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# On the Interplays between Generalisation and Optimisation: a PAC-Bayes Approach

# Acknowledgements

TODO

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# List of Notations

### General

| | |
|---|---|
| $a$ | A scalar (integer or real) |
| $\mathbb{R}$ | The set of real numbers |
| $\mathbb{R}^d$ | The euclidean set of dimension $d$ |
| $\|\cdot\|$ | a norm of an euclidean set |
| $\mathrm{dist}\,(\cdot,\cdot)$ | A distance on a Polish space. |
| $\mathbb{N}$ | The set of natural numbers |
| $\nabla f$ | the gradient of a function $f : \mathbb{R}^d \to \mathbb{R}$ |

### Statistical Learning Theory

| | |
|---|---|
| $\mathcal{Z}$ | Data space. In supervised learning, $\mathcal{Z} = (\mathcal{X}, \mathcal{Y})$ with $\mathcal{X}, \mathcal{Y}$ input and label spaces |
| $\mathbf{z}$ | A datum of $\mathcal{Z}$, in supervised learning $\mathbf{z} = (\mathbf{x}, y)$ with $\mathbf{x}$ input and $y$ label |
| $\mathcal{S}$ | Learning sample $\mathcal{S} = \{\mathbf{z}_i\}_{i\geq 1}$ |
| $\mathcal{D}_\mathcal{S}$ | Distribution of $\mathcal{S}$ |
| $\mathcal{S}_m$ | Restriction of $\mathcal{S}$ to its $m$ first data $\mathcal{S}_m = \{\mathbf{z}_i\}_{i=1\cdots m}$ |
| $\mathcal{D}$ | For *i.i.d.* $\mathcal{S}$, distribution of a single datum on $\mathcal{Z}$ |
| $\mathcal{D}^m$ | For *i.i.d.* $\mathcal{S}$, distribution of $\mathcal{S}_m$ |
| $\mathcal{T}$ | For *i.i.d.* $\mathcal{S}$, Test set drawn from $\mathcal{D}$ |
| $\mathcal{H}$ | The set of hypotheses |
| $h$ | A hypothesis $h \in \mathcal{H}$ |
| $\ell$ | Loss function $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}$ |

### Probability Theory

| | |
|---|---|
| $\mathbb{E}_{X\sim\nu}[\cdot]$ | The expectation *w.r.t.* the random variable $X \sim \nu$ |
| $\mathbb{P}_{X\sim\nu}[\cdot]$ | The probability *w.r.t.* the random variable $X \sim \nu$ |
| $\mathbb{1}[a]$ | Indicator function; returns $1$ if $a$ is true and $0$ otherwise |
| $(\mathcal{F}_i)_{i\geq 1}$ | Filtration adapted to $\mathcal{S}$ |
| $\mathbb{E}_i[\cdot]$ | Conditional expectation *w.r.t.* $\mathcal{F}_i$, *i.e.* $\mathbb{E}_i[\cdot] := \mathbb{E}[\cdot \mid \mathcal{F}_i]$ |
| $\mathcal{N}(\mu, \Sigma)$ | Gaussian distribution on $\mathbb{R}^d$ with mean $\mu$ and covariance matrix $\Sigma$ |

## PAC-Bayes framework

| | |
|---|---|
| $\mathcal{M}(\mathcal{H})$ | Set of Probability densities *w.r.t.* the reference measure on $\mathcal{H}$ |
| $\mathrm{Q}$ | Posterior distribution $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$ on $\mathcal{H}$ |
| $\mathrm{P}$ | Prior distribution $\mathrm{P} \in \mathcal{M}(\mathcal{H})$ on $\mathcal{H}$ |
| $\mathrm{KL}(\mathrm{Q}\|\mathrm{P})$ | Kullback-Leibler (KL) divergence between $\mathrm{Q}$ and $\mathrm{P}$ |
| $D_\alpha(\mathrm{Q}\|\mathrm{P})$ | Rényi Divergence between $\mathrm{Q}$ and $\mathrm{P}$ |
| $\mathsf{R}_{\mathcal{D}}(h)$ | Population Risk of $h \in \mathcal{H}$ *w.r.t.* $\mathcal{D}$, *i.e.* $\mathsf{R}_{\mathcal{D}}(h) := \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\ell(h, \mathbf{z})]$ |
| $\hat{\mathsf{R}}_{\mathcal{S}_m}(h)$ | Empirical Risk on $\mathcal{S}_m$, *i.e.* $\hat{\mathsf{R}}_{\mathcal{S}_m}(h) \dfrac{1}{m}\sum_{i=1}^{m} \ell(h, \mathbf{z}_i)$ |
| $\Delta_{\mathcal{S}_m}(h)$ | Generalisation gap $\Delta_{\mathcal{S}_m}(h) := \mathsf{R}_{\mathcal{D}}(h) - \hat{\mathsf{R}}_{\mathcal{S}_m}(h)$ |
| $\mathsf{R}_{\mathcal{D}}(\mathrm{Q})$ | Expected population risk *w.r.t.* $\mathrm{Q}$, *i.e.* $\mathsf{R}_{\mathcal{D}}(\mathrm{Q}) := \mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}_{\mathcal{D}}(\mathrm{Q})]$ |
| $\hat{\mathsf{R}}_{\mathcal{S}_m}(\mathrm{Q})$ | Expected empirical risk *w.r.t.* $\mathrm{Q}$, $\hat{\mathsf{R}}_{\mathcal{S}_m}(\mathrm{Q}) := \mathbb{E}_{h\sim\mathrm{Q}}\left[\hat{\mathsf{R}}_{\mathcal{S}_m}(\mathrm{Q})\right]$ |
| $\Delta_{\mathcal{S}_m}(\mathrm{Q})$ | Expected generalisation gap *w.r.t.* $\mathrm{Q}$, $\Delta_{\mathcal{S}_m}(\mathrm{Q}) := \mathbb{E}_{h\sim\mathrm{Q}}[\Delta_{\mathcal{S}_m}(h)]$ |
| $\mathrm{P}_{-f(h)}$ | Gibbs posterior associated to prior $\mathrm{P}$ and function $f : \mathcal{H} \to \mathbb{R}$ |

## Optimal transport

| | |
|---|---|
| $\mathrm{W}_1$ | The $1$-Wasserstein distance |
| $\mathrm{W}_2$ | The $2$-Wasserstein distance |
| $\Gamma(\mathrm{Q}, \mathrm{P})$ | Set of all coupling distribution on $\mathcal{H}^2$ whose marginals are $\mathrm{Q}$ and $\mathrm{P}$. |

# List of Publications

## Conference article

Paul Viallard, Maxime Haddouche, Umut Simsekli, and Benjamin Guedj. Learning via Wasserstein-Based High Probability Generalisation Bounds. *Advances in Neural Information Processing Systems (NeurIPS)*. (2023).

Maxime Haddouche and Benjamin Guedj. Online PAC-Bayes Learning. *Advances in Neural Information Processing Systems (NeurIPS)*. (2022).

## Journal article

Maxime Haddouche and Benjamin Guedj. PAC-Bayes Generalisation Bounds for Heavy-Tailed Losses through Supermartingales. *Transactions on Machine Learning Research*. (2023).

## Research Report

Maxime Haddouche and Benjamin Guedj. Wasserstein PAC-Bayes Learning: A Bridge Between Generalisation and Optimisation. *arXiv*. abs/2304.07048. (2023).

Maxime Haddouche, Benjamin Guedj, and Olivier Wintenberger. Optimistic Dynamic Regret Bounds. (2023). arXiv: 2301.07530 [cs.LG].

Pierre Jobic, Maxime Haddouche, and Benjamin Guedj. Federated Learning with Nonvacuous Generalisation Bounds. (2023). arXiv: 2310.11203 [cs.LG].

Maxime Haddouche, Benjamin Guedj, and John Shawe-Taylor. Upper and Lower Bounds on the Performance of Kernel PCA. (2020). arXiv: 2012.10369 [cs.LG].

# Préambule: Apprentissage humain, Apprentissage Machine et Généralisation

Ce manuscrit étudie la question de la capacité de *généralisation* des algorithmes d'apprentissage machine. Pour comprendre la généralisation, il faut d'abord appréhender l'*apprentissage*, prenons donc le luxe, pour un bref instant, d'oublier les machines pour se concentrer sur l'apprentissage en ce qu'il a de plus humain.

**Appréhender l'apprentissage humain.** Un être apprenant, en premier lieu, va se structurer autour d'expériences, vécues ou transmises par autrui et va ensuite en bénéficier via diverses modalités. Il peut, par exemple, considérer une expérience médiée comme vraie (le feu brûle) et agir en fonction de ce postulat alors qu'à l'opposé, la réitération ou la négation de cette même experience peuvent être symptomatiques d'une valeur de vérité nulle. Ces scénarios peuvent tout aussi bien apparaître pour une expérience vécue (hallucinations). Cette première dichotomie quant au traitement de l'information est intrinsèquement liée à une question clairement énoncée : est-ce que le feu brûle? Puis-je me fier à mes sens ou ai-je halluciné ? Dans ces cas de figure, l'apprentissage a eu lieu à travers l'assujettissement de l'expérience à sa valeur de vérité par rapport à une question simple (ici à deux issues). Cette vision peut facilement s'étendre à une arborescence finie de possibles pour des questions à choix multiples. En effet, on peut étendre la question de la brûlure comme suit: quelle est l'intensité de la brûlure en fonction de la température du feu? On peut dès lors établir une multitude de réponses représentant divers degrés de brûlure.
Néanmoins, de nombreuses questions ne peuvent se réduire à un nombre fini de possibilités. Par exemple, qu'est-ce que le feu? Pour répondre à cette question, il est néanmoins possible d'exploiter de multiples facettes d'expériences (feu de bois, brindille, roche) pour proposer le feu comme étant la réaction chimique de l'oxygène de l'air avec un matériau combustible, un apport d'énergie servant de déclencheur.
Il est alors légitime de se demander pourquoi l'apprenant a eu besoin de comprendre la vraie nature du feu. Cette compréhension fondamentale des choses émerge de considérations pratiques : comment ne plus avoir froid? Peut-on manger de la viande autrement que crue pour diminuer les risques de maladie? Il faut alors de multiples interactions avec l'environnement pour générer des expériences et ensuite apprendre d'elles pour répondre graduellement à un besoin complexe (comment faire un feu pour se réchauffer?).

Ainsi, par cette analyse préliminaire, nous avons trouvé plusieurs prémices de compréhension de l'apprentissage chez l'homme.

- Comment l'apprentissage se formalise-t-il structurellement ? L'apprenant doit abâtardir l'expérience à des questions simples pour acquérir des certitudes primaires. Ces dernières acquises, il est possible d'atteindre des questions complexes en imbriquant de plus en plus de considérations élémentaires.

- D'où provient le besoin d'apprendre ? D'un point de vue pratique, l'émergence de ces questions complexes dérive bien souvent d'un rapport de l'être à son environnement, permettant d'élaborer des objectifs contextuels. L'apprenant devient alors graduellement capable de répondre à des besoins complexes par une succession d'actions simples.

**De l'apprentissage humain à l'apprentissage machine.** L'apprentissage machine s'est structuré autour de deux approches, une première symbolique qui tire profit des extrapolations humaines pour apprendre à la machine à manipuler une axiomatique et une seconde, statistique, qui consiste à fournir bon nombre d'expériences à la machine pour lui faire apprendre par de multiples exemples empiriques. Nous allons nous focaliser sur la seconde approche car, elle sous-tend une large partie de la recherche moderne. Cette méthode requiert de nombreuses expériences transmises à la machine qui en extrait les connaissances à travers des procédures optimisatoires. Plus précisément, la connaissance extraite dépend de la question posée ainsi que sa traduction mathématique. Nous pouvons alors relever des parallèles avec l'apprentissage humain décrit plus haut: il faut des expériences et une question pour réduire le réel à quelque chose d'apprenable. Pour aller plus loin, la variétés des scenarii d'apprentissages humain décrits au dessus ont une correspondance dans l'apprentssage machine moderne: à la question "Le feu brûle-t-il?" on peut associer l'apprentissage supervisé qui traite apprend sur des questions à choix multiples. A la question "qu'est-ce que le feu?", on peut associer l'apprentissage non-supervisé qui va chercher, dans le cas du clustering (ou regroupement), des similitudes non-induites par la question entre diverses expériences. Finalement, quant à l'interaction avec l'environnement et la question "puis-je faire un feu?", elle est associée à l'apprentissage par renforcement qui étudie l'apprentissage d'un agent qui interagit avec son environnement.

**Comprendre la généralisation depuis l'apprentissage.** La généralisation peut être vue comme la capacité d'exploiter l'apprentissage d'une expérience au delà de cette dernière. Cela englobe une compréhension théorique et axiomatique d'un phénomène bien au delà de l'expérience en elle même, *i.e.* une extrapolation fructueuse ou bien la capacité à exploiter la connaissance acquise pour une situation inédite, présentant des similitudes avec divers vécus, *i.e.* interpoler des expériences.

Ce double aspect de la généralisation se retrouve aussi bien chez l'homme que la machine sous diverses modalités. Les réseaux de neurones profonds, qui sont le fer de lance de l'apprentissage machine moderne, se basent sur des espaces de dimension finie pour apprendre, ce qui revient à dire qu'un problème peut être appris à travers un nombre fini de principes fondateurs. Le nombre de principes pouvant être augmentés autant que les capacités numériques le permettent, nous dirons alors que les réseaux de neurones ont une puissance discrète de généralisation. Etant donné que les méthodes d'apprentissage machine sont corrêlées à leur pendantes humaines, on peut alors se demander si la puissance de généralisation (et même d'apprentissage) humaine est également discrète. Cette afirmation semble cavalière, car même s'il est possible de supposer que la part consciente de l'esprit humain raisonne à horizon finie et a une puissance dénombrable (transmise d'ailleurs à la machine, apprenant selon des modalités humaines), cette dimension occulte la quantité d'information sans cesse captée et filtrée par notre cerveau ainsi que son assimilation inconsciente, relevant autant de la pensée abstraite que du biologique peut potentiellement générer une puissance de généralisation relevant d'un infini plus large et ainsi fournir une puissance de généralisation continue (relevant davantage de la ligne que du point). Dès lors, comment penser la généralisation chez l'homme alors que, mathématiquement, nos intuitions les plus simples nous font défaut lorsque cette puissance continue intervient (la boule de rayon 1 n'est pas compacte en dimension infinie, Riesz, 1955)? On peut également se demander si l'extrapolation existe dans de telles structures ou si tout revient à interpoler (Hasson *et al.*, 2020).

