A General Framework for the Disintegration of PAC-Bayesian Bounds
Paul Viallard, Pascal Germain, Amaury Habrard, Emilie Morvant

To cite this version:
Paul Viallard, Pascal Germain, Amaury Habrard, Emilie Morvant. A General Framework for the Disintegration of PAC-Bayesian Bounds. 2021. hal-03143025v2

HAL Id: hal-03143025
https://hal.archives-ouvertes.fr/hal-03143025v2
Preprint submitted on 8 Oct 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
A General Framework for the Disintegration of PAC-Bayesian Bounds

Paul Viallard$^1$, Pascal Germain$^2$, Amaury Habrard$^1$, and Emilie Morvant$^1$

$^1$Univ Lyon, UJM-Saint-Etienne, CNRS, Institut d Optique Graduate School, Laboratoire Hubert Curien UMR 5516, F-42023, SAINT-ETIENNE, France
$^2$Département d’informatique et de génie logiciel, Université Laval, Québec, Canada

Abstract
PAC-Bayesian bounds are known to be tight and informative when studying the generalization ability of randomized classifiers. However, when applied to some family of deterministic models such as neural networks, they require a loose and costly derandomization step. As an alternative to this step, we introduce new PAC-Bayesian generalization bounds that have the originality to provide disintegrated bounds, i.e., they give guarantees over one single hypothesis instead of the usual averaged analysis. Our bounds are easily optimizable and can be used to design learning algorithms. We illustrate the interest of our result on neural networks and show a significant practical improvement over the state-of-the-art framework.

Introduction
PAC-Bayesian theory (Shawe-Taylor and Williamson, 1997; McAllester, 1998) provides a powerful framework for analyzing the generalization ability of machine learning models such as linear classifiers (Germain et al., 2009), SVM (Ambroladze et al., 2006) or neural networks (Dziugaite and Roy, 2017). PAC-Bayesian analyses usually take the form of bounds on the average risk of a randomized classifier with respect to a learned posterior distribution given a chosen prior distribution defined over a set of hypotheses. While such bounds are very effective for analyzing stochastic classifiers, some machine learning methods need nevertheless guarantees on deterministic models. In this case, a derandomization step of the bound is required. Different forms of derandomization have been introduced in the literature for specific settings. Among them, Langford and Shawe-Taylor (2002) propose a derandomization for Gaussian posteriors over linear classifiers: thanks to the Gaussian symmetry, a bound on the risk of the maximum a posteriori (deterministic) classifier is obtainable from the bound on the average risk of the randomized classifier. Also relying on Gaussian posteriors, Letarte et al. (2019) derived a PAC-Bayes bound for a very specific deterministic network architecture using sign functions as activations. Another line of works derandomizes neural networks (Neyshabur et al., 2018; Nagarajan and Kolter, 2019a). While being technically different, it starts from PAC-Bayesian guarantees on the randomized classifier and use an “output perturbation” bound to convert a guarantee from a random classifier to the mean classifier. These works highlight the need of a general framework for the derandomization of classic PAC-Bayesian bounds.

In this paper, we focus on another kind of derandomization, sometimes referred to as disintegration of the PAC-Bayesian bound, and first proposed by Catoni (2007, Th.1.2.7) and Blanchard and Fleuret (2007): Instead of bounding the average risk of a randomized classifier with respect to the posterior distribution, the disintegrated PAC-Bayesian bounds upper-bound the risk of a sampled (unique) classifier from the posterior distribution. Despite their interest in derandomizing PAC-Bayesian bounds, this kind of bounds have only received little study in the literature; especially we can cite the recent work of Rivasplata et al. (2020, Th.1(ii)) who derived a general disintegrated PAC-Bayesian theorem. Moreover, these bounds have never been used in practice. Driven by machine learning practical purposes, our objective is twofold: To derive new tight disintegrated PAC-Bayesian bounds (i) that directly derandomize any type of classifiers without any other additional step and with (almost) no impact on the guarantee, (ii) that can be easily optimized to learn classifiers with strong guarantees. Our main contribution has a practical objective: Providing a new general framework based on the Rényi divergence allowing efficient learning. We also derive an information-theoretic bound giving interesting new insights on disintegration procedures. Note that for the sake of readability we deferred to the technical appendix the proofs of our theoretical results.

Setting and basics
General notations. We tackle supervised classification tasks with $X$ the input space, $Y$ the label set, and $D$ an unknown data distribution on $X \times Y=\mathcal{Z}$. An example is denoted by $z=(x, y) \in \mathcal{Z}$, and the learning sample $S=\{z_i\}_{i=1}^m$ is constituted by $m$ examples drawn i.i.d. from $D$; the distribution of such a $m$-sample being $D^m$. We consider a hypothesis set $\mathcal{H}$ of functions $h :X \to Y$. The learner aims to find $h \in H$ that assigns a label $y$ to an input $x$ as accurately as possible. Given an example $z$ and a hypothesis $h$, we assess the quality of the prediction of $h$ with a loss function $\ell : \mathcal{H} \times \mathcal{Z} \to [0,1]$ evaluating to which extent the prediction is accurate. Given the loss $\ell$, the true risk $R_D(h)$ of a hypothesis $h$ on the distribution $D$ and its empirical counterpart $R_S(h)$ estimated on $S$ are defined as

$$R_D(h) \triangleq \mathbb{E}_{z \sim D} \ell(h, z) , \quad \text{and} \quad R_S(h) \triangleq \frac{1}{m} \sum_{i=1}^m \ell(h, z_i).$$
Then, we want to find the hypothesis from $\mathcal{H}$ that minimizes $R_D(h)$, that is, however, not computable since $D$ is unknown. In practice we can consider the Empirical Risk Minimization (ERM) principle that looks for a hypothesis minimizing $R_S(h)$. Generalization guarantees over unseen data from $D$ can be obtained by quantifying how much the empirical risk $R_S(h)$ is a good estimate of $R_D(h)$. The statistical machine learning theory (e.g., Vapnik, 2000) studies the conditions of consistency and convergence of ERM towards the true value. This kind of result is called generalization bounds, often referred to as PAC (Probably Approximately Correct) bounds (Valiant, 1984), and take the form:

$$
\mathbb{P}_{S \sim D^m}\left[ R_D(h) - R_S(h) \leq \epsilon\left(\frac{1}{2}, \frac{1}{m}, \mathcal{H}\right) \right] \geq 1 - \delta.
$$

Put into words, with high probability (1−δ) on the random choice of $S$, we obtain good generalization properties when the deviation between the true risk $R_D(h)$ and its empirical estimate $R_S(h)$ is low, i.e., $\epsilon\left(\frac{1}{2}, \frac{1}{m}, \mathcal{H}\right)$ should be as small as possible. The function $\epsilon$ depends on 3 quantities: (i) the number of examples $m$ for statistical precision, (ii) the hypothesis set $\mathcal{H}$ for assessing how its specificities influence generalization, (iii) the parameter confidence $\delta$. We now recall 3 classic bounds with a focus on the PAC-Bayesian theory at the heart of our contribution.

**Uniform convergence bound.** A first classical type of generalization bounds is referred to as Uniform Convergence bounds based on a measure of complexity of the set $\mathcal{H}$ and stand for all the hypotheses of $\mathcal{H}$. Among the most renowned complexity measure, we can cite the VC-dimension or the Rademacher complexity. This type of bound takes the form

$$
\mathbb{P}_{S \sim D^m}\left[ \sup_{h \in \mathcal{H}} |R_D(h) - R_S(h)| \leq \epsilon\left(\frac{1}{2}, \frac{1}{m}, \mathcal{H}\right) \right] \geq 1 - \delta.
$$

This bound holds for all $h \in \mathcal{H}$, including the best, but also the worst. The worst-case analysis makes hard to obtain a non-vacuous bound with $\epsilon\left(\frac{1}{2}, \frac{1}{m}, \mathcal{H}\right)<1$. The ability of such bounds to explain the generalization of deep learning has been recently challenged (Nagarajan and Kolter, 2019b).

**Algorithmic-Dependent Bound.** Other bounds depend on the learning algorithm (Bousquet and Elisseeff, 2002; Xu and Mannor, 2012), and directly involve some particularities of the learning algorithm $L$. This allows obtaining bounds that stand for a single hypothesis $h_{L(S)}$, the one learned with $L$ from the learning sample $S$. The form of such bounds is

$$
\mathbb{P}_{S \sim D^m}\left[ |R_D(h_{L(S)}) - R_S(h_{L(S)})| \leq \epsilon\left(\frac{1}{2}, \frac{1}{m}, L\right) \right] \geq 1 - \delta.
$$

**PAC-Bayesian Bound.** This paper leverages on PAC-Bayes bounds that stand in the PAC framework but borrow inspiration from the Bayesian probabilistic view that deals with randomness and uncertainty in machine learning (McAllester, 1998). That being said, considering the set $\mathcal{M}(\mathcal{H})$ of probability measures on $\mathcal{H}$, a PAC-Bayesian generalization bound is a bound in expectation over the hypothesis set $\mathcal{H}$ and involves a prior distribution $P \in \mathcal{M}(\mathcal{H})$ on $\mathcal{H}$ and a posterior distribution $Q \in \mathcal{M}(\mathcal{H})$ on $\mathcal{H}$ learned from $S$. The form of such a bound is

$$
\mathbb{P}_{S \sim D^m}\left[ \forall Q, \mathbb{E}_{h \sim Q} [R_D(h) - R_S(h)] \leq \epsilon\left(\frac{1}{2}, \frac{1}{m}, \mathcal{H}\right) \right] \geq 1 - \delta.
$$

We recall below the classical PAC-Bayesian theorem in a slightly different form from the usual one: From Theorem 1, $\phi(h,S) = \mathbb{E}(\phi(h,S))$ gives the usual form of the bounds.

**Theorem 1 (General PAC-Bayes bounds).** For any distribution $D$ on $\mathcal{Z}$, for any hypothesis set $\mathcal{H}$, for any prior distribution $P$ on $\mathcal{H}$, for any $\phi : \mathcal{H} \times Z^m \to \mathbb{R}^+$, for any $\delta > 0$ we have

$$
\mathbb{P}_{S \sim D^m}\left( \forall Q, \mathbb{E}_{h \sim Q} \ln(\phi(h,S)) \leq \frac{\text{KL}(Q \| P) + \ln\left(\frac{1}{\delta}\right)}{\delta} \right) \geq 1 - \delta,
$$

and

$$
\mathbb{P}_{S \sim D^m}\left( \forall Q, \mathbb{E}_{h \sim Q} \ln(\phi(h,S)) \leq \frac{\text{KL}(Q \| P) + \ln\left(\frac{1}{\delta}\right)}{\delta} \right) \geq 1 - \delta,
$$

with $D_{\alpha}(Q \| P) \triangleq \frac{1}{\alpha \mathbb{E}_{h \sim P} \ln\left(\frac{Q(h)}{P(h)}\right)^\alpha}$ the Rényi divergence $(\alpha > 1)$ and $\text{KL}(Q \| P) \triangleq \mathbb{E}_{h \sim P} \ln\left(\frac{Q(h)}{P(h)}\right)$ the KL-divergence.

Equation (0.2) is more general than Equation (0.1) since the Rényi divergence can be seen as a generalization of the KL-divergence: When $\alpha$ tends to 1, then $D_{\alpha}(Q \| P)$ tends to $\text{KL}(Q \| P)$. The advantage of these bounds is that they are general since they can be seen as the starting points for deriving different forms of bounds by first, instantiating $\phi$ to capture a deviation between the true and empirical risks, second, upper-bounding the term $\mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P} \phi(h,S)$. For instance, with $\phi(h,S) = e^{m2[L_D(h)-R_S(h)]^2}$ we retrieve from Equation (0.1) the form of McAllester (1998):

$$
\mathbb{E}_{h \sim Q} R_D(h) \leq \mathbb{E}_{h \sim Q} R_S(h) + \sqrt{\frac{\text{KL}(Q \| P) + \ln\left(\frac{2\sqrt{m}}{\delta}\right)}{2m}}.
$$

This bound illustrates the trade-off between the average empirical risk and the bound. Another example, leading to a slightly tighter but less interpretable bound, is the Seeger (2002); Maurer (2004)'s bound that we retrieve with $\phi(h,S) = e^{m\textrm{kl}(R_D(h)||R_S(h))}$ and $\textrm{kl}[q||p] = q \ln \frac{q}{p} + (1-q) \ln \frac{1-q}{1-p}$:

$$
\mathbb{E}_{h \sim Q} \text{kl}(R_S(h)||R_D(h)) \leq \frac{\text{KL}(Q \| P) + \ln\left(\frac{2\sqrt{m}}{\delta}\right)}{m}.
$$

Such PAC-Bayesian bounds are known to be tight, but they stand for a randomized classifier by nature (due to the expectation on $\mathcal{H}$). A key issue for usual machine learning tasks is then the derandomization of the bounds to obtain a guarantee for a deterministic classifier. In some cases, this derandomization is a result of the structure of the hypotheses such as for randomized linear classifier that can be directly expressed as one deterministic linear classifier (Germain et al.,
However, in other cases the derandomization is much more complex and specific to a class of hypothesis, such as for neural networks (e.g., Neyshabur et al. (2018), Nagarajan and Kolter (2019b, Ap. J)).

In the following, we state our contribution: A general de-randomization framework for desintegrating PAC-Bayesian bounds into a bound for a single hypothesis from $\mathcal{H}$.

