Dirac-delta function (Friedman, 1990), \( \delta_{\theta_0} : \Theta \rightarrow \mathbb{R}^+ \) with parameter \( \theta_0 \in \Theta \), is a generalized function with the following property

\[
\int \delta_{\theta_0}(\theta)f(\theta)d\theta = f(\theta_0)
\]  

for any continuous function \( f : \Theta \rightarrow \mathbb{R} \). The Dirac-delta function also defines the density function of a probability distribution because it is positive and, by the above property, \( \int \delta_{\theta_0}(\theta)d\theta = 1 \). This Dirac-delta distribution is a degenerated probability distribution which always samples the same value \( \theta_0 \) because \( \delta_{\theta_0}(\theta) = 0 \) if \( \theta \neq \theta_0 \). We also have that the entropy of a Dirac-delta distribution is minus infinity, \( H(\delta_{\theta_0}) = -\infty \) because \( \ln \delta_{\theta_0}(\theta_0) = \infty \) (Friedman, 1990).

\[^3\text{For the sake of simplicity, when computing code lengths we obviate rounding terms and always consider the natural logarithm.}\]
3 The learning problem

We approach the following learning problem. There is a computing machine, called the learner, which is observing the outside world through a digital sensor.

**Assumption 1.** The sensor readings \( \{x_1, x_2, \ldots\} \) are i.i.d from an unknown but fixed distribution \( \nu(x) \), known as the data generative distribution.

There is another machine, called the receiver, connected to the learner through a noiseless channel. The learner wants to send to the receiver the information it is getting from the outside world. As the communication channel between them has a limited bandwidth, the learner must compress the information before sending it to the receiver.

For compressing the sensor information, the learner chooses a parametric probability distribution family \( P = \{ p(x|\theta) : \theta \in \Theta \subseteq R^M \} \), and wants to build a Bayesian mixture code for computing the code length of an observation \( x \in X \), denoted by \( \bar{\ell}(x, \rho) \),

\[
\bar{\ell}(x, \rho) = \ln \frac{1}{E_{\rho(\theta)}[p(x|\theta)]}
\]

where \( \rho \), a probability distribution over \( \Theta \), is the mixture distribution of the Bayesian code.

We denote \( \bar{L}(\rho) \) the expected code length of the Bayesian mixture code defined by \( \rho \),

\[
\bar{L}(\rho) = E_{\nu(x)}[\bar{\ell}(x, \rho)]
\]

The learning problem we study in this paper is how the learner, using only a finite set of i.i.d. observations \( D \), can find a mixture distribution \( \rho \) which minimizes this expected code length for the observations coming from \( \nu(x) \), i.e. the outside world.

\[
\rho^* = \arg \min_{\rho} \bar{L}(\rho)
\]

As the learner has a limited memory capacity, this imposes several restrictions when learning. The first one is on the number of parameters \( M \) defining the distribution \( p(x|\Theta) \). In that way, we are under limited modelling capacity because more powerful models tend to require a higher number of parameters, which we need to store in memory. For example, [Sutskever & Hinton 2008] shows that deep sigmoid neural networks can approximate any distribution over binary vectors to arbitrary accuracy, even when the width of each layer is limited to the length of the binary vectors, but these networks need exponential depth. So, a key assumption in this work is the following,

**Assumption 2.** The learner operates under model miss-specification, \( \nu \notin P \).

Moreover, we also assume that the model class is non-identifiable,

**Assumption 3.** The model class \( P \) is non-identifiable. And we denote \( \Omega_{\theta_0} \), the set of parameters which defines the same distribution than \( \theta_0 \), i.e. if \( \theta' \in \Omega_{\theta_0} \subseteq \Theta \) then \( \forall x \in X \ p(x|\theta_0) = p(x|\theta') \).
Another consequence derived for the limited memory capacity of the learner is an upper bound on the maximum code length the learner can assign to any observation \( x \) in the support of the distribution \( \nu \), denoted by \( \text{supp}(\nu) = \{ x \in X : \nu(x) > 0 \} \). In this way, we assume that

**Assumption 4.** The learner operates in a setting where \( \forall x \in \text{supp}(\nu), \forall \theta \in \Theta \)

\[
0 \leq \ln \frac{1}{p(x|\theta)} \leq B,
\]

where \( B > 0 \) is the upper bound.

Although this assumption is violated in many statistical learning settings, we argue this is not the case in many real machine learning settings. We have to consider that the sensor readings are always finite-precision numbers, which implies that the norm of the input vectors \( |x| \) is bounded. In Appendix A we provide a formal treatment of this fact, which is not included here for the sake of simplicity. In Appendix B we show how we can easily define many standard machine learning models satisfying Assumption 4 by using this bounded norm assumption over the input vectors and, also, by the fact that we are free to constrain the parameter space \( \Theta \).

Finally, the learner has always to choose a uniquely decodable code [Cover & Thomas, 2012] to guarantee an error-free communication with the receiver. We should note that these learning settings guarantee that because they satisfy the Kraft inequality [Cover & Thomas, 2012],

\[
\int e^{-\tilde{L}(\rho)} d\mathbf{x} = \int E_{\rho(\theta)}[p(x|\theta)] d\mathbf{x} = \int p(x) d\mathbf{x} = 1.
\]

Finally, as commented in the introduction, we should note that this learning problem, as stated in Equation (8), is equivalent to the minimization problem involving the KL distance between the data generative distribution \( \nu(x) \) and the predictive posterior \( E_{\rho(\theta)}[p(x|\theta)] \) defined by \( \rho \), as stated in Equation (1). They are equivalent because this KL distance can be expressed in the following form,

\[
KL(\nu(x), E_{\rho(\theta)}[p(x|\theta)]) = \bar{L}(\rho) - H(\nu)
\]

where \( H(\nu) \) denotes the entropy of \( \nu(x) \). As this entropy is constant wrt to \( \rho \), minimize this KL distance over \( \rho \) is equivalent to minimize \( \bar{L}(\rho) \), i.e. the expected code-length a Bayesian mixture code.

### 4 The three gaps of learning

We describe here the three gaps the learner should overcome to optimally solve the learning problem describe in the previous section (Equation (8)). These three gaps are associated to the following three inequalities,

\[
H(\nu) \leq \bar{L}(\rho) \leq \bar{L}_J(\rho) \leq \bar{L}_{PB}(D, \rho)
\]
where $H(\nu)$ denotes the entropy of the data generative distribution, $\bar{L}(\rho)$ the expected code length of the Bayesian mixture code defined by the mixture distribution $\rho$, $\bar{L}_j(\rho)$ is the so-called Jensen bound which depends of $\rho$, and $\bar{L}(D, \rho)$ is the PAC-Bayes bound which depends of $\rho$ and the observed data set $D$.

The learner has to minimize $\bar{L}(\rho)$ to maximize the level of compression of the observations coming from the outside world that are sent to the receiver. But the learner can not perform this minimization over $\bar{L}(\rho)$ directly because it has no access to the data generative distribution $\nu$. So, the learning strategy is to upper bound this function with some other function which depends on the observed data set $D$, which is $\bar{L}_{PB}(D, \rho)$ in this case. The learner will then perform the minimization over this function $\bar{L}_{PB}(D, \rho)$ with the hope that by minimizing it, it will also minimize the $\bar{L}(\rho)$ function. In the next sections, we detail this learning strategy and present and analyze these bounding functions, their associated gaps and which role they play in the learning process.

### 4.1 The Kullback-Leibler gap

From information theory (Cover & Thomas 2012), we know that the expected code length is bounded below from the entropy of the data generative distribution, denoted by $H(\nu)$. The following result shows that this is also the case here.

**Theorem 2.** Let us denote $H(\nu)$ the entropy of the distribution $\nu(x)$, then we have that for any mixture distribution $\rho$ on $\Theta$,

$$H(\nu) \leq \bar{L}(\rho),$$

where the equality only holds if the data generative distribution $\nu(x)$ and the posterior predictive distribution $p(x) = \mathbb{E}_{\rho(\theta)}[p(x|\theta)]$ are equal.

**Proof.** As we have that the KL distance between $\nu(x)$ and $p(x)$ is always greater or equal than zero, we also have that

$$KL(\nu(x), p(x)) = \mathbb{E}_{\nu(x)}[\ln \nu(x)] + \mathbb{E}_{\nu(x)}[\frac{1}{\mathbb{E}_{\rho(\theta)}[p(x|\theta)]}]$$

$$= -H(\nu(x)) + \mathbb{E}_{\nu(x)}[\bar{\ell}(x, \rho)]$$

$$= -H(\nu(x)) + \bar{L}(\rho) \geq 0$$

and the statement follows from the last inequality. \qed

We define the **Kullback-Leibler gap** as the difference between the expected code length achieve by the mixture distribution $\rho^*$ minimizing $\bar{L}$ (see Equation (8)) and the overall optimal code length defined by the entropy of $\nu$, $H(\nu)$. And this gap corresponds to the Kullback-Leibler distance between the data generative distribution $\nu(x)$ and the posterior predictive distribution $p(x)$,

$$KL(\nu(x), \mathbb{E}_{\rho^*(\theta)}[p(x|\theta)]) = \bar{L}(\rho^*) - H(\nu).$$

(9)
The KL gap is null under perfect model specification

Under perfect model specification (i.e. $\nu \in \mathcal{P}$), the following result shows that an optimal mixture distribution $\rho$ would be a Dirac-delta distribution centered in the parameter vector matching the data generative distribution.

**Lemma 2.** Under perfect model specification (i.e. $\nu \in \mathcal{P}$), by definition, there exist a $\theta^*_\nu \in \Theta$, such that $\nu(x) = p(x|\theta^*_\nu)$. In this case, the mixture distribution $\rho^*_\nu$ defined as a Dirac-delta distribution centered in this parameter vector:

$$\rho^*_\nu(\theta) = \delta_{\theta^*_\nu}(\theta),$$

is a minimizer of $\bar{L}$, and

$$H(\nu) = \bar{L}(\rho^*) = \bar{L}(\rho^*_\nu),$$

where $\rho^*$ is a minimizer of $\bar{L}$, as defined in Equation (8). And we can say that $\rho^*_\nu$ is an optimal mixture distribution because it achieves the best possible expected code-length, which is $H(\nu)$.

**Proof.** If $\nu(x) = p(x|\theta^*_\nu)$, then KL distance between $\nu(x)$ and $p(x|\theta^*_\nu)$ is equal to zero and the equality $H(\nu) = \bar{L}(\rho^*)$ follows from Equation (9). Then, we have $H(\nu) = L(\rho^*) \leq L(\rho)$ for any $\rho$, where the inequality follows from Theorem 2. In consequence, $\rho^*_\nu$ is a global minimizer of $\bar{L}$. □

The above result can be extended to distributions $\rho$ over the non-identifiable parameters in $\Omega_{\theta^*_\nu}$.

**Corollary 1.** Any distribution $\rho'$ whose support is contained in $\Omega_{\theta^*_\nu}$, i.e. $\text{supp}(\rho') \subseteq \Omega_{\theta^*_\nu}$, is a global minimizer of $\bar{L}$, and

$$H(\nu) = \bar{L}(\rho^*) = \bar{L}(\rho').$$

**Proof.** By definition we have that if $\theta' \in \text{supp}(\rho') \subseteq \Omega_{\theta^*_\nu}$, then $\forall x \in X \ p(x|\theta^*_\nu) = p(x|\theta')$. In consequence, $E_{\rho'/(\theta)}[\nu(x|\theta)] = p(x|\theta^*_\nu) = E_{\rho^*_\nu/(\theta)}[\nu(x|\theta)]$, which implies that $\bar{L}(\rho^*_\nu) = \bar{L}(\rho')$. □

So, the KL gap is null under perfect model specification.