**Quid de la généralisation en apprentissage machine de nos jours?** Qu'espérer alors des réseaux de neurones artificiels et de leur capacité de généralisation relativement à l'humain? Les théorèmes d'approximations universels (voir *e.g.* Lu *et al.*, 2017; Park *et al.*, 2021) assurent que les réseaux de neurones sont capables d'approximer n'importe quelle fonction vivant dans un espace à la puissance du continu (*e.g.* l'espace de Banach des fonctions continues à support compact qui n'admet pas de base dénombrable), faisant de ces structures des candidats prometteurs pour appréhender les mécanismes humains de généralisation. Les approximations prodiguées par ces machines seront, dans un avenir proche, potentiellement suffisamment puissantes pour donner l'illusion d'une capacité de généralisation humaine. Néanmoins, il demeure bon de garder en tête que, si la thèse d'une inégalité fondamentale de nature entre les puissances de généralisation humaine et machine est avérée, alors les réseaux de neurones artificiels n'atteindront jamais pleinement les capacités de compréhension du monde de leurs homologues biologiques. Reste que la qualité de leurs approximations font de ces structures des assistants de valeur, enrichissant les capacités de chacun. Mieux comprendre la puissance de généralisation machine, être capable de la quantifier, d'identifier les mécanismes qui la favorisent sont les objets de ce manuscrit.

# Preamble: Human Learning, Machine Learning and Generalisation

This manuscript tackles the notion of *generalisation* a notion built upon the general notion of *learning*. For a brief moment, let's take the luxury of forgetting about machines and concentrate on learning at its most human.

**Apprehending human learning** A human being (here a learner) is structured around experiences, either lived or passed on by others.

The learner then benefits from these experiences in various ways, for instance, by considering a mediated experience to be true (fire burns) and acting according to this. On the contrary, reiteration or denial of this same information may be symptoms of zero truth value. These scenarios can just as easily appear for a lived experience (the question of hallucinations). This first dichotomy in information processing is intrinsically linked to a clearly stated question: does fire burn? Can I trust my senses or have I hallucinated? In these cases, learning has taken place by reducing the intrinsic complexity of an experience to its truth value *w.r.t.* a simple question (in this case with two outcomes). This vision can easily be extended to a finite tree of possibilities through multiple-choice questions. Indeed, we can extend the burning question as follows: what is the intensity of the burn as a function of the temperature of the fire? We can then establish a multitude of answers representing various degrees of burn.

However, many questions cannot be reduced to a finite number of possibilities. For example, what is fire? To answer this question, it is nevertheless possible to exploit multiple facets of experience (wood, twig, rock fire) to propose that fire is the chemical reaction of oxygen in the air with a combustible material, with a supply of energy serving as the trigger.

Then, a legitimate question is: why has mankind understood the nature of fire? This fundamental understanding emerged from practical considerations: how can we stop being cold? Can we eat meat other than raw to reduce the risk of illness? It then takes multiple interactions with the environment to generate experiences and then learn from them to gradually respond to a complex need (how to make a fire to keep yourself warm?).

Thus, through this preliminary analysis, we have found several premises of understanding human learning.

- How is learning formalised structurally? The learner must base the experience on simple questions to acquire primary certainties. These latter acquired, it is possible to reach complex questions by interweaving more and more elementary considerations.
- Where does the need to learn come from? From a practical point of view, the emergence of these complex questions often arises from a relationship between the being and its environment, making it possible to develop contextual objectives. The learner then gradually becomes capable of responding to complex needs through a succession of simple actions.

**From human to machine learning** Machine learning has been structured around two approaches, the first is symbolic and takes advantage of human extrapolations to teach the machine to manipulate an axiomatic, while the second is statistical, and consists of providing the machine with a large number of experiments so that it learns from multiple empirical examples. We are going to focus on the second approach because it underpins a large part of modern research. This method requires a large number of experiments to be transmitted to the machine, which then extracts the knowledge through optimising procedures. More precisely, the knowledge extracted depends on the question posed and its mathematical translation. We can see parallels with human learning described above: you need experiments and a question to reduce reality to something learnable. To go a step further, the variety of human learning scenarios described above can be applied to modern machine learning: the question "Does fire burn?" can be associated with supervised learning, which learns from multiple-choice questions. The question "What is fire?" can be associated with unsupervised learning, which, in the case of clustering, looks for similarities between numerous experiments that are not induced by the question. Finally, the question "Can I make a fire?" can be linked to reinforcement learning which focuses on the evolution of an agent learning from its interaction with the environement.

**From learning to generalisation.** Generalisation can be seen as the ability to exploit learning from experience beyond that experience. This encompasses a theoretical and axiomatic understanding of a phenomenon, *i.e.* a fruitful extrapolation, or the ability to exploit the knowledge acquired for a new, yet showing similarities, situations *i.e.* to interpolate experiences.
This dual aspect of generalisation can be found in both humans and machines in a variety of ways. Deep neural networks, which are the spearhead of modern machine learning, are based on finite-dimensional learning spaces, which means that a problem can be learned through a finite number of founding principles. Since the number of principles can be increased as far as numerical capacity allows, we can say that neural networks have discrete generalising power. Given that machine learning methods are

correlated with their human counterparts, we might then ask whether the power of human generalisation (and even learning) is also discrete. This assertion is somewhat bold as even it is assumable that the conscious part of the human mind reasons on a finite horizon and has a discrete generalisation power (transmitted, moreover, to the machine, which learns according to human methods), this dimension obscures the quantity of information constantly captured and filtered by our brain, as well as its unconscious assimilation, In other words, the fact that our brain is as much a part of abstract thought as it is of biological thought can potentially generate a generalisation power that relates to a wider infinity and thus provide a continuous generalisation power (relating more to the line than to the point). So how can we think about generalisation in humans when, mathematically, our simplest intuitions fail us when this continuous power is involved (the ball of radius 1 is not compact in infinite dimension, Riesz, 1955)? We might also ask whether extrapolation exists in such structures or whether it all boils down to interpolation (Hasson *et al.*, 2020).

**What to expect from generalisation in modern machine learning?** So what can we expect from artificial neural networks and their ability to generalise to humans? Universal approximation theorems (see *e.g.* Lu *et al.*, 2017; Park *et al.*, 2021) ensure that neural networks are capable of approximating any function living in a space to the power of the continuum (*e.g.* the space of continuous functions with compact support which does not admit a countable base as a Banach space), making these structures promising candidates for partially understanding human generalisation mechanisms. In the near future, machine approximations will potentially be powerful enough to give the illusion of human generalisation capacity. Nevertheless, it is worth bearing in mind that, if the thesis of a fundamental inequality in nature between the powers of human and machine generalisation is confirmed, then artificial neural networks will never fully attain the world-understanding capacities of their human counterparts. It is stll worth noticing artificial neural nets ability to approximate this human intelligence makes these structures valuable assistants, enriching the capabilities of any individual. That being said, this manuscript aims to provide a better understanding of generalisation in machine learning, quantifying and indentifying the mechanisms that promote it.
JURY:
Rapporteurs: Alquier (sur)/Chopin (moins)
Membres: Seldin (rapporteur mais peut etre pas fou pour le rapport)/ Pascal Germain (rapporteur) Gérard (si Pierre pas dispo), John Shawe-Taylor (examinateur), Emilie Morvant (présidente) + le Maitre + Arnak Dalalyan (trop proche?), Alessandro Rudi
CHALLENGE HERE: being very rigorous on the lit review.

# 1 PAC-Bayes Learning, a field of many paradigms

## Contents



## 1.1 A brief introduction to statistical learning

Statistical learning (Vapnik, 1999; James *et al.*, 2013) quantifies and identifies how learning algorithms, trained on a specific task using a finite training dataset, generalise to novel, unseen datum. More precisely, an agent has to learn how to answer a question, formalised as a *learning problem* being a tuple $(\mathcal{H}, \mathcal{Z}, \ell)$ composed of a *predictor space* on which evolves the agent during the learning process, a *data space* $\mathcal{Z}$ and a *loss function* being the mathematical formulation of the question. Such a minimalistic structure is convenient to encompass a broad range of real-life learning scenarii. To learn, the agent has access to a *training dataset* $\mathcal{S}_m = (\mathbf{z}_i)_{i=1\cdots m}$. The most classical way to learn from $\mathcal{S}_m$ is the empirical risk minimisation (ERM), minimising the *empirical risk* $\hat{\mathrm{R}}_{\mathcal{S}_m} := \frac{1}{m}\sum_{i=1}^{m} \ell(h, \mathbf{z}_i)$. In this setting, when $\mathcal{S}_m$ is *i.i.d.* (following the distribution $\mathcal{D}$), two facets of generalisation are commonly studied in statistical learning for an agent $h \in \mathcal{H}$.

- First, the *population risk* $\mathrm{R}_{\mathcal{D}}(h) := \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\ell(h, \mathbf{z})]$ focus on the average performance of our learning agent *w.r.t.* any new situation $\mathbf{z} \in \mathcal{D}$, independent of $\mathcal{S}_m$, possibly faced by the agent. A small population risk ensure then efficient generalisation.

- Second, the *generalisation gap* $\Delta_{\mathcal{S}_m}(h) := \mathrm{R}_D(h) - \hat{\mathrm{R}}_{\mathcal{S}_m}(h)$ evaluate the coherence between the empirical risk and the population one. Having a small generalisation gap ensure that the generalisation ability of the agent has the same magnitude than its training performance.

Note that the population risk is a stronger notion of generalisation than the generalisation gap. However, a small generalisation gap (in absolute value) as well as a small empirical risk is enough to ensure a good population risk. Given that modern optimisation algorithm often yield small empirical risk, the generalisation gap has received a particular attention in statistical learning.

**Generalisation bounds.** Generalisation bounds are inequalities controlling the generalisation gap (or the population risk) by various quantities depending either on $\mathcal{H}, \mathcal{Z}$ or $\mathcal{S}_m$. We propose below general patterns usually involved in generalisation bounds for an agent $h_{\mathcal{S}_m} \in \mathcal{H}$ depending on $\mathcal{S}_m$ (for instance the output of the ERM).
**Expected generalisation bound.** For any training set $\mathcal{S}_m$:

$$\mathbb{E}_{\mathcal{S}_m}\left[\Delta_{\mathcal{S}_m}(h_{\mathcal{S}_m})\right] \leq f\left(\textsc{Complexity}, \frac{1}{m}\right). \tag{1.1}$$

**High-probability generalisation bounds.** For any training set $\mathcal{S}_m$, with probability $1-\delta$ pver the draw of $\mathcal{S}_m$:

$$\Delta_{\mathcal{S}_m}(h_{\mathcal{S}_m}) \leq f\left(\textsc{Complexity}, \frac{1}{m}, \log\frac{1}{\delta}\right). \tag{1.2}$$

The nature of $f$ and the Complexity term depend on the facet of the complexity of the learning problem we aim to focus. Celebrated examples are for instance the dimension of $\mathcal{H}$, if euclidean, the VC dimension of $\mathcal{H}$ (Vapnik, 2000), the Rademacher complexity (Bartlett and Mendelson, 2001, 2002), the stability parameter of a learning algorithm (Bousquet and Elisseeff, 2000) or the subgaussian diameter of $\mathcal{Z}$ (Kontorovich, 2014). Another approach relies on the Bayesian learning paradigm, deriving *posterior* knowledge from data and prior modelling of the environment. Then, the Complexity can be borrowed from information theory (Cover and Thomas, 2001), *e.g.* mutual information (Neal, 2012), or from optimal transport, *e.g.* Wasserstein distances (Wang *et al.*, 2019; Rodriguez-Galvez *et al.*, 2021).
Those two approaches have various benefits. A notable strength of expected bounds is that they may reach fast convergence rates (*i.e.* faster than $\frac{1}{\sqrt{m}}$) contrary to high-probability one, even when $\mathcal{H}$ is a singleton thanks to the central limit theorem (Grunwald *et al.*, 2021). However, expected bounds often involves a theoretical Complexity which cannot be estimated in practice and may be hard to interpret while high probability bounds may be fully empirical and can be considered with small confidence parameter $\delta$ as it is attenuated by a logarithm.

**How to choose the complexity term ? An introductory example.** There is no evidence proving that a certain notion of complexity is preferrable to another. The

choice of COMPLEXITY may however be driven by practical considerations, emerging from the learning problem of interest. To illustrate this point, let us focus on the following example, providing two learning problems which differs only from the predictor space $\mathcal{H}$ and which have very different interactions with the VC dimension.

**Example 1.1.1** (VC dimension of multilayer perceptrons)**.** Consider a supervised learning problem where $\mathcal{Z} = \mathbb{R}^k \times \mathcal{Y}$ with $\mathcal{Y} = \{0, 1\}$, $k$ smaller than $m$ and with loss $\ell(h, (x, y)) = \mathbb{1}\{h(x) \neq y\}$. First, assume that $\mathcal{H}$ is the set of linear classifiers; *i.e.* $\mathcal{H}_1 := \{h_\theta(x) = sgn(\langle \theta, x \rangle)\}$, where $sgn(a)$ denotes the sign of $a$. In this case, using the VC dimension may lead to non-vacuous generalisation bounds (VAPNIK, 2000).
However, in modern machine learning, deep neural networks are often considered, let us first define a celebrated class of deep neural networks.

> **Definition 1.1.1** (Multlilayer perceptron)**.** A multilayer perceptron with depth $K$ and architecture $\{N_1, \cdots, N_K\}$, denoted as $h_{\mathbf{w}}(\mathbf{x}) := W h^K(\cdots h^1(\mathbf{x})) + b$, is composed of $K$ layers $h^1(\cdot), \ldots, h^K(\cdot)$. $W \in \mathbb{R}^{|\mathcal{Y}| \times N_K}$ and $b \in \mathbb{R}^{N_K}$ are the weight matrix and the bias of the last layer, and the $i$-th layer $h^i$, composed of $N_i$ nodes, is defined by $h^i(\mathbf{x}) := \sigma_i(W_i \mathbf{x} + b_i)$, where $W_i \in \mathbb{R}^{N_i \times N_{i-1}}$ and the bias $b_i \in \mathbb{R}^{N_i}$ are its weight matrix and bias respectively; $\sigma_i : \mathbb{R}^{N_i} \to \mathbb{R}^{N_i}$ is an activation function. The weights $\mathbf{w} = \mathrm{vec}(\{W, W_K, \ldots, W_1, b, b_K, \ldots, b_1\})$ represent the vectorisation of all parameters of the network.

Now, consider the learning problem with the same $\mathcal{Z}, \ell$ as above, but with $\mathcal{H}_2$ being the set of multilayer perceptrons *w.r.t.* a fixed depth $K$ and architecture $\{N_1, \cdots, N_K\}$. To be consistent with modern practice, assume also that we are in the *overparametrised setting*, meaning that the space $\mathcal{H}_2$ has a dimension $d$ far greater than $m$. In this case, VC dimension fails to explain the good generalisation ability (seen in practice) of multilayer perceptrons (BARTLETT and MAASS, 2003).

Understanding the generalisation ability of deep neural networks remains nowadays a major challenge and in what follows, we focus on a modern branch of learning theory which provided non-vacuous bounds of the generalisation ability of deep neural networks: PAC-Bayes learning.