**Disintegrated PAC-Bayesian theorems**

**Form of a disintegrated PAC-Bayes bound.** First, we recall another kind of bound introduced by Blanchard and Fleuret (2007) and Catoni (2007, Th.1.2.7) and referred to as the disintegrated PAC-Bayesian bound; Its form is

$$\mathbb{P}_{S \sim \mathcal{D}^m, h \sim Q_{S}} \left[ |R_{\mathcal{D}}(h) - R_{S}(h)| \leq \epsilon \left( \frac{1}{\delta} \frac{1}{m}, Q_{S} \right) \right] \geq 1 - \delta.$$  

This kind of generalization bound allows one to derandomize the usual PAC-Bayes bounds as follows. Instead of considering a bound that stands for all the posterior distributions on $\mathcal{H}$ as usually done in PAC-Bayes (Theorem 1), we propose to consider only the posterior distribution $Q_{S}$ obtained through a deterministic algorithm taking the learning sample $S$ as input. More formally, we consider a deterministic algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})$ chosen a priori which (i) takes a learning sample $S \in \mathcal{Z}^m$ as input and (ii) outputs a data-dependent distribution $Q_{S} = A(S)$ from the set $\mathcal{M}(\mathcal{H})$ of all possible probability measures on $\mathcal{H}$. Then, the above bound stands for a unique hypothesis $h \sim Q_{S}$ instead of a randomized classifier: The individual risks are no longer averaged over the random choice of the learning sample $S \sim \mathcal{D}^m$ and the hypothesis $h \sim Q_{S}$. Under this principle, we present in the following two new general disintegrated PAC-Bayesian bounds in Theorems 2 and 4. Importantly, they have the advantage to be instantiation for neural networks.

**Disintegrated PAC-Bayesian bounds with the Rényi divergence.** In the same spirit as Equation (0.2) our first result stated below can be seen as a general bound depending on the Rényi divergence $D_{\alpha}(Q_{S} || P)$ of order $\alpha > 1$.

**Theorem 2** (Disintegrated PAC-Bayes Bound). For any distribution $\mathcal{D}$ on $\mathcal{Z}$, for any hypothesis set $\mathcal{H}$, for any prior distribution $P$ on $\mathcal{H}$, for any $\phi : \mathcal{H} \times \mathcal{Z}^m \rightarrow \mathbb{R}^+$, for any $\alpha > 1$, for any $\delta > 0$, for any algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})$, we have

$$\mathbb{P}_{S \sim \mathcal{D}^m, h \sim Q_{S}} \left[ \frac{\alpha}{\alpha - 1} \ln \left( \phi(h, S) \right) \leq \frac{2}{\alpha - 1} \ln \frac{2}{\delta} + D_{\alpha}(Q_{S} || P) \right] + \ln \left[ \mathbb{E}_{S' \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right] \geq 1 - \delta,$$

where $Q_{S} = A(S)$ is output by the deterministic algorithm $A$.

**Proof sketch (see Appendix for details).** First, note that $Q_{S}$ is obtained with algorithm $A$ from $S$. Then, applying Markov’s inequality on $\phi(h, S)$ with the random variable (r.v.) $h$ and using Hölder’s inequality to introduce $D_{\alpha}(Q_{S} || P)$, we have with probability at least $1 - 2/\delta$ on $S \sim \mathcal{D}^m$ and $h \sim Q_{S}$

$$\frac{\alpha}{\alpha - 1} \ln \left( \phi(h, S) \right) \leq \frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim Q_{S}} \phi(h', S) \right)$$

$$\leq - D_{\alpha}(Q_{S} || P) + \frac{\alpha}{\alpha - 1} \ln \frac{2}{\delta} + \ln \left( \mathbb{E}_{h' \sim P} \phi(h', S)^{\frac{1}{\alpha - 1}} \right).$$

By applying again Markov’s inequality on $\phi(h, S)$ with the r.v. $S$, we have with probability at least $1 - 2/\delta$ on $S \sim \mathcal{D}^m$ and $h \sim Q_{S}$

$$\ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right) \leq \ln \left( \frac{2}{\delta} \mathbb{E}_{S' \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right).$$

By combining the two bounds with a union bound argument, we obtain the desired result.

Note that Hölder’s inequality is used differently in the classic PAC-Bayes bound’s proof. Indeed, in Bégia et al. (2016, Th. 8), the change of measure (based on Hölder’s inequality) is key to obtain a bound that holds for all posterior $Q$ with high probability, while our bound holds for a unique posterior $Q_{S}$ dependent on the sample $S$. In fact, we use Hölder’s inequality to make appear a prior $P$ independent from $S$, a crucial point for our bound instantiated in Corollary 6. Compared to Equation (0.2), our bound requires an additional term $\ln 2 + \frac{\alpha}{\alpha - 1} \ln \frac{2}{\delta}$. However, by taking $\phi(h, S) = n \mathbb{E}_{S \sim \mathcal{D}^m} R_{\mathcal{D}}(h) / R_{S}(h)$ and $\alpha = 2$, the term $\ln \frac{2}{\delta}$ is multiplied by $\frac{1}{m}$, allowing us to obtain a reasonable overhead to “derandomize” a bound into a disintegrated one. For instance, if $m = 5, 000$ (reasonable sample size) and $\delta = 0.5$, we have $\frac{1}{m} \ln \frac{2}{\delta} \approx 0.002$.

We instanciate below Theorem 2 for $\alpha \rightarrow 1^+$ and $\alpha \rightarrow +\infty$.

**Corollary 3.** Under the assumptions of Theorem 2, when $\alpha \rightarrow 1^+$, with probability at least $1 - \delta$ we have

$$\ln \phi(h, S) \leq \frac{2}{\delta} + \ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right).$$

When $\alpha \rightarrow +\infty$, with probability at least $1 - \delta$ we have

$$\ln \phi(h, S) \leq \ln \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}}$$

where $\mathbb{E}sup$ is the essential supremum.

This corollary illustrates that the parameter $\alpha$ controls the trade-off between the Rényi divergence $D_{\alpha}(Q_{S} || P)$ and $\ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right)$. Indeed, when $\alpha \rightarrow 1^+$, the Rényi divergence vanishes while the other term converges toward $\ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right)$, roughly speaking the maximal value possible for the second term. On the other hand, when $\alpha \rightarrow +\infty$, the Rényi divergence increases and converges toward $\ln \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}}$, and the other term decreases toward $\ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h', S')^{\frac{1}{\alpha - 1}} \right)$.

For the sake of comparison, we recall the bound of Rivasplata et al. (2020, Th.1(ii)), that is more general than the
bounds of Blanchard and Fleuret (2007) and Catoni (2007):
\[
\mathbb{P}_{S \sim \mathcal{D}^m, h \sim \mathcal{Q}_S} \left( \ln \phi(h, S) \right) \leq \\
\mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{Q}_S} \left( \ln \frac{\mathcal{Q}_S(h)}{\mathcal{P}(h)} + \frac{1}{\delta} \mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S') \right) \geq 1 - \delta. \tag{0.4}
\]

Our bound has a worse dependence in \(\delta\), which is the price we pay for a general result with a divergence. Indeed, the main difference with Equation (0.4) is that our bound involves the Rényi divergence \(D_\alpha(Q_S || P)\) between the prior \(P\) and the posterior \(Q_S\). In contrast, the term \(\ln \mathcal{Q}_S(h) / \mathcal{P}(h)\) (also involved in the bounds of Catoni (2007); Blanchard and Fleuret (2007)) can be seen as a “disintegrated1 KL-divergence” depending only on the sampled \(h \sim \mathcal{Q}_S\). Overall, from the properties of the Rényi divergence (van Erven and Harremos, 2014), our bound is expected to be looser. However, as we show in our experiment, the divergence term of Equation (0.4) makes it harder to optimize since it can be subject to a high variance. Optimizing our bound with \(D_\alpha(Q_S || P)\) makes the procedure more stable and efficient which is thus more interesting in practice, allowing us to get better empirical results.

We now provide a parametrized version of our bound enlarging its practical scope. In the PAC-Bayes literature, parametrized bounds have been introduced (e.g., Catoni (2007); Thiemann et al. (2017)) to control the trade-off between the empirical risk and the divergence along with the additional term. We follow a similar approach to introduce a version of a disintegrated Rényi divergence-based bound that has the advantage to be parametrizable.

**Theorem 4** (Parametrizable Disintegrated PAC-Bayes Bound). Under the same assumptions than Theorem 2, we have
\[
\mathbb{P}_{S \sim \mathcal{D}^m, h \sim \mathcal{Q}_S} \left( \forall \lambda > 0, \ln \phi(h, S) \right) \leq \\
\mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{Q}_S} \left( \frac{\lambda}{2} D_2(Q_S || P) + \frac{8}{2\lambda\delta^3} \mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S')^2 \right) \geq 1 - \delta.
\]

Of note, \(e^{D_2(Q_S || P)}\) is closely related to the \(\chi^2\) distance: \(e^{D_2(Q_S || P)} - 1 = \chi^2(Q_S || P)\). An asset of Theorem 4 is the parameter \(\lambda\) controlling the trade-off between the exponentiated Rényi divergence \(e^{D_2(Q_S || P)}\) and \(\frac{1}{\delta} \mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S')^2\). Our bound is valid for all \(\lambda > 0\), then from a practical view we can select the parameter to minimize the bound (and control the possible numerical instability due to \(e^{D_2(Q_S || P)}\)). Despite this algorithmic advantage, for a given \(P\) and \(Q_S\), Proposition 5 shows the optimal bound of Theorem 4 is the bound of Theorem 2.

**Proposition 5.** For any distribution \(\mathcal{D}\) on \(\mathcal{Z}\), for any hypothesis set \(\mathcal{H}\), for any prior distribution \(P\) on \(\mathcal{H}\), for any \(\delta > 0\) and for any algorithm \(A : \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})\), let
\[
\lambda^* = \arg \min_{\lambda > 0} \mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S')^2.
\]

\[
\lambda^* = \sqrt{\frac{\mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S')^2}{\delta \exp(D_2(Q_S || P))}}. \tag{0.5}
\]

In other words, the optimal \(\lambda^*\) gives the same bound for Theorems 2 and 4.

So far we have introduced theoretical results allowing to derandomize PAC-Bayesian bounds through a disintegration approach. Our bounds are general and can be instantiated to different settings. In the next section, we illustrate the instantiation and usefulness of Theorem 2 on neural networks.

**The disintegration in action**

**Specialization to neural network classifiers.** We consider neural networks (NN) parametrized by a weight vector \(w \in \mathbb{R}^d\) and overparametrized, i.e., \(d \gg m\). We aim at learning the weights of the NN leading to the lowest true risk. Practitioners usually proceed by epochs2 and obtain one “intermediate” NN after each epoch. Then, they select the best “intermediate” NN associated with the lowest validation risk. We translate this practice into our PAC-Bayesian setting by considering one prior per epoch. Given \(T\) epochs, we hence have \(T\) priors \(P_t = \{P_t\}_{t=1}^T\), where \(\forall t \in \{1, \ldots, T\}, P_t = \mathcal{N}(\nu_t, \sigma^2 I_d)\) is a Gaussian distribution centered at \(\nu_t\), the weight vector associated with the \(t\)-th “intermediate” NN, with a covariance matrix of \(\sigma^2 I_d\) (where \(I_d\) is the \(d \times d\)-dimensional identity matrix). Assuming the \(T\) priors are learned from a set \(S_{\text{prior}}\) such that \(S_{\text{prior}} \cap S = \emptyset\), then Corollaries 6 and 7 will guide us to learn a posterior \(Q_S = \mathcal{N}(w, \sigma^2 I_d)\) from the best prior on \(S\) (we give more details on the procedure after the forthcoming corollaries).

We instantiate Theorem 2 to this setting in Corollary 6. For the sake of comparison, we instantiate in Corollary 7 the Rivspla et al. (2020)’s bound (recalled in Equation (0.4)) in Equation (0.5), and the ones of Blanchard and Fleuret (2007) and Catoni (2007) respectively in Equations (0.6) and (0.7).

**Corollary 6.** For any distribution \(\mathcal{D}\) on \(\mathcal{Z}\), for any set \(\mathcal{H}\), for any set \(\mathcal{P}\) of \(T\) priors on \(\mathcal{H}\), for any algo. \(A : \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})\),
for any loss $\ell: \mathcal{H} \times Z \to [0, 1]$, for any $\delta > 0$, we have

$$\mathbb{P}_{S\sim D^m, h\sim Q_S} \left( \forall \mathcal{P}_t \in \mathcal{P}, \text{ kl}(R_S(h)||R_D(h)) \leq \frac{1}{m} \left[ \frac{\|w-v_t\|_2^2}{2\sigma^2} + \frac{16T\sqrt{m}}{\delta^3} \right] \right) \geq 1-\delta,$$

where $\text{kl}(a||b) = a \ln \frac{a}{b} + (1-a) \ln \frac{1-a}{1-b}$.

**Corollary 7.** Under Corollary 6’s assumptions, with probability at least $1-\delta$ over $S\sim D^m$ and $h\sim Q_S$, we have $\forall \mathcal{P}_t \in \mathcal{P}$

$$\text{kl}(R_S(h)||R_D(h)) \leq \frac{1}{m} \left[ \frac{\|w+e-v_t\|_2^2 - \|e\|_2^2}{2\sigma^2} + \frac{16T\sqrt{m}}{\delta^3} \right], \quad (0.5)$$

$$\text{kl}(R_S(h)||R_D(h)) \leq \frac{1}{m} \left[ \frac{m+1}{m} \frac{\|w+e-v_t\|_2^2 - \|e\|_2^2}{2\sigma^2} + \frac{Tm+T}{\delta^3} \right], \quad (0.6)$$

$$\forall c \in C, R_D(h) \leq \frac{1}{1-e^{-\text{kl}(R_S(h)||R_D(h))}} - \frac{1}{1-e^{-\text{kl}(c||R_D(h))}}, \quad (0.7)$$

where $e \sim N(0, \sigma^2 I_d)$ is a Gaussian noise s.t. $w+e$ are the weights of $h\sim Q_S$ with $Q_S=N(w, \sigma^2 I_d)$, and $C$ is a set of hyperparameters fixed a priori.