The role of the KL gap in learning

The KL gap defines the first limitation the learner encounters when learning. First, there is a lower bound limit on the quality of the coding the learner can achieve. And this limit is defined by the entropy of the data generative distribution, i.e. the nature of the outside world. But the KL gap tells us about the loss the learner incurs when learning under a limited modeling capacity (c.f. Assumption 2), which is caused from the inherently limited memory capacity of the learner. So, the only way to address this gap is by increasing the modeling and memory capacity of the learner.
4.2 The Jensen gap

In this section, we analyze the consequences on the learning strategy defined at the beginning of Section 4 when employing Jensen bounds, i.e. the consequences of having to move an expectation out of a function. In the first part, we start by analyzing what happens when we try to minimize standard (first-order) Jensen bounds. And, in the second part, we repeat this same analysis for second-order Jensen bounds. We then show that the Jensen gap is null under perfect model specification, i.e. there are no consequences for applying Jensen bounds in this case, and we finish this section discussing the implications of this gap on learning.

First-order Jensen bounds

Let us denote $L(\theta)$ the expected code-length achieved by the parameter $\theta$,

$$L(\theta) = E_{\nu(x)}[\ln \frac{1}{p(x|\theta)}].$$

As the logarithm function is a convex function, we can apply Jensen inequality to derive an upper bound over $\bar{L}(\rho)$ using the expected value of $L(\theta)$ wrt to $\rho$.

Let us denote $\bar{L}_J(\rho)$ the so-called first-order Jensen bound.

$$\bar{L}_J(\rho) = E_{\rho(\theta)}[L(\theta)]$$

Then, we have that

**Lemma 3.** Any distribution $\rho$ over $\Theta$ satisfies the following inequality,

$$H(\nu) \leq \bar{L}(\rho) \leq \bar{L}_J(\rho).$$

**Proof.** This result is a straightforward application of the Jensen inequality over the $\bar{L}(\rho)$ function,

$$\bar{L}(\rho) = -E_{\nu(x)}[\ln E_{\rho(\theta)}[p(x|\theta)]]$$

$$\leq -E_{\nu(x)}[E_{\rho(\theta)}[\ln p(x|\theta)]]$$

$$= E_{\rho(\theta)}[E_{\nu(x)}[\ln \frac{1}{p(x|\theta)}]]$$

□

Due to model non-identifiability, there could potentially be many different minimisers of the Jensen bound, but the following two results clearly characterize a mixture distribution $\rho$ attaining a minimum,

**Lemma 4.** Let us define $\theta^*_J$ a minimizer of $L(\theta)$,

$$\theta^*_J = \arg \min_{\theta} L(\theta)$$
The mixture distribution \( \rho^*_J \) defined as a Dirac-delta distribution center around \( \theta^*_J \),

\( \rho^*_J(\theta) = \delta_{\theta^*_J}(\theta) \) is a minimizer of the Jensen bound,

\[
\rho^*_J = \arg\min_{\rho} \bar{L}_J(\rho),
\]

and the density \( p(x|\theta^*_J) \) minimizes the KL-distance with respect to \( v(x) \),

\[
\theta^*_J = \arg\min_{\theta} KL(v(x), p(x|\theta))
\]

**Proof.** We first have that \( L(\theta) = E_{v(x)}[\ln \frac{1}{p(x|\theta)}] \geq 0 \) because, due to Assumption 4, \( \ln \frac{1}{p(x|\theta)} \geq 0 \). We also have that \( \int L(\theta)\rho(\theta)d\theta \geq \min_{\theta} L(\theta) \int \rho(\theta)d\theta \), because \( L(\theta) \geq 0 \). In consequence, \( E_{\rho(\theta)}[L(\theta)] \geq L(\theta^*_J) \). So, \( \rho^*_J(\theta) = \delta_{\theta^*_J}(\theta) \) will always be a minimizer of the Jensen bound, because \( E_{\rho(\theta)}[L(\theta)] \geq L(\theta^*_J) = E_{\rho^*_J(\theta)}[L(\theta)] \). The last KL equality of this lemma follows because \( KL(v(x), p(x|\theta)) = -H(v) + L(\theta) \), and \( H(v) \) is constant wrt to \( \theta \), so it does not influence the minimization. \( \square \)

**Corollary 2.** Any distribution \( \rho' \) whose support is contained in \( \Omega_{\theta^*_J} \), i.e. \( \text{supp}(\rho') \subseteq \Omega_{\theta^*_J} \), is a minimizer of the Jensen bound \( \bar{L}_J(\rho) \).

**Proof.** By definition we have that if \( \theta' \in \text{supp}(\rho^*_J) \subseteq \Omega_{\theta^*_J} \), then \( \forall x \in X \ p(x|\theta^*_J) = p(x|\theta') \). In consequence, \( E_{\rho'(\theta)}[L(\theta)] = L(\theta^*_J) = E_{\rho^*_J(\theta)}[L(\theta)] \). \( \square \)

In this sense, we define the Jensen GAP as the loss in the expected code-length the learner incurs when using \( \rho^*_J \) instead of \( \rho^* \) for coding,

\[
\bar{L}(\rho^*_J) - \bar{L}(\rho^*)
\]

**Second-order Jensen bounds**

Here, we exploit a recent result \( \text{[Liao & Berg, 2019]} \) for deriving a tighter (second-order) Jensen bound. We will refer to this bound as the second-order Jensen bound, or the Jensen\(^2\) bound, denoted by \( \bar{L}_{J^2}(\rho) \),

\[
\bar{L}_{J^2}(\rho) = E_{\rho(\theta)}[L(\theta)] - \nabla(\rho) \tag{11}
\]

where \( \nabla(\rho) \) denotes the expected (normalized) variance of \( p(x|\theta) \) wrt \( \rho(\theta) \),

\[
\nabla(\rho) = E_{v(x)}\left[ \frac{1}{2\max_{\theta} p(x|\theta)^2} E_{\rho(\theta)}[(p(x|\theta)-p(x))^2] \right].
\]

where the maximization operation has to be performed only over the support of \( \rho \). The following result proves that \( \bar{L}_{J^2}(\rho) \) also bounds the \( \bar{L}(\rho) \) function.

**Theorem 3.** Any distribution \( \rho \) over \( \Theta \) satisfies the following inequality,

\[
H(\nu) \leq \bar{L}(\rho) \leq \bar{L}_{J^2}(\rho).
\]

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Figure 1: Graphical description of the three gaps of learning for a toy example. The ρ distribution can be defined with a single parameter between 0 and 1. In the model miss-specification case, there exists a ρ distribution achieving the optimal code-length, but the Jensen bound is minimized with a Dirac-delta distribution (i.e. ρ = 1). While the minimum of the Jensen^2 bound achieves a much better result. In the case of perfect model specification, everything is much simpler and both the Jensen and the Jensen^2 bound achieve optimal results.
Proof. Applying Taylor’s theorem to $\ln y$ about $\mu$ with a mean-value form of the remainder gives,

$$
\ln y = \ln \mu + \frac{1}{\mu} (y - \mu) - \frac{1}{2g(y)^2} (y - \mu)^2,
$$

where $g(y)$ is a real value between $y$ and $\mu$. Therefore,

$$
E_{\rho(\theta)}[\ln p(x|\theta)] = \ln E_{\rho(\theta)}[p(x|\theta)] - E_{\rho(\theta)}\left[\frac{1}{2g(p(x|\theta))^2} (p(x|\theta) - p(x))^2\right]
$$

Rearranging we have

$$
- \ln E_{\rho(\theta)}[p(x|\theta)] = -E_{\rho(\theta)}[\ln p(x|\theta)] - E_{\rho(\theta)}\left[\frac{1}{2g(p(x|\theta))^2} (p(x|\theta) - p(x))^2\right]
\leq -E_{\rho(\theta)}[\ln p(x|\theta)] - \frac{1}{2\max_{\theta} p(x|\theta)^2} E_{\rho(\theta)}[(p(x|\theta) - p(x))^2],
$$

where the inequality is derived from that fact $(p(x|\theta) - p(x))^2$ is always positive and $g(p(x|\theta))$, which is a real number between $p(x|\theta)$ and $E_{\rho(\theta)}[p(x|\theta)]$, is upper bounded by $\max_{\theta} p(x|\theta)$, where the max operation is over the support of $\rho$.

Finally, the result of the theorem is derived by taking expectation wrt $\nu(x)$ on both sides of the above inequality. $\square$

We can see that the Jensen$^2$ bound is a tighter bound than the Jensen bound because it introduces a quadratic or variance term which is always positive. This will avoid the problems of the first-order Jensen bound, and when minimizing this new bound we will not have to end up in a Dirac-delta distribution because the variance term will push the minimum away for this extreme solution. Figure[1] graphically illustrates this situation for a probabilistic model, both in the case of perfect model specification and model miss-specification.

The following result will show that the Jensen$^2$ bound is not affected by model identifiability (c.f. Assumption[3]). I.e., we can not trick the minimization of the Jensen$^2$ bound by getting $\rho^*_y$, which minimizes the Jensen bound $L_2(\rho)$, and then expand the support of $\rho^*_y$ to other parameters defining the same probability density, i.e. $\Omega_{\theta^*_y}$, because the variance term of the Jensen$^2$ bound is, even in this case, zero. This is formalized in the following result.

Lemma 5. For any distribution $\rho'$ such that, $\text{supp}(\rho') \subseteq \Omega_{\theta^*_y}$, the variance term of the Jensen$^2$ bound is equal to zero, $\forall (\rho') = 0$.

Proof. Because $\text{supp}(\rho') \subseteq \Omega_{\theta^*_y}$, we have that $E_{\rho'([\theta])}[p(x|\theta)] = p(x|\theta^*_y)$. In consequence, $E_{\rho'([\theta])}[p(x|\theta)] = E_{\rho'([\theta])}[p(x|\theta)] = 0$ because $p(x|\theta) = p(x|\theta^*_y)$ for any $\theta \in \text{supp}(\rho')$. So, $\forall (\rho') = 0$. $\square$

The following result tell us that the expected code-length of a mixture distribution $\rho$ minimizing the Jensen$^2$ bound is always at least as good as the mixture distribution minimizing the Jensen bound.
Lemma 6. Let us denote $\rho_2^*$ and $\rho_J^*$ two mixtures distribution minimizing the Jensen\textsuperscript{2} bound, $L_{J_2}(\rho)$, and the Jensen bound, $L_J(\rho)$, respectively. The following inequalities hold

\[ H(\nu) \leq \bar{L}(\rho^*) \leq \bar{L}(\rho_{J_2}^*) \leq \bar{L}(\rho_J^*). \]

Proof. Let us define $\Delta$ the space of all the mixture distributions $\rho$ which are a Dirac-delta distribution. Then, we have that the minimum of the Jensen\textsuperscript{2} bound for all the mixture distributions $\rho \in \Delta$ can be written as,

\[ \min_{\rho \in \Delta} \mathbb{E}_{\nu(\theta)}[L(\theta)] - \mathbb{V}(\rho) = \min_{\rho \in \Delta} \mathbb{E}_{\rho(\theta)}[L(\theta)] = \mathbb{E}_{\nu(\theta)}[L(\theta)], \]

where the first inequality follows because if $\rho \in \Delta$ then $\mathbb{V}(\rho) = 0$, and the second equality follows from Lemma 4. We also have that

\[ \mathbb{E}_{\rho_{J_2}^*(\theta)}[L(\theta)] - \mathbb{V}(\rho_{J_2}^*) \leq \mathbb{E}_{\rho_{J_2}^*(\theta)}[L(\theta)] \]

because, by definition, the left hand side of the inequality is the minimum of the Jensen\textsuperscript{2} bound for all the mixture distributions $\rho$, while the right hand side of the inequality is the minimum of the Jensen\textsuperscript{2} bound but only for those mixture distributions $\rho \in \Delta$.