## 1.2 An information-theoretic exposition of PAC-Bayes learning

PAC-Bayes learning is a recent branch of learning theory which emerged in the late 90s via the seminal work of (SHAWE-TAYLOR and WILLIAMSON, 1997; MCALLESTER,

1998, 1999, 2003) and later pursued by (Catoni, 2003, 2007). Modern surveys are available to describe the various advances in the field (Guedj, 2019; Hellström *et al.*, 2023; Alquier, 2024). Similarly to the various subfields of statistical learning described in Section 1.1, PAC-Bayes theory provide generalisation bounds involving a Complexity term apprehending a facet of the complexity of the learning problem. In PAC-Bayes, this term is inspired from the Bayesian learning paradigm of designing a *posterior* knowledge of the learning problem based on both training data and a *prior* knowledge of the considered situation. A concrete example of Bayesian learning would be an explorer mapping an ill-known territory. The explorer has to adapt the existing maps at its disposal before exploration to its discoveries. Doing so, he creates an *a posteriori* map imbricating the benefits of both the prior knowledge alongside its findings. From a mathematical perspective, the Bayes approach relies on the Bayes formula, providing an update recipe from a prior distribution $\mathrm{P} \in \mathcal{M}(\mathcal{H})$ over the predictor space $\mathcal{H}$ to a posterior $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$ through a likelihood. On the contrary, PAC-Bayes, while inspired from the Bayesian philosophy, does not relies on the Bayes formula but instead on tools from information theory. This general approach benefits from additional flexibility as PAC-Bayes can be linked and applied to Bayesian learning (see Guedj, 2019) but also blurs the notion of prior and posterior distributions, now independent of the fundamental Bayes formula. We further develop those points through two celebrated high-probability bounds: the McAllester and Catoni ones.

## Two fundamental results

The McAllester's bound (McAllester, 2003) enriched with Maurer's trick (Maurer, 2004) and Catoni's bound (Alquier *et al.*, 2016, Theorem 4.1, being a relaxation of Catoni, 2007, Theorem 1.2.6) are probably the most known high-probability PAC-Bayes bounds. We recall them in Proposition 1.2.1.

**Proposition 1.2.1** (McAllester and Catoni's bounds)**.** Assume $\mathcal{S}_m$ to be *i.i.d.*.
**McAllester's bound, (Maurer, 2004, Theorem 5).** For any $\delta \in (0,1), \ell \in [0,1]$, any data-free prior $\mathrm{P} \in \mathcal{M}(\mathcal{H})$, with probability at least $1-\delta$, for any posterior $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$,

$$\Delta_{\mathcal{S}_m}(\mathrm{Q}) \leq \sqrt{\frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \ln \frac{2\sqrt{m}}{\delta}}{2m}}. \tag{1.3}$$

**Catoni's bound, (Alquier *et al.*, 2016, Theorem 4.1).** For any $\lambda \in \mathbb{R}/\{0\}, \delta \in (0,1), \ell$ being $\sigma^2$-subgaussian and a data-free prior $\mathrm{P}$, with probability at least $1-\delta$ over $\mathcal{S}$, for any $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$,

$$\Delta_{\mathcal{S}_m}(\mathrm{Q}) \leq \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(1/\delta)}{\lambda} + \frac{\lambda\sigma^2}{2m}. \tag{1.4}$$

For both results, $\Delta_{\mathcal{S}_m}(\mathrm{Q})$ denotes the expected generalisation gap *w.r.t.* $\mathrm{Q}$ and $\mathrm{KL}$ denotes the Kullback-Leibler divergence.

Recall that a random variable $X$ is $\sigma^2$-subgaussian if for any $\lambda \in \mathbb{R}$, $\mathbb{E}[\exp(\lambda(X - \mathbb{E}[X]))] \leq \exp\left(\frac{\lambda^2\sigma^2}{2}\right)$ and that any loss $\ell \in [0, C]$ is $C$-subgaussian. Both McAllester and Catoni bounds fit the general shape of (1.2). In both cases, $\textsc{Complexity} = \mathrm{KL}(\mathrm{Q},\mathrm{P})$ and $f$ varies. The immediate link with the Bayesian philosophy of learning is that the prior has to be data-free. However, (1.3) and (1.4) are both valid simultaneously for any posterior, which is strictly more general than considering the Bayesian posterior. Note that if $\lambda$ is optimised, then Catoni's bound would boil down to an upgraded McAllester bound without the $\log(\sqrt{m})$ term, but such an optimisation is not feasible as $\lambda$ has to be chosen independently of the dataset $\mathcal{S}_m$. Note that this gap has been recently filled by Dupuis and Şimşekli (2024, Theorem 33). While the theoretical links between those two bounds are clear, they involve two different toolboxes: McAllester's bound heavily relies on the KL divergence between Bernoullis alongisde calculation tricks exploiting the boundedness of the loss while the original Catoni's bound (Catoni, 2007, Theorem 1.2.6) exploits tools from statistical physics. The relaxation (1.4) proposed here is reachable by a few key arguments, involved in a vast majority of PAC-Bayes proofs. We propose it below for pedagogical purpose.

*Proof of Equation* (1.4). Note that the first part of the proof holds for a large part of PAC-Bayes literature.

**A generic pattern for PAC-Bayes bounds.** This part is designed upon two cornerstones, retrievable in many existing results: the change of measure inequality (Csiszár, 1975; Donsker and Varadhan, 1976 – see also Banerjee, 2006; Guedj, 2019 for a proof) and Markov's inequality.

**Lemma 1.2.1** (Change of measure inequality)**.** For any measurable function $\psi : \mathcal{H} \to \mathbb{R}$ and any distributions $\mathrm{Q}, \mathrm{P}$ on $\mathcal{H}$:

$$\mathbb{E}_{h\sim\mathrm{Q}}[\psi(h)] \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log\left(\mathbb{E}_{h\sim\mathrm{P}}[\exp(\psi(h))]\right).$$

For a given $\lambda > 0$, the change of measure inequality is then applied to a certain

function $f_m : \mathcal{H} \to \mathbb{R}$, possibly involving $\mathcal{S}_m$: for all posteriors $Q$,

$$\mathbb{E}_{h\sim \mathrm{Q}}[f_m(h)] \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log\left(\mathbb{E}_{h\sim \mathrm{P}}[\exp(f_m(h))]\right). \tag{1.5}$$

To deal with the random variable $X(\mathcal{S}_m) := \mathbb{E}_{h\sim \mathrm{P}}[\exp(f_m(h))]$, our second building block is Markov's inequality $\left(\mathbb{P}(X > a) \leq \frac{\mathbb{E}[X]}{a}\right)$ which we apply for a fixed $\delta \in (0,1)$ on $X(\mathcal{S}_m)$ with $a = \mathbb{E}_{\mathcal{S}_m}[X(\mathcal{S}_m)]/\delta$. Taking the complementary event gives that for any $m$, with probability at least $1-\delta$ over the sample $\mathcal{S}_m$, $X(\mathcal{S}_m) \leq \mathbb{E}_{\mathcal{S}_m}[X(\mathcal{S}_m)]/\delta$, thus:

$$\mathbb{E}_{h\sim \mathrm{Q}}[f_m(h)] \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(1/\delta) + \log\left(\mathbb{E}_{h\sim P}\mathbb{E}_{\mathcal{S}_m}[\exp(f_m(h))]\right). \tag{1.6}$$

Note that in (1.6), we swapped the two expectations in the last term thanks to Fubini's theorem and the fact that $\mathrm{P}$ is data-free.

**Proving Catoni's bound.** Now, we take $f_m(h) = \lambda\Delta_{\mathcal{S}_m}$ and consider for any $h \in \mathcal{H}$, $A(h) = \mathbb{E}_{\mathcal{S}_m}[\exp(f_m(h))]$.
Note that, given $\mathcal{S}_m$ is iid,

$$A(h) = \prod_{i=1}^{m} \mathbb{E}_{\mathcal{S}_m}\left[\exp\left(\frac{\lambda}{m}(\mathsf{R}_{\mathcal{D}}(h) - \ell(h,\mathbf{z}_i))\right)\right],$$

and thanks to Heoffding's lemma alongside $\ell$ being $\sigma^2$-subgaussian,

$$A(h) \leq \prod_{i=1}^{m} \exp\left(\frac{\lambda^2\sigma^2}{2m^2}\right) = \exp\left(\frac{\lambda^2\sigma^2}{2m}\right).$$

Plugging this upper bound in (1.6) and dividing by $\lambda$ concludes the proof. ■

The generic pattern (1.6), allows to retrieve many PAC-Bayes bounds, starting with McAllester's one, where $f_m = kl(\mathsf{R}_{\mathcal{D}}(h), \hat{\mathsf{R}}_{\mathcal{S}_m}(h))$, $kl$ being the KL divergence between Bernoullis and completing with the subtle calculations of Maurer (2004). This pattern is also valid, for instance, for the results of Germain *et al.* (2009), the Bernstein PAC-Bayesian bounds of Tolstikhin and Seldin (2013) and Mhammedi *et al.* (2019) and many other results, *e.g.* Thiemann *et al.* (2017), Guedj and Robbiano (2018), Holland (2019), and Wu and Seldin (2022). This then pins two major points for a large part of PAC-Bayes literature:

1. Interpreting PAC-Bayes from a Bayesian point of view is legitimated by the change of measure inequality, yet the KL divergence. More generally, this property allows interpreting PAC-Bayes under a more general information-theoretic paradigm, where relevant prior information is transferred to the posterior (here

by absolute continuity to keep the KL finite). This information-theoretic vision is also retrieved in in-expectation PAC-Bayes bounds, where mutual information can be considered instead of KL divergence (Russo and Zou, 2016; Xu and Raginsky, 2017; Hellström and Durisi, 2020; Steinke and Zakynthinou, 2020; Grunwald *et al.*, 2021; Hellström and Durisi, 2022).

2. The statistical properties of the learning problem are linked to the exponential moment coming from the change of measure inequality, this often implies the strong assumptions of Proposition 1.2.1: data-free prior, bounded or subgaussian losses (sometimes attenuated to subexponentiality Catoni, 2004).

**A theory suited for Example 1.1.1?** The two previous points show that Proposition 1.2.1 holds for learning problem with light-tailed losses (often bounded), *i.i.d.* data, encompassing classification tasks for instance. Then, PAC-Bayes learning seems suited to understand, on such problems, the McAllester and Catoni bounds are suited to the learning problem $(\mathcal{H}_2, \mathcal{Z}, \ell)$ of Example 1.1.1.
However, the question of their tightness is unsolved as we do not know the behavior of the KL term in practice. Furthermore the question of which distribution $\mathrm{Q}$ should be taken in Proposition 1.2.1 remains open. Hopefully, PAC-Bayes bounds can be transformed into learning algorithms.

# 1.3 From theory to learning algorithms

## Algorithms associated to McAllester and Catoni bounds

A shared particularity of McAllester and Catoni bounds is that they are both fully empirical. Then it is possible to minimise them in practice and thus, deriving new theory-driven learning algorithms which are expected to have at worse, a small generalisation gap and at best, a small population risk. More precisely, learning algorithms associated to Proposition 1.2.1 are stated below:

$$\mathrm{Q}_M := \operatorname*{argmin}_{\mathrm{Q}\in\mathcal{C}} \hat{\mathrm{R}}_{\mathcal{S}_m}(\mathrm{Q}) + \sqrt{\frac{\mathrm{KL}(\mathrm{Q},\mathrm{P})}{2m}}. \tag{1.7}$$

For any $\lambda > 0$,

$$\mathrm{Q}_C := \operatorname*{argmin}_{\mathrm{Q}\in\mathcal{C}} \hat{\mathrm{R}}_{\mathcal{S}_m}(\mathrm{Q}) + \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P})}{\lambda}. \tag{1.8}$$

In both cases, $\mathcal{C} \subseteq \mathcal{M}(\mathcal{H})$ is the class of distributions on which we optimise. The choice of $\mathcal{C}$ can come from a priori knowledge of the problem or from optimisation concerns to make the KL divergence tractable.

Knowing Catoni's bound is a relaxation of McAllester's one, it seems more natural to consider $\mathrm{Q}_M$ over $\mathrm{Q}_C$. However, the presence of a square root in (1.7) can be challenging for practical optimisation. We illustrate this below.

**Example 1.3.1** (A celebrated class of measures for PAC-Bayes algorithms)**.** Consider the case where, for a given $\sigma > 0$, $\mathcal{C} = \{\mathcal{N}(\mu, \sigma^2\mathrm{Id}) \mid \mu \in \mathbb{R}^d\}$. Then the for any $\mathrm{P} = \mathcal{N}(\mu_1, \sigma^2\mathrm{Id}), \mathrm{Q} = \mathcal{N}(\mu_2, \sigma^2\mathrm{Id})$, $\mathrm{KL}(\mathrm{Q}, \mathrm{P}) = \frac{\|\mu_1 - \mu_2\|^2}{2\sigma^2}$. Then, optimising (1.7) in this case implies to lose the strong convexity of the KL divergence while it is retained for (1.8).

Another practical advantage of (1.8) over (1.7) emerges when $\mathcal{C} = \mathcal{M}(\mathcal{H})$. In this case, Catoni's bound admits a closed form solution, while McAllester's one should be numerically optimised on all the space of distributions, which is not feasible. This closed form, extracted from Catoni (2003, Section 5.1), is recalled below.

$$\text{When } \mathcal{C} = \mathcal{M}(\mathcal{H}),\ d\mathrm{Q}_C(h) = \frac{\exp(-\lambda \hat{\mathrm{R}}_{\mathcal{S}_m}(h))}{\mathbb{E}_{h\sim \mathrm{P}}[\exp(-\lambda \hat{\mathrm{R}}_{\mathcal{S}_m}(h))]} d\mathrm{P}(h) \tag{1.9}$$

Then, $\mathrm{Q}_C = \mathrm{P}_{-\lambda \hat{\mathrm{R}}_{\mathcal{S}_m}}$ is the *Gibbs posterior* associated to $\mathrm{P}, \lambda \hat{\mathrm{R}}_{\mathcal{S}_m}$. By introducing Gibbs posterior in statistical learning, Catoni (2007) draws a theoretical link between statistical physics and learning theory. Unfortunately, Gibbs posteriors often require Monte Carlo methods to be implemented, which can be time-consuming. Below, we then focus on PAC-Bayes algorithms working on a subset $\mathcal{C}$ of $\mathcal{M}(\mathcal{H})$.

## Instantiation and efficiency of PAC-Bayesian algorithms

**A general pattern for PAC-Bayesian algorithms** The introductory examples (1.7),(1.8) unveil a general design for any KL-based PAC-Bayesian algorithm, satisfying a trade-off between *(i)* the empirical risk, showing that the learner has to fit the training dataset, and *(ii)* a *regulariser* being a function of $\mathrm{KL}(\mathrm{Q}, \mathrm{P})$. This regulariser ensures that, during training, the learner will not overfit on training data. This training ensures a good generalisation ability as long as the associated generalisation bound is small.
While the conceptual ins and outs of PAC-Bayes algorithms are getting clearer, two unanswered questions remains:

1. How are those algorithms instantiated in practice?
2. Are these algorithms efficient and do they come with non-vacuous theoretical guarantees?