Experiments we performed involve the direct minimization of Corollary 6 (or any other bounds of Corollary 7). To obtain a tight bound, the divergence between one prior $\mathcal{P}_t \in \mathcal{P}$ and $Q_S$ must be low, i.e., $\|w-v_t\|_2^2$ or $\|w+e-v_t\|_2^2 - \|e\|_2^2$ has to be low. However, this can be challenging with NNs since $d \gg m$. One solution is to split the learning sample into 2 non-overlapping subsets $S_{\text{prior}}$ and $S$, where $S_{\text{prior}}$ is used to learn the prior, while $S$ is used both to learn the posterior and compute the bound. Hence, if we “pre-learn” a good enough prior $\mathcal{P}_t \in \mathcal{P}$ from $S_{\text{prior}}$, then we can expect to have a low $\|w-v_t\|_2^2$.

### Training Method

The original training set is split in two distinct subsets: $S_{\text{prior}}$ and $S$. The training has two phases.

1. **The prior distribution $\mathcal{P}$ is “pre-learned” with $S_{\text{prior}}$ and selected by early stopping the algorithm with $S$ as validation set (from an arbitrary learning algorithm $A_{\text{prior}}$).**
2. **Given $S$ and $\mathcal{P}$, we learn the posterior $Q_S$ with the algorithm $A$ (defined a priori).**

At first sight, the selection of the prior weights with $S$ by early stopping may appear to be “cheating”. However, this procedure can be seen as: 1) first constructing $\mathcal{P}$ from the $T$ “intermediate” NNs learned after each epoch from $S_{\text{prior}}$, 2) optimizing the bound with the prior that leads to the best risk on $S$. This gives a statistically valid result, since Corollaries 6 is valid for every $\mathcal{P}_t \in \mathcal{P}$, we can thus select the one we want, in particular the best one on $S$. Usually, practitioners consider this “best” prior as the final NN. In our case, the advantage is that we refine this “best” prior on $S$ to learn the posterior $Q_S$. Note that Pérez-Ortiz et al. (2020) have already introduced tight generalization bounds with data-dependent priors for—non-derandomized—stochastic NNs. Nevertheless, our training method to learn the prior differs greatly since 1) we learn $T$ NNs (i.e., $T$ priors) instead of only one, 2) we also fix the variance of the Gaussian in the posterior $Q_S$. Hence, to the best of our knowledge, our training method for the prior is new.

### A note about stochastic neural networks.

Due to its stochastic nature, PAC-Bayesian theory has been explored to study stochastic NNs (e.g., Dziugaite and Roy (2017; 2018); Zhou et al. (2019); Pérez-Ortiz et al. (2020)). In Corollary 8 below, we instantiate the bound of Equation (0.1) for stochastic NNs to empirically compare the stochastic and the deterministic NNs associated with prior(s) and posterior distributions. We recall that, in this paper, a deterministic NN is a single $h$ sampled from the posterior distribution $Q_S=N(w, \sigma^2 I_d)$ output by the algorithm $A$. This means that for each example the label prediction is performed by the same deterministic NN: The one parametrized by the weights $w \in \mathbb{R}^d$. Conversely, the stochastic NN associated with a posterior distribution $Q=N(w, \sigma^2 I_d)$ predicts the label of a given example by (i) first sampling $h$ according to $Q$ (i.e., the NN parametrized by $w \in \mathbb{R}^d$), (ii) then returning the label predicted by $h$. Thus, the result of the stochastic NN is the expected risk value $\mathbb{E}_{h \sim Q} R_D(h)$, where the expectation is taken over all $h$ sampled from $Q$. We compute the empirical risk of the stochastic NN from a Monte Carlo approximation: (i) if we sample $n$ weight vectors, and (ii) we average the risk over the $n$ associated NNs; We denote by $Q^n$ the distribution of such $n$-sample. In this context, we propose the following randomized PAC-Bayesian bound.

**Corollary 8.** For any distribution $D$ on $Z$, for any $\mathcal{H}$, for any set $\mathcal{P}$ of $T$ priors on $\mathcal{H}$, for any loss $\ell: \mathcal{H} \times Z \to [0, 1]$, for any $\delta > 0$, with probability at least $1-\delta$ over $S\sim D^m$ and $\{h_1, \ldots, h_n\} \sim Q^n$, we have simultaneously $\forall \mathcal{P}_t \in \mathcal{P}, \forall Q$,

$$\text{kl} \left( \mathbb{E}_{h \sim Q} R_S(h) || \mathbb{E}_{h \sim Q} R_D(h) \right) \leq \frac{1}{m} \left[ \frac{\|w-v_t\|_2^2 + \frac{16T\sqrt{m}}{\delta^3}}{2\sigma^2} \right], \quad (0.8)$$

and

$$\text{kl} \left( \frac{1}{n} \sum_{i=1}^{n} R_S(h_i) || \mathbb{E}_{h \sim Q} R_S(h) \right) \leq \frac{1}{n} \ln \frac{4}{\delta}. \quad (0.9)$$

This result shows two key features that allow considering it as an adapted baseline for a fair comparison between disintegrated and classical PAC-Bayesian bounds, thus between deterministic and stochastic NNs. On the one hand, it involves the same terms as Corollary 6. On the other hand, it is close to the bound of Pérez-Ortiz et al. (2020, Sec. 6.2), since (i) we adapt the KL-divergence to our setting (i.e., $\text{KL}(Q||\mathcal{P})=\frac{1}{m^2} \|w-v_t\|_2^2$), (ii) the bound holds for $T$ priors thanks to a union bound argument.

---

3The stochastic classifier is called Gibbs classifier in PAC-Bayes.
Experiments on neural networks

In this section, we do not seek state-of-the-art performance, in fact, we have a twofold objective: (i) We show that our disintegrated bound of Corollary 6 is tighter and more stable than the of Corollary 7 based on Rivasplata et al. (2020), Blanchard and Fleuret (2007) and Catoni (2007). (ii) We highlight that our disintegrated bound associated with the deterministic NN is tighter than the randomized bound associated with the stochastic NN (Corollary 8).

Training method. We follow our Training Method in which we integrate the direct minimization of the bounds. We refer as ours the training method based on our bound of Corollary 6 (stochastic denotes the randomized associated bound), as Rivasplata the one based on Equation (0.5), as BLANCHARD the one based on Equation (0.6), and as CATONI the one based on Equation (0.7). First of all, we replace the non-differentiable 0-1 loss by a surrogate for which the bounds still hold: The bounded cross entropy loss (Dziugaite and Roy, 2018). This latter is defined in a multiclass setting with \( y \in \{1, 2, \ldots \} \) by

\[
\ell(h, (x, y)) = - \frac{1}{y} \ln[H_t(y)] + \ln[H_t(y)] \in [0, 1]
\]

where \( h[y] \) is the \( y \)-th output of the NN, and \( \forall y \in [0, 1], \Phi(p) = e^{-2z} + (1 - 2e^{-2z})p \) (set \( Z = 4 \)). That being said, to learn the best prior

\[
P \in \mathbf{P}
\]

and the posterior \( \mathcal{Q}_S \), we run our Training Method with two gradient descent-based algorithms \( A_{prior} \) and \( A \).

In phase 1) algorithm \( A_{prior} \) learns from \( S_{prior} \) the \( T \) priors \( P_1, \ldots, P_T \) in \( \mathcal{P} \) (i.e., during \( T \) epochs) by minimizing the bounded cross entropy loss. In other words, at the end of the epoch \( t \), the weights \( \omega \) of the classifier are used to define the prior \( P_t = N(\omega, \sigma^2 I_D) \). Then, the best prior \( \mathcal{P} \) \( \mathcal{P} \) is selected by early stopping on \( S \). In phase 2), given \( S \) and \( \mathcal{P} \), algorithm \( A \) integrates the direct optimization of the bounds with the bounded cross entropy loss.

Optimization procedure. Let \( \omega \) be the mean vector of a Gaussian distribution used as NN weights that we are optimizing. In phases 1) and 2), at each iteration of the optimizer (i.e., Adam in our case), we sample a noise \( \epsilon \sim \mathcal{N}(0, \sigma^2 I_D) \). Then, we forward the examples of the mini-batch in the NN parametrized by the weights \( \omega + \epsilon \) and we update \( \omega \) according to the bounded cross entropy loss. Note that during phase 1), at the end of each epoch \( t \), \( P_t = N(\omega, \sigma^2 I_D) \) and finally at the end of phase 2), we have \( \mathcal{Q}_S = \mathcal{N}(\omega, \sigma^2 I_D) \).

Datasets and experimental setting. We perform our experimental study on 3 datasets. As a sanity check, we...
use the MNIST dataset (LeCun et al., 1998) and Fashion-MNIST (Xiao et al., 2017). We also consider a more complex dataset: CIFAR-10 (Krizhevsky, 2009). For the (Fashion-)MNIST datasets we train a variant of the All Convolutional Network (Springenberg et al., 2015), and for CIFAR we train a ResNet network (He et al., 2016). We divide each original train set into 2 independent subsets \( S_{\text{prior}} \) and \( S \) (with a split of 50%/50%); The test sets denoted \( T \) remain the original ones. For ours, rivasplata, Blanchard and Catoni, i.e., for each disintegrated bound, we report in Table 1 the test risk \( R_T(h) \) and the bound values with the associated train risk \( R_S(h) \) and the divergence value (the Rényi divergence \( D_2(\mathbb{Q}_S||\mathbb{P}) = \frac{1}{2\alpha} \mathbb{E}[\|w - v_i\|_2^2] \) for ours and the disintegrated KL-divergence \( \ln \mathbb{Q}_P(h) = \mathbb{E}[\|w + e - v_i\|_2^2 - \|e\|_2^2] \) for the others; note the latter can be negative). The values are averaged over 400 deterministic NNs sampled from \( \mathbb{Q}_S \) for two learning rates (10^{-4} and 10^{-6}) and different values for \( \sigma \in \{10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}\} \); We fixed the set of hyperparameters for catoni as \( C = \{10^{k_i} | k_i = -3, -2, \ldots, 3\} \) (the other optimizer parameters are set to their default values). We additionally report as stochastic (Corollary 8) the randomized bound value and KL-divergence \( \ln \mathbb{Q}_P(h) = \mathbb{E}[\|w - v_i\|_2^2] \) associated with the model learned by ours, meaning that \( n = 400 \) and that the test risk reported for ours also corresponds to the risk of the stochastic NN approximated with these 400 NNs.

**Analysis of the results.** First of all, ours leads to more precise bounds than the randomized stochastic. This imprecision is due to the non-avoidable sampling according to \( Q \) done in the randomized PAC-Bayesian bound of Corollary 8 (the higher \( n \), the tighter is the bound). Thus, using a disintegrated PAC-Bayesian bound avoids sampling a large number of NNs to obtain a low risk. This confirms that our framework makes sense.

Moreover, ours leads in average to the tightest bound 20 times over 24. An important point to remark is that ours behaves differently than rivasplata, Blanchard and Catoni. Indeed, for both learning rates, when \( \sigma^2 \) decreases the value of our bound remains low; while the others increase drastically due to the explosion of the disintegrated KL-divergence term. Concretely, the disintegrated KL-divergence in Corollary 7 involves the noise \( e \) through \( \|w + e - v_i\|_2^2 - \|e\|_2^2 \) (our divergence simply computes \( \|w - v_i\|_2^2 \)). Then, the sampled noise during the optimization procedure \( e \) has an influence on the disintegrated KL-divergence making it to prone to high variations and thus to a certain level of instability. This makes the objective function to optimize (i.e., the bound) subjects to high variations during the optimization, implying higher final bound values. Hence, the Rényi divergence has a certain advantage compared to the disintegrated KL-divergence since it does not depend on the sampled noise \( e \).

**Toward information-theoretic bounds**

Before concluding, we propose another interpretation of the disintegration procedure through Theorem 9 below. Actually, the Rényi divergence between \( \mathbb{P} \) and \( \mathbb{Q} \) is sensitive to the choice of the learning sample \( S \). When the posterior \( \mathbb{Q} \) learned from \( S \) differs greatly from the prior \( \mathbb{P} \) the divergence is high. To avoid such behavior, we consider the Sibson’s mutual information (Verdú, 2015) which is a measure of dependence between the random variables \( S \in \mathbb{Z}^m \) and \( h \in \mathcal{H} \). It involves an expectation over all the learning samples of a given size \( m \) and is defined for a given \( \alpha > 1 \) by

\[
I_\alpha(h; S) \triangleq \min_{\mathbb{P} \in \mathcal{M} \mathcal{H}} \frac{1}{\alpha - 1} \ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \frac{\mathbb{Q}_S(h)}{\mathbb{P}(h)} \right)^\alpha.
\]

The higher \( I_\alpha(h; S) \), the higher the correlation is, meaning that the sampling of \( h \) is highly dependent on the choice of \( S \). This measure has two interesting properties: It generalizes the mutual information (Verdú, 2015), and it can be related to the Rényi divergence. Indeed, let \( \rho(h, S) = Q_S(h) \times D^m(S) \), resp. \( \pi(h, S) = P(h) \times D^m(S) \), be the probability of sampling both \( S \sim D^m \) and \( h \sim Q_S \), resp. \( S \sim D^m \) and \( h \sim P \). Then we can write:

\[
I_\alpha(h; S) = \min_{\mathbb{P} \in \mathcal{M} \mathcal{H}} \frac{1}{\alpha - 1} \ln \left( \mathbb{E}_{S \sim \mathcal{D}^m} \frac{\mathbb{Q}_S(h)D^m(S)}{\mathbb{P}(h)D^m(S)} \right)^\alpha = \min_{\mathbb{P} \in \mathcal{M} \mathcal{H}} D_\alpha(\rho(\cdot | \pi)) \tag{0.10}
\]