By chaining the above inequality with the Jensen\textsuperscript{2} bound inequality of Theorem 3, we have

\[ \bar{L}(\rho_{J_2}^*) \leq \mathbb{E}_{\rho_{J_2}^*(\theta)}[L(\theta)] \]

Finally, we have that,

\[ \mathbb{E}_{\rho_J^*(\theta)}[L(\theta)] = L(\theta_J^*) = \mathbb{E}_{\nu(x)}[\ln \frac{1}{\hat{p}(x|\theta_J^*)}] = \mathbb{E}_{\nu(x)}[\ln \frac{1}{\mathbb{E}_{\rho_{J_2}^*(\theta)}[p(x|\theta)]}] = \bar{L}(\rho_J^*), \]

where first equality follows from the property of Dirac-delta distributions (see Equation 5), the second equality follows from the definition of $L(\theta)$, the third equality follows again from the property of Dirac-delta distributions, and the last equality follows from the definition of $\bar{L}$.

The inequality $H(\nu) \leq \bar{L}(\rho^*)$ follows from Theorem 2 and $\bar{L}(\rho^*) \leq \bar{L}(\rho_{J_2}^*)$ follows because, by definition, $\rho^*$ is a global minimizer of $\bar{L}$. \qed

We define the Jensen gap in this case as the loss incurred by the application of this Jensen\textsuperscript{2} bound as,

\[ \bar{L}(\rho_{J_2}^*) - \bar{L}(\rho^*) \]

i.e. the difference between the expected code-length achieved by they mixture distribution $\rho_{J_2}^*$, minimizing the Jensen\textsuperscript{2} bound and the expected code-length achieved by the optimal mixture distribution $\rho^*$. Figure 1 graphically illustrates this gap for a toy probabilistic model.
The Jensen gap is null under perfect model specification

In the case of perfect model specification, we have that both the Jensen bound and Jensen² bound are tight, and that \( \rho_J^* \) and \( \rho_J^2 \) are optimal.

**Lemma 7.** If \( \nu \in \mathcal{P} \), then we have,

\[
H(\nu) = \bar{L}(\rho^*) = \bar{L}(\rho_J^2) = \bar{L}(\rho_J^*),
\]

and, then, \( \rho_J^* \) and \( \rho_J^2 \) are both optimal mixture distributions.

**Proof.** If \( \nu \in \mathcal{P} \), then, by definition, \( \min_{\theta} KL(\nu(x), p(x|\theta)) = 0 \). In consequence, \( KL(\nu(x), p(x|\theta_J^*)) = 0 \) because \( \theta_J^* \) is a minimizer of this KL distance according to Lemma 4. Then, by Equation (9), we have \( H(\nu) = \bar{L}(\rho^*) \). And \( \bar{L}(\rho_J^2) = \bar{L}(\rho_J^*) \) because of Lemma 2. Finally, the lemma statement follows by also considering Lemma 6 which states that \( H(\nu) \leq \bar{L}(\rho^*) \leq \bar{L}(\rho_J^*), \) \( \bar{L}(\rho_J^2) \leq \bar{L}(\rho_J^*) \). \( \square \)

Lemma 7 shows that the Jensen gap is null under perfect model specification. So, minimizing the Jensen² bound will provide the same result than the minimization of the Jensen bound, and both will be optimal. Again, this is graphically illustrated in Figure 1 for a toy probabilistic model.

**The role of the Jensen gap in learning**

This gap defines a second limitation the learner encounters when learning. It comes directly from the cost of moving and expectation out of a function. We have seen in this section that first-order Jensen bounds can induce the learner to pick up a suboptimal solution. The introduction of a second-order bound alleviates this problem and leads to better solutions (see Lemma 6). The size of this gap and the quality of the learning is going to depend on the quality of the Jensen bound we employ. The only way to address this gap is by using tighter Jensen bounds. Later, in Section 5.1, we will introduce a new second-order Jensen bound which is tighter, but more elaborated, than the second-order Jensen bound described here and which leads to better learning algorithms.

### 4.3 The PAC-Bayes gap

In this last step, we introduce the PAC-Bayes bound. As we saw on Section 2.2, PAC-Bayes bounds are not deterministic, they are probabilistic in the sense that they only hold with a given probability \( 1 - \xi \), with \( \xi \in (0, 1) \), over draws of the training data \( D \sim \nu^n(x) \).

The PAC-Bayes bound for \( \bar{L}_J(\rho) \) follows directly from the application of Theorem 1. We denote \( \bar{L}_{PB}(D, \rho) \) to this first-order PAC-Bayes bound, which is defined as,

\[
\bar{L}_{PB}(D, \rho) = \frac{B}{1 - e^{-B}} \left( \mathbb{E}_{\rho(\theta)}[\bar{L}(D, \theta)] + \frac{KL(\rho, \pi) + \ln \frac{1}{\xi}}{n} \right)
\]
where $\pi$ is a prior distribution over $\Theta$, $B$ is the bound of the log-loss (see Assumption 4), and $\hat{L}(D, \theta)$ is the empirical log-loss of $\theta$.

$$
\hat{L}(D, \theta) = \frac{1}{n} \sum_{i=1}^{n} \ln \frac{1}{p(x_i|\theta)} = -\frac{1}{n} \ln p(D|\theta)
$$

Then, we prove that $\hat{L}_{PB}(D, \rho)$ bounds $\hat{L}_f(\rho)$.

**Lemma 8.** For any prior distribution $\pi$ over $\Theta$ and for any $\xi \in (0, 1)$, with probability at least $1 - \xi$ over draws of training data $D \sim \nu^n(x)$, for all mixture distribution $\rho$ over $\Theta$, $H(\nu) \leq \hat{L}(\rho) \leq \hat{L}_{PB}(D, \rho)$

**Proof.** It follows directly from the application of Theorem 1 to the normalized loss $\frac{1}{B} \ell(x, \theta) = \frac{1}{B} \ln \frac{1}{p(\theta|x)}$. □

The derivation of the PAC-Bayes bound for $\hat{L}_{PB}(D, \rho)$ is a bit more involved. We need first to rewrite the $\hat{L}_{PB}(\rho)$ function.

**Lemma 9.** For any distribution $\rho$ over $\Theta$, the Jensen’s bound can be expressed as follows,

$$
\hat{L}_{PB}(\rho) = \mathbb{E}_{\rho(\theta, \theta')}[\mathbb{E}_{\nu(x)}[\ell(x, \theta, \theta')]],
$$

where $\theta, \theta' \in \Theta$, $\rho(\theta, \theta') = p(\theta)p(\theta')$, and $\ell(x, \theta, \theta')$ is defined as

$$
\ell(x, \theta, \theta') = \ln \frac{1}{p(x|\theta)} - \frac{1}{2 \max_{\theta} p(x|\theta)^2} (p(x|\theta)^2 - p(x|\theta)p(x|\theta')),
$$

**Proof.** The proof is straightforward by applying first this equality,

$$
\mathbb{E}_{p(x|\theta)}[p(x|\theta) - p(x)]^2 = \mathbb{E}_{p(x|\theta)}[p(x|\theta)^2] - \mathbb{E}_{p(x|\theta)}[p(x|\theta)]^2,
$$

and, after that, the following equality,

$$
\mathbb{E}_{p(x|\theta)}[p(x|\theta)p(x|\theta')] = \mathbb{E}_{p(x|\theta)}[p(x|\theta)]\mathbb{E}_{p(x|\theta)}[p(x|\theta')] = \mathbb{E}_{p(x|\theta)}[p(x|\theta)]^2
$$

□

To introduce this new second-order PAC-Bayes bound we again apply Theorem 1 to the $\hat{L}_{PB}(\rho)$ expression given in Lemma 9. This second-order PAC-Bayes bound, denoted by $\tilde{L}_{PB^2}(D, \rho)$, can be expressed as follows,

$$
\tilde{L}_{PB^2}(D, \rho) = \frac{B}{1 - e^{-B-1}} (\mathbb{E}_{p(x|\theta)}[\hat{L}(D, \theta)] - \tilde{V}(D, \rho) + \frac{2KL(p, \pi) + \ln \frac{1}{\xi}}{n}) + A
$$

where $A = \frac{1}{2}(\frac{B+1}{1 - e^{-B-1}} - 1)$ and $\tilde{V}(D, \rho)$ denote the empirical (normalized) variance of $p(x|\theta)$ wrt $\rho(\theta)$,

$$
\tilde{V}(D, \rho) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2 \max_{\theta} p(x_i|\theta)^2} \mathbb{E}_{p(x|\theta)}[(p(x_i|\theta) - p(x_i))^2]
$$

The following result also contains the three gaps of learning in the form of three chained inequalities,
Theorem 4. For any prior distribution \( \pi \) over \( \Theta \) and for any \( \xi \in (0, 1) \), with probability at least \( 1 - \xi \) over draws of training data \( D \sim \nu^x(x) \), for all mixture distribution \( \rho \) over \( \Theta \),

\[
H(\nu) \leq \bar{L}(\rho) \leq \bar{L}_{PB}(D, \rho)
\]

Proof. We start proving that \( \ell(x, \theta, \theta') \in [B - 1/2, B + 1/2] \). First, \( \ln \frac{1}{p(x|\theta)} \in [0, B] \) due to Assumption 4. Second, we have that \( \frac{1}{2} p(x|\theta')(p(x|\theta) - p(x|\theta')) \in [-1/2, 1/2] \), and dividing this quantity by \( \max p(x|\theta)^2 \) does not change this interval.

Now, we can apply Theorem 1 to the normalized loss \( \ell(x, \theta, \theta') \). And we have that for any prior distribution \( \pi \) over \( \Theta \), such that \( \pi(\theta, \theta') = \pi(\theta)\pi(\theta') \), and for any \( \xi \in (0, 1) \), with probability at least \( 1 - \xi \) over draws of training data \( D \sim \nu^x(x) \), for all mixture distribution \( \rho \) over \( \Theta \), such that \( \rho(\theta, \theta') = \rho(\theta)\rho(\theta') \),

\[
\mathbb{E}_{\rho(\theta')}[\frac{L(\theta, \theta') + 1/2}{B + 1}] \leq \frac{1}{1 - e^{-c}} \left( CE_{\rho(\theta)}[\frac{L(D, \theta, \theta') + 1/2}{B + 1}] + nKL(\rho, \pi) + \ln \frac{1}{\xi} \right),
\]

where \( L(\theta, \theta') \) is the expected value of \( \ell(x, \theta, \theta') \) wrt \( \nu(x) \), and \( L(D, \theta, \theta') \) is the empirical expectation of \( L(\theta, \theta') \). The PAC-Bayes bound is obtained by taking \( B = C + 1 \), rearranging terms, by applying Lemma 9, and by the following equality \( KL(\rho(\theta, \theta'), \pi(\theta, \theta')) = 2KL(\rho(\theta), \pi(\theta)) \).