**Instantiating a PAC-Bayes algorithm** In practice, using a single prior $\mathrm{P}$ usually does not work, but it remains theoretically possible to consider a finite set of priors. Indeed, if one wants to consider $k$ priors, then it is possible to consider $k$ PAC-Bayes bounds holding for each of those priors with probability at least $1-\frac{\delta}{k}$ and then consider a union bound, such a set of priors is called a grid. This method has been widely used in many PAC-Bayes work with clever grids, deteriorating initial bounds at the cost of supplementary $\log(n)$ or $\log\log(n)$ (divided by $m$), see *e.g.* Alquier (2024). This can also be used, for Catoni-typed algorithms, to the parameter $\lambda$. In both cases, considering grids allows to optimise on both the prior, the posterior (and possibly $\lambda$ when involved) and then taking the closest value of those optimised parameters on the grid to still obtain theoretical guarantees. Another technique to ensure a good prior is to sacrifice a part of the training set to pre-train $\mathrm{P}$. Doing so, the prior is then data-dependent and yields tighter bounds alongside increased performance (Perez-Ortiz *et al.*, 2021a,c).

**Efficiency of PAC-Bayes algorithms on supervised learning problems.** The work of Dziugaite and Roy (2017) showed that optimising (1.7) when $\mathcal{C}$ is a class of Gaussian measures for the weights of a deep neural network yields non-vacuous generalisation bound, meaning that the generalisation benefits of PAC-Bayesian training on deep nets can be theoretically ensured. Note that PAC-Bayesian bounds can also be used to quantify the generalisation ability of other learning algorithms, but the bound value is then suboptimal. Dziugaite and Roy (2017) used the toolbox described in the 'instantiation' paragraph, alongside a preliminary use of Stochastic Gradient Descent (SGD) to update $\mathrm{Q}$ before the PAC-Bayes training algorithm. This promising work paved the way to various extensions, providing non-vacuous guarantees for a wide range PAC-Bayes algorithms (Letarte *et al.*, 2019; Rivasplata *et al.*, 2019; Dziugaite *et al.*, 2021; Perez-Ortiz *et al.*, 2021a,b,c; Biggs and Guedj, 2022a, 2023), showing that the PAC-Bayes toolbox provides elements of answer to understand the generalisation ability of neural networks. Beyond generalisation guarantees, PAC-Bayes bounds are also useful to propose original training methods, even if the associated guarantees are vacuous (Biggs and Guedj, 2021, 2022b). Another important empirical use is to exploit PAC-Bayes bounds as correlation measures, to see whether a decrease of the bound is related to an increased generalisation ability of the learner. For instance Neyshabur *et al.* (2017) used McAllester's bound (1.3) as a 'flatness' measure and showed that it correlates well with a good generalisation ability for a few learning problems. This conclusion has been extended to a wider range of problems in Dziugaite *et al.* (2020) and Jiang *et al.* (2020).

**PAC-Bayes algorithms beyond supervised learning.** While supervised learning is a widely used to perform experiments in PAC-Bayes (often involving celebrated datasets

such as MNIST or CIFAR-10), the McAllester bound holds for any learning problem with bounded loss, going beyond this setting. This theoretical flexibility has been exploited to derive PAC-Bayesian algorithm for various learning settings reinforcement learning (Fard and Pineau, 2010), multi-armed bandits (Seldin *et al.*, 2011, 2012b; Sakhi *et al.*, 2023), meta-learning (Amit and Meir, 2018; Ding *et al.*, 2021; Farid and Majumdar, 2021; Rothfuss *et al.*, 2021, 2022) to name but a few.

**Is Example 1.1.1 tackled now?** (Dziugaite and Roy, 2017) and following works have provided a positive answer by obtaining non-vacuous guarantees (sometimes tight) for $(\mathcal{H}_2, \mathcal{Z}, \ell)$ of Example 1.1.1 for various $\mathcal{Z}$ (being, *e.g.*, set of images for MNIST CIFAR-10 etc...). To obtain such guarantees, a PAC-Bayesian training needs to be performed to minimise its associated theoretical bound. That being said, several questions then legitimately emerge.

- Modern machine learning often implies learning problems where assumptions such as bounded (or subgaussian) losses or *i.i.d.* data do not hold. Is PAC-Bayes theory extendable beyond those assumptions?
- As shown in Dziugaite and Roy (2017), the PAC-Bayesian training is often combined to another procedure (*e.g.* ERM) to yield non-vacuous bounds. However, PAC-Bayes bounds do not bring the theoretical understanding of such additional methods, often outputting deterministic predictors (*i.e.* Dirac distributions). This kind of predictor is not allowed in (1.3), (1.4). Is it possible to obtain PAC-Bayes bounds valid for such methods?

## 1.4 An optimisation perspective of PAC-Bayes

The questions raised at the end of the previous part are important as they underline a gap between the information-theoretic approach of PAC-Bayes bounds and practical optimisation. A supplementary example of this is the grid required in practice to optimise the prior (and/or $\lambda$ in Catoni's bound). Indeed this hybrid solution is required to roughly fit theory,(exploiting a single prior) and practice (optimising freely the prior on a continuous space), while not being truly adapted to any of these settings. This then raises the following fundamental question:

**Can we think PAC-Bayes learning from an optimisation perspective?**

The elements of answer to this question are multiple. First, one can mix PAC-Bayes argument with geometric properties of optimisation procedure to obtain generalisation bounds designed for specific algorithms exploiting their geometric properties and assumptions, including but not limited to, SGD, Langevin dynamics (London, 2017;

Dziugaite and Roy, 2018a; Neu *et al.*, 2021; Clerico *et al.*, 2022; Haghifam *et al.*, 2023; Zhou *et al.*, 2023). Those works shows both convergence properties as well as minimax rates, showing the impact of PAC-Bayes learning to provide a better theoretical understanding of the generalisation ability of concrete algorithms.
A second approach consists in describe general principles that should be satisfied by the various terms and assumptions in PAC-Bayes when looking at this through the prism of optimisation. We propose such an analysis below.

**An optimisation-driven view of PAC-Bayes**

- **Statistical assumptions.** While $\ell$ satisfies desirable geometric properties (convexity, gradient lipschitz ...), no statistical assumption is needed to have optimisation algorithms with convergence properties, on then may wonder about the generalisation abilities of the reached empirical minima. It happens that the output of two runs of a stochastic optimisation algorithm on the same training set may vary a lot, for instance, the specific case of SGD shows that heavy-tailed behaviour (see *e.g.* Şimşekli *et al.*, 2019; Zhang *et al.*, 2020; Gürbüzbalaban *et al.*, 2021) may emerge in practice. Given such behaviours, generalisation bounds, from an optimisation point of view, should hold with weak statistical assumptions on the dataset, possibly at the cost of additional geometric assumptions on the loss.

- **The role of the prior.** The information-theoretic approach justifies the Bayesian view of the prior, as discussed earlier. In this spirit it is also possible to sacrifice a part of the training set (*i.e.* of the available information) to enrich $\mathrm{P}$. Doing so, we accept to not understand what happens during the training of $\mathrm{P}$ and thus, to explain partially the efficiency of an information-theoretic training. Those two visions (Bayesian prior or data-dependent prior) are not easily linked to optimisation concerns as the first one would be linked to a 'good' initialisation, something we cannot know in advance, while the second makes little sense as $\mathrm{P}$ is obtained through a first, unexplained, optimisation process which is necessary to understand the efficiency of the second part of training, outputting $\mathrm{Q}$. From an optimisation stance, we suggest to assign only two possible roles to $\mathrm{P}$: *(i)* the initialisation of the optimisation algorithm, then its impact should be attenuated through the learning process and *(ii)* a minimiser we aim to reach through optimisation. In this case, its impact is crucial as it translates the speed of convergence of our learning algorithms.

- **The place of stochastic predictors.** Involving a KL divergence as a complexity brings a particular focus on stochastic predictors, drawn from a distribution $\mathrm{Q}$. Classical PAC-Bayes bounds usually focus on the average performance of such a predictor (hence the expectation over $\mathrm{Q}$ in (1.3),(1.4)), but recent extensions

directly proposed guarantees for a single draw over $\mathrm{Q}$ (Rivasplata *et al.*, 2020; Viallard *et al.*, 2023a). However, involving a KL implies that $\mathrm{Q}$ has to be absolutely continuous *w.r.t.* $\mathrm{P}$, meaning that the support of $\mathrm{Q}$ cannot go beyond the one of $\mathrm{P}$: this excludes the case of Dirac distributions, *i.e.* deterministic predictors. This is a clear limitation of the information-theoretic approach, as many learning algorithms outputs a deterministic predictor and thus, should be avoided to be in line with common practice in optimisation.

Those three points, while not necessarily considered explicitly through the lens of optimisation have been recently challenged.

### PAC-Bayes beyond the usual setting

Recall that according to what we saw in McAllester's bound (1.3) and Catoni's one (1.4), we denote by usual setting a bound holding for *i.i.d.* $\mathcal{S}_m$, with bounded or subgaussian losses and involving a KL divergence as Complexity term. Many works overcame at least one of this assumption as precised below.

**Beyond *i.i.d.* data** The work of Fard and Pineau (2010) established links between reinforcement learning and PAC-Bayes theory. This naturally led to the study of PAC-Bayesian bound for martingales instead of *i.i.d.* data (Seldin *et al.*, 2011, 2012a,b). Also, PAC-Bayesian bound for lifelong learning (Pentina and Lampert, 2014; Flynn *et al.*, 2022) challenged also the *i.i.d.* assumption. We also denote that the PAC-Bayes bound for meta learning (Amit and Meir, 2018; Ding *et al.*, 2021; Farid and Majumdar, 2021; Rothfuss *et al.*, 2021, 2022) consider independent but non-identically distributed datasets (corresponding to different tasks).

**Avoiding light-tailed losses.** Light-tailed losses encompass bounded, subgaussian, subexponential losses. Deriving PAC-Bayes bound for heavy-tailed losses, starting from Audibert and Catoni (2011) which provided PAC-Bayes bounds for least square estimators with heavy-tailed random variables. Their results was suboptimal with respect to the intrinsic dimension and was followed by further works from Catoni (2016) and Catoni and Giulini (2017). More recently, this question has been addressed in the works of Alquier and Guedj (2018), Holland (2019), Kuzborskij and Szepesvári (2019), and Haddouche *et al.* (2021), extending PAC-Bayes to heavy-tailed losses under additional technical assumptions.

**Towards data-dependent priors.** The work of (Catoni, 2007; Lever *et al.*, 2010, 2013) proposed priors, not directly data-dependent, but depending of the data distribution $\mathcal{D}$ when *i.i.d.* data are considered. can be informed by the data-generating distribution, Parrado-Hernández *et al.* (2012), Oneto *et al.* (2016), Dziugaite

and Roy (2017), and Mhammedi *et al.* (2019) also obtained PAC-Bayes bound with data-dependent priors by infusing directly data in the prior (and sacrificing a part of the dataset). The drawback of this method is that, in practice, such a prior allows tighter bounds, but at the cost of a reduced theoretical understanding as the prior is in practice often learned via ERM, and the PAC-Bayes bound hardly gives insights on what happens during this pre-training. Furthermore, if this pre-training has already made the bound converge to a minimum generalising well, then the PAC-Bayes training has no effect and the associated bound is no more than a test bound (the case $\mathrm{Q} = \mathrm{P}$). It has been shown for instance in (Perez-Ortiz *et al.*, 2021a) that when $\mathrm{P}$ is trained with a consequent fraction of data, then the generalisation performance of the pre-trained $\mathrm{P}$ was roughly the same than $\mathrm{Q}$, obtained from $\mathrm{P}$ after a PAC-Bayesian training. It is then unclear how impacting are PAC-Bayes methods compared to a test bound in this case. To alleviate this issue, another original route (Dziugaite and Roy, 2018b) exploits differential privacy to replace the data-free prior by a differentially private one, making possible to consider the prior as the learning objective (in their case a Gibbs posterior).

**Beyond KL divergence.** Several works allowed to extend PAC-Bayes beyond KL divergences. The most investigated route is to focus on the more general class of $f$-divergence, which include, *e.g.*, KL, $\chi^2$, Rényi divergences among others (Alquier and Guedj, 2018; Ohnishi and Honorio, 2021; Picard-Weibel and Guedj, 2022; Viallard *et al.*, 2023a). However, $f$-divergences still implies absolute continuity of $\mathrm{Q}$ *w.r.t.* $\mathrm{P}$. Another route recently emerged (Amit *et al.*, 2022), replacing $f$-divergences by integral probability metrics (IPMs), finally allowing Dirac distribution in PAC-Bayes.
These works have sometimes been explicitly driven by optimisation considerations (Dziugaite and Roy, 2018b involved differential privacy to numerically tighten their bound without sacrificing data). However, in many cases, the information-theoretic vision of PAC-Bayes remained majoritary. In what follows, the contributions of this manuscript are designed *w.r.t.* the optimisation view of PAC-Bayes detailed above.

### Contributions of this thesis

The contributions of this manuscript are motivated by optimisation considerations and are structured as follows:

- In Chapter 2, we propose novel PAC-Bayes bounds for martingales, batch learning, with an application to multi-armed bandits. Those bounds are anytime-valid (*i.e.* for any dataset size simultaneously) and holds at the sole assumption of finite order 2 moments on both the posterior and the data distribution. Such weak statistical assumptions make these results applicable, for instance, for

heavy-tailed SGD or many learning problems where optimisation procedure are performed regardless of the training set noise.

- Chapter 3 introduces *Online PAC-Bayes learning*, proposing theoretical bounds and learning algorithms involving a sequence of pairs $(\mathrm{Q}_i, \mathrm{P}_i)$, evolving through the optimisation process. Contrary to PAC-Bayes in a batch setting, the impact of $\mathrm{P} = \mathrm{P}_1$ is attenuated during the learning process, making Online PAC-Bayes useful when there is no prior information available, which is consistent with the vision of $\mathrm{P}$ as initialisation of a learning algorithm, while being only applicable, for now, to stochastic predictors as a KL divergence is involved.

- Chapter 4 still consider the prior as an initialisation point, but this time, considering batch learning algorithms. It is shown that the impact of the prior is attenuated by *flat minima*, *i.e.* minima such that their neighbourhood nearly minimises the loss. More generally, this chapter exhibits theoretical links between flat minima and generalisation and thus draw links between the benefits of a successful optimisation process (small gradients) and generalisation.

- Considering $\mathrm{P}$ as the learning objective allows to draw more explicit links between optimisation and generalisation. In Chapter 5, it is shown that the convergence guarantees of *Bures-Wasserstein SGD*, a SGD-like algorithm on Gaussian measure spaces, can be directly incorporated within PAC-Bayes bounds, yielding interpretable results. This is possible by exploiting *Wasserstein PAC-Bayes learning*, which uses as $\textsc{Complexity}$ term a 1-Wasserstein distance, allowing to trade statistical assumptions to geometric ones such as lipschtz or gradient-lipschitz losses.

- Wasserstein PAC-Bayes learning can also be exploited when $\mathrm{P}$ is seen as an initialisation point. In Chapter 6, we propose Wasserstein PAC-Bayes algorithms with associated theoretical bound for both batch and online learning. A notable strength of these methods is that they hold for deterministic predictors (Dirac distributions), making PAC-Bayes in line with a large part of optimisation algorithms.