From Verdú (2015) the optimal prior \( \mathbb{P}^* \) minimizing Equation (0.10) is a distribution-dependent prior:

\[
\mathbb{P}^*(h) = \frac{\left[ \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{Q}_S(h)^\alpha \right]^{\frac{1}{\alpha - 1}}}{\mathbb{E}_{h \sim \mathcal{P}} \left[ \mathbb{E}_{S \sim \mathcal{D}^m} \mathbb{Q}_S(h)^\alpha \right]^{\frac{1}{\alpha - 1}}}.
\]

This leads an Information-Theoretic generalization bound:

**Theorem 9** (Disintegrated Information-Theoretic Bound). For any \( \mathcal{D} \) on \( \mathcal{Z} \), for any \( \mathcal{H} \), for any function \( \phi: \mathcal{H} \times \mathcal{Z}^m \rightarrow \mathbb{R}^+ \), for any \( \alpha > 1 \), for any algorithm \( A: \mathcal{Z}^m \rightarrow \mathcal{M} \mathcal{H} \), we have

\[
P_{S \sim \mathcal{D}^m, h \sim \mathbb{Q}_S} \left( \frac{\alpha}{\alpha - 1} \ln \phi(h, S) \right) \leq I_\alpha(h'; S') + \ln \left( \frac{1}{\delta \alpha - 1} \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathbb{P}^*} \phi(h', S')^{\frac{\alpha - 1}{\alpha}} \right) \geq 1 - \delta.
\]

Note that Esposito et al. (2020, Cor.4) introduced a bound based on the Sibson’s mutual information, but, as discussed in the Appendix, Theorem 9 leads to a tighter bound. From a theoretical view, Theorem 9 brings a different philosophy than the disintegrated PAC-Bayes bounds. Indeed, in Theorems 2 and 4, given \( S \), the Rényi divergence \( D_\alpha(\mathbb{Q}_S || \mathbb{P}) \) suggests that the learned posterior \( \mathbb{Q}_S \) should be close enough to the prior \( \mathbb{P} \) to get a low bound. While in Theorem 9, the Sibson’s Mutual Information \( I_\alpha(h'; S') \) suggests that the random variable \( h \) has to be not too much correlated to \( S \) on average. However, the bound of Theorem 9 is not computable in practice due notably to the sample expectation over the unknown distribution \( \mathcal{D} \) in \( I_\alpha \). An exciting line of future works could be to study how we can make use of Theorem 9 in practice.

---

\[^7\text{We provide a mutual information-based bound in Appendix.}\]
Conclusion
We provide new and general disintegrated PAC-Bayesian bounds providing some novel perspectives in the formalization of derandomized PAC-Bayesian bounds, allowing some parametrization and offering nice opportunities for the analysis and optimization of deterministic classifiers. We notably illustrate the interest of our theoretical result on neural networks. Future work includes specializations to specific architectures and models, and the use of the perspectives carried by Theorem 9. Lastly, about ethical aspects, while our work is mainly theoretical, its practical applications require to follow the required ethical principles related in the machine learning field.

References


A General Framework for the Disintegration of PAC-Bayesian Bounds

Appendix

This Appendix is structured as follows. We give the proof of Theorem 2, Corollary 3, Theorem 4, Proposition 5, Corollary 6, Corollary 7, and Corollary 8. We also discuss the minimization and the evaluation of the bounds introduced in the different corollaries. Additionally, we provide more details on our experimental setup. The last section is devoted to Theorem 9.

Proof of Theorem 2

Theorem 2. For any distribution \( D \) on \( Z \), for any hypothesis set \( H \), for any prior distribution \( P \) on \( H \), for any function \( \phi : H \times Z \rightarrow \mathbb{R}^+ \), for any \( \alpha > 1 \), for any deterministic algorithm \( A : Z^m \rightarrow \mathcal{M}(H) \), we have

\[
\mathbb{P}_{S \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq \frac{2\alpha - 1}{\alpha - 1} \ln \left( \frac{\mathbb{E}_{h' \sim P} Q_{S}(h') \phi(h', S)}{\mathbb{E}_{h' \sim P} Q_{S}(h')} \right) \right] \geq 1 - \frac{\delta}{\alpha - 1}.
\]

where \( Q_S \) is output by \( A \), i.e., \( Q_S \approx A(S) \).

Proof. For any sample \( S \) and deterministic algorithm \( A \) fixed which allow us to obtain the distribution \( Q_S \), note that \( \phi(h, S) \) is a non-negative random variable. Hence, from Markov’s inequality we have

\[
\mathbb{P}_{h \sim Q_S} \left[ \phi(h, S) \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right] \geq 1 - \frac{\delta}{\delta} \iff \mathbb{E}_{h \sim Q_S} I \left[ \phi(h, S) \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right] \geq 1 - \frac{\delta}{\delta}.
\]

Taking the expectation over \( S \sim D^m \) to both sides of the inequality gives

\[
\mathbb{E}_{S \sim D^m, h \sim Q_S} \mathbb{P} \left[ \phi(h, S) \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right] \geq 1 - \frac{\delta}{\delta} \iff \mathbb{E}_{S \sim D^m, h \sim Q_S} \mathbb{P} \left[ \phi(h, S) \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right] \geq 1 - \frac{\delta}{\delta}.
\]

Taking the logarithm to both sides of the equality and multiplying by \( \frac{\alpha}{\alpha - 1} > 0 \), we obtain

\[
\mathbb{E}_{S \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq \frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right) \right] \geq 1 - \frac{\delta}{\delta}.
\]

We develop the right side of the inequality in the indicator function and make the expectation of the hypothesis over the prior distribution \( P \) appears. Indeed, we have

\[
\forall P \in \mathcal{M}(H), \quad \frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right) = \frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \frac{Q_{S}(h') \phi(h', S)}{P(h')} \right) = \frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim P} \frac{Q_{S}(h')}{P(h')} \phi(h', S) \right).
\]

Remark that \( \frac{1}{s} + \frac{1}{s} = 1 \) with \( r = \alpha \) and \( s = \frac{\alpha}{\alpha - 1} \). Hence, we can apply Hölder’s inequality:

\[
\mathbb{E}_{h' \sim P} \frac{Q_{S}(h')}{P(h')} \phi(h', S) \leq \left[ \mathbb{E}_{h' \sim P} \left( \frac{Q_{S}(h')}{P(h')} \right)^r \right]^\frac{1}{r} \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^{s} \right]^{\frac{s}{r}}.
\]

Then, by taking the logarithm; adding \( \ln \left( \frac{2}{\delta} \right) \) and multiplying by \( \frac{\alpha}{\alpha - 1} > 0 \) to both sides of the inequality, we obtain

\[
\frac{\alpha}{\alpha - 1} \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim P} \frac{Q_{S}(h')}{P(h')} \phi(h', S) \right) \leq \frac{1}{\alpha - 1} \ln \left( \mathbb{E}_{h' \sim P} \left( \frac{Q_{S}(h')}{P(h')} \right)^{\alpha} \right) + \frac{\alpha}{\alpha - 1} \ln \left( \mathbb{E}_{h' \sim P} \phi(h', S)^{s} \right) = D_{\alpha}(Q_S || P) + \frac{\alpha}{\alpha - 1} \ln \left( \mathbb{E}_{h' \sim P} \phi(h', S)^{s} \right).
\]

From this inequality, we can deduce that

\[
\mathbb{P}_{S \sim D^m, h \sim Q_S} \left[ \forall P \in \mathcal{M}(H), \quad \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq D_{\alpha}(Q_S || P) + \frac{\alpha}{\alpha - 1} \ln \left( \mathbb{E}_{h' \sim P} \phi(h', S)^{s} \right) \right] \geq 1 - \frac{\delta}{\delta} \quad (\ref{inequality})
\]
Note that $\mathbb{E}_{h \sim \mathcal{P}} \phi(h', S)$ is a non-negative random variable, hence, we apply Markov’s inequality to have

$$
\mathbb{P}_{S \sim \mathcal{D}^m} \left[ \mathbb{E}_{h \sim \mathcal{P}} \phi(h', S)^{\frac{\alpha}{1 - \alpha}} \right] \leq \frac{2}{\delta} \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \geq 1 - \frac{\delta}{2}.
$$

Since the inequality does not depend on the random variable $h \sim Q_S$, we have

$$
\mathbb{P}_{S \sim \mathcal{D}^m, h \sim Q_S} \left[ \mathbb{E}_{h \sim \mathcal{P}} \phi(h', S)^{\frac{\alpha}{1 - \alpha}} \right] \leq \frac{2}{\delta} \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \geq 1 - \frac{\delta}{2}.
$$

Taking the logarithm to both sides of the inequality and adding $\frac{\alpha}{1 - \alpha} \ln \frac{2}{\delta}$ give us

$$
\mathbb{P}_{S \sim \mathcal{D}^m, h \sim Q_S} \left[ \mathbb{E}_{h \sim \mathcal{P}} \phi(h', S)^{\frac{\alpha}{1 - \alpha}} \right] \leq \frac{2}{\delta} \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \geq 1 - \frac{\delta}{2} \iff 
$$

Combining Equation (12) with a union bound gives us the desired result.

Proof of Corollary 3

Corollary 3 Under the assumptions of Theorem 2, when $\alpha \rightarrow 1^+$, with probability at least $1 - \delta$ we have

$$
\ln \phi(h, S) \leq \ln \frac{2}{\delta} + \ln \left[ \text{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S') \right].
$$

When $\alpha \rightarrow +\infty$, with probability at least $1 - \delta$ we have

$$
\ln \phi(h, S) \leq \ln \text{esssup}_{h' \in \mathcal{H}} \left( \frac{\mathcal{Q}_S(h')}{\mathcal{P}(h')} \right) + \ln \left[ \frac{4}{\delta^2} \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S') \right],
$$

where $	ext{esssup}$ is the essential supremum.

Proof. Starting from Theorem 2 and rearranging, we have

$$
\mathbb{P}_{S \sim \mathcal{D}^m, h \sim Q_S} \left[ \ln \left( \mathbb{E}_{h \sim \mathcal{P}} \phi(h, S) \right) \right] \leq \frac{2\alpha - 1}{\alpha} \ln \frac{2}{\delta} + \frac{\alpha - 1}{\alpha} D_\alpha(Q_S \| \mathcal{P}) + \ln \left[ \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \right] \geq 1 - \delta.
$$

Then, we will prove the case when $\alpha \rightarrow 1$ and $\alpha \rightarrow +\infty$ separately.

When $\alpha \rightarrow 1$. First, we have $\lim_{\alpha \rightarrow 1^+} \frac{2\alpha - 1}{\alpha} \ln \frac{2}{\alpha} = \ln \frac{2}{\delta}$ and $\lim_{\alpha \rightarrow 1^+} \frac{\alpha - 1}{\alpha} D_\alpha(Q_S \| \mathcal{P}) = 0$.

Furthermore, note that

$$
\|\phi\|_{\frac{\alpha}{1 - \alpha}} = \left[ \mathbb{E}_{S \sim \mathcal{D}^m, h \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \right]^{\frac{\alpha - 1}{\alpha - 1}} = \left[ \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \right]^{\frac{\alpha - 1}{\alpha - 1}}
$$

is the $L_{\frac{\alpha}{1 - \alpha}}$-norm of the function $\phi : \mathcal{H} \times \mathcal{Z}^m \rightarrow \mathbb{R}^+$, where $\lim_{\alpha \rightarrow 1^+} \|\phi\|_{\frac{\alpha}{1 - \alpha}} = \lim_{\alpha' \rightarrow +\infty} \|\phi\|_{\alpha'}$ (since we have $\lim_{\alpha \rightarrow 1^+} \frac{\alpha}{\alpha - 1} = (\lim_{\alpha \rightarrow 1} \alpha)(\lim_{\alpha \rightarrow 1} \frac{1}{\alpha - 1}) = +\infty$). Then, it is well known that

$$
\|\phi\|_{\infty} = \lim_{\alpha' \rightarrow +\infty} \|\phi\|_{\alpha'} = \text{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S').
$$

Hence, we have

$$
\lim_{\alpha \rightarrow 1} \ln \left[ \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \right] = \ln \left[ \lim_{\alpha \rightarrow 1} \left[ \mathbb{E}_{S' \sim \mathcal{D}^m, h' \sim \mathcal{P}} \phi(h', S')^{\frac{\alpha}{1 - \alpha}} \right]^{\frac{\alpha - 1}{\alpha - 1}} \right] = \ln \left( \lim_{\alpha \rightarrow 1} \|\phi\|_{\frac{\alpha}{1 - \alpha}} \right) = \ln \left( \lim_{\alpha' \rightarrow +\infty} \|\phi\|_{\alpha'} \right) = \ln \left( \text{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S') \right).
$$
Finally, we can deduce that
\[
\lim_{\alpha \to 1} \left[ \frac{2\alpha-1}{\alpha} \ln \frac{2}{\delta} + \frac{\alpha-1}{\alpha} D_\alpha(Q_S \| P) + \ln \left( \left[ \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S') \right]^{1-\alpha} \right) \right] = \ln \frac{2}{\delta} + \ln \left( \operatorname{esssup}_{S' \in Z, h' \in \mathcal{H}} \phi(h', S') \right).
\]

When \( \alpha \to +\infty \). First, we have \( \lim_{\alpha \to +\infty} \frac{2\alpha-1}{\alpha} \ln \frac{2}{\delta} = \ln \frac{2}{\delta} \left(2 - \lim_{\alpha \to +\infty} \frac{1}{\alpha}\right) = 2 \) and \( \lim_{\alpha \to +\infty} \|\phi\|_{\frac{1}{\alpha}} = \lim_{\alpha \to +\infty} \|\phi\|_{\frac{1}{\alpha}} = 1 \). Hence, we have
\[
\lim_{\alpha \to +\infty} \ln \left( \left[ \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S') \right]^{\frac{1}{\alpha}} \right) = \ln \left( \lim_{\alpha \to +\infty} \left[ \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S') \right]^{\frac{1}{\alpha}} \right) = \ln \left( \lim_{\alpha \to +\infty} \|\phi\|_{\frac{1}{\alpha}} \right) = \ln \left( \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S') \right).
\]