We now define the following two functions, which contain only those non-constant terms in the PAC-Bayes bounds wrt \( \rho \),

\[
\mathcal{L}_{PB}(D, \rho) = \mathbb{E}_{\rho(\theta)}[\bar{L}(D, \theta)] + \frac{1}{n}KL(\rho, \pi) \quad (12)
\]

\[
\mathcal{L}_{PB}(D, \rho) = \mathbb{E}_{\rho(\theta)}[\bar{L}(D, \theta)] - \bar{V}(D, \rho) + \frac{2}{n}KL(\rho, \pi) \quad (13)
\]

So, the \( \rho \) mixture distributions minimizing \( \mathcal{L}_{PB}(D, \rho) \) and \( \mathcal{L}_{PB}(D, \rho) \) are the same than the ones minimizing \( L_{PB}(D, \rho) \) and \( L_{PB}(D, \rho) \), respectively.

In this case, the first-order PAC-Bayes gap is defined as the loss in the expected code-length that the learner incurs when coding using the distribution minimizing the first-order PAC-Bayes bound, \( \rho_{PB} = \arg\min \mathcal{L}_{PB}(D, \rho) \), and the expected code length of the optimal mixture distribution \( \rho^* \),

\[
\bar{L}(\rho_{PB}) - \bar{L}(\rho^*)
\]

And the same definition applies to the \( \bar{L}_{PB}(D, \rho) \) bound. Note, the PAC-Bayes gap is related to the concept of excess risk and different from the generalization error, which involves the difference between \( L_{PB}(D, \rho) \) and \( L(\rho) \) for a given \( \rho \) distribution.

By the strong law of large numbers, we have, with probability 1, that

\[
\lim_{n \to \infty} \mathcal{L}_{PB}(D, \rho) = \bar{L}(\rho)
\]

\[
\lim_{n \to \infty} \bar{L}_{PB}(D, \rho) = \bar{L}(\rho),
\]

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Under the assumption of uniform convergence in probability for the above sequences, we have that the PAC-Bayes gap converges in probability to the Jensen GAP in the large sample limit, because the minimum of $\bar{L}_{PB}(D, \rho)$ will converge, in probability, to the minimum of $L_{J}(\rho)$. And the same applies for $\bar{L}_{PB}^2(D, \rho)$ and $L_{J}^2(\rho)$. So, $\rho^\star_{PB}$ will converge in the large sample limit to a Dirac-delta distribution centered around the parameter $\theta^\star_{J}$ which defines the probabilistic model $p(x|\theta^\star_{J})$ closest to the data generative distribution $\nu(x)$ in terms of KL distance (see Lemma 4). However, this will not be the case of $\rho^\star_{PB}^2$ (except in some pathological situations) because the variance term will push the minimum away from a Dirac-delta distribution. And, according to Lemma 6, the latter will always provide better coding schemes than the former.

**The PAC-Bayes gap is null in the large sample limit under perfect model specification**

According to Corollary 1 and Lemma 7 both the KL gap and Jensen gap are null. It means that, in this case, the only remaining gap is the PAC-Bayes gap. The use of second-order Jensen bounds would not make any difference because is also tight and attain the same minimum than the first-order Jensen bound under perfect model specification (see Lemma 7). As we have discussed above, in the large sample limit, and under the assumption of uniform convergence, the PAC-Bayes gap converges in probability to the Jensen GAP. So, the PAC-Bayes gap is also null under perfect model specification in the large sample limit. And the optimal $\rho$ distribution will be a Dirac-delta distribution centered around the parameter defining the data generative distribution (see Lemma 4).

**Bayesian Learning under model miss-specification**

Under the assumptions stated in Section 3, this work shows new insights over the optimality of the Bayesian posterior $p(\theta|D)$ for making predictions through the posterior predictive distribution. The following result shows that the Bayesian posterior minimizes the first-order PAC-Bayes bound $L_{PB}(D, \rho)$ defined in Lemma 8.

**Lemma 10.** The Bayesian posterior $p(\theta|D)$ is the distribution over $\Theta$ which minimizes the first-order PAC-Bayes bound, $L_{PB}(D, \rho)$,

$$p(\theta|D) = \arg \min_{\rho} \bar{L}_{PB}(D, \rho)$$

**Proof.** As stated in Lemma 1, the Bayesian posterior $p(\theta|D)$ can be defined as the distribution $q$ over $\Theta$ maximizing the evidence lower bound function, $\mathcal{L}(D, q)$,

$$p(\theta|D) = \arg \max_{q} \mathcal{L}(D, q) = \arg \max_{q} \mathbb{E}_{q(\theta)}[\ln p(D|\theta)] - KL(q, \pi),$$

But, at the same time, we have that the $\bar{L}_{PB}(D, \rho)$ (see Equation 12) can be expressed as,

$$\bar{L}_{PB}(D, \rho) = \mathbb{E}_{q(\rho)}[-\frac{1}{n} \ln p(D|\theta)] + \frac{KL(\rho, \pi)}{n}$$
So, $\tilde{L}_{PB}(D, \rho) = -\frac{1}{n} L(D, \rho)$ and the Bayesian posterior can also be characterized as the distribution $\rho$ over $\Theta$ minimizing $\tilde{L}_{PB}(D, \rho)$, which is equivalent to minimize the first-order PAC-Bayes bound function $L_{PB}(D, \rho)$. \hfill \Box

In that way, the analysis performed in this work helps us to better understand the limitations of the Bayesian posterior for building predictive posterior distributions under model miss-specification.

The main limitation of Bayesian learning is that the Bayesian posterior minimizes a PAC-Bayes bound over a first-order Jensen bound. That means that the Bayesian posterior will tend to concentrate on a single parameter in the presence of large data samples, which are the standard settings in machine learning today. We have seen that this is optimal under perfect model specification, but it is suboptimal when the data generative distribution and the model family do not match.

The role of the PAC-Bayes gap in learning

This is a well known gap in the machine literature [McAllester 1999, Yang et al., 2019]. This gap defines the last limitation the learner has to overcome when learning. PAC-Bayes gap defines the loss the learner incurs when learning from a finite data sample. As discussed in the previous sections, under some assumptions, this gap converges to the Jensen gap in the large sample limit. So, under model miss-specification, we can not guarantee perfect learning even in the large sample limit. We should note that addressing this gap requires to solve an optimization problem. This is another limitation the learner suffers, because solving this minimization over an unconstrained probability distribution space is not feasible under constrained computational resources. In the next section, we introduce a family of learning algorithms which can solve the minimization of this gap trading-off computational complexity with the quality of the solution.

5 Learning by minimizing second-order PAC-Bayes bounds

In this section, we introduce a new family of learning algorithms based on the minimization of the second-order PAC-Bayes bound presented in the previous section. Minimizing this second-order PAC-Bayes bound is a sound approach to learning because is a way to minimize the generalization log-loss or, equivalently, the expected code-length of a Bayesian mixture code. We should note this approach is equivalent to maximize the generalization capacity of the predictive posterior, $E_{\rho(\theta)}[\ln p(x|\theta)]$, i.e. maximizing the predictive log-likelihood over the unseen data.

We define the PAC$^2$-Bayesian posterior, $\rho(\theta|D)$, as the mixture distribution $\rho$ over $\Theta$ which minimizes the second-order PAC-Bayes bound, $L_{PB^2}(\rho)$,

\[
\rho(\theta|x) = \arg \min_{\rho} L_{PB^2}(\rho)
\]

\[
= \arg \min_{\rho} \tilde{L}_{PB^2}(\rho)
\]

\[
= \arg \min_{\rho} E_{\rho(\theta)}[\tilde{L}(D, \rho)] - \hat{V}(D, \rho) + 2KL(\rho, \pi) \tag{14}
\]
Figure 2: **Perfect Model Specification:** The data generative model, $\nu(y|x)$, is a linear model plus noise, $y \sim \mathcal{N}(\mu = 1 + x, \sigma^2 = 1)$. The probabilistic model, $p(y|x, \theta)$ is $y \sim \mathcal{N}(\mu = \theta_0 + \theta_1 x, \sigma^2 = 1)$. The prior $\pi(\theta)$ is a standard Normal distribution. We learn from 100 samples. The Bayesian posterior $p(\theta|D)$ is a bidimensional Normal distribution and can be exactly computed. The PAC$^2$-Bayesian posteriors $\rho(\theta|D)$ and $\rho_h(\theta|D)$ are computed using a bidimensional Normal distribution approximation family. The expected log-likelihood of the posterior predictive distribution, estimated over 10000 samples, is $-1.43$, $-1.41$, $-1.42$ and $-1.42$ for the MAP model, the Bayesian model and the $\rho(\theta|D)$ and $\rho_h(\theta|D)$ models, respectively. The uncertainty in the predictions is computed by random sampling first from $\theta \sim \rho(\theta)$ and then from $y \sim p(y|x, \theta)$ for 100 times. We plot the predictive mean plus/minus two standard deviations. We distinguish between *epistemic uncertainty* which comes from the uncertainty in $\rho(\theta)$ and *aleatory uncertainty* which comes from the uncertainty in $p(y|x, \theta)$. 
Note that, as discussed in Section 4.3, the Bayesian posterior $p(\theta|D)$ can be defined as the mixture distribution $\rho$ over $\Theta$ which minimizes the first-order PAC-Bayes bound, $\bar{L}_{PB}(\rho)$ (see Equation (10)). In that sense, the difference between the PAC$^2$-Bayesian posterior $\rho(\theta|x)$ and the (PAC-)Bayesian posterior $p(\theta|D)$ simply stems from the kind of Jensen bound, first or second order, we use to bound the expected code-length of the Bayesian mixture code.

By using standard results from variational inference and exploiting the representation provided in Lemma 9, we can build the following iterative algorithm which converges to the PAC$^2$-Bayesian posterior $\rho(\theta|x)$ as defined in Equation (14),

$$
\rho_{t+1}(\theta|D) = \frac{\pi(\theta)}{Z} \exp \left( \sum_{i=1}^{n} \ln p(x_i|\theta) + \frac{p(x_i|\theta)^2 - p(x_i|\theta) \mathbb{E}_{\rho_{t}(\theta|D)}[p(x_i|\theta)]}{2 \max_{\theta} p(x_i|\theta)^2} \right)
$$

(15)

5.1 PAC$^2$-Variational Learning and tighter Jensen bounds

Although Equation (15) provides an iterative updating equation which converges to the optimal PAC$^2$-Bayesian posterior $\rho(\theta|D)$, computing the normalization constant $Z$ in this equation is usually intractable for many relevant probabilistic models. Fortunately, Equation (14) directly resembles standard variational inference methods (see Section 2.1).

So, like in variational inference, we can choose a tractable family of $\rho(\theta|\lambda)$ distributions parametrized by some parameter vector $\lambda$, for which we can tractably solve the optimization problem of Equation (14). Then, we can resort to variational inference literature (Zhang et al., 2018) to choose tractable probability distribution families for $\rho$ as well as efficient optimization methods.