To conclude this introduction we recap in Figures 1.1 and 1.2 the classical information-theoretic vision of PAC-Bayes alongside the original optimisation view proposed above.

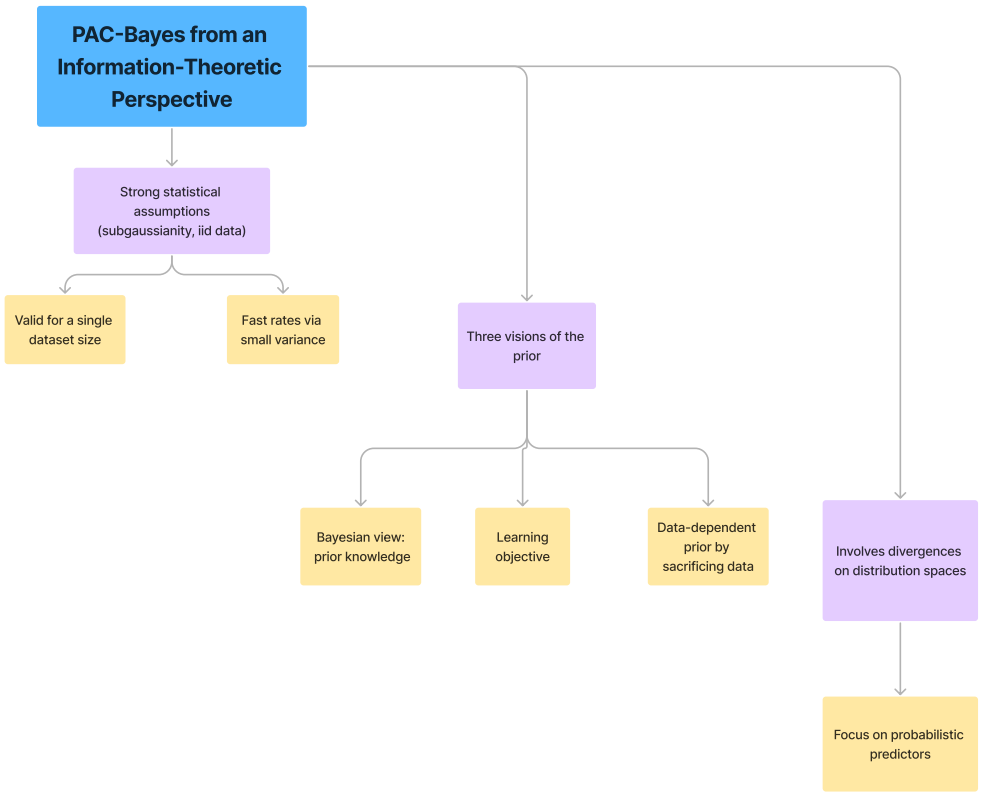


***Figure 1.1.*** *Recap of the information-theoretic vision of PAC-Bayes.*

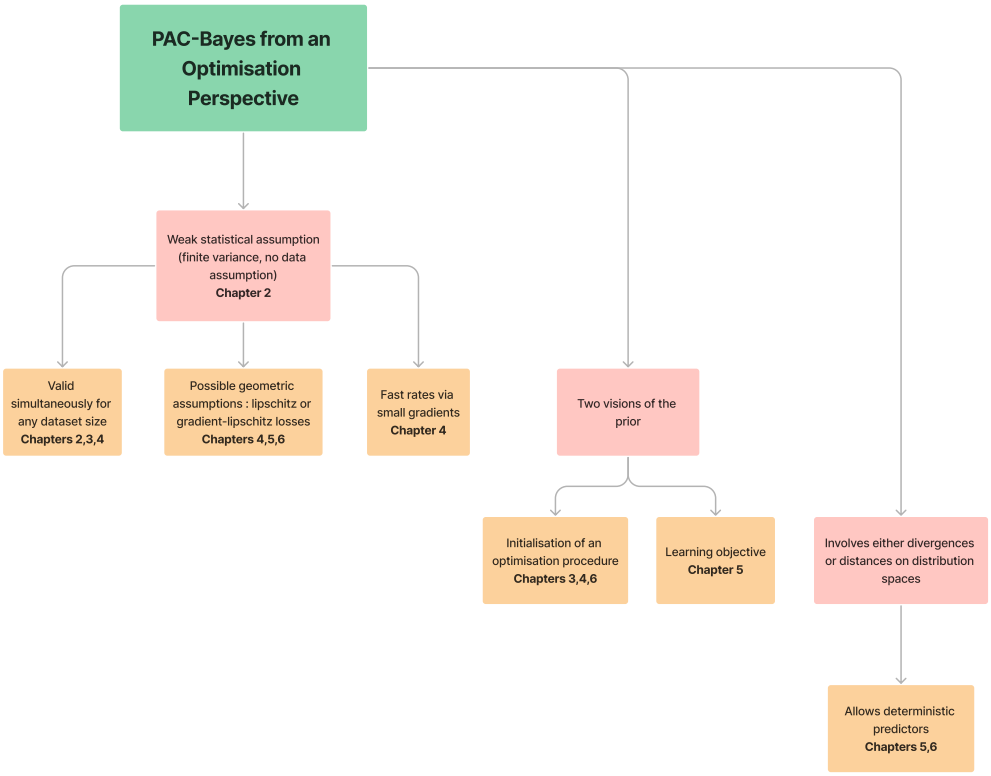


***Figure 1.2.*** *Recap of the optimisation vision of PAC-Bayes and where those views are exploited in the manuscript.*

# 2

# PAC-Bayes with Weak Statistical Assumptions: Generalisation Bounds for Martingales and Heavy-Tailed losses

**This chapter is based on the following paper**

Maxime Haddouche and Benjamin Guedj. PAC-Bayes Generalisation Bounds for Heavy-Tailed Losses through Supermartingales. *Transactions on Machine Learning Research*. (2023)

## Contents




**Abstract**

Chapter 2 provide PAC-Bayes bounds holding with weak statistical assumptions (finite variance), this is promising to encompass various learning situations involving optimisation algorithms such as heavy-tailed SGD (Gürbüzbalaban *et al.*, 2021) where assumptions such as bounded or subgaussian losses do not hold. Furthermore those results go beyond *i.i.d.* assumption on $\mathcal{S}$ and holds for all datasets $(\mathcal{S}_m)_{m\geq 1}$ simultaneously. Such a flexible setting is in line with various optimisation frameworks, where new data can be available after the beginning of the learning process and be incorporated on-the-fly to the ongoing

training, regardless of their potential correlation with previous data. Then, the theoretical results proposed in this chapter are a promising step toward practical settings where data may exhibit heavy-tailed behaviours and the loss function to be unbounded.

## 2.1 Introduction

In Chapter 1, McAllester's and Catoni's bound (McAllester, 2003; Catoni, 2007) have been presented as key theoretical results with practical repercussions through their associated learning algorithm. However, the bounded or subgaussian assumption on the loss makes those results limited to tackle many real-life situations, which are limiting in practice. Indeed, from an optimisation perspective, as stated in Section 1.4 of Chapter 1, generalisation bounds should hold with weak statistical assumptions to make PAC-Bayes general enough to be used for learning settings where data are potentially heavy-tailed. Several works already proposed routes to overcome the boundedness constraint: Catoni (2004, Chapter 5) already proposed PAC-Bayes bounds for classification tasks and regressions ones with quadratic loss under a subexponential assumption. This technique has later been exploited in Alquier and Biau (2013) for the single-index model, and by Guedj and Alquier (2013) for nonparametric sparse additive regression, both under the assumption that the noise is subexponential. However all these works are dealing with light-tailed losses. Alquier and Guedj (2018), Holland (2019), Kuzborskij and Szepesvári (2019), and Haddouche *et al.* (2021) proposed extensions beyond light-tailed losses. This chapter stands in the continuation of this spirit while developing and exploiting a novel technical toolbox. To better highlight the novelty of our approach, we first present the two classical building blocks of PAC-Bayes.

### 2.1.1 Understanding PAC-Bayes: a celebrated route of proof

In the following subsection, we exploit again, for the sake of pedagagogy, the general pattern of proof for PAC-Bayes bounds described in Equation (1.4) to prove Catoni's bound.

#### 2.1.1.1 Two essential building blocks for a preliminary bound

For the rest of this section, similarly to Chapter 1, we assume access to a non-negative loss function $\ell(h, z)$ taking as argument a predictor $h \in \mathcal{H}$ and data $z \in \mathcal{Z}$ (think of $z$ as a pair input-output $(x, y)$ for supervised learning problems, or as a single datum $x$ in unsupervised learning). We also assume access to a $m$-sized sample $\mathcal{S}_m = (z_1, ..., z_m) \in \mathcal{Z}^m$. $\mathcal{S}_m$ is then used to learn a posterior distribution $\mathrm{Q}$ on $\mathcal{H}$, from a prior $\mathrm{P}$.

PAC-Bayesian proofs are built upon two cornerstones. The first one is the change of measure inequality, recalled in Lemma 1.2.1. This property is applied to a certain function $f_m : \mathcal{Z}^m \times \mathcal{H} \to \mathbb{R}$ of the data and a candidate predictor: for all posteriors $\mathrm{Q}$,

$$\mathbb{E}_{h\sim\mathrm{Q}}[f_m(\mathcal{S}_m, h)] \leq \mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log\left(\mathbb{E}_{h\sim\mathrm{P}}[\exp(f_m(\mathcal{S}_m, h))]\right). \tag{2.1}$$

To deal with the random variable $X(\mathcal{S}_m) := \mathbb{E}_{h\sim\mathrm{P}}[\exp(f_m(\mathcal{S}_m, h))]$, our second building block is Markov's inequality $\left(\mathbb{P}(X > a) \leq \frac{\mathbb{E}[X]}{a}\right)$ which we apply for a fixed $\delta \in (0, 1)$ on $X(\mathcal{S}_m)$ with $a = \mathbb{E}_{\mathcal{S}_m}[X(\mathcal{S}_m)]/\delta$. Taking the complementary event gives that for any $m$, with probability at least $1-\delta$ over the sample $\mathcal{S}_m$, $X(\mathcal{S}_m) \leq \mathbb{E}_{\mathcal{S}_m}[X(\mathcal{S}_m)]/\delta$, thus:

$$\mathbb{E}_{h\sim\mathrm{Q}}[f_m(\mathcal{S}_m, h)] \leq \mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(1/\delta) + \log\left(\mathbb{E}_{h\sim\mathrm{P}}\mathbb{E}_{\mathcal{S}_m}[\exp(f_m(\mathcal{S}_m, h))]\right). \tag{2.2}$$

#### 2.1.1.2 From preliminary to complete bounds

From the preliminary result of Equation (2.2), there exists several ways to obtain PAC-Bayesian generalisation bounds, all being tied to specific choices of $f$ and the assumptions on the dataset $\mathcal{S}_m$. However, they all rely on the control of an exponential moment implied by Markov's inequality: this is a strong constraint which has been at the heart of the classical assumption appearing in PAC-Bayes learning. For instance, McAllester's bound (1.3) and Catoni's bound (1.4), exploits in particular, a data-free prior, an *i.i.d.* assumption on $\mathcal{S}_m$ and a light-tailed loss. Most of the existing results stand with those assumptions (see *e.g.*, Catoni, 2007; Germain *et al.*, 2009; Guedj and Alquier, 2013; Tolstikhin and Seldin, 2013; Guedj and Robbiano, 2018; Mhammedi *et al.*, 2019; Wu and Seldin, 2022). Indeed, in many of these works, either a boundedness or a subgaussian assumption on the loss is used. Catoni (2004) extended PAC-Bayes learning to the subexponential case. Many works tried to mitigate at least one of the following three assumptions.

- **Data-free priors.** With an alternative set of techniques, Catoni (2007) obtained bounds with localised (*i.e.*, data-dependent) priors. More recently, Lever *et al.* (2010), Parrado-Hernández *et al.* (2012), Lever *et al.* (2013), Oneto *et al.* (2016), Dziugaite and Roy (2017), and Mhammedi *et al.* (2019) also obtained PAC-Bayes bound with data-dependent priors.
- **The *i.i.d.* assumption on $\mathcal{S}_m$.** The work of Fard and Pineau (2010) established links between reinforcement learning and PAC-Bayes theory. This naturally led to the study of PAC-Bayesian bound for martingales instead of iid data (Seldin *et al.*, 2011, 2012a,b).

- **Light-tailed loss.** PAC-Bayes bounds for heavy-tailed losses (*i.e.*, without subgaussian or subexponential assumptions) have been studied. Audibert and Catoni (2011) provide PAC-Bayes bounds for least square estimators with heavy-tailed random variables. Their results was suboptimal with respect to the intrinsic dimension and was followed by further works from Catoni (2016). More recently, this question has been adressed in the works of Alquier and Guedj (2018), Holland (2019), Kuzborskij and Szepesvári (2019), and Haddouche *et al.* (2021), extending PAC-Bayes to heavy-tailed losses under additional technical assumptions.

Several questions then legitimately arise.

**Can we avoid these three assumptions simultaneously?** The answer is yes: for instance the work of Rivasplata *et al.* (2020) proposed a preliminary PAC-Bayes bound holding with none of the three assumptions listed above. Building on their theorem, Haddouche and Guedj (2022) only exploited a bounded loss assumption to derive a PAC-Bayesian framework for online learning, requiring no assumption on data and allowing data (history in their context)-dependent priors.

**Can we obtain PAC-Bayes bounds without the change of measure inequality?** Yes, for instance Alquier and Guedj (2018) proposed PAC-Bayes bounds involving $f$-divergences and exploiting Holder's inequality instead of Lemma 1.2.1. More recently, Ohnishi and Honorio (2021) and Picard-Weibel and Guedj (2022) developed a broader discussion about generalising the change of measure inequality for a wide range of $f$-divergences. We note also that Germain *et al.* (2009) proposed a version of the classical route of proof stated above avoiding the use of the change of measure inequality. This comes at the cost of additional technical assumptions (see Haddouche *et al.*, 2021, Theorem 1 for a statement of the theorem in a proper measure-theoretic framework).

**Can we avoid Markov's inequality?** We mentioned above that several works avoided the change of measure inequality to obtain PAC-Bayesian bounds, but can we do the same with Markov's inequality? This is of interest as avoiding Markov could avoid assumptions such as subgaussiannity to provide PAC-Bayes bound. The answer is yes but this is a rare breed. To the best of our knowledge, only two papers are explicitly not using Markov's inequality: Kakade *et al.* (2008) obtained a PAC-Bayes bound using results on Rademacher complexity based on the McDiarmid concentration inequality, and Kuzborskij and Szepesvári (2019) exploited a concentration inequality from De la Peña *et al.* (2009), up to a technical assumption to obtain results for unbounded losses. Both of those works do not require a bound on an exponential moment to hold.

### 2.1.2 Originality of our approach

Avoiding Markov's inequality appears challenging in PAC-Bayes but leads to fruitful results as those in Kuzborskij and Szepesvári (2019).
In this work, we exploit a generalisation of Markov's inequality for supermartingales: Ville's inequality (as noticed by Doob 1939). This result has, to our knowledge, never been used in PAC-Bayes before.