Moreover, by rearranging the terms in \( \frac{\alpha-1}{\alpha} D_\alpha(Q_S \| P) \), we have
\[
\frac{\alpha-1}{\alpha} D_\alpha(Q_S \| P) = \frac{1}{\alpha} \ln \left( \mathbb{E}_{h \sim P} \frac{Q_S(h)}{P(h)} \right)^{\alpha} = \ln \left( \left[ \mathbb{E}_{h \sim P} \frac{Q_S(h)}{P(h)} \right]^{\alpha} \right) = \ln \left( \left[ \mathbb{E}_{h \sim P} \Delta(h)^{\alpha} \right]^{\frac{1}{\alpha}} \right) = \ln \left( \left[ \mathbb{E}_{h \sim P} \frac{Q_S(h)}{P(h)} \right]^{\frac{1}{\alpha}} \right).
\]

where \( \|\Delta\|_{\alpha} \) is the \( L^\alpha \)-norm of the function \( \Delta \) defined as \( \Delta(h) = \frac{Q_S(h)}{P(h)} \). Hence, we have
\[
\lim_{\alpha \to +\infty} \frac{\alpha-1}{\alpha} D_\alpha(Q_S \| P) = \lim_{\alpha \to +\infty} \ln(\|\Delta\|_{\alpha}) = \ln \left( \lim_{\alpha \to +\infty} (\|\Delta\|_{\alpha}) \right) = \ln (\|\Delta\|_{\infty}) = \ln \left( \operatorname{esssup}_{h \in \mathcal{H}} \Delta(h) \right) = \ln \left( \operatorname{esssup}_{h \in \mathcal{H}} \frac{Q_S(h)}{P(h)} \right).
\]

Finally, we can deduce that
\[
\lim_{\alpha \to +\infty} \left[ \frac{2\alpha-1}{\alpha} \ln \frac{2}{\delta} + \frac{\alpha-1}{\alpha} D_\alpha(Q_S \| P) + \ln \left( \left[ \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S') \right]^{\frac{1}{\alpha}} \right) \right] = \ln \operatorname{esssup}_{h' \in \mathcal{H}} \frac{Q_S(h')}{P(h')} + \ln \frac{4}{\delta^2} \mathbb{E}_{S' \sim D} \mathbb{E}_{h' \sim p} \phi(h', S').
\]

\[\Box\]

**Proof of Theorem 4**

For the sake of completeness, we first prove an upper bound on \( \sqrt{ab} \) (see e.g., Thiemann et al., 2017).

**Lemma 10.** For any \( a > 0, b > 0 \), we have
\[
\sqrt{\frac{a}{b}} = \inf_{\lambda > 0} \left( \frac{a}{\lambda} + \lambda b \right), \quad 2\sqrt{ab} = \inf_{\lambda > 0} \left( \frac{a}{\lambda} + \lambda b \right) \quad \text{and} \quad \forall \lambda > 0, \sqrt{ab} \leq \frac{1}{2} \left( \frac{a}{\lambda} + \lambda b \right).
\]

**Proof.** Let \( f(\lambda) = (\frac{a}{\lambda} + \lambda b) \). The first and second derivatives of \( f \) w.r.t. \( \lambda \) is
\[
\frac{\partial f}{\partial \lambda}(\lambda) = \left( b - \frac{a}{\lambda^2} \right) \quad \text{and} \quad \frac{\partial^2 f}{\partial \lambda^2}(\lambda) = \frac{2a}{\lambda^3}.
\]

Hence, for \( \lambda > 0 \), we have \( \frac{\partial f}{\partial \lambda}(\lambda) > 0 \); \( f \) is strictly convex and admit a unique minimum. Solving \( \frac{\partial f}{\partial \lambda}(\lambda) = 0 \) we have \( \lambda^* = \frac{2a}{b} \). Additionally, \( f(\lambda^*) = 2\sqrt{ab} \) which proves the claim. \[\Box\]
We can now prove Theorem 4 with Lemma 10.

**Theorem 4.** For any distribution $D$ on $Z$, for any hypothesis set $H$, for any prior distribution $P$ on $H$, for any function $\phi : H \times Z^m \to \mathbb{R}^+$, for any deterministic algorithm $A : Z^m \to \mathcal{M}(H)$, we have

$$
\Pr_{S \sim D^m, h \sim Q_S} \left[ \forall \lambda > 0, \ln(\phi(h, S)) \leq \ln \left( \frac{1}{2} \left[ \lambda e^{D_2(Q_S \| P)} + \frac{8}{\lambda \delta^2} \mathbb{E}_{S \sim D^m, h \sim P} \phi(h', S')^2 \right] \right) \right] \geq 1 - \delta,
$$

where $Q_S \triangleq A(S)$.

**Proof.** The proof is similar to the one of Theorem 2. Given a sample $S$ and a deterministic algorithm $A$ (which allow us to obtain the distribution $Q_S$), the value $\phi(h, S)$ is a non-negative random variable. Hence, from Markov’s inequality we have

$$
\Pr_{h \sim Q_S} \left[ \phi(h, S) \leq \frac{2}{\delta} h' \sim Q_S \phi(h', S) \right] \geq 1 - \frac{\delta}{2} \iff \mathbb{E}_{h \sim Q_S} \left[ \phi(h, S) \right] \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \geq 1 - \frac{\delta}{2}.
$$

Taking the expectation over $S \sim D^m$ to both sides of the inequality gives

$$
\mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \left[ \phi(h, S) \right] \geq 1 - \frac{\delta}{2} \iff \Pr_{S \sim D^m, h \sim Q_S} \left[ \phi(h, S) \leq \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right] \geq 1 - \frac{\delta}{2}.
$$

Using the fact that Lemma 10 with $a = \frac{1}{\delta} \phi(h', S)^2$ and $b = \frac{Q_S(h')^2}{P(h')}$, we have

$$
\forall P \in \mathcal{M}(H), \forall \lambda > 0, \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) = \mathbb{E}_{h' \sim P} \sqrt{\frac{Q_S(h')^2}{P(h')}^2 + \frac{4}{\lambda \delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2} \leq \frac{1}{2} \left[ \lambda \mathbb{E}_{h' \sim P} \left( \frac{Q_S(h')}{P(h')} \right)^2 + \frac{4}{\lambda \delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \right].
$$

Then, taking the logarithm to both sides of the inequality, we obtain

$$
\forall \lambda > 0, \ln \left( \frac{2}{\delta} \mathbb{E}_{h' \sim Q_S} \phi(h', S) \right) \leq \ln \left( \frac{1}{2} \left[ \lambda \mathbb{E}_{h' \sim P} \left( \frac{Q_S(h')}{P(h')} \right)^2 + \frac{4}{\lambda \delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \right] \right) = \ln \left( \frac{1}{2} \left[ \lambda \exp(D_2(Q_S \| P)) + \frac{4}{\lambda \delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \right] \right).
$$

Hence, we can deduce that

$$
\Pr_{S \sim D^m, h \sim Q_S} \left[ \forall P \in \mathcal{M}(H), \forall \lambda > 0, \ln(\phi(h, S)) \leq \ln \left( \frac{1}{2} \left[ \lambda e^{D_2(Q_S \| P)} + \frac{4}{\lambda \delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \right] \right) \right] \geq 1 - \frac{\delta}{2}.
$$

(13)

Note that $\mathbb{E}_{h' \sim P} \phi(h', S)^2$ is a non-negative random variable, hence, we apply Markov’s inequality:

$$
\Pr_{S \sim D^m} \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq \frac{2}{\delta} \mathbb{E}_{S \sim D^m, h \sim P} \phi(h', S')^2 \right] \geq 1 - \frac{\delta}{2}.
$$

Since the inequality does not depend on the random variable $h \sim Q_S$, we have

$$
\Pr_{S \sim D^m} \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq \frac{2}{\delta} \mathbb{E}_{S \sim D^m, h \sim P} \phi(h', S')^2 \right] = \mathbb{E}_{S \sim D^m, h \sim P} \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq \frac{2}{\delta} \mathbb{E}_{S \sim D^m, h \sim P} \phi(h', S')^2 \right] = \Pr_{S \sim D^m, h \sim Q_S} \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq \frac{2}{\delta} \mathbb{E}_{S \sim D^m, h \sim P} \phi(h', S')^2 \right].
$$

Technical Report

13
Additionally, note that multiplying by \(\frac{4}{2\lambda^2} > 0\), adding \(\frac{4}{2\lambda^2} \exp(D_2(Q_S\|P))\), and taking the logarithm to both sides of the inequality results in the same indicator function. Indeed,

\[
I \left[ \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq 2 \frac{E}{\delta} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right]
= I \left[ \forall \lambda > 0, 2 \frac{E}{\delta^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \leq \frac{8}{2\lambda^2} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right]
= I \left[ \forall \lambda > 0, \ln \left( \frac{4}{2\lambda^2} \exp(D_2(Q_S\|P)) + \frac{4}{2\lambda^2} \mathbb{E}_{h' \sim P} \phi(h', S)^2 \right) \leq \ln \left( \frac{8}{2\lambda^2} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right) \right].
\]

Hence, we can deduce that

\[
\forall \lambda > 0, \ln \left( \frac{1}{2} \lambda \exp(D_2(Q_S\|P)) + \frac{8}{2\lambda^2} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right) \leq \ln \left( \frac{1}{2} \lambda \exp(D_2(Q_S\|P)) + \frac{8}{2\lambda^2} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right) \geq 1 - \frac{4}{\lambda^2}.
\]

Combining Equation (13) and Equation (14) with a union bound gives us the desired result. \(\square\)

**Proposition 5.** For any distribution \(D\) on \(\mathcal{Z}\), for any hypothesis set \(\mathcal{H}\), for any prior distribution \(P\) on \(\mathcal{H}\), for any function \(\phi: \mathcal{H} \times \mathcal{Z}^m \rightarrow \mathbb{R}^+\) and for any deterministic algorithm \(A: \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})\), let

\[
\lambda^* = \arg \min_{\lambda > 0} \left( \frac{1}{2} \lambda \exp(D_2(Q_S\|P)) + \frac{8}{2\lambda^2} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right),
\]

then

\[
2 \ln \left( \frac{\lambda^*}{2} \exp(D_2(Q_S\|P)) + \frac{8 \phi(h', S')^2}{2\lambda^*} \right) = D_2(Q_S\|P) + \ln \left( \frac{8}{2\lambda^*} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2 \right),
\]

where \(\lambda^* = \sqrt{\frac{8 \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2}{\delta^3 \exp(D_2(Q_S\|P))}}\).

**Proof.** We first prove the closed form of \(\lambda^*\), then, we compute the difference between the two bounds. For the sake of clarity, let \(d = \exp(D_2(Q_S\|P))\), and \(p = \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h', S')^2\) and \(f(\lambda) = \ln \left( \frac{1}{2} \lambda + \frac{8}{2\lambda^2} \right)\). We can find the first and second derivatives of \(f\) w.r.t. \(\lambda\), indeed, we have

\[
\frac{\partial f}{\partial \lambda} (\lambda) = \frac{\delta^3 \lambda^2 d - 8p}{\delta^3 \lambda^3 d + 8\lambda p} \quad \text{and} \quad \frac{\partial^2 f}{\partial \lambda^2} (\lambda) = \frac{-[\delta^3 \lambda^2 d] + 32 \lambda p^2}{(\delta^3 \lambda^3 d + 8\lambda p)^2}.
\]

Furthermore, when \(\frac{\partial f}{\partial \lambda} (\lambda) = 0\), we have \(\lambda = \sqrt{\frac{8p}{\delta^3 d}}\), and we can prove that the associated minimum is unique (i.e., \(\lambda = \lambda^*\)) by studying the function. Actually, we have \(\frac{\partial^2 f}{\partial \lambda^2} (\lambda) > 0 \Leftrightarrow \delta^3 \lambda^2 d - 8p(2 + \sqrt{5}) > 0 \Leftrightarrow 0 < \delta^3 \lambda^2 d < 8p(2 + \sqrt{5}) \Leftrightarrow 0 < \lambda < \frac{8p}{\delta^3 d \sqrt{2 + \sqrt{5}}}\).

Hence, for \(\lambda \in \left[0, \sqrt{\frac{8p}{\delta^3 d \sqrt{2 + \sqrt{5}}}}\right]\), \(f\) is strictly convex and \(\lambda^*\) is the unique minimizer on that interval. Furthermore, from the first derivative, we know that

\[
\frac{\partial f}{\partial \lambda} (\lambda) > 0 \Leftrightarrow \lambda > \sqrt{\frac{8p}{\delta^3 d}}.
\]

Hence, \(f\) is strictly increasing on \(\left[\sqrt{\frac{8p}{\delta^3 d}}, +\infty\right]\), hence, \(\lambda^* = \sqrt{\frac{8p}{\delta^3 d}}\) is the unique minimizer on \([0, +\infty]\).

Lastly, substituting \(\lambda\) by \(\lambda^*\) in the right term of the inequality in Theorem 4 gives the equality. \(\square\)
Proof of Corollary 6

We introduce Theorem 2', which takes into account a set of priors \( P \) while Theorem 2 handles a unique prior \( \mathcal{P} \).