Another relevant point we explore here is the use of other (second-order) Jensen bounds which are tighter than the one considered in Theorem 3. As discusses in Section 4.2, the Jensen gap can be a significant barrier when learning, so the use of tighter (second-order) Jensen bounds can potentially lead to better learning algorithms. In that sense, we recommend to use the following Jensen bound proposed in (Liao & Berg, 2019) which can be written as,

$$
\ln \mathbb{E}_{\rho(\theta)}[p(x|\theta)] \geq \mathbb{E}_{\rho(\theta)}[\ln p(x|\theta)] + \nabla_h(x, \rho)
$$

(16)

where $\nabla_h(x, \rho)$ is defined as

$$
\nabla_h(x, \rho) = h(m_x, \mu_x) \mathbb{E}_{\rho(\theta)}[(p(x|\theta) - p(x))^2],
$$

and $\mu_x = \mathbb{E}_{p(\theta)}[p(x|\theta)]$, $m_x = \max_{\theta} p(x|\theta)$, while $h(m, \mu)$ is defined as

$$
h(m, \mu) = \frac{\ln \mu - \ln m}{(m - \mu)^2} + \frac{1}{\mu(m - \mu)},
$$

(17)

This bound is tighter because (Liao & Berg, 2019)

$$
\forall x \in \mathcal{X} \quad h(m_x, \mu_x) \geq \frac{1}{2 \max_{\theta} p(x|\theta)^2}.
$$

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Figure 3: **Model Miss-Specification**: The data generative model, $\nu(y|x)$, is a linear model plus noise, $y \sim \mathcal{N}(\mu = 1 + x, \sigma^2 = 5)$. The probabilistic model, $p(y|x, \theta)$ is $y \sim \mathcal{N}(\mu = \theta_0 + \theta_1 x, \sigma^2 = 1)$. So, the probabilistic model is miss-specified, but note how model miss-specification mainly affects to the parameter $\theta_0$. The experimental settings are equal to the ones of Figure 2. The estimated expected log-likelihood of the posterior predictive distribution is -13.63, -13.01, -9.43 and -6.15 for the MAP model, the Bayesian model and the two PAC$^2$-Bayesian models $\rho(\theta|D)$ and $\rho_{h}(\theta|D)$, respectively.
We define the PAC²-Variational algorithm to any method which minimizes over \( \lambda \) the following objective function,

\[
\bar{L}_{P\!B^2}(\lambda) = \mathbb{E}_{\rho(\theta|\lambda)}[\hat{L}(D)] - \hat{V}_h(D, \rho) + \frac{2}{n} KL(\rho, \pi),
\]

(18)

where \( \hat{V}_h(D, \rho) = \frac{1}{n} \sum_{i=1}^{n} V_h(x_i, \rho) \).

We will refer to the distribution minimizing the above functional as the PAC²-posterior, denoted \( \rho_h(\theta|D) \), to differentiate it from the distribution minimizing \( \bar{L}_{P\!B^2}(\lambda) \), which is denoted \( \rho(\theta|D) \). But, unless otherwise stated, we will use the tighter version as the default one. We consider both solutions to illustrate how tighter Jensen bounds give rise to better learning algorithms. In summary, we consider a first-order Jensen bound and two second-order Jensen bounds for deriving learning algorithms.

Appendix C discusses a numerically stable algorithm, exploiting the representation provided in Lemma 9, to perform optimization over this kind of objective functions using modern black-box variational methods (Zhang et al., 2018).

Note that, instead of considering the minimization of second-order PAC-Bayes bounds, we consider the minimization of first-order PAC-Bayes bounds \( \bar{L}_{P\!B}(D, \rho) \) (see Equation (4.3)) over a tractable family of \( \rho(\theta|\lambda) \) distributions, we would directly arrive to standard variational methods (see Section 2.1 and note that \( \bar{L}_{P\!B}(D, \rho) = -\frac{1}{n} L(D, \rho) \), where \( L(D, \rho) \) is defined in Equation (4)). So, standard variational methods can also be interpreted as learning algorithms which find the mixture distribution \( \rho \), within a tractable family, minimizing the first-order PAC-Bayes bound over the expected code-length of a Bayesian mixture code.

Now that we have a method to compute the (approximate) PAC²-Bayesian posterior, we present in Figures 2 and 3 how it differs from the Bayesian posterior in a simple toy example under perfect model specification and model miss-specification, respectively. While Figure 4 exemplifies the use of this approach over a simple neural network on a toy data set.

5.2 Maximum a Posteriori estimation (and empirical risk minimization) under model miss-specification

By definition, the maximum a posteriori estimate (MAP) equals the mode of the Bayesian posterior distribution. This estimate can be computed by solving the following maximization problem,

\[
\theta_{MAP} = \arg \max_{\theta} \sum_{i=1}^{n} \ln p(x_i|\theta) + \ln \pi(\theta).
\]

We can see that this approach is equivalent to finding a two-part coding scheme (see Section 2.3).

By employing a Dirac-delta distribution centred around the MAP estimate, \( \rho(\theta) = \delta_{\theta_{MAP}}(\theta) \) we can build our predictive posterior, \( p(x) \), as

\[
\mathbb{E}_{\delta_{\theta_{MAP}}(\theta)}[p(x|\theta)] = p(x|\theta_{MAP})
\]

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Learning under Perfect Model Specification

![Variational Inference](image1)

![PAC$^2$-Variational Learning](image2)

Learning under Model Miss-Specification

![Variational Inference](image3)

![PAC$^2$-Variational Learning](image4)

Figure 4: PAC$^2$-Variational Learning: Data generative model, $\nu(y|x)$, is a sinusoidal function plus Gaussian noise, $y = s(x) + \epsilon$, $\epsilon \sim N(0, \sigma^2)$, with $\sigma^2 = 1$ and $\sigma^2 = 10$ for the first and second row, respectively. The probabilistic model $p(y|x, \theta)$ is $y = f_{\theta}(x) + \epsilon$, $\epsilon \sim N(0, \sigma^2 = 1)$, where $f$ is a neural network parametrized by $\theta$, with one hidden layer with 20 units and softplus activation able to approximate $s(x)$. The prior $\pi(\theta)$ is a standard Normal distribution. 10000 training samples. The Bayesian posterior and the PAC$^2$-Bayesian posterior $\rho_h(\theta|D)$ are computed with the Variational Inference (see Equation (4)) and the PAC$^2$-Variational inference algorithms (see Equation (18)), respectively, using a fully factorized mean field Normal distribution as approximation family. Under perfect model specification, the expected log-likelihood of the posteriors predictive distribution, estimated over 10000 samples, is -1.42, -1.42, -1.43 and -1.43 for the MAP model, the Variational model and for the two PAC$^2$-Variational models, $\rho(\theta|D)$ and $\rho_h(\theta|D)$, respectively. Under model miss-specification, the expected log-likelihood of the posteriors predictive distribution is -50.44, -50.20, -34.86 and -26.50, respectively. Uncertainty estimations are computed as in Figure 2.
We can also try to compute the PAC-Bayes bound of the MAP estimate. But this approach will fail because the entropy of this Dirac-delta distribution is minus infinity, 

\[ H(\delta_{\theta_{\text{MAP}}}) = -\infty, \]

and the PAC-Bayes bound become useless. However, by including the following assumption, we can perform a PAC-Bayesian analysis of single point estimates.

**Assumption 5.** The support of the prior distribution that the learner employs only includes finite-precision parameters. It means that the support of the distribution \( \pi \) is contained in \( \Theta_F \), which denotes the space of real number vectors of dimension \( M \) that can be represented under a finite-precision scheme using \( F \) bits to encode each element of the vector. So, we have that \( \text{supp}(\pi) \subseteq \Theta_F \subseteq \Theta \subseteq \mathbb{R}^M \). So, the number of bits needed to store a parameter vector \( \theta \) is \( MF \) bits.

We denote \( \pi_F \) any prior distribution satisfying the above assumption. This prior distribution can be mathematically defined as a mixture of Dirac-delta distributions,

\[
\pi_F(\theta) = \sum_{\theta' \in \Theta_F} w_{\theta'} \delta_{\theta'}(\theta)
\]

where \( w_{\theta'} \) are positive scalars values parametrizing this prior distribution. They satisfy that \( w_{\theta'} \geq 0 \) and \( \sum_{\theta' \in \Theta_F} w_{\theta'} = 1 \). This is a valid density function because \( \pi_F(\theta) \geq 0 \) and

\[
\int \pi_F(\theta) d\theta = \sum_{\theta' \in \Theta_F} w_{\theta'} \int \delta_{\theta'}(\theta)d\theta = \sum_{\theta' \in \Theta_F} w_{\theta'} = 1
\]

We should also note that we can compute the KL distance between a Dirac-delta distribution \( \delta_{\theta'}(\theta) \) and \( \pi_F(\theta) \) if \( \theta' \in \Theta_F \),

\[
KL(\delta_{\theta'}, \pi_F) = \ln \frac{\delta_{\theta'}(\theta')}{\pi_F(\theta')} = \ln \frac{\delta_{\theta'}(\theta')}{w_{\theta'} \delta_{\theta'}(\theta')} = -\ln w_{\theta'}
\]

Under this assumption, we can compute the PAC-Bayes bound of point estimates.

**Theorem 5.** Under Assumptions 1-6, for any prior distribution \( \pi_F \) over \( \Theta \) and for any \( \xi \in (0, 1) \), with probability at least \( 1 - \xi \) over draws of training data \( D \sim \nu^n(x) \), for any \( \theta \in \Theta \),

\[
E_{\nu(x)}[\ln \frac{1}{p(x|\theta)}] \leq \frac{B}{1 - e^{-B}} \left( \hat{L}(D, \theta) - \frac{\ln \pi_F(\theta) + \ln \xi}{n} \right),
\]

where \( \ln \pi_F(\theta) = \ln w_{\theta} \) if \( \theta \in \Theta_F \) and \( \ln \pi_F(\theta) = -\infty \) if \( \theta \notin \Theta_F \).

**Proof.** This result is obtained by applying Lemma 8 over \( \rho \) distributions defined as Dirac-delta distributions, \( \delta_{\theta} \). This result applies to Dirac-delta distributions because we can compute expectations from Dirac-delta distributions, and the KL distance between a Dirac-delta distribution and \( \pi_F(\theta) \) is well defined, as we showed above. More precisely, we first have that if \( \theta \notin \Theta_F \), then \( \text{supp}(\rho) \nsubseteq \text{supp}(\pi_F) \) and \( KL(\rho, \pi_F) = \infty \) and the bound holds because is completely vacuous. Finally, we obtain the bound when \( \theta \in \Theta_F \), because \( KL(\delta_{\theta}, \pi_F) = \ln w_{\theta} \).

\[ \square \]
Under Assumptions 1-5 we can see that the MAP estimate will be quite close to the parameter minimizing the above bound. So, the above result shows why we need to include a prior, or a regularizer, when learning point estimates because it is a way to improve the generalization capacity of our estimate.