**Lemma 2.1.1** (Ville's maximal inequality for supermartingales)**.** Let $(\mathcal{F}_t)$ be a filtration adapted to $(Z_t)$, a non-negative super-martingale with $Z_0 = 1$ almost surely, *i.e.* $(Z_t)_{t\geq 1}$ is a discrete process such that for any $t \in \mathbb{N}$, $\mathbb{E}\left[Z_t \mid \mathcal{F}_{t-1}\right] \leq Z_{t-1}$ a.s., $t \geq 1$, then, for any $0 < \delta < 1$, it holds

$$\mathbb{P}\left(\exists T \geq 1 : Z_T > \delta^{-1}\right) \leq \delta.$$

*Proof.* We apply the optional stopping theorem (Durrett, 2019, Thm 4.8.4) with Markov's inequality defining the stopping time $i = \inf\{t > 1 : \ Z_t > \delta^{-1}\}$ so that

$$\mathbb{P}\left(\exists t \geq 1 : Z_t > \delta^{-1}\right) = \mathbb{P}\left(Z_i > \delta^{-1}\right) \leq \mathbb{E}\left[Z_i\right]\delta \leq \mathbb{E}\left[Z_0\right]\delta \leq \delta.$$

■

A major interest of Ville's result is that it holds for a countable sequence of random variables simultaneously. This point is new in PAC-Bayes and will allow us to obtain bounds holding for a countable (not necessarily finite) dataset $\mathcal{S}$.

**On which supermartingale do we apply Ville's bound ?** To fully exploit Lemma 2.1.1, we now take a countable dataset $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1} \in \mathcal{Z}^{\mathbb{N}}$. Recall that, because we use the change of measure inequality, we have to deal with the following exponential random variable appearing in Eq. (2.1) for any $m \geq 1$:

$$Z_m := \mathbb{E}_{h\sim \mathrm{P}}[\exp(f_m(\mathcal{S}, h))].$$

Our goal is to choose a sequence of functions $f_m : \mathcal{Z}^{\mathbb{N}} \times \mathcal{H} \to \mathbb{R}$ such that $(Z_m)_{m\geq 1}$ is a supermartingale. A way to do so comes from Bercu and Touati (2008).

**Lemma 2.1.2** (Towards the design of a supermartingale)**.** Let $(M_m)$ be a locally square-integrable martingale with respect to the filtration $(\mathcal{F}_m)$. For all $\eta \in \mathbb{R}$ and $m \geq 0$, one has:

$$\mathbb{E}\left[\exp\left(\eta\Delta M_m - \frac{\eta^2}{2}\left(\Delta[M]_m + \Delta\langle M\rangle_m\right)\right) \mid \mathcal{F}_{m-1}\right] \leq 1,$$

where $\Delta M_m = M_m - M_{m-1}, \Delta[M]_m = \Delta M_m^2$ and $\Delta\langle M\rangle_m = \mathbb{E}\left[\Delta M_m^2 \mid \mathcal{F}_{m-1}\right]$. We define $V_m(\eta) = \exp\left(\eta M_m - \frac{\eta^2}{2}\left([M]_m + \langle M\rangle_m\right)\right)$. Then, for all $\eta \in \mathbb{R}, (V_m(\eta))$ is a positive supermartingale with $\mathbb{E}\left[V_m(\eta)\right] \leq 1$ where $[M]_m(h) := \sum_{i=1}^m \Delta[M]_m, \langle M\rangle_m(h) := \sum_{i=1}^m \Delta\langle M\rangle_m$.

In the sequel, this lemma will be helpful to design a supermartingale (*i.e.*, to choose a relevant $f_m$ for any $m$) without further assumption.

### 2.1.3 Contributions and outline

By avoiding Markov, a key message of (Kuzborskij and Szepesvári, 2019) is that, for learning problems with independent data, PAC-Bayes learning only requires the control of order 2 moment on losses to be used with convergence guarantees. This is strictly less restrictive than the classical subgaussian/subgamma assumptions appearing in the major part of the literature.
We successfully prove this fact remains even for non-independent data: we only need to control order 2 (conditional) moments to perform PAC-Bayes learning. We focus in this chapter on the PAC-Bayesian framework for martingales (Seldin *et al.*, 2011, 2012a,b). We then provide a novel PAC-Bayesian bound holding for data-free priors and unbounded martingales. From this, we recover in PAC-Bayes bounds for unbounded losses and iid data as a significant particular case. We also propose an extension of Seldin *et al.* (2012a)'s result for multi-armed bandits.
More precisely, Section 2.2.1 contains our novel PAC-Bayes bound for unbounded martingales and Section 2.2.3 contains an immediate corollary for learning theory with iid data. We eventually apply our main result for martingales in Section 2.3 to the setting of multi-armed bandit. Doing so, we provably extend a result of Seldin *et al.* (2012a) to the case of unbounded rewards.
Appendix C.1 gathers more details on PAC-Bayes, we draw in Appendix C.2 a detailed comparison between our new results and a few classical ones. We show that adapting our bounds to the assumptions made in those papers allows to recover similar or improved bounds. We defer to Appendix C.3 the proofs of Sections 2.2.3 and 2.3.

## 2.2 A PAC-Bayesian bound for unbounded martingales

### 2.2.1 Main result

A line of work led by Seldin *et al.* (2011, 2012a,b) provided PAC-Bayes bounds for almost surely bounded martingales. We provably extend the remits of their result to

the case of unbounded martingales.

**Framework** Our framework is close to the one of SELDIN *et al.*, 2012a: we assume having access to a countable dataset $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1} \in$ with no restriction on the distribution of $\mathcal{S}$ (in particular the $\mathbf{z}_i$ can depend on each others). We denote for any $m$, $\mathcal{S}_m := (\mathbf{z}_i)_{i=1..m}$ the restriction of $\mathcal{S}$ to its $m$ first points. $(\mathcal{F}_i)_{i\geq 0}$ is a filtration adapted to $\mathcal{S}$. We denote for any $i \in \mathbb{N}$ $\mathbb{E}_{i-1}[.] := \mathbb{E}[. \mid \mathcal{F}_{i-1}]$. We also precise the space $\mathcal{H}$ to be an index (or a hypothesis) space, possibly uncountably infinite. Let $\{X_1(\mathcal{S}_1, h), X_2(\mathcal{S}_2, h), \cdots : h \in \mathcal{H}\}$ be martingale difference sequences, meaning that for any $m \geq 1, h \in \mathcal{H}$, $\mathbb{E}_{m-1}\left[X_m(\mathcal{S}_m, h)\right] = 0$.
For any $h \in \mathcal{H}$, let $M_m(h) = \sum_{i=1}^m X_i(S_i, h)$ be martingales corresponding to the martingale difference sequences and we define, as in BERCU and TOUATI (2008), the following

$$[M]_m(h) := \sum_{i=1}^m X_i(\mathcal{S}_i, h)^2,$$

$$\langle M\rangle_m(h) = \sum_{i=1}^m \mathbb{E}_{i-1}\left[X_i(\mathcal{S}_i, h)^2\right].$$

For a distribution $\mathrm{Q}$ over $\mathcal{H}$ define weighted averages of the martingales with respect to $\mathrm{Q}$ as $M_m(\mathrm{Q}) = \mathbb{E}_{h\sim\mathrm{Q}}\left[M_m(h)\right]$ (similar definitions hold for $[M]_m(\mathrm{Q}), \langle M\rangle_m(\mathrm{Q})$).
**Main result.** We now present the main result of this section where we succesfully avoid the boundedness assumption on martingales. This relaxation comes at the cost of additional variance terms $[M]_m, \langle M\rangle_m$.

**Theorem 2.2.1** (A PAC-Bayesian bound for unbounded martingales)**.** For any data-free prior $\mathrm{P} \in \mathcal{M}(\mathcal{H})$, any $\lambda > 0$, any collection of martingales $(M_m(h))_{m\geq 1}$ indexed by $h \in \mathcal{H}$, the following holds with probability $1-\delta$ over the sample $\mathcal{S} = (\mathbf{z}_i)_{i\in\mathbb{N}}$, for all $m \in \mathbb{N}/\{0\}$, $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$:

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(2/\delta)}{\lambda} + \frac{\lambda}{2}\left([M]_m(\mathrm{Q}) + \langle M\rangle_m(\mathrm{Q})\right).$$

Proof lies in Section 2.2.2.
**Analysis of the bound.** This theorem involves several terms. The change of measure inequality introduces the KL divergence term, the approximation term $\log(2/\delta)$ comes from Ville's inequality (instead of Markov in classical PAC-Bayes). Finally, the terms $[M]_m(\mathrm{Q}), \langle M\rangle_m(\mathrm{Q})$ come from our choice of supermartingale as suggested by BERCU and TOUATI (2008). The term $[M]_m(\mathrm{Q})$ can be interpreted as an empirical variance term while $\langle M\rangle_m(\mathrm{Q})$ is its theoretical counterpart. Note that $\langle M\rangle_m(\mathrm{Q})$ also appears in SELDIN *et al.* (2012a, Theorem 1).

We recall that this general result stands with no assumption on the martingale difference sequence $(X_i)_{i\geq 1}$ and holds uniformly on all $m \geq 1$. Those two points are, to the best of our knowledge, new within the PAC-Bayes literature. We discuss in Section 2.2.3 and appendix C.2 more concrete instantiations.

**Comparison with literature.** The closest result from Th. 2.2.1 is the PAC-Bayes Bernstein inequality of SELDIN *et al.*, 2012a. Our bound is a natural extension of theirs as their result only involves the variance term (not the empirical one), but requires two additional assumptions:

1. Bounded variations of the martingale difference sequence: $\forall m, \exists C_m \in \mathbb{R}^2$ such that a.s. for all $h$ $|X_m(\mathcal{S}_m, h)| \leq C_m$.
2. Restriction on the range of the $\lambda$: $\forall m, \lambda_m \leq 1/C_m$.

SELDIN *et al.* (2012a) need those assumptions to ensure the *Bernstein assumption* which states that for any $h$, $\mathbb{E}[\exp(\lambda M_m(h) - \frac{\lambda^2}{2}\langle M\rangle_m(h))] \leq 1$. Our proof technique do not require the Bernstein assumption (and so none of the two conditions described above, which allow us to deal with unbounded martingales) as we exploit the supermartingale structure to obtain our results. More precisely, the price to pay to avoid the Bernstein assumption is to consider the empirical variance term $[M]_m(h)$ and to prove that $\left(\exp\left(\lambda M_m - \frac{\lambda^2}{2}\left([M]_m + \langle M\rangle_m\right)\right)\right)_{m\geq 1}$ is a supermartingale using Lemma 2.1.1 and Lemma 2.1.2 (see Section 2.2.2 for the complete proof). A broader discussion is detailed in appendix C.2.

## 2.2.2 Proof of Theorem 2.2.1

*Proof of Theorem 2.2.1.* We fix $\eta \in \mathbb{R}$ and we consider the function $f_m$ to be for all $(\mathcal{S}, h)$:

$$\begin{aligned} f_m(\mathcal{S}, h) &:= \eta M_m(h) - \frac{\eta^2}{2}\left([M]_m(h) + \langle M\rangle_m(h)\right) \\ &= \sum_{i=1}^{m} \eta \Delta M_i(h) - \frac{\eta^2}{2}(\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)), \end{aligned}$$

where $\Delta M_i(h) = X_i(\mathcal{S}_i, h), \quad \Delta[M]_i(h) = X_i(\mathcal{S}_i, h)^2, \quad \Delta\langle M\rangle_i(h) = \mathbb{E}_{i-1}\left[X_i(\mathcal{S}_i, h)^2\right]$.
For the sake of clarity, we dropped the dependency in $\mathcal{S}$ of $M_m$. Note that, given the definition of $M_m$, $M_m(h)$ is $\mathcal{F}_m$ measurable for any fixed $h$.
Let $\mathrm{P}$ a fixed data-free prior, we first apply the change of measure inequality to

obtain $\forall m \in \mathbb{N}, \forall \mathrm{Q} \in \mathcal{M}(\mathcal{H})$:

$$\mathbb{E}_{h\sim\mathrm{Q}}[f_m(\mathcal{S},h)] \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log\left(\underbrace{\mathbb{E}_{h\sim\mathrm{P}}\left[\exp(f_m(\mathcal{S},h))\right]}_{:=Z_m}\right),$$

with the convention $f_0 = 0$. We now have to show that $(Z_m)_m$ is a supermartingale with $Z_0 = 1$. To do so remark that for any $m$, because $\mathrm{P}$ is data free one has the following result.

**Lemma 2.2.1.** For any data-free prior $\mathrm{P}$, any $\sigma$-algebra $\mathcal{F}$ belonging to the filtration $(\mathcal{F}_i)_{i\geq 0}$, any nonnegative function $f$ taking as argument the sample $\mathcal{S}$ and a predictor $h$, one has almost surely:

$$\mathbb{E}\left[\mathbb{E}_{h\sim\mathrm{P}}[f(\mathcal{S},h)] \mid \mathcal{F}\right] = \mathbb{E}_{h\sim\mathrm{P}}\left[\mathbb{E}[f(\mathcal{S},h) \mid \mathcal{F}]\right].$$

*Proof of Lemma 2.2.1.* Let $A$ be a $\mathcal{F}$-measurable event. We want to show that

$$\mathbb{E}\left[\mathbb{E}_{h\sim \mathrm{P}}[f(\mathcal{S},h)]\mathbb{1}_A\right] = \mathbb{E}\left[\mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}[f(\mathcal{S},h)\mid \mathcal{F}]\right]\mathbb{1}_A\right],$$

where the first expectation in each term is taken over $\mathcal{S}$. Note that it is possible to take this expectation thanks to the Kolomogorov's extension theorem (see *e.g.* Tao, 2011, Thm 2.4.4) which ensure the existence of a probability space for the discrete-time stochastic process $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1}$.
Thus, this is enough to conclude that

$$\mathbb{E}\left[\mathbb{E}_{h\sim \mathrm{P}}[f(\mathcal{S},h)] \mid \mathcal{F}\right] = \mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}[f(\mathcal{S},h)\mid \mathcal{F}]\right],$$

by definition of the conditional expectation. To do so, notice that because $f(\mathcal{S},h)\mathbb{1}_A$ is a nonnegative function, and that $\mathrm{P}$ is data-free, we can apply the classical Fubini-Tonelli theorem.

$$\mathbb{E}\left[\mathbb{E}_{h\sim \mathrm{P}}[f(\mathcal{S},h)]\mathbb{1}_A\right] = \mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}\left[f(\mathcal{S},h)\mathbb{1}_A\right]\right].$$

One now conditions by $\mathcal{F}$ and use the fact that $\mathbb{1}_A$ is $\mathcal{F}$-measurable:

$$= \mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}\left[\mathbb{E}\left[f(\mathcal{S},h)\mid \mathcal{F}\right]\mathbb{1}_A\right]\right].$$

We finally re-apply Fubini-Tonelli to re-intervert the expectations:

$$= \mathbb{E}\left[\mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}\left[f(\mathcal{S},h)\mid \mathcal{F}\right]\mathbb{1}_A\right]\right].$$