**Theorem 2'.** For any distribution \( D \) on \( Z \), for any hypothesis set \( \mathcal{H} \), for any priors \( \{P_t\}_{t=1}^T \) of \( T \) prior \( \mathcal{P} \) on \( \mathcal{H} \), for any function \( \phi : \mathcal{H} \times Z^m \rightarrow \mathbb{R}^+ \), for any \( \alpha > 1 \), for any deterministic algorithm \( A : Z^m \rightarrow \mathcal{M}(\mathcal{H}) \), we have

\[
S \sim D^m, h \sim Q_S \quad \mathbb{P}_S \left[ \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq D_a(Q_S \| \mathcal{P}) + \alpha \frac{2}{\alpha - 1} \ln \frac{2T}{\delta} + \ln \left( \mathbb{E}_{S' \sim D^m} \phi(h', S')^{\frac{1}{\alpha - 1}} \right) \right] \geq 1 - \delta.
\]

**Proof.** The proof is essentially the same as Theorem 2. Indeed, we first derive the same equation as Equation (11), we have

\[
\forall P \in \mathcal{M}(\mathcal{H}), \quad \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq D_a(Q_S \| \mathcal{P}) + \alpha \frac{2}{\alpha - 1} \ln \frac{2T}{\delta} + \ln \left( \mathbb{E}_{S' \sim D^m} \phi(h', S')^{\frac{1}{\alpha - 1}} \right) \geq 1 - \frac{\delta}{2}.
\]

Then, we apply Markov’s inequality (as in Theorem 2) \( T \) times with the \( T \) priors \( P_t \) belonging to \( \mathcal{P} \), however, we set the confidence to \( \frac{\delta}{2T} \) instead of \( \frac{\delta}{2} \), we have

\[
\mathbb{P}_S \left[ \frac{\alpha}{\alpha - 1} \ln (\phi(h, S)) \leq D_a(Q_S \| \mathcal{P}) + \alpha \frac{2}{\alpha - 1} \ln \frac{2T}{\delta} + \ln \left( \mathbb{E}_{S' \sim D^m} \phi(h', S')^{\frac{1}{\alpha - 1}} \right) \right] \geq 1 - \frac{\delta}{2T}.
\]

Finally, combining the \( T + 1 \) bounds with a union bound gives us the desired result. \( \square \)

We now prove Corollary 6 from Theorem 2'.

**Corollary 6.** For any distribution \( D \) on \( Z \), for any hypothesis set \( \mathcal{H} \), for any priors \( \{P_t\}_{t=1}^T \) of \( T \) prior \( \mathcal{P} \) on \( \mathcal{H} \), for any algorithm \( A : Z^m \rightarrow \mathcal{M}(\mathcal{H}) \), for any loss \( l : \mathcal{H} \times Z \rightarrow [0, 1] \), we have

\[
S \sim D^m, h \sim Q_S \quad \mathbb{P}_S \left[ \forall P_t \in \mathcal{P}, \quad \text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ \frac{\|w - v\|^2_2}{\sigma^2} \frac{\delta}{2} + \ln \left( 16T \sqrt{m} \right) \right] \right] \geq 1 - \delta.
\]

**Proof.** We instantiate Theorem 2' with \( \phi(h, S) = \exp \left( \frac{\alpha - 1}{\alpha} \text{kl}(R_S(h) \| R_D(h)) \right) \) and \( \alpha = 2 \); we have with probability at least \( 1 - \delta \) over \( S \sim D^m \) and \( h \sim Q_S \), for all prior \( P_t \in \mathcal{P} \)

\[
\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ D_2(Q_S \| P_t) + \ln \left( \frac{8T}{\delta^3} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P_t} e^{\alpha \text{kl}(R_S(h') \| R_D(h'))} \right) \right].
\]

From Maurer (2004) we upper-bound \( \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P_t} e^{\alpha \text{kl}(R_S(h') \| R_D(h'))} \) by \( 2 \sqrt{m} \) for each prior \( P_t \). Hence, we have, for all prior \( P_t \in \mathcal{P} \)

\[
\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ D_2(Q_S \| P_t) + \ln \left( \frac{16T \sqrt{m}}{\delta^3} \right) \right].
\]

Additionally, the Rényi divergence \( D_2(Q_S \| P_t) \) between two multivariate Gaussians \( Q_S = \mathcal{N}(w, \sigma^2 I_d) \) and \( P_t = \mathcal{N}(v_t, \sigma^2 I_d) \) is well known: its closed-form solution is \( D_2(Q_S \| P_t) = \frac{\|w - v_t\|^2_2}{2\sigma^2} \) (see, for example, (Gil et al., 2013)). \( \square \)

**Proof of Corollary 7**

We first prove the following lemma in order to prove Corollary 7.

**Lemma 11.** If \( Q_S = \mathcal{N}(w, \sigma^2 I_d) \) and \( \mathcal{P} = \mathcal{N}(v, \sigma^2 I_d) \), we have

\[
\ln \frac{Q_S(h)}{P(h)} = \frac{1}{2\sigma^2} \left[ \|w + \epsilon - v\|^2_2 - \|\epsilon\|^2_2 \right],
\]

where \( \epsilon \sim \mathcal{N}(0, \sigma^2 I_d) \) is a Gaussian noise such that \( w + \epsilon \) are the weights of \( h \sim Q_S \) with \( Q_S = \mathcal{N}(w, \sigma^2 I_d) \).

**Proof.** The probability density functions of \( Q_S \) and \( P \) for \( h \sim Q_S \) (with the weights \( w + \epsilon \)) can be rewritten as

\[
Q_S(h) = \left[ \frac{1}{\sigma \sqrt{2\pi}} \right]^d \exp \left( -\frac{1}{2\sigma^2} \|\epsilon\|^2_2 \right) \quad \text{and} \quad P(h) = \left[ \frac{1}{\sigma \sqrt{2\pi}} \right]^d \exp \left( -\frac{1}{2\sigma^2} \|w + \epsilon - v\|^2_2 \right).
\]

We can derive a closed-form expression of \( \ln \frac{Q_S(h)}{P(h)} \). Indeed, we have

\[
\ln \frac{Q_S(h)}{P(h)} = \ln |Q_S(h)| - \ln |P(h)|
\]

\[
= \ln \left( \left[ \frac{1}{\sigma \sqrt{2\pi}} \right]^d \exp \left( -\frac{1}{2\sigma^2} \|\epsilon\|^2_2 \right) \right) - \ln \left( \left[ \frac{1}{\sigma \sqrt{2\pi}} \right]^d \exp \left( -\frac{1}{2\sigma^2} \|w + \epsilon - v\|^2_2 \right) \right)
\]

\[
= -\frac{1}{2\sigma^2} \|\epsilon\|^2_2 + \frac{1}{2\sigma^2} \|w + \epsilon - v\|^2_2 = \frac{1}{2\sigma^2} \left( \|w + \epsilon - v\|^2_2 - \|\epsilon\|^2_2 \right).
\]

\( \square \)
We can now prove Corollary 7.

**Corollary 7.** Under Corollary 6’s assumptions, with probability at least 1 − δ over $S \sim D^m$ and $h \sim Q_S$, we have $\forall P_t \in P$

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ \frac{\|w + \epsilon - v_i\|^2}{2\sigma^2} \ln \left( 1 + \frac{2T\sqrt{m}}{\delta} \right) \right],$$

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ \frac{m+1}{m} \frac{\|w + \epsilon - v_i\|^2 - \|\epsilon\|^2}{2\sigma^2} + \ln \left( Tm + T \right) \right],$$

$$\forall e \in C, R_P(h) \leq \frac{1 - e}{1 - e^{-e}},$$

where $\epsilon \sim N(0, \sigma^2 I_d)$ is a Gaussian noise s.t. $w + \epsilon$ are the weights of $h \sim Q_S$ with $Q_S = N(w, \sigma^2 I_d)$, and $C$ is a set of hyperparameters fixed a priori.

**Proof.** We will prove separately the three bounds. The proofs share the same proof technique.

**Equation (0.5).** We instantiate Theorem 1(i) of Rivasplata et al. (2020) with $\phi(h, S) = \exp[\text{ml}(R_S(h) \| R_D(h))]$, however, we apply the theorem $T$ times for each prior $P_t \in P$ (with a confidence $\frac{T}{T}$ instead of $\delta$). Hence, for each prior $P_t \in P$, we have with probability at least $1 - \frac{T}{T}$ over the random choice of $S \sim D^m$ and $h \sim Q_S$

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ \ln \left( \frac{Q_S(h)}{P_t(h)} \right) + \ln \left( \frac{T}{\delta} \sum_{S \sim D^m, h \sim P} e^{\text{ml}(R_{g'}(h') \| R_D(h'))} \right) \right].$$

From Maurer (2004), we upper-bound $E_{S \sim D^m, h \sim P} e^{\text{ml}(R_{g'}(h') \| R_D(h'))}$ by $2\sqrt{m}$ and using Lemma 11 we rewrite the disintegrated KL divergence. Finally, a union bound argument on the $T$ bounds gives us the claim.

**Equation (0.6).** We apply $T$ times Proposition 3.1 of Blanchard and Fleuret (2007) with a confidence $\frac{T}{T}$ instead of $\delta$ and with their parameter $k$ defined as $k = m$. Hence, for each prior $P_t \in P$, we have with probability at least $1 - \frac{T}{T}$ over the random choice of $S \sim D^m$ and $h \sim Q_S$

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ (1 + \frac{1}{m}) \ln \left( \frac{Q_S(h)}{P_t(h)} \right) + \ln \left( T(m+1) \right) \right].$$

From Lemma 11 and a union bound argument on the $T$ bounds, we obtain the claim.

**Equation (0.7).** We apply $T|C|$ times Theorem 1.2.7 of Catoni (2007) with a confidence $\frac{T}{T|C|}$ instead of $\delta$. For each prior $P_t \in P$ and hyperparameter $c \in C$, we have with probability at least $1 - \frac{T}{T|C|}$ over the random choice of $S \sim D^m$ and $h \sim Q_S$

$$R_D(h) \leq \frac{1}{1 - e^{-e}} \left[ 1 - \exp \left( -cR_S(h) - \frac{1}{m} \ln \left( \frac{Q_S(h)}{P_t(h)} \right) + \ln \left( T|C| \right) \right) \right].$$

From Lemma 11 and a union bound argument on the $T$ bounds, we obtain the claim.

**Proof of Corollary 8.** For any distribution $D$ on $Z$, for any hypothesis set $H$, for any priors’ set $P = \{P_t\}_{t=1}^T$ of $T$ priors $P$ on $H$, for any loss $\ell : H \times Z \rightarrow \{0, 1\}$ we have, with probability at least $1 - \delta$ over the random choice of $S \sim D^m$ and $\{h_1, \ldots, h_n\} \sim Q^n$, we have simultaneously

$$\text{kl} \left( \frac{1}{n} \sum_{i=1}^n R_S(h_i) \| R_S(h) \right) \leq \frac{1}{n} \ln \frac{4}{\delta}, \quad \text{(Equation (0.9))}$$

and, for all prior $P_t \in P$, for all posterior $Q$,

$$\text{kl} \left( \mathbb{E}_{h \sim Q} R_S(h) \| R_D(h) \right) \leq \frac{1}{m} \left[ \frac{w + \epsilon - v_i}{2\sigma^2} + \ln \left( \frac{4T\sqrt{m}}{\delta} \right) \right]. \quad \text{(Equation (0.8))}$$

Technical Report 16
Proof. We instantiate Equation (0.3) (and apply Jensen’s inequality on the right side of the inequation) for each prior \( \mathcal{P}_t \) with \( Q = \mathcal{N}(\mathbf{w}, \sigma^2 \mathbf{I}_d) \) and \( \mathcal{P}_t = \mathcal{N}(\mathbf{v}_t, \sigma^2 \mathbf{I}_d) \) with a confidence \( \frac{\delta}{m} \) instead of \( \delta \). Indeed, for each prior \( \mathcal{P}_t \), with probability at least \( 1 - \frac{\delta}{m} \) over the random choice of \( \mathcal{S} \sim \mathcal{D}^m \), we have for all posterior \( Q \) on \( \mathcal{H} \),

\[
\text{kl} \left( \mathbb{E}_{h \sim Q} R_S(h) \| \mathbb{E}_{h \sim Q} R_{\mathcal{D}}(h) \right) \leq \frac{1}{m} \left[ \text{KL}(Q\|P_t) + \ln \frac{4T\sqrt{m}}{\delta} \right].
\]

Note that the closed form solution of the KL divergence between the Gaussian distributions \( Q \) and \( \mathcal{P}_t \) is well known, we have

\[
\text{KL}(Q\|P_t) = \frac{\|w - v_t\|^2}{2\sigma^2}.
\]

Then, by applying a union bound argument over the \( T \) bounds obtained with the \( T \) priors \( \mathcal{P}_t \), we have with probability at least \( 1 - \frac{\delta}{m} \) over the random choice of \( \mathcal{S} \sim \mathcal{D}^m \), for all prior \( \mathcal{P}_t \in \mathcal{P} \), for all posterior \( Q \)

\[
\text{kl} \left( \mathbb{E}_{h \sim Q} R_S(h) \| \mathbb{E}_{h \sim Q} R_{\mathcal{D}}(h) \right) \leq \frac{1}{m} \left[ \frac{\|w - v_t\|^2}{2\sigma^2} + \ln \frac{4T\sqrt{m}}{\delta} \right].
\] (Equation (0.8))

Additionally, we obtained Equation (0.9) by a direct application the Theorem 2.2 of Dziugaite and Roy (2017) (with confidence \( \frac{\delta}{m} \) instead of \( \delta \)). Finally, from a union bound of the two bounds in Equations (0.9) and (0.8) gives the claimed result.