But the above result also shows that the MAP estimate arises from the minimization of the PAC-Bayes bound, $L_{PB}(\rho)$, over the constrained space of Dirac-delta distributions, $\rho(\theta) = \delta_{\theta_0}(\theta)$. At the same time, in large sample settings, the MAP estimate should be quite close to the minimum of the second-order PAC-Bayes bound, $L_{PB2}(\rho)$, over the same constrained space of Dirac-delta distributions, because the variance term of Dirac-delta distribution $\nabla(\delta_{\theta_0}(\theta))$ is always null. In that sense, the use of point estimates (i.e. Dirac-delta distributions) to define predictive posteriors is suboptimal because we only optimize the PAC-Bayes bounds over a highly constrained space of $\rho$ distributions. Note that the empirical risk minimizer (ERM) equals the MAP estimate when using the $-\ln p(x|\theta)$ as loss function and the log-prior $\ln \pi(\theta)$ as regularizer. So, the ERM can be also interpreted from this point of view.

At the same time, we have seen that with large data samples, the Bayesian posterior tends to approximate a Dirac-delta distribution concentrating all its probability mass around the MAP parameter. So, in large data samples, a Bayesian approach may do not provide significant gains in terms of prediction performance if the Dirac-delta distributions centred around the MAP/ERM estimates become very good approximations of the Bayesian posterior. This work suggests that if, instead of using the Bayesian posterior, we employed the PAC$^2$-Bayesian posterior, then the performance differences wrt MAP/ERM estimates could be significant in the case of model miss-specification.

Finally, note that Assumption 5 induces a non-continuous and non-differentiable bound due to the $\ln \pi_F(\theta)$ term. But in a computer, any implemented statistical distribution $\pi(\theta)$ (e.g. a Normal distribution) can be seen as an approximation for its finite-precision counter-part, $\pi_F(\theta)$. So, we can employ this continuous and differentiable approximation $\ln \pi(\theta)$ as a proxy to perform gradient-based optimization over the bounds involving the term $\ln \pi_F(\theta)$. Note that, at each step, our optimization algorithm will end up in a parameter in $\Theta_F$ because they are the only ones which can be represented in the computer.

5.3 PAC$^2$-Ensemble Learning

Ensemble models (Dietterich 2000) are based on the combination of the predictions of a group of models to obtain predictions that are more accurate than the predictions of any single model of the group alone. This work provides a simple explanation of why the combination of multiple models can give rise to better performance. It also provides a sound explanation of why the so-called diversity of the ensemble is key to have powerful ensembles (Kuncheva & Whitaker 2003). Finally, we present a novel ensemble learning algorithm.

Let us denote $\{\theta_j\}_{1 \leq j \leq E}$ a set of $E$ parameter vectors describing $E$ different models, $\{p(x|\theta_j)\}_{1 \leq j \leq E}$. Let us assume we compute the combine prediction of these

---

4They are not equal because the parameter minimizing the bound of Theorem 5 will always belong to $\Theta_F$. 

Figure 5: Ensemble Learning under Model Miss-Specification: Same experimental settings than in Figure 4. But now the probabilistic model \( p(y|x, \theta) \) is an ensemble model with three components \( y = \sum_{j=1}^{3} f_{\theta_j}(x) + \epsilon_j, \quad \epsilon_j \sim \mathcal{N}(0, \sigma^2 = 1) \), where each \( f_{\theta_j} \) is again a neural network with one hidden layer with 20 units and softplus activation able to approximate \( s(x) \). The PAC\(^2\)-ensemble model \( \rho_{h}(\theta|D) \) is learned by maximizing Equation (21), while the \( \rho(\theta|D) \) version is learned using the looser Jensen bound presented in Theorem 3. The expected log-likelihood of the posteriors predictive distribution is -51.35, -39.16 and -15.88 for the PAC-ensemble model and for the two PAC\(^2\)-ensemble models \( \rho(\theta|D) \) and \( \rho_{h}(\theta|D) \), respectively.
models as the average of the individual predictions\(^5\),

\[ p_E(x) = \frac{1}{E} \sum_{j=1}^{E} p(x|\theta_j) \]  

(19)

Note that the \( p_E(x) \) can be seen as a predictive posterior distribution \( E \rho_E(\theta) [p(x|\theta)] \) where \( \rho_E \) is defined as a mixture of Dirac-delta distributions centered around the parameters \( \{\theta_j\}_{1 \leq j \leq E} \).

\[ \rho_E(\theta) = \sum_{j=1}^{E} \frac{1}{E} \delta_{\theta_j}(\theta) \]  

(20)

The PAC-Bayes bound of the prediction capacity of a single model was given in Theorem 5. The following result provides a second-order PAC-Bayes bound over the prediction capacity of an ensemble of models.

**Theorem 6.** Under Assumptions 1-6, for any prior distribution \( \pi_F \) over \( \Theta \) and for any \( \xi \in (0, 1) \), with probability at least \( 1 - \xi \) over draws of training data \( D \sim \nu^n(x) \), for any \( \{\theta_j\}_{1 \leq j \leq E} \subset \Theta \)

\[
\bar{L}(\rho_E) \leq \frac{B + 1}{1 - e^{-B-1}} \left( \frac{1}{E} \sum_{j=1}^{E} \hat{L}(D, \theta_j) - \hat{V}_E(D, \{\theta_j\}) \right) - \frac{1}{E} \sum_{j=1}^{E} \ln \pi_F(\theta_j) + \ln \frac{\xi}{n} + A,
\]

where \( \hat{V}_E(D, \{\theta_j\}) \) is the empirical variance term of the PAC\(^2\)-Bayes bound.

**Proof.** This result simply follows by considering Theorem 4 given a mixture distribution \( \rho_E \) as defined in Equation (20). And noting that \( KL(\rho_E, \pi_F) = -\frac{1}{E} \sum_{j=1}^{E} \ln \pi_F(\theta_j) \) in this case.

So, according to Theorems 5 and 6 we should prefer an ensemble over a single model if,

\[
\frac{1}{E} \sum_{j=1}^{E} \hat{L}(D, \theta_j) - \hat{V}_E(D, \{\theta_j\}) - \frac{1}{E} \sum_{j=1}^{E} \ln \pi_F(\theta_j) < \max_j \hat{L}(D, \theta_j) - \ln \pi_F(\theta_j)
\]

Note how \( \hat{V}_E \) is a measure of the diversity of the ensemble [Kuncheva & Whitaker, 2003], and note that when creating optimal ensembles we need to trade-off how well we fit the data (i.e. low values for \( \hat{L}(D, \theta_j) \)) while also maintaining high diversity (i.e. high \( \hat{V}_E \) values) to make the ensemble works (i.e. reduces the generalization bound given in Theorem 6). This is a clear explanation about why ensembles need diversity to generalize better, but it is out the scope of the this paper to further explore this claim.

\(^5\)This analysis can be easily extended to weighted predictions too.
Theorem 6 shows how to design a learning algorithm for building ensembles by minimizing the generalization upper bound. The algorithm we propose, called the **PAC\textsuperscript{2}-ensemble learning algorithm**, is simply based on a gradient-based optimization of the \(\{\theta_j\}_{1 \leq j \leq E}\) parameters of the following objective function, denoted as \(\bar{L}_E(\theta_1, \ldots, \theta_E)\),

\[
\begin{align*}
\sum_{j=1}^{E} \sum_{i=1}^{n} \left( -\ln p(x_i | \theta_j) - h(m_{x_i}, p_E(x_i)) (p(x_i | \theta_j) - p_E(x_i))^2 - \ln \pi(\theta_j) \right) \\
\end{align*}
\]

where \(m_{x_i} = \max_j p(x_i | \theta_j)\), and \(h(m, \mu)\) is the function defined in Equation (17) to exploit the tighter Jensen bound defined in Equation (16). Appendix C discusses a numerically stable algorithm to perform gradient-based optimization over this objective function.

This ensemble learning algorithm can also be interpreted as a particle-based variational inference algorithm (Liu & Wang, 2016). In these algorithms, a set of parameters \(\{\theta_j\}_{1 \leq j \leq E}\) are used to define a posterior, which is \(\rho_E(\theta)\) in this case.

Note that we can similarly derive an ensemble learning algorithm by adapting this same analysis to first-order PAC-Bayes bounds. In that case, the objective function to optimize would be

\[
\sum_{j=1}^{E} \sum_{i=1}^{n} -\ln p(x_i | \theta_j) - \ln \pi(\theta_j). 
\]

By inspecting this objective function, we can easily understand the limitations of this approach. We refer to the minimization of this function as the **PAC-ensemble learning algorithm**. We introduce it simply to illustrate the main differences that arise in learning algorithms when we consider second-order PAC-Bayes bounds instead of standard first-order PAC-Bayes bounds.

Figures 5 and 6 illustrate these algorithms on two different toy data samples.

### 5.4 Flat minima and generalization

This work may offer a simple explanation to the empirically observed phenomenon that parameters in a flat minimum generalizes better than parameters in a sharp minimum (Hochreiter & Schmidhuber, 1997; Keskar et al., 2016; Zhang et al., 2016). Figure 7 shows a simple experiment fitting a feed-forward neural network with one hidden layer with 20 hidden units, \(y = f(\theta(x)) + \epsilon, \epsilon \sim \mathcal{N}(0, 0.01)\), i.e. the same network used in the previous figures but where the noise level is strongly reduced to encourage stronger fit to the data points. This network has a total of 80 parameters. We randomly generate 25 data points for a linear model with white noise (\(\sigma^2 = 2\)). For fitting the network we employ a MAP, Variational and the two PAC\textsuperscript{2}-Variational models \(\rho(\theta | D)\) and \(\rho_h(\theta | D)\), respectively, and we let the optimizer run for 10000 iterations. We plot the results of the learned curves in Figure 7. The Variational and the MAP approach provide similar results with clear signs of overfitting. However, the PAC\textsuperscript{2}-Variational models provide a fairly good estimation, especially \(\rho_h(\theta | D)\) which is based on a tighter second-order Jensen bound, even though we are in a situation where the number of parameters is much larger than the number of data points.
Figure 6: Ensemble Learning over Multimodal Data: Same settings than in previous Figures 4 and 5. But now the data generative function is a mixture of two sinusoidal functions (i.e. multimodal data) with $\sigma^2 = 1$. The expected log-likelihood of the posteriors predictive distribution is -18.86, -8.54, -13.31 and -4.00 for the Variational, PAC$^2$-Variational model $\rho_h(\theta|D)$ and for two PAC$^2$-ensemble models $\rho(\theta|D)$ and $\rho_h(\theta|D)$, respectively.
Figure 7: Flat minima and generalization I. Same settings than in previous Figures 4 and 5. But now the data generative distribution is a linear model plus noise, $y \sim \mathcal{N}(\mu = 1 + x, \sigma^2 = 2)$, from which we sample 25 data points. See Section 5.4 for details.

We look at how flat was the convergence point of each algorithm. For that purpose, we apply white noise ($\sigma^2 = 0.01$) perturbations to the mode/MAP parameters obtained with the four approaches. In the presence of a flat minimum, we should expect that the minus log-prob of the training data with the perturbed weights is similar to the minus log-prob of the training data with the mode/MAP parameters. While in a sharp minimum we should expect the opposite situation, perturbed weights should lead to much worse solutions than the solution with the mode parameters. Figure 8 shows the histograms of the log-prob for 100 perturbed weights for each of the four approaches. This figure shows that PAC$^2$-Variational approaches converge to much flatter minima than the others, where the perturbed weights can lead to solutions almost 3 times worse.