This concludes the proof of Lemma 2.2.1. ■

We then use Lemma 2.2.1 with $f = \exp(f_m)$ and $\mathcal{F} = \mathcal{F}_{m-1}$ to obtain:

$$\begin{aligned}\mathbb{E}_{m-1}[Z_m] &= \mathbb{E}_{h\sim \mathrm{P}}\left[\mathbb{E}_{m-1}[(\exp(f_m(\mathcal{S},h))]\right] \\ &= \mathbb{E}_{h\sim \mathrm{P}}\left[\exp(f_{m-1}(\mathcal{S},h))\mathbb{E}_{m-1}\left[\exp(\eta\Delta M_m(h) - \frac{\eta^2}{2}(\Delta[M]_m(h) + \Delta\langle M\rangle_m(h))\right]\right],\end{aligned}$$

with $f_{m-1}(\mathcal{S},h) = \sum_{i=1}^{m-1}\eta(\Delta M_i(h)) - \frac{\eta^2}{2}(\Delta[M]_i(h) + \Delta\langle M\rangle_i(h))$. Using Lemma 2.1.2 ensures that for any $h$,

$$\mathbb{E}_{m-1}[\exp(\eta\Delta M_m(h) - \frac{\eta^2}{2}(\Delta[M]_m(h) + \Delta\langle M\rangle_m(h))] \leq 1,$$

thus we have

$$\mathbb{E}_{m-1}[Z_m] \leq \mathbb{E}_{h\sim \mathrm{P}}\left[\exp(f_{m-1}(\mathcal{S},h))\right] = Z_{m-1}.$$

Thus $(Z_m)_m$ is a nonnegative supermartingale with $Z_0 = 1$. We can use Ville's inequality (Lemma 2.1.1) which states that

$$\mathbb{P}_S\left(\exists m \geq 1 : Z_m > \delta^{-1}\right) \leq \delta.$$

Thus, with probability $1-\delta$ over $\mathcal{S}$, for all $m \in \mathbb{N}, Z_m \leq 1/\delta$. We then have the following intermediary result. For all $\mathrm{P}$ a data-free prior, $\eta \in \mathbb{R}$, with probability $1-\delta$ over $\mathcal{S}$, for all $m > 0, \mathrm{Q} \in \mathcal{M}(\mathcal{H})$

$$\eta M_m(\mathrm{Q}) \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(1/\delta) + \frac{\eta^2}{2}\left([M]_m(\mathrm{Q}) + \langle M\rangle_m(\mathrm{Q})\right)], \tag{2.3}$$

recalling that $M_m(\mathrm{Q}) = \mathbb{E}_{h\sim\mathrm{Q}}[M_m(h)]$, and that similar definitons hold for $[M]_m(\mathrm{Q}), \langle M\rangle_m(\mathrm{Q})$. Thus, applying the bound with $\eta = \pm\lambda$ ($\lambda > 0$) and taking an union bound gives, with probability $1-\delta$ over $\mathcal{S}$, for any $m \in \mathbb{N}$, $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$

$$\lambda\left|M_m(\mathrm{Q})\right| \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(2/\delta) + \frac{\lambda^2}{2}\left([M]_m(\mathrm{Q}) + \langle M\rangle_m(\mathrm{Q})\right)].$$

Dividing by $\lambda$ concludes the proof. ■

### 2.2.3 A corollary: Batch learning with iid data and unbounded losses

In this section, we instantiate Theorem 2.2.1 onto a learning theory framework with iid data. We show that our bound encompasses several results of literature as particular cases.

**Framework** We consider a *learning problem* specified by a tuple $(\mathcal{H}, \mathcal{Z}, \ell)$ consisting of a set $\mathcal{H}$ of predictors, the data space $\mathcal{Z}$, and a loss function $\ell : \mathcal{H}\times\mathcal{Z} \to \mathbb{R}^+$. We consider a countable dataset $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1} \in \mathcal{Z}^{\mathbb{N}}$ and assume that sequence is *i.i.d.* following the distribution $\mathcal{D}$. We also denote by $\mathcal{M}(\mathcal{H})$ is the set of probabilities on $\mathcal{H}$.

**Definitions** Similarly to Chapter 1, the *population risk* $\mathrm{R}$ of a predictor $h \in \mathcal{H}$ is $\forall h, \mathrm{R}(h) = \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\ell(h,\mathbf{z})]$, the *empirical error* of $h$ is $\forall h, \hat{\mathrm{R}}_{\mathcal{S}_m}(h) = \frac{1}{m}\sum_{i=1}^m \ell(h,z_i)$ and finally the *quadratic generalisation error* $V$ of $h$ is $\forall h, Quad(h) = \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\ell(h,z)^2]$. We also denote by *generalisation gap* for any $h$ the quantity $\mathrm{R}(h) - \hat{\mathrm{R}}_{\mathcal{S}_m}(h)$.

**Main result.** We now state the main result of this section. This bound is a corollary of Theorem 2.2.1 and fills the gap with learning theory.

**Theorem 2.2.2** (A PAC-Bayes bound for batch learning with heavy-tailed losses)**.** For any data-free prior $P \in \mathcal{M}(\mathcal{H})$, any $\lambda > 0$ the following holds with probability $1-\delta$ over the sample $\mathcal{S} = (\mathbf{z}_i)_{i\in\mathbb{N}}$, for all $m \in \mathbb{N}/\{0\}$, $Q \in \mathcal{M}(\mathcal{H})$

$$\mathbb{E}_{h\sim \mathrm{Q}}[\mathrm{R}(h)] \leq \mathbb{E}_{h\sim \mathrm{Q}}\left[\hat{\mathrm{R}}_{\mathcal{S}_m}(h) + \frac{\lambda}{2m}\sum_{i=1}^{m}\ell(h,z_i)^2\right] + \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(2/\delta)}{\lambda m} + \frac{\lambda}{2}\mathbb{E}_{h\sim \mathrm{Q}}[\mathrm{Quad}(h)].$$

Proof is furnished in Appendix C.3.

**About the choice of $\lambda$.** A novelty in this theorem is that the bound holds *simultaneously on all* $m > 0$ – this is due to the use of Ville's inequality. This sheds a new light on the choice of $\lambda$. Indeed, taking a localised $\lambda$ depending on a given sample size (e.g. $\lambda_m = 1/\sqrt{m}$) ensures convergence guarantees for the expected generalisation gap. Doing so, our bound matches the usual PAC-Bayes literature (i.e. a bound holding with high probability for a single $m$). However the novelty brought by Theorem 2.2.2 is that our bound holds for unbounded losses for all times simultaneously. This suggests that taking a sample size-dependent $\lambda$ may not be the best answer. We detail an instance of this fact below when one thinks of $\lambda$ as a parameter of an optimisation objective. Indeed, our bound suggests a new optimisation objective for unbounded losses which is for any $m > 0$:

$$\mathrm{argmin}_{\mathrm{Q}}\, \mathbb{E}_{h\sim \mathrm{Q}}\left[\frac{1}{m}\sum_{i=1}^{m}\left(\ell(h,z_i) + \frac{\lambda}{2}\ell(h,z_i)^2\right)\right] + \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P})}{\lambda m}. \tag{2.4}$$

Equation (2.4) differs from the classical objective of Catoni (2007, Thm 1.2.6) (described in (1.8)) on the additional quadratic term $\frac{\lambda}{2}\ell(h,z_i)^2$. Note that this objective implies a bound on the theoretical order 2 moment to be meaningful as we do not include it in our objective. Note that this constraint is less restrictive than Catoni's objective which requires a bounded loss. This objective stresses the role of the parameter $\lambda$ as being involved in a new explicit tradeoff between the KL term and the efficiency on training data.
Also, this optimisation objective is valid for any sample size $m$, this means that our $\lambda$ should not depend on certain dataset size but should be fixed in order to ensure a learning algorithm with generalisation guarantees at all time. This draws a parallel with Stochastic Gradient Descent with fixed learning step.

**About the underlying assumptions in this bound.** Our result is empirical (all terms can be computer or approximated) at the exception of the term $\mathbb{E}_{h\sim\mathrm{Q}}[\mathrm{Quad}(h)]$. This invites to choose carefully the class of posteriors, in order to bound this second-order moment with minimal assumptions. For instance, if we consider the particular case of the quadratic loss $\ell(h,z)=(h-z)^2$, then we only need to assume that our data have a finite variance if we restrict our posteriors to have both bounded means and variance. This assumption is striclty less restrictive than the classical subgaussian/subgamma assumption classically appearing in the literature.

**Comparison with literature.** Back to the bounded case, we note that instantiating the boundedness assumption in Th. 2.2.2 make us recover the result of Alquier *et al.* (2016, Theorem 4.1) for the subgaussian case. We also remark that instantiating the HYPE condition conditioning Haddouche *et al.* (2021, Theorem 3) allow us to improve their result as we transformed the control of an exponential moment into one on a second-order moment. More details are gathered in Appendix C.2. We also compare Theorem 2.2.2 to Kuzborskij and Szepesvári (2019, Theorem 3) which is a PAC-Bayes bound for unbounded losses obtained through a concentration inequality from De la Peña *et al.* (2009). They arrived to what they denote as semi-empirical inequalities which also involve empirical and theoretical variance terms (and not an exponential moment).Their bound holds for independent data and a single posterior. First of all, note that Theorem 2.2.2 holds for any posterior, which is strictly more general. Note also that our bound is a straightforward corollary of Theorem 2.2.1 which holds for any martingale (thus for any data distribution in a learning theory framework) and so, exploits a different toolbox than Kuzborskij and Szepesvári (2019) (control of a supermartingale vs. concentration bounds for independent data). We insist that a fundamental novelty in our work is to extend the conclusion of Kuzborskij and Szepesvári, 2019 to the case of non-independent data: it is possible to perform PAC-Bayes learning for unbounded losses at the expense of the control of second-order moments. Note also that their bound is slightly tighter than ours as their result is Theorem 2.2.2 being optimised in $\lambda$ (which is something we cannot do as the resulting $\lambda$ would be data-dependent).

## 2.3 Application to the multi-armed bandit problem

We exploit our main result in the context of the multi-armed bandit problem – we adopt the framework of Seldin *et al.* (2012a).

**Framework.** Let $\mathcal{A}$ be a set of actions of size $|\mathcal{A}|=K<+\infty$ and $a\in\mathcal{A}$ be an action. At each round $i$, the environment furnishes a reward function $R_i:\mathcal{A}\to\mathbb{R}$ which associate a reward $R_i(a)$ to the arm $a$. Assuming the $R_i$s are iid, we denote for any $a$, the *expected reward for action* $a$ to be $R(a)=\mathbb{E}_{R_1}[R_1(a)]$. At each round $i$,

the player executes an action $A_i$ according to a policy $\pi_i$. We then set the filtration $(\mathcal{F}_i)_{i\geq 1}$ to be $\mathcal{F}_i = \sigma\left(\{\pi_j, A_j, R_j \mid 1 \leq j \leq m\}\right)$.

**Assumptions.** We suppose here that $(R_i)_{i\geq 1}$ is an iid sequence and that at each time $i$, $A_i$ and $R_i$ are independent and that $\pi_i$ is $\mathcal{F}_{i-1}$ measurable. This means that the player is not aware of the rewards each round and performs its current move with regards to the past.
We also add two technical assumptions. First, the order two moment of the expected reward is uniformly bounded: $\sup_{a\in\mathcal{A}} \mathbb{E}_{R_1}[R_1(a)^2] \leq C$. This assumption is strictly less restrictive than the boundedness assumption made in SELDIN *et al.*, 2012a. Similarly to this work, we also assume that there exists a sequence $(\varepsilon_i)_{i\geq 1}$ such that $\inf_{a\in\mathcal{A}} \pi_i(a) \geq \varepsilon_i$. We say that $(\pi_i)_{i\geq 1}$ is *bounded from below by* $(\varepsilon_i)_{i\geq 1}$.

**Definitions.** For $i \geq 1$ and $a \in \{1, \ldots, K\}$, define a set of random variables $(R_i^a)_{i\geq 1}$ (*the importance weighted samples*, SUTTON and BARTO, 2018)

$$R_i^a := \begin{cases} \frac{1}{\pi_i(a)} R_i, & \text{if } A_i = a, \\ 0, & \text{otherwise.} \end{cases}$$

We define for any time $m$: $\hat{R}_m(a) = \frac{1}{m}\sum_{i=1}^t R_i^a$. Observe that for all $i$, $\mathbb{E}\left[R_i^a \mid \mathcal{F}_{i-1}\right] = R(a)$ and $\mathbb{E}[\hat{R}_m(a)] = R(a)$. Let $a^*$ be the "best" action (the action with the highest expected reward, if there are multiple "best" actions pick any of them). Define the *expected and empirical per-round regrets* as

$$\Delta(a) = R\left(a^*\right) - R(a), \quad \hat{\Delta}_m(a) = \hat{R}_m\left(a^*\right) - \hat{R}_m(a).$$

Observe that $m\left(\hat{\Delta}_m(a) - \Delta(a)\right)$ forms a martingale. Let

$$V_m(a) = \sum_{i=1}^m \mathbb{E}\left[\left(R_i^{a^*} - R_i^a - \left[R\left(a^*\right) - R(a)\right]\right)^2 \mid \mathcal{F}_{i-1}\right]$$

be the cumulative variance of this martingale and

$$\hat{V}_m(a) = \sum_{i=1}^m \left(R_i^{a^*} - R_i^a - \left[R\left(a^*\right) - R(a)\right]\right)^2$$

its empirical counterpart. We denote for any distribution $\mathrm{Q}$ over $\mathcal{A}$, $\Delta(\mathrm{Q}) = \mathbb{E}_{a\sim\mathrm{Q}}[\Delta(a)]$, $V_m(\mathrm{Q}) = \mathbb{E}_{a\sim\mathrm{Q}}[V_m(a)]$, similar definitions hold for $\hat{\Delta}_m(\mathrm{Q}), \hat{V}_m(\mathrm{Q})$. We can now state the main result of this section – its proof is deferred to Appendix C.3.

**Theorem 2.3.1** (PAC-Bayes bounds for heavy-tailed rewards)**.** For any $m \geq 1$, any history-dependent policy sequence $(\pi_i)_{i\geq 1}$ bounded from below by $(\varepsilon_i)_{i\geq 1}$, we have with probability $1-\delta$, for all posterior $\mathrm{Q}$

$$\left|\Delta(\mathrm{Q}) - \hat{\Delta}_m(\mathrm{Q})\right| \leq 2\sqrt{\frac{\left(1+\frac{2K}{\delta}\right)\left(\log(K)+\log(4/\delta)\right)}{m\varepsilon_m}}.$$

To the best of our knowledge, this result is the first PAC-Bayesian guarantees for multi-armed bandits with unbounded rewards. The proposed bound is as tight as Theorem 2.3 of Seldin *et al.* (2012a), up to a factor $(e-2)$ transformed into $\left(1+\frac{2K}{\delta}\right)$ (which is a huge dependency in $K$) within the square root. Note that our result comes at the price of the localisation: Theorem 2.3 of Seldin *et al.* (2012a) proposes a bound holding uniformly for all time $m$ while our approach only holds for a single time $m$.
We believe there is room for improvement in Th. 2.3.1. Indeed, the current approach is naive as it consists in bounding crudely with high probability the empirical variance. Such a naive trick impeach us to consider all times simultaneously. Indeed, in its current form, taking an union bound on Theorem 2.3.1 is costful as we have a dependency in $1/\delta$ in our result (instead of $\log(1/\delta)$ in Seldin *et al.*, 2012a): this would destroy the convergence rate. The question of dealing more subtly with the empirical variance term is left as an open question.