\section*{Evaluation and Minimization of the Bounds in Corollaries 6, 7 and 8}

We optimize and evaluate the bounds of the corollaries (except Eq. (0.7)) thanks to the inverse binary kl divergence defined as

\[
\text{kl}^{-1}(q|\psi) = \max \left\{ p \in (0,1) \mid \text{kl}(q|p) \leq \psi \right\},
\]

where \( q \) is typically the empirical risk and \( \psi \) the PAC-Bayesian bound. Here, the function \( \text{kl}^{-1}(q|\psi) \) outputs the worst true risk \( p \) where the inequality \( \text{kl}(q|p) \leq \psi \) holds. We can actually instantiate \( p, q \) and \( \psi \) for the different corollaries. Indeed, we have

\[
R_{\mathcal{D}}(h) \leq \text{kl}^{-1}\left( R_S(h) \left| \frac{1}{m} \left[ \frac{\|w - v_t\|^2}{\sigma^2} + \ln \frac{4T\sqrt{m}}{\delta} \right] \right. \right),
\]

Corollary 6

\[
R_{\mathcal{D}}(h) \leq \text{kl}^{-1}\left( R_S(h) \left| \frac{1}{m} \left[ \frac{\|w + \epsilon - v_t\|^2 - \|\epsilon\|^2}{2\sigma^2} + \ln \frac{2T\sqrt{m}}{\delta} \right] \right. \right),
\]

Equation (0.5)

\[
R_{\mathcal{D}}(h) \leq \text{kl}^{-1}\left( R_S(h) \left| \frac{1}{m} \left( \frac{1}{m} + \frac{1}{m} \right) \left[ \frac{\|w + \epsilon - v_t\|^2 - \|\epsilon\|^2}{2\sigma^2} \right] + \frac{\ln T(m+1)}{\delta} \right. \right),
\]

Equation (0.6)

\[
\mathbb{E}_{h \sim Q} R_{\mathcal{D}}(h) \leq \text{kl}^{-1}\left( \frac{1}{n} \sum_{i=1}^{n} R_S(h_i) \left| \frac{1}{n} \ln \frac{4}{\delta} \right. \right) \left| \frac{1}{m} \left[ \frac{\|w - v_t\|^2}{2\sigma^2} + \ln \frac{4T\sqrt{m}}{\delta} \right] \right),
\]

Corollary 8

Hence, \( \text{kl}^{-1} \) has to be evaluated in order to obtain the value of the upper-bound on \( R_{\mathcal{D}}(h) \) or \( \mathbb{E}_{h \sim Q} R_{\mathcal{D}}(h) \): the evaluation of \( \text{kl}^{-1}(q|\psi) \) is performed by the bisection method. From these new formulation of the bounds, we can remark that the objective is to minimize the function \( \text{kl}^{-1}(q|\psi) \) in order to minimize the true risk \( p \). To do so, Reeb et al. (2018) introduced an analytical expression of the derivative of \( \text{kl}^{-1} \) with respect to the empirical risk \( q \) and the PAC-Bayesian bound \( \psi \). The two partial derivatives are defined in the following way:

\[
\frac{\partial \text{kl}^{-1}(q|\psi)}{\partial q} = \frac{\ln \frac{1 - q}{1 - \text{kl}^{-1}(q|\psi)}}{1 - \text{kl}^{-1}(q|\psi)} - \ln \frac{q}{\text{kl}^{-1}(q|\psi)}, \quad \text{and} \quad \frac{\partial \text{kl}^{-1}(q|\psi)}{\partial \psi} = \frac{1}{1 - \text{kl}^{-1}(q|\psi) - \text{kl}^{-1}(q|\psi)}.
\]

Note that these partial derivatives need the evaluation of \( \text{kl}^{-1}(q|\psi) \) for a given empirical risk \( q \) and a PAC-Bayesian bound \( \psi \). Then, by computing the derivatives of \( q \) and \( \psi \) with respect to the parameters and by using the chain rule of differentiation, a library like PyTorch (see Paszke et al. (2019)) can compute automatically the derivatives of \( \text{kl}^{-1} \) with respect to the parameters.
At each iteration in phase 2), after sampling the noise $\epsilon$, the algorithm update the weights $\omega$ (i.e., the hypothesis $h$) by optimizing

$$
\text{kl}^{-1}\left( R_S(h) \left[ \frac{1}{m} \left[ \frac{||\omega-v_t||^2}{\sigma^2} + \ln \frac{2T \sqrt{m}}{\delta^3} \right] \right] \right),
$$

Objective function for Corollary 6

$$
\text{kl}^{-1}\left( R_S(h) \left[ \frac{1}{m} \left[ \frac{||\omega+\epsilon-v_t||^2 - ||\epsilon||^2}{2\sigma^2} + \ln \frac{2T \sqrt{m}}{\delta^3} \right] \right] \right),
$$

Objective function for Equation (0.5)

$$
\text{kl}^{-1}\left( R_S(h) \left[ \frac{1}{m} \left[ \left( 1 + \frac{1}{m} \right) \frac{||w+\epsilon-v_t||^2 - ||\epsilon||^2}{2\sigma^2} + \ln \frac{T(m+1)}{\delta} \right] \right] \right),
$$

Objective function for Equation (0.6)

with the bounded cross entropy loss $\ell(h, (x, y)) = -\frac{1}{Z} \ln(\Phi(h[y]))$ (see Dziugaite and Roy (2018)).

To optimize Equation (0.7), we (a) initialize $c \in \mathbb{C}$ with the one that performs best on the first mini-batch and (b) optimize by gradient descent the parameter. Note that the loss is the bounded cross entropy loss $\ell(h, (x, y)) = -\frac{1}{Z} \ln(\Phi(h[y]))$ of Dziugaite and Roy (2018) during the optimization. To evaluate Equation (0.7), we take $c \in \mathbb{C}$ that leads to the tightest bound.

**Experiments**

We give more details on the architectures and the hyperparameters that we consider in the experiments.

**Training the MNIST-like datasets.** We train a variant of the All Convolutional Network of Springenberg et al. (2015). The model is a 3-hidden layers convolutional network with 96 channels. We use $5 \times 5$ convolutions with a padding of size 1, and a stride of size 1 everywhere except on the second convolution where we use a stride of size 2. We adopt the Leaky ReLU activation functions after each convolution. Lastly, we use a global average pooling of size $8 \times 8$ in order to obtain the desired output size. Furthermore, the weights are initialized with Xavier Normal initializer while the biases are left initialized with the default initializer. We learn the prior weights by using Adam optimizer for 100 epochs with a learning rate of 0.001 and a batch size of 32. Moreover, the posterior weights are learned for one epoch with the same batch size and optimizer (except that the learning rate is different).

**Training the CIFAR datasets.** We train ResNet-20, i.e., a ResNet network from He et al. (2016) with 20 layers. The weights are initialized with Kaiming Normal initializer and the initialization of the bias is the default one. The prior weights are learned for 100 epochs and the posterior weights for 10 epochs with a batch size of 32 by using Adam optimizer as well. Additionally, the learning rate to learn the prior for CIFAR-10 is .01.

**About Theorem 9**

This section is devoted to (i) the proof of a bound that is easier to interpret than Theorem 9, (ii) the proof of Theorem 9 and (iii) a discussion about Theorem 9.

**A bound easier to interpret**

Since the mutual information is well known, a bound based on this quantity will be more interpretable than the one with the Sibson’s. Hence, we propose a mutual-information-based bound in Theorem 13. However, in order to prove this theorem, we need to prove Lemma 12.

**Lemma 12.** For any distribution $D$ on $Z$, for any hypothesis set $H$, for any function $\phi : H \times Z^m \rightarrow [1, +\infty[$, for any deterministic algorithm $A : Z^m \rightarrow M(H)$, we have

$$
\mathbb{P}_{S \sim D^m, h \sim Q_S} \left[ \forall P \in M(H), \ln \phi(h, S) \leq \frac{1}{\delta} \left[ \mathbb{E}_{S \sim D^m} \text{KL}(Q_S || P) + \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P} \phi(h, S) \right) \right] \right] \geq 1 - \delta.
$$
Proof. By developing $\mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \phi(h, S)$, we have for all prior $P \in \mathcal{M}(H)$

\[
\mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \phi(h, S) = \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{Q_S(h)P(h)}{\mathcal{P}(h)Q_S(h)} \phi(h, S)
\]

\[
= \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \left[ \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{Q_S(h)}{\mathcal{P}(h)} + \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{\mathcal{P}(h)}{Q_S(h)} \phi(h, S) \right]
\]

\[
= \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) + \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{\mathcal{P}(h)}{Q_S(h)} \phi(h, S).
\]

From Jensen’s inequality, we have for all prior $P \in \mathcal{M}(H)$

\[
\mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) + \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{\mathcal{P}(h)}{Q_S(h)} \phi(h, S) \leq \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) + \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{\mathcal{P}(h)}{Q_S(h)} \phi(h, S)
\]

\[
= \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) + \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P} \phi(h, S).
\]

(15)

Since we assume in this case that $\phi(h, S) \geq 1$ for all $h \in H$ and $S \in Z^m$, we have $\ln \phi(h, S) \geq 0$; we can apply Markov’s inequality to obtain

\[
\mathbb{P}_{S \sim D^m, h \sim Q_S} \left[ \ln \phi(h, S) \leq \frac{1}{\delta} \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \phi(h, S) \right] \geq 1 - \delta.
\]

(16)

Then, from Equations (15) and (16), we can deduce that stated result.

We are now ready to prove Theorem 13.

Theorem 13. For any distribution $D$ on $Z$, for any hypothesis set $H$, for any function $\phi : H \times Z^m \rightarrow [1, +\infty]$, for any deterministic algorithm $A : Z^m \rightarrow \mathcal{M}(H)$, we have

\[
\mathbb{E}_{S \sim D^m} \mathbb{P}_{h \sim Q_S} \left[ \ln \phi(h, S) \leq \frac{1}{\delta} \left( I(h; S) + \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P^*} \phi(h, S) \right) \right) \right] \geq 1 - \delta,
\]

where $P^*$ is defined such that $P^*(h) = \mathbb{E}_{S \sim D^m} Q_{S'}(h)$ and $I(h; S) = \min_{P \in \mathcal{M}(H)} \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P)$.

Proof. Note that the mutual information is defined by $I(h; S) = \min_{P \in \mathcal{M}(H)} \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P)$. Hence, to prove Theorem 13, we have to instantiate Lemma 12 with the optimal prior, i.e., the prior $P$ which minimizes $\mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P)$. The optimal prior is well-known: for the sake of completeness, we derive it. First, we have

\[
\mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) = \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{Q_S(h)}{P(h)}
\]

\[
= \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{Q_S(h)\mathbb{E}_{S' \sim D^m} Q_{S'}(h)}{P(h)\mathbb{E}_{S' \sim D^m} Q_{S'}(h)}
\]

\[
= \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \left( \frac{Q_S(h)}{\mathbb{E}_{S' \sim D^m} Q_{S'}(h)} \right) + \mathbb{E}_{h \sim Q_S} \ln \frac{\mathbb{E}_{S' \sim D^m} Q_{S'}(h)}{P(h)}.
\]

Hence,

\[
\text{argmin}_{P \in \mathcal{M}(H)} \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P) = \text{argmin}_{P \in \mathcal{M}(H)} \left[ \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim Q_S} \ln \frac{Q_S(h)}{\mathbb{E}_{S' \sim D^m} Q_{S'}(h)} + \mathbb{E}_{h \sim Q_S} \ln \frac{\mathbb{E}_{S' \sim D^m} Q_{S'}(h)}{P(h)} \right]
\]

\[
= \text{argmin}_{P \in \mathcal{M}(H)} \left[ \mathbb{E}_{h \sim Q_S} \ln \frac{\mathbb{E}_{S' \sim D^m} Q_{S'}(h)}{P(h)} \right] = P^*,
\]

where $P^*(h) = \mathbb{E}_{S' \sim D^m} Q_{S'}(h)$. Note that $P^*$ is defined from the data distribution $D$, hence, $P^*$ is a valid prior when instantiating Lemma 12 with $P^*$. Then, we have with prob. at least $1 - \delta$ over $S \sim D^m$ and $h \sim Q_S$

\[
\ln \phi(h, S) \leq \frac{1}{\delta} \left[ \mathbb{E}_{S \sim D^m} \text{KL}(Q_S \| P^*) + \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{P}_{h \sim P} \phi(h, S) \right) \right]
\]

\[
= \frac{1}{\delta} \left[ I(h; S) + \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{P}_{h \sim P} \phi(h, S) \right) \right].
\]

As you can remark, this bound is looser than Theorem 9 which is based on the Sibson’s mutual information. For example, when we instantiate this bound with $\phi(h, S) = \exp \left[ m \ln |R_S(h)||R_D(h)| \right]$, the bound will be multiplied by $\frac{1}{m}$, while the bound of Theorem 9 is only multiplied by $\frac{1}{m}$ (but we add the term $\frac{1}{m} \ln \frac{1}{\delta}$ to the bound which is small even for small $m$).
Proof of Theorem 9

We first introduce Lemma 14 in order to prove Theorem 9.

Lemma 14. For any distribution \( D \) on \( Z \), for any hypothesis set \( H \), for any prior distribution \( P \) on \( H \), for any function \( \phi : H \times Z^m \rightarrow \mathbb{R}^+ \), for any \( \alpha > 1 \), for any deterministic algorithm \( A : Z^m \rightarrow \mathcal{M}(H) \), we have

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] \leq D_\alpha(\rho||\pi) + \ln \left( \frac{1}{\delta} \frac{1}{\delta \sim D^m, h \sim P} \mathbb{E}_{h \sim p} Q_{S'(h') \sim Q_S(h')} \phi(h', S') \right)^{\frac{1}{\alpha-1}} \geq 1 - \delta.
\]

where \( \rho(h,S) = Q_S(h) \times D^m(S); \ (h,S) \sim P(h) \times D^m(S) \) and \( Q_S \triangleq A(S) \).