We know that the $\hat{V}_h$ term of the PAC$^2$-Variational functional (see Equation (14)) induces the optimization algorithm to converge to local minimum with large $\hat{V}_h$ values. Our hypothesis is that $\hat{V}_h$ might be connected with the flatness of the local optima. (Yang et al., 2019, Definition 4.1) provides a similar quantity to measure the flatness of a local minimum. In the above example, the $\hat{V}_h$ value of the local minimum found by the Variational and the two PAC$^2$-Variational approaches is 111.6, 166.06 and 290.0, respectively.
respectively. According to this work, generalization under model mis-specification involves jointly optimize the data fit term $\mathbb{E}_p[L(D, \theta)]$ and the variance term $\hat{V}_h$, not only the former. It is beyond the scope of the paper to thoroughly study this problem.

Figure 8: Flat minima and generalization II: Sensitivity analysis for the results of Figure 7. Histograms reflect the variability of the log-probability of the data to small perturbations of the convergence point. High variability is associated to sharp minima. Low variability is associated to flat minima. The x axis scale is minus the log-prob of the training data for the mode parameter plus/minus 3 times this quantity. The Pearson variation coefficient is 22.26%, 35.90%, 0.62% and 1.55% for the MAP, Variational and the two PAC$^2$-Variational models, respectively. See Section 5.4 for details.

5.5 PAC$^2$-Bayesian learning with general loss functions

Here we present a simple extension to perform PAC$^2$-Bayesian learning with general loss functions. Without loss of generality, we assume we have now a supervised classification problem. So, we assume we have a data set $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ where the samples are i.i.d. distributed according to some unknown but fixed distribution $\nu(x, y)$. We also assume that $\ell(y, y')$ defines a general bounded loss function taking values in the interval $[0, B]$, and $g_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ is our model class parametrized
by $\theta \in \Theta$. Abusing the notation to make it more compact, we denote $\ell(y, x, \theta) = \ell(y, g_{\theta}(x))$.

Learning under (regularized) empirical risk minimization (ERM) consists on solving the following minimization problem,

$$
\theta^* = \arg \min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, x_i, \theta) - \frac{\ln \pi(\theta)}{n},
$$

where, without loss of generality, $-\ln \pi(\theta)$ plays the role of the regularizer.

When a new observation $x$ arrives, under ERM, we provide the following prediction,

$$
y^* = \arg \min_{y \in \mathcal{Y}} \ell(y, x, \theta^*).
$$

The PAC^2-Bayesian extension to this framework starts by defining the so-called posterior average loss, denoted $\bar{\ell}(y, x, \rho)$,

$$
\bar{\ell}(y, x, \rho) = \ln \frac{1}{\mathbb{E}_{\rho(\theta)}[e^{-\ell(y, x, \theta)}]}.
$$

The posterior average loss $\bar{\ell}$ can be seen as a log-sum-exp operation to smooth out the individual losses $\ell(y, x, \theta)$. E.g. if $\ell(y, x, \theta)$ is defined as the 0-1 loss and $\rho$ is a uniform mixture of Dirac-delta distributions, as defined in Equation (20), we have that $\arg \min_y \bar{\ell}(y, x, \rho)$ corresponds to a majority voting scheme.

Then, we can define the expected posterior average loss, denoted $\bar{L}(\rho)$, as

$$
\bar{L}(\rho) = \mathbb{E}_{\nu(y, x)}[\bar{\ell}(y, x, \rho)].
$$

And the learning problem we aim to solve is again to find a mixture distribution $\rho$ which minimizes $\bar{L}(\rho)$,

$$
\rho^* = \arg \min_{\rho} \bar{L}(\rho).
$$

The predictions for a new arriving observation $x$ are now made in the following way,

$$
y^* = \arg \min_{y \in \mathcal{Y}} \bar{\ell}(y, x, \rho^*).
$$

Under these settings, we can repeat the whole analysis performed in Section 4 and derived the same learning algorithms presented in Section 5. The key considerations for doing that are:

- The Jensen bounds employed in this work applies to $\ln \mathbb{E}_{\rho(\theta)}[f(\theta)]$ where $f$ is any general smooth function from $\Theta$ to $\mathcal{R}$ (Liao & Berg, 2019).
- The PAC-Bayes bounds employed in this work applies to general bounded losses (Catoni, 2007) and, in this case, we have that $\ell(y, x, \theta)$ and $e^{-\ell(y, x, \theta)}$ are both bounded.
The rest of the relevant quantities needed for this task are the following ones,

\[
L(\theta) = \mathbb{E}_{\nu(y,x)}[\ell(y, x, \theta)]
\]

\[
V(\rho) = \mathbb{E}_{\nu(y,x)}\left[ \frac{1}{2 \max_{\theta} e^{-2\ell(y,x,\theta)}} \mathbb{E}_{\rho(\theta)}[\left(e^{-\ell(y,x,\theta)} - \mathbb{E}_{\rho(\theta)}[e^{-\ell(y,x,\theta)}]\right)^2] \right],
\]

It is out the scope of this paper to further explore this extension to general loss functions.

6 Related Work

6.1 PAC-Bayes Theory

PAC-Bayes theory [Catoni, 2007] and the approach presented here differ in that they do not try to answer the same question. While PAC-Bayes focused on bounding the expected log-loss, \[\mathbb{E}_{\nu(x)}[-\ln p(x|\theta)]]\], the focus of this approach is to bound the expected code-length of a Bayesian mixture code, \[\mathbb{E}_{\nu(x)}[-\ln \mathbb{E}_{\rho(\theta)}[p(x|\theta)]]\]. However, both quantities are closely related, as we have seen in this work, because the former is an upper-bound of the latter. Under the assumption of perfect model specification and bounded log-loss, we showed in Lemma 7 that the expected log-loss is a tight upper-bound of the expected code-length of a Bayesian mixture code. So, standard PAC-Bayes bounds are also optimal bounds of the expected code-length of a Bayesian mixture code in case of perfect model specification. But, to the best of our knowledge, this has not been acknowledged in the literature.

The relation of Bayesian learning and PAC-Bayes theory has been previously explored [Germain et al., 2016]. But this work shows that this relationship was only partially explored under the implicit assumption of perfect model specification. And these authors were not aware of this relevant distinction.

The use of some kind of variance term in the PAC-Bayes bound has previously appeared in the literature [Yang et al., 2019; Tolstikhin & Seldin, 2013], but they have a different formulation than the variance term used here. And, in general, their focus is on bounding the generalization error of a Gibbs classifier, which is different from the goal of this work.

PAC-Bayes bounds have also been provided for ensembles of classification models [Lorenzen et al., 2019]. But they focus on bounding the generalization error of majority voting. Although these bounds include some terms measuring the discrepancy/uncorrelation among predictors, the bounds and the algorithms presented here are different.

6.2 Generalized Bayesian Algorithms

That standard Bayesian inference can behave suboptimally if the model is wrong has been previously studied in the literature [Grünwald, 2012; Grünwald et al., 2017; Grünwald, 2018]. The propose approached to address this issue, known as Safe Bayesian, introduces a tempered likelihood which gives rise to a new Bayesian posterior,

\[
p_\nu(\theta|D) \propto p(D|\theta)^\gamma p(\theta)
\]
where $\eta \geq 0$ is known as the learning rate. $\eta = 1$ gives rise to the Bayesian posterior, but the recommendation is to use smaller $\eta$ values. Actually in [Gr"unwald, 2012], an algorithm is presented to automatically compute this learning rate. These works show that this approach defines posteriors which are more consistent and which provide better predictive performance when empirically evaluated.

Although these previous works described inconsistency issues in Bayesian learning under model miss-specification, their focus were not analyze the generalization prediction capacity of the Bayesian posterior under these settings. Our work can theoretically explain why using a tempered log-likelihood with $\eta < 1$ can give better predictions under model miss-specification. $p_{\eta}(\theta|D)$ can be seen as the solution to the following maximization problem,

$$p_{\eta}(\theta|D) = \arg \max_{\rho} \eta \mathbb{E}_{\rho}[\ln p(D|\theta)] - KL(\rho, \pi).$$

It is clear than when $\eta < 1$ the weight of the data log-likelihood term is smaller, then the optimal $\rho$ will be closer to $\pi$, and $p_{\eta}(\theta|D)$ will be less concentrated around the MAP estimate (i.e. higher entropy). Looking at Equation (14) we can see that this posterior, if $\eta$ is carefully chosen, can provide better prediction performance, just because a less concentrated posterior will have a higher variance term $\hat{V}(D, \rho)$.

### 6.3 Minimum Description Length

One of the main differences between the framework considered here and the MDL principle (see Section 2.3) is that, under the MDL principle, there are no assumptions about the data-generating process. In this section, we try to establish a connection between these two frameworks.

Let us assume we have a finite data set $D^* = \{x_1, \ldots, x_N\}$ we want to compress. However, we only have access to a subset of this data set $D$, randomly extracted with replacement from $D^*$. If we define $\nu(x)$ as the empirical probability distribution of $D^*$, we have that $D$ is formed from i.i.d. samples coming from $\nu(x)$.

Then, under the assumptions stated in Section 3 we can interpret the PAC$^2$-Bayes approach as selecting the Bayesian mixture code which minimizes an upper-bound over the code-length for $D^*$, where this upper-bound only depends of the observed data set $D$, which is a random subsample with replacement from $D^*$. Our model miss-specification assumption can be seen here as making no assumptions about the data-generative process of $D^*$.

### 7 Conclusions and Future Works

This work provides a novel theoretical analysis of the problem of learning from i.i.d. data under model miss-specification. This theoretical analysis provides several key insights which have to be considered when designing a learning algorithm in these settings.

First, we show that under perfect model specification there is only a single gap we have to care about, the PAC-Bayes gap, which stems from the problem of learning from a finite data sample.
However, under model misspecification, things are more complex because we have to care about another two gaps. The KL gap which defines the loss of having to learn with a model which is not expressive enough to capture all the patterns of the data. And the Jensen gap, which defines the loss associated with taking an expectation out of a function. We show that this last gap can induce suboptimal solutions when considering standard first-order Jensen bounds. But, we also show that the use of tighter second-order Jensen bounds can lead us to more optimal solutions.

Using this analysis, we describe how the Bayesian posterior is derived after employing a standard first-order Jensen bound for bounding the generalization error. In consequence, the Bayesian posterior has a suboptimal behaviour when defining predictive distributions under model misspecification and large data samples because it tends to concentrate all its mass around a single parameter vector.

Under perfect model specification and large data samples, we do not find strong reasons to consider (finite or infinite) ensemble models when making predictions. But we provide strong theoretical arguments showing that this is not the case under model misspecification. We believe that the current situation in which Bayesian approaches are not consistently providing state-of-the-art performance in many machine learning tasks can be at least partly explained by this analysis.

Finally, we derive new learning algorithms which are directly based on the theoretical tools presented in this work. In the case of the ensemble learning algorithm, we arrive at a clear explanation about why ensembles need diversity to generalize better. We also provide novel hypotheses for the empirically observed phenomenon that shows that parameters in flat minima generalize better than parameters in sharp minima.

Future works should empirically validate the analysis and algorithms presented in this work.

### A Finite-Precision Sensor Readings

In this work, we also consider the so-called digital sensor assumption which states that the sensor readings are composed by finite-precision numbers,

**Assumption 6.** The sensor provides readings in the form of vectors of real numbers under finite-precision representation. It means that the support of the distribution $\nu$ is contained in $X_F$, which denotes the space of real number vectors of dimension $K$ that can be represented under a finite-precision scheme using $F$ bits to encode each element of the vector. So, we have that $\text{supp}(\nu) \subseteq X_F \subseteq \mathcal{X} \subseteq \mathbb{R}^K$. Then, the number of bits needed to store a sensor reading is $K F$ bits.

Mathematically, $\nu(x)$ can be defined as a probability mass function satisfying,

$$E_{\nu(x)}[g(x)] = \sum_{x_j \in X_F} w_{x_j} g(x_j)$$

(23)

where the $w_{x_j}$ are positive scalar values parameterizing the distribution. They satisfy that $w_{x_j} \geq 0$ and $\sum_{x_j \in X_F} w_{x_j} = 1$. 

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Under this assumption, the code-length of an observation $x_j \in X_F$ is defined by

$$\bar{\ell}(x_j, \rho) = \ln \frac{1}{\mathbb{E}_{\rho(\theta)}[p(x_j|\theta)]]}$$

(24)

where, abusing notation, we define $p(x_j|\theta) = \int_{j\Delta}^{(j+1)\Delta} p(x|\theta)dx$, and $\Delta$ is the width of the bins associated to the quantization into finite-precision numbers of a continuous variable over real-vectors.)

By using this new definition of code-length, the rest of quantities (e.g. $\bar{L}(\rho)$) are equally defined.

We also have that this scheme defines uniquely decodable codes because the Kraft inequality (Cover & Thomas, 2012) is also satisfied,

$$\sum_{x_j \in X_F} e^{-\bar{\ell}(x_j, \rho)} = \sum_{x_j \in X_F} \mathbb{E}_{\rho(\theta)}[p(x_j|\theta)] = \sum_{x_j \in X_F} \int_{j\Delta}^{(j+1)\Delta} p(x)dx = \int p(x)dx = 1$$

(25)

The only result which needs to be revised in the light of this new assumption is Theorem 2.

**Theorem 7.** Let us denote $H(\nu)$ the entropy of the distribution $\nu(x)$, then we have that for any mixture distribution $\rho$ on $\Theta$,

$$H(\nu) \leq \bar{L}(\rho),$$

where the equality only holds if the data generative distribution $\nu(x)$ and the posterior predictive distribution $p(x) = \mathbb{E}_{\rho(\theta)}[p(x|\theta)]$ are equal.

**Proof.** We first have to prove that $KL(\nu(x), p(x)) \geq 0$. We have that,

$$KL(\nu(x), p(x)) = \mathbb{E}_{\nu(x)}[-\ln \frac{p(x)}{\nu(x)}]$$

$$= \sum_{x_j \in X_F} -w_{x_j} \ln \frac{p(x_j)}{w_{x_j}}$$

$$\geq -\ln \sum_{x_j \in X_F} w_{x_j} \frac{p(x_j)}{w_{x_j}}$$

$$= -\ln \sum_{x_j \in X_F} p(x_j)$$

$$= 0$$

where the equality of second line follows form Equation (23), the inequality of the third line is the Jensen inequality, and the last inequality follows from Equation (25).

---

$^6$ $\Delta$ can indexed by $j$, $\Delta_j$, to cover float-precision numbers and/or the extreme of the integral.
As we have proved that the KL distance between $\nu(x)$ and $p(x)$ is always greater or equal than zero, we also have

$$KL(\nu(x), p(x)) = \mathbb{E}_{\nu(x)}[\ln \nu(x)] + \mathbb{E}_{p(x)}\left[\frac{1}{\mathbb{E}_{p(\theta)}[p(x|\theta)]}\right]$$

$$= -H(\nu(x)) + \mathbb{E}_{\nu(x)}[\ell(x, \rho)]$$

$$= -H(\nu(x)) + \bar{L}(\rho) \geq 0$$

and the statement follows from the last inequality. $\Box$

### B Bounded Log-Loss

Here we show how we can easily bound the log-loss of many standard machine-learning models. We do that by simply constraining the parameter space $\Theta$ because, according to Assumption 6, the input space $\mathcal{X}_F$ is just a (large) finite set and, in consequence, the norm of its elements is bounded.

- **Logistic Regression**: We have that $\forall y \in \{0, 1\}, \forall x \in \mathcal{X}_F$,

$$\ln \left(\frac{1}{p(y|x, \theta)}\right) = \ln(1 + e^{\theta^T x}) \leq \ln(1 + e^{||\theta||\cdot||x||})$$

where $|| \cdot ||$ denotes the Euclidean norm. The first equality follows from the definition of logistic regression, second equality follows because the exponential function is a monotonic function, and the last one follows from the Cauchy-Schwarz inequality. Moreover, we have that $||x||$ is bounded because $x \in \mathcal{X}_F$ is a finite-precision real vector whose norm is bounded (i.e. $\mathcal{X}_F$ is a finite set). So, if we define a parameter space $\Theta$ where the norm of any $\theta \in \Theta$ is bounded, we have that the log-loss of a logistic regression model is also bounded too.

- **Multi-Class Logistic Regression**: We have that $\forall y \in \{1, \ldots, R\}, \forall x \in \mathcal{X}_F$,

$$\ln \left(\frac{1}{p(y=r|x, \theta, \theta_1, \ldots, \theta_R)}\right) = -\ln \left(\sum_{i=1}^{R} e^{\theta_i^T x}\right) = \ln \left(\sum_{i=1}^{R} e^{(\theta_i - \theta_r)^T x}\right),$$

and, by following the same reasoning that with the logistic regression model, we can show this log-loss is bounded if the Euclidean norm of any $\theta \in \Theta$ is bounded.

- **Multi-Linear Regression**: We have that $\forall (y, x) \in \mathcal{X}_F$, and some precision matrix $M$,

$$\ln \left(\frac{1}{p(y|x, \theta, M)}\right) \leq (y - \theta^T x)^T M (y - \theta^T x) + A \leq ||y - \theta^T x||_M + A,$$

Note $\mathcal{X}_F$, as defined in Assumption 6, denotes the space of real vectors that can be represented with a finite precision scheme using $F$ bits to encode each element of the vector.
where the first inequality follows from the log-likelihood of a multivariate Normal with precision matrix $M$, and $A$ is some constant bounding the log-determinant of $M^{-1}$ plus some constant terms. The second inequality follows because $(y - \theta^T x)^T M (y - \theta^T x) \geq 0$ because $M$ is a positive semi-definite matrix and we can apply the Cauchy-Schwarz inequality where $\| \cdot \|_M$ denotes the weighted norm according to $M$, i.e. $\|z\|_M = \sqrt{z^T M z}$. Again, if the the log-determinant of $M^{-1}$ is bounded and the norm of any $\theta \in \Theta$ is bounded, then this log-loss is bounded because the norms of $y$ and $x$ are also bounded because they are finite-precision real vectors.

- **Multi-Layered Neural networks** over cross-entropy and mean-square error loss functions have bounded log-loss if the space of weights $\Theta$ is bounded. This happens because the loss depends on the activation of the neurons of the last and/or previous layers. So, the norm of this activation vector is bounded and the previous analyses apply here.

- **Variational Autoencoders**: In general, this model also has bounded log-loss if we consider a bounded parameter space $\Theta$ and that the support of $p(z)$ is bounded too. Then $- \ln p(x | z, \theta)$ is bounded from the analysis in the previous points. Finally, because

$$- \ln p(x | \theta) \leq -E_{p(z)} [\ln p(x | z, \theta)],$$

due to Jensen inequality, we can conclude that the log-loss of a VAE would be bounded too.

We can get rid off of the condition that the support of $p(z)$ is bounded if the output of the decoder network in the VAE only depends on the activations of the neurons of the last layer. In this case, the norm of the activations is always bounded and we do not need to bound the support of $p(z)$.

Following this reasoning, we think that, properly constraining the parameter space $\Theta$, we can build many machine learning models with bounded log-loss because, due to Assumption 6 the input space is always bounded.

### C PAC$^2$-Variational Learning

PAC$^2$-Variational Inference is based on the optimization of Equation (18). This optimization is not feasible in this current formulation. By employing the expression provided in Lemma 9 and multiplying and dividing the term $\bar{V}_h$ by $2 \max_{\theta} p(x | \theta)^2$, we can re-express Equation (18) as follows,

$$\mathcal{L}_{P_{H_h}}(\lambda) = E_{p(\theta, \theta' | \lambda)} \left[ \frac{1}{n} \sum_{i=1}^{n} - \ln p(x_i | \theta) - h(\alpha_{x_i}) \bar{V}(x_i, \theta, \theta') \right] + \frac{2}{n} KL(\rho, \pi)$$

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where \( \rho(\theta, \theta' | \lambda) = \rho(\theta | \lambda) \rho(\theta' | \lambda) \) and

\[
\begin{align*}
\alpha_{\lambda, i} & = \max_j (\ln p(x_i | \theta_j) + \ln p(x_i | \theta'_j)) + \epsilon \\
\mu_{\lambda, i} & = \ln \sum_j \exp(\ln p(x_i | \theta_j)) - \ln E \\
\alpha_{\lambda, i} & = \mu_{\lambda, i} - m_{\lambda, i} \\
h(\alpha_{\lambda, i}) & = \frac{\alpha_{\lambda, i}}{(1 - \exp(\alpha_{\lambda, i}))^2} + \frac{1}{\exp(\alpha_{\lambda, i})(1 - \exp(\alpha_{\lambda, i}))}.
\end{align*}
\]

with \( \epsilon > 0 \).

We can minimize \( \tilde{L}_{PB}^2 (\lambda) \) using any gradient-based optimizing algorithm. Unbiased estimates of the gradient of \( \tilde{L}_{PB}^2 (\lambda) \) can be computed using appropriate Monte-Carlo gradient estimation methods (Mohamed et al., 2019). We apply stop-gradient operation over \( m_{\lambda, i} \) and \( h(\alpha_{\lambda, i}) \) to avoid problems deriving a max or a log-sum-exp operation.

## D PAC\(^2\)-Ensemble Learning

PAC\(^2\)-Ensemble Learning is done by minimizing Equation (21). We now show how to express this function in a numerically stable way,

\[
\begin{align*}
\sum_j \sum_k \sum_i - \ln p(x_i | \theta_j) \\
& - h(\alpha_{\lambda, i}) \exp(2 \ln p(x_i | \theta_j) - 2m_{\lambda, i}) \\
& + h(\alpha_{\lambda, i}) \exp(\ln p(x_i | \theta_j) + \ln p(x_i | \theta_k) - 2m_{\lambda, i}) \\
& - \ln \pi(\theta_j)
\end{align*}
\]

where we also need the following definitions

\[
\begin{align*}
m_{\lambda, i} & = \max_j \ln p(x_i | \theta_j) \\
\mu_{\lambda, i} & = \ln \sum_j \exp(\ln p(x_i | \theta_j)) - \ln E \\
\alpha_{\lambda, i} & = \mu_{\lambda, i} - m_{\lambda, i} \\
h(\alpha_{\lambda, i}) & = \frac{\alpha_{\lambda, i}}{(1 - \exp(\alpha_{\lambda, i}))^2} + \frac{1}{\exp(\alpha_{\lambda, i})(1 - \exp(\alpha_{\lambda, i}))}.
\end{align*}
\]

Again, we apply stop-gradient operation over \( m_{\lambda, i} \) and \( h(\alpha_{\lambda, i}) \) to avoid problems deriving a max or a log-sum-exp operation.

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\( ^8 \epsilon = 0.1 \) in the reported experiments.
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