Proof. For any deterministic algorithm \( A \) fixed which allow us to obtain the distribution \( Q_S \) from a sample \( S \), note that \( \phi(h,S) \) is a non-negative random variable. From Markov’s inequality, we have

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] \leq \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \geq 1 - \delta.
\]

Taking the logarithm to both sides of the equality and multiplying by \( \frac{\alpha}{\alpha-1} > 0 \), we have

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] \leq \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \geq 1 - \delta.
\]

We develop the right side of the inequality in the indicator function and make the expectation of the hypothesis over the distribution \( P \) appears; for all \( P \in \mathcal{M}(H) \),

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] = \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln \left( \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \right) \right]
\]

Then, remark that \( \frac{1}{\delta} + \frac{1}{\delta} = 1 \) where \( r = \alpha \) and \( s = \frac{s}{\alpha-1} \). Hence, Hölder’s inequality gives

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln \left( \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \right) \right] \leq \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \alpha \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}}.
\]

Taking the log, adding \( \ln(\frac{1}{\delta}) \), and multiplying by \( \frac{\alpha}{\alpha-1} > 0 \) to both sides of the inequality, we have

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln \left( \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \right) \right]
\]

\[
\leq \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln \left( \frac{1}{\delta} \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \left( Q_{S'}(h') / P(h') \right) \phi(h', S') \right) \right]^{\frac{\alpha-1}{\alpha}}
\]

\[
= \frac{1}{\alpha} \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \left( Q_{S'}(h') / P(h') \right) \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}}.
\]

Hence, we can deduce that

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] \leq \frac{1}{\alpha} \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \mathbb{E}_{\delta' \sim D^m} \mathbb{E}_{h' \sim Q_{S'}} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} 
\]

where by definition we have \( D_\alpha(\rho||\pi) = \frac{1}{\alpha-1} \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ Q_{S'}(h') / P(h') \right]^{\frac{\alpha-1}{\alpha}} \).

From Lemma 14, we prove Theorem 9.

Theorem 9. For any distribution \( D \) on \( Z \), for any hypothesis set \( H \), for any function \( \phi : H \times Z^m \rightarrow \mathbb{R}^+ \), for any \( \alpha > 1 \), for any deterministic algorithm \( A : Z^m \rightarrow \mathcal{M}(H) \), we have

\[
\mathbb{E}_{\delta \sim D^m, h \sim Q_S} \left[ \frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \right] \leq I_\alpha(h'; S') + \ln \left( \frac{1}{\delta} \mathbb{E}_{\delta \sim D^m, h \sim Q_S} \phi(h', S') \right) \geq 1 - \delta.
\]

where \( Q_S \triangleq A(S) \).
Proof. Note that Sibson’s mutual information is defined as $I_\alpha(h;S) = \min_{P \in \mathcal{M}(H)} D_\alpha(\rho||\pi)$. Hence, in order to prove Theorem 9, we have to instantiate Lemma 14 with the optimal prior, i.e., the prior $P$ which minimizes $D_\alpha(\rho||\pi)$. Actually, this optimal prior has a closed-form solution (Verdú, 2015). For the sake of completeness, we derive it. First, we have

\[
D_\alpha(\rho||\pi) = \frac{1}{\alpha-1} \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P} \left[ \frac{Q_S(h)}{P(h)} \right]^\alpha \right) = \frac{1}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \left[ \frac{Q_S(h)^\alpha}{P(h)} \right] \right) = \frac{1}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \left[ \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha \right] P(h)^{-\alpha} \right) = \frac{\alpha}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \left[ \frac{1}{\mathbb{E}_{S \sim D^m} Q_S(h)^\alpha} \right] \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha P(h)^{-\alpha} \right) + \frac{1}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \frac{1}{P(h)} \left[ \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha P(h)^{-\alpha} \right] \right) = \frac{\alpha}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \left[ \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha \right] \right) + D_\alpha(\mathcal{P}^*||\mathcal{P}),
\]

where $\mathcal{P}^*(h) = \left[ \frac{\mathbb{E}_{S \sim D^m} Q_S(h)^\alpha}{\mathbb{E}_{S' \sim D^m} Q_{S'}(h')^\alpha} \right]$. From these equalities and using the fact that $D_\alpha(\mathcal{P}^*||\mathcal{P})$ is minimal (i.e., equal to zero) when $\mathcal{P}^* = \mathcal{P}$, we can deduce that

\[
\arg\min_{P \in \mathcal{M}(H)} D_\alpha(\rho||\pi) = \arg\min_{P \in \mathcal{M}(H)} \left[ \frac{\alpha}{\alpha-1} \ln \left( \mathbb{E}_{h \sim P} \left[ \mathbb{E}_{S \sim D^m} Q_S(h)^\alpha \right] \right) + D_\alpha(\mathcal{P}^*||\mathcal{P}) \right] = \arg\min_{P \in \mathcal{M}(H)} D_\alpha(\mathcal{P}^*||\mathcal{P}) = \mathcal{P}^*.
\]

Note that $\mathcal{P}^*$ is defined from the data distribution $D$, hence, $\mathcal{P}^*$ is a valid prior when instantiating Lemma 14 with $\mathcal{P}^*$. Then, we have with prob. at least $1-\delta$ over $S \sim D^m$ and $h \sim Q_S$

\[
\frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \leq D_\alpha(\rho||\pi^*) + \ln \left( \frac{1}{\delta^{1-\alpha}} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h',S')^{\frac{1}{\delta^{1-\alpha}}} \right) = I_\alpha(h';S') + \ln \left( \frac{1}{\delta^{1-\alpha}} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h',S')^{\frac{1}{\delta^{1-\alpha}}} \right),
\]

where $\pi^*(h, S) = \mathcal{P}^*(h) \times D^m(S)$.

\[\boxed{}\]

**About Theorem 9**

For the sake of comparison, we introduce the following corollary of Theorem 9.

**Corollary 15.** Under the assumptions of Theorem 9, when $\alpha \rightarrow 1^+$, with probability at least $1-\delta$ we have

\[
\ln \phi(h,S) \leq \frac{1}{\delta} + \ln \left( \operatorname{esssup}_{S' \in \mathcal{S}, h' \in \mathcal{H}} \phi(h',S') \right).
\]

When $\alpha \rightarrow +\infty$, with probability at least $1-\delta$ we have

\[
\ln \phi(h,S) \leq \ln \left( \operatorname{esssup}_{S' \in \mathcal{S}, h' \in \mathcal{H}} \frac{Q_S(h)}{\mathcal{P}^*(h)} \right) + \ln \left( \frac{1}{\delta^{1-\alpha}} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h',S')^{\frac{1}{\delta^{1-\alpha}}} \right),
\]

where $\operatorname{esssup}$ is the essential supremum.

**Proof.** The proof is similar to Corollary 3. Starting from Theorem 9 and rearranging, we have

\[
\frac{\alpha}{\alpha-1} \ln(\phi(h,S)) \leq \frac{\alpha}{\alpha-1} I_\alpha(h';S') + \frac{1}{\delta} + \ln \left( \frac{1}{\delta^{1-\alpha}} \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P} \phi(h',S')^{\frac{1}{\delta^{1-\alpha}}} \right) \geq 1-\delta,
\]

Then, we will prove separately the case when $\alpha \rightarrow 1$ and $\alpha \rightarrow +\infty$. 

Technical Report 21
When $\alpha \to 1$. First, we have $\lim_{\alpha \to 1} \frac{1}{\alpha} I_\alpha(h'; S') = 0$. Furthermore, note that

$$\|\phi\|_{\alpha^{-1}} = \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} = \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}}$$

is the $L^{\frac{1}{\alpha}}$-norm of the function $\phi : \mathcal{H} \times \mathcal{Z}^m \to \mathbb{R}^+$, where $\lim_{\alpha \to 1} \|\phi\|_{\alpha^{-1}} = \lim_{\alpha' \to +\infty} \|\phi\|_{\alpha'}$ (since we have $\lim_{\alpha \to 1} \frac{1}{\alpha} = (\lim_{\alpha \to 1} \alpha)(\lim_{\alpha \to 1} \frac{1}{\alpha^{-1}}) = +\infty$). Then, it is well known that

$$\|\phi\|_{\infty} = \lim_{\alpha' \to +\infty} \|\phi\|_{\alpha} = \operatorname{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S').$$

Hence, we have

$$\lim_{\alpha \to 1} \ln \left( \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right) = \ln \left( \lim_{\alpha \to 1} \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right)$$

$$= \ln \left( \lim_{\alpha \to 1} \|\phi\|_{\alpha^{-1}} \right) = \ln \left( \lim_{\alpha' \to +\infty} \|\phi\|_{\alpha'} \right)$$

$$= \ln \left( \lim_{\alpha \to 1} \|\phi\|_{\infty} \right) = \ln \left( \operatorname{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S') \right).$$

Finally, we can deduce that

$$\lim_{\alpha \to 1} \left[ \frac{1}{\alpha} I_\alpha(h'; S') + \frac{1}{\delta} + \ln \left( \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right) \right] = \ln \frac{1}{\delta} + \ln \left( \operatorname{esssup}_{S' \in \mathcal{Z}, h' \in \mathcal{H}} \phi(h', S') \right).$$

When $\alpha \to +\infty$. First, we have $\lim_{\alpha \to +\infty} \|\phi\|_{\alpha^{-1}} = \lim_{\alpha' \to 1} \|\phi\|_{\alpha'} = \|\phi\|_1$. Hence, we have

$$\lim_{\alpha \to +\infty} \ln \left( \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right) = \ln \left( \lim_{\alpha \to +\infty} \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right)$$

$$= \ln \left( \lim_{\alpha \to +\infty} \|\phi\|_{\alpha^{-1}} \right) = \ln \left( \lim_{\alpha' \to 1} \|\phi\|_{\alpha'} \right)$$

$$= \ln \left( \|\phi\|_1 \right) = \ln \left( \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right).$$

Moreover, by rearranging the terms in $\frac{1}{\alpha} I_\alpha(h'; S')$, we have

$$\frac{1}{\alpha} I_\alpha(h'; S') = \frac{1}{\alpha} \ln \left( \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P^*} \frac{Q_S(h)}{P^*(h)} \right) = \ln \left( \left[ \mathbb{E}_{S \sim D^m} \mathbb{E}_{h \sim P} \left( \frac{Q_S(h)}{P^*(h)} \right) \right]^{\frac{1}{\alpha}} \right) = \ln \left( \left[ \mathbb{E}_{h \sim P} \Delta(h)^{\frac{1}{\alpha}} \right]^{\frac{1}{\alpha}} \right) = \ln(\|\Delta\|_\alpha),$$

where $\|\Delta\|_\alpha$ is the $L^\alpha$-norm of the function $\Delta$ defined as $\Delta(h) = \frac{Q_S(h)}{P^*(h)}$. Hence, we have

$$\lim_{\alpha \to +\infty} \frac{1}{\alpha} I_\alpha(h'; S') = \lim_{\alpha \to +\infty} \ln(\|\Delta\|_\alpha) = \ln \left( \operatorname{esssup}_{S \in \mathcal{S}, h \in \mathcal{H}} \Delta(h) \right) = \ln \left( \operatorname{esssup}_{S \in \mathcal{S}, h \in \mathcal{H}} \frac{Q_S(h)}{P^*(h)} \right).$$

Finally, we can deduce that

$$\lim_{\alpha \to 1} \left[ \frac{1}{\alpha} I_\alpha(h'; S') + \frac{1}{\delta} + \ln \left( \left[ \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right]^{\frac{\alpha-1}{\alpha}} \right) \right] = \ln \left( \operatorname{esssup}_{S \in \mathcal{S}, h \in \mathcal{H}} \frac{Q_S(h)}{P^*(h)} \right) + \ln \left( \mathbb{E}_{S' \sim D^m} \mathbb{E}_{h' \sim P^*} \phi(h', S') \right).$$
As for Theorem 2, this corollary illustrates a trade-off introduced by $\alpha$ between the Sibson’s mutual information $I_\alpha(h';S')$ and the term $\ln(\mathbb{E}_{S' \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} \phi(h',S'))$.

Furthermore, Esposito et al. (2020, Cor.4) introduced a bound involving the Sibson’s mutual information. Their bound holds with probability at least $1-\delta$ over $S \sim \mathcal{D}^m$ and $h \sim Q_S$:

$$2(R_S(h) - R_D(h))^2 \leq \frac{1}{m} \left[ I_\alpha(h';S') + \ln \frac{2}{\delta^\alpha} \right].$$

(.17)

Hence, we compare Equation (17) with the equations of the following corollary.

**Corollary 16.** For any distribution $\mathcal{D}$ on $Z$, for any hypothesis set $\mathcal{H}$, for any deterministic algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{M}(\mathcal{H})$, with probability at least $1-\delta$ over $S \sim \mathcal{D}^m$ and $h \sim Q_S$, we have

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ I_\alpha(h';S') + \ln \frac{2}{\delta^\alpha} \right]$$

and

$$2(R_S(h) - R_D(h))^2 \leq \frac{1}{m} \left[ I_\alpha(h';S') + \ln \frac{2}{\delta^\alpha} \right].$$

(.18)

(.19)

**Proof.** First of all, we instantiate Theorem 9 with $\phi(h,S) = \exp\left[ \frac{\alpha-1}{\alpha} \text{mkl}(R_S(h) \| R_D(h)) \right]$, we have (by rearranging the terms)

$$\text{kl}(R_S(h) \| R_D(h)) \leq \frac{1}{m} \left[ I_\alpha(h';S') + \ln \left( \mathbb{E}_{S' \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} e^{\text{mkl}(R_{S'}(h') \| R_D(h'))} \right) \right].$$

Then, from Maurer (2004), we upper-bound $\mathbb{E}_{S' \sim \mathcal{D}^m} \mathbb{E}_{h' \sim P} e^{\text{mkl}(R_{S'}(h') \| R_D(h'))}$ by $2\sqrt{m}$ to obtain Equation (18). Finally, to obtain Equation (19), we apply Pinsker’s inequality, i.e., $2(R_S(h) - R_D(h))^2 \leq \text{kl}(R_S(h) \| R_D(h))$ on Equation (18).

Equation (19) is slightly looser than Equation (17) since it involves an extra term of $\frac{1}{m} \ln \sqrt{m}$. However, Equation (18) is tighter than Equation (17) when $\text{kl}(R_S(h) \| R_D(h)) - 2(R_S(h) - R_D(h))^2 \geq \frac{1}{m} \ln \sqrt{m}$ (which becomes more frequent as $m$ grows).