## 2.4 Conclusion

**A first step towards an optimisation perspective of PAC-Bayes** We showed that it is possible to generalise the PAC-Bayes toolbox to unbounded martingales and heavy-tailed losses (resp. learning problem with unbounded losses for batch/online learning), the solely implicit assumption being the existence of second order moments on the martingale difference sequence (resp. on the loss function) which is reasonable as many PAC-Bayes bound lies on assumptions on exponential moments (*e.g.* the subgaussian assumption) to work.
**Current Limitations.** Doing so, we made a first step towards concrete optimisation perspective of PAC-Bayes by showing generalisation bounds are attainable with weak statistical assumptions and thus, compatible with many practical settings where optimisation is performed. However, Chapter 2 still presents some strong links with the information-theoretic approach such as: *(i)* the presence of a prior $\mathrm{P}$ in Theorem 2.2.2 which does no fit the optimisation views of the prior (see Figure 1.2), and *(ii)* the presence of a KL divergence, suggesting an information-theoretic perspective of learning. Point *(i)* will be later developed in Chapters 3, 4 and 6 when $\mathrm{P}$ is seen as an

initialisation point and in Chapter 5 when $\mathrm{P}$ is the learning objective. *(ii)* will be later developed in Chapters 5 and 6.

**Extensions of this work.** The supermartingale framework presented here are extracted from Haddouche and Guedj (2023a) and has inspired many follow-up works. Chugg *et al.* (2023) extended the approach of this chapter to other supermartingales as well as reversed submartingales, allowing to recover a vast majority of existing PAC-Bayes literature, also, Rodriguez-Galvez *et al.* (2023) tightened the theorems presented here by allowing the optimisation in $\lambda$. The tools presented in this work (*e.g.* Ville's inequality) are also useful to obtain fast rate PAC-Bayes bounds based on the coin-betting approach Jang *et al.* (2023) and Kuzborskij *et al.* (2024). The coin-betting approach originally in online learning (Orabona and Pál, 2016). In Chapter 3, we take a deeper focus on online learning, showing that an online approach of PAC-Bayes is possible, and allows to consider prior distribution as an initialisation point of a learning algorithm.

# 3 Mitigating Initialisation Impact by Real-Time Control: Online PAC-Bayes Learning

**This chapter is based on the following papers**

Maxime Haddouche and Benjamin Guedj. Online PAC-Bayes Learning. *Advances in Neural Information Processing Systems (NeurIPS)*. (2022)
Maxime Haddouche and Benjamin Guedj. PAC-Bayes Generalisation Bounds for Heavy-Tailed Losses through Supermartingales. *Transactions on Machine Learning Research*. (2023)

## Contents




**Abstract**

While Chapter 2 showed weak statistical assumptions were reachable in PAC-Bayes, allowing its use in a wide range of concrete optimisation settings, the role of the prior $\mathrm{P}$ remains untreated. To tackle this issue, we propose here to consider $\mathrm{P}$ as the initialisation point of a learning algorithm. Then, to attenuate its impact in PAC-Bayes procedures, we develop *Online PAC-Bayes learning*, which consider a sequence $(\mathrm{Q}_i, \mathrm{P}_i)_{i=1\cdots m}$ of pairs (posterior,prior) evolving through time. Thus, the impact of initialisation $\mathrm{P} = \mathrm{P}_1$ is attenuated through the evolution of $\mathrm{P}_i$ during the learning phase. We develop the first Online PAC-Bayes bounds and propose experiments showing that online PAC-Bayes outperforms SGD in several cases.

## 3.1 Introduction

Batch learning is somewhat the dominant learning paradigm in which we aim to design the best predictor by collecting a training dataset which is then used for inference or prediction. Classical algorithms such as SVMs (see Cristianini, Shawe-Taylor, *et al.*, 2000, among many others) or feedforward neural networks (Svozil *et al.*, 1997) are popular examples of efficient batch learning. While the mathematics of batch learning constitute a vivid and well understood research field, in practice this might not be aligned with the way practitionners collect data, which can be sequential when too much information is available at a given time (*e.g.* the number of micro-transactions made in finance on a daily basis). Indeed batch learning is not designed to properly handle dynamic systems.

Online learning (OL) (Zinkevich, 2003; Shalev-Shwartz, 2012; Hazan, 2016) fills this gap by treating data as a continuous stream with a potentially changing learning goal. OL has been studied with convex optimisation tools and the celebrated notion of regret which measures the discrepancy between the cumulative sum of losses for a specific algorithm at each datum and the optimal strategy. It led to many fruitful results comparing the efficiency of prediction for optimisation algorithms such that Online Gradient Descent (OGD), Online Newton Step through static regret (Zinkevich, 2003; Hazan *et al.*, 2007). OL is flexible enough to incorporate external expert advice onto classical algorithms with the optimistic point of view that such advices are useful for training (Rakhlin and Sridharan, 2013; Rakhlin and Sridharan, n.d.) and then having optimistic regret bounds. Modern extensions also allow to compare to moving strategies through dynamic regret (see e.g. Yang *et al.*, 2016; Zhao *et al.*, 2020; Zhang *et al.*, n.d.). However, this notion of regret has been challenged recently: for instance, Wintenberger (2021) chose to control an expected cumulative loss through PAC inequalities in order to deal with the case of stochastic loss functions.

While OL tackles learning problems going beyond batch learning, it can also be used as a tool to understand stochastic methods in batch learning, such as SGD, where data are picked sequentially. Then, obtaining generalisation bounds tailored for OL is also of interest to understand the evolution of generalisation ability of stochastic batch algorithms. In the context of PAC-Bayes, it is then natural to ask whether in online learning could either explain better the evolution in-training of the generalisation ability or provide online variants of classical algorithms (*e.g.* (1.7), (1.8)). In both cases, the online paradigm allows to focus less on the prior $\mathrm{P}$ and more on its evolution, being consistent with the optimisation view of the prior as an intialisation point (see Figure 1.2).

**Our contributions.** Our goal is to provide a general online framework for PAC-Bayesian learning. Our main contribution (Th. 3.2.1 in section 3.2) is a general bound which is then used to derive several online PAC-Bayesian results (as developed in sections 3.3 and 3.4). More specifically, we derive two types of bounds, *online PAC-*

*Bayesian training and test bounds*. Training bounds exhibit online procedures while the test bound provide efficiency guarantees. We propose then several algorithms with their associated training and test bounds as well as a short series of experiments to evaluate the consistency of our online PAC-Bayesian approach. Our efficiency criterion is not the classical regret but an expected cumulative loss close to the one of WINTENBERGER (2021). More precisely, section 3.3 propose a stable yet time-consuming Gibbs-based algorithm, while section 3.4 proposes time efficient yet volatile algorithms. We emphasize that our PAC-Bayesian results only require a bounded loss to hold: no assumption is made on the data distribution, priors can be data-dependent and we do not require any convexity assumption on the loss, as commonly assumed in the OL framework.

**Outline.** section 3.2 introduces the theoretical framework as well as our main result. section 3.3 presents an online PAC-Bayesian algorithm and draws links between PAC-Bayes and OL results. section 3.4 details online PAC-Bayesian disintegrated procedures with reduced computational time and section 3.5 gathers supporting experiments. We include reminders on OL and PAC-Bayes in **????**. **??** provide disucssion about our main result. All proofs are deferred to appendix C.3.

## 3.2 An online PAC-Bayesian bound

We establish a novel PAC-Bayesian theorem (which in turn will be particularised in section 3.3) which overcomes the classical limitation of data-independent prior and iid data. We call our main result an *online PAC-Bayesian bound* as it allows to consider a sequence of priors which may depend on the past and a sequence of posteriors that can dynamically evolve as well. Indeed, we follow the online learning paradigm which considers a continous stream of data that the algorithm has to process on the fly, adjusting its outputs at each time step w.r.t. the arrival of new data and the past. In the PAC-Bayesian framework, this paradigm translates as follows: from an initial (still data independent) prior $Q_1 = P$ and a data sample $S = (z_1, ..., z_m)$, we design a sequence of posterior $(Q_i)_{1 \leq i \leq m}$ where $Q_i = f(Q_1, ..., Q_{i-1}, z_i)$.

**Framework.** Consider a data space $\mathcal{Z}$ (which can be only inputs or pairs of inputs/outputs). We fix an integer $m > 0$ and our data sample $S \in \mathcal{Z}^m$ is drawn from an unknown distribution $\mu$. We do not make any assumption on $\mu$. We set a sequence of priors, starting with $P_1 = P$ a data-free distribution and $(P_i)_{i \geq 2}$ such that for each $i$, $P_i$ is $\mathcal{F}_{i-1}$ measurable where $(\mathcal{F}_i)_{i \geq 0}$ is an adapted filtration to $S$. For $P, Q \in \mathcal{M}_1(\mathcal{H})$, the notation $P \ll Q$ indicates that $Q$ is absolutely continuous wrt $P$ (i.e. $Q(A) = 0$ if $P(A) = 0$ for measurable $A \subset \mathcal{H}$). We also denote by $Q_i$ our sequence of candidate posteriors. There is no restriction on what $Q_i$ could be. In what follows we fix a filtration $(\mathcal{F}_i)_{i \geq 0}$ and we denote by $\mathrm{KL}$ the Kullback-Leibler divergence between two distributions.

We consider a predictor space $\mathcal{H}$ and a loss funtion $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}^+$ bounded by a real constant $K > 0$. This loss defines the (potentially moving) learning objective. We denote by $\mathcal{M}_1(\mathcal{H})$ the set of all probability distributions on $\mathcal{H}$. We now introduce the notion of *stochastic kernel* (RIVASPLATA *et al.*, 2020) which formalise properly data-dependent measures within the PAC-Bayes framework. First, for a fixed predictor space $\mathcal{H}$, we set $\Sigma_{\mathcal{H}}$ to be the considered $\sigma$-algebra on $\mathcal{H}$.

**Definition 3.2.1** (Stochastic kernels)**.** A *stochastic kernel* from $\mathcal{S} = \mathcal{Z}^m$ to $\mathcal{H}$ is defined as a mapping $Q : \mathcal{Z}^m \times \Sigma_{\mathcal{H}} \to [0; 1]$ where

- For any $B \in \Sigma_{\mathcal{H}}$, the function $S = (z_1, ..., z_m) \mapsto Q(S, B)$ is measurable,
- For any $S \in \mathcal{Z}^m$, the function $B \mapsto Q(S, B)$ is a probability measure over $\mathcal{H}$.

We denote by $\texttt{Stoch}(\mathcal{S}, \mathcal{H})$ the set of all stochastic kernels from $\mathcal{S}$ to $\mathcal{H}$ and for a fixed $S$, we set $Q_S := Q(S, .)$ the data-dependent prior associated to the sample $S$ through Q.

From now, to refer to a distribution $Q_S$ depending on a dataset $S$, we introduce a stochastic kernel $Q(., .)$ such that $Q_S = Q(S, .)$. Note that this notation is perfectly suited to the case when $Q_S$ is obtained from an algorithmic procedure $A$. In this case the stochastic kernel $Q$ of interest is the learning algorithm $A$. We use this notion to characterise our sequence of priors.

**Definition 3.2.2.** We say that a sequence of stochastic kernels $(P_i)_{i=1..m}$ is an ***online predictive sequence*** if (i) for all $i \geq 1, S \in \mathcal{Z}^m, P_i(S, .)$ is $\mathcal{F}_{i-1}$ measurable and (ii) for all $i \geq 2$, $P_i(S, .) \gg P_{i-1}(S, .)$.

Note that (ii) implies that for all $i, P_i(S, .) \gg P_1(S, .)$ with $P_1(S, .)$ a data-free measure (yet a classical prior in the PAC-Bayesian theory).
We can now state our main result.

**Theorem 3.2.1.** For any distribution $\mu$ over $\mathcal{Z}^m$, any $\lambda > 0$ and any online predictive sequence (used as priors) $(P_i)$, for any sequence of stochastic kernels $(Q_i)$ we have with probability $1 - \delta$ over the sample $S \sim \mu$, the following, holding for the data-dependent measures $Q_{i,S} := Q_i(S, .), P_{i,S} := P_i(S, .)$ :

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim Q_{i,S}} \left[ \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \right] \leq \sum_{i=1}^{m} \mathbb{E}_{h_i \sim Q_{i,S}} \left[ \ell(h_i, z_i) \right] + \frac{\mathrm{KL}(Q_{i,S} \| P_{i,S})}{\lambda} + \frac{\lambda m K^2}{2} + \frac{\log(1/\delta)}{\lambda}.$$

**Remark 3.2.1.** For the sake of clarity, we assimilate in what follows the stochastic kernels $Q_i, P_i$ to the data-dependent distributions $Q_i(S,.), P_i(S,.)$. Then, an online predictive sequence is also assimilated to a sequence of data-dependent distributions. Concretely this leads to the switch of notation $Q_{i,S} \to Q_i$ in Th. 3.2.1. The reason of this switch is that, even though stochastic kernel is the right theoretical structure to state our main result, we consider in sections 3.3 and 3.4 practical algorithmic extensions which focus only on data-dependent distributions, hence the need to alleviate our notations.

The proof is deferred to section 3.7.1. See **??** for context and discussions.

**A batch to online conversion.** First, we remark that our bound slightly exceeds the OL framework: indeed, it would require our posterior sequence to be an online predictive sequence as well, which is not the case here (for any $i$, the distribution $Q_{i,S}$ can depend on the whole dataset ). This is a consequence of our proof method (see section 3.7.1), which is classically denoted as a "batch to online" conversion (in opposition to the "online to batch" procedures as in Dekel and Singer, 2005). In other words, we exploited PAC-Bayesian tools designed for a fixed batch of data to obtain a dynamic result. This is why we refer to our bound as online as it allows to consider sequences of priors and posteriors that can dynamically evolve.

**Analysis of the different terms in the bound.** Our PAC-Bayesian bound formally differs in many points from the classical ones. On the left-hand side of the bound, the sum of the averaged expected loss conditioned to the past appears. Having such a sum of expectations instead of a single one is necessary to assess the quality of all our predictions. Indeed, because data may be dependent, one can not consider a single expectation as in the iid case. We also stress that taking an online predictive sequence as priors leads to control losses conditioned to the past, which differs from classical PAC-Bayes results designed to bound the expected loss. This term, while original in the PAC-Bayesian framework (to the best of our knowledge) recently appeared (in a modified form) in Wintenberger (2021, Prop 3). See **??** for further disucssions.

On the right hand-side of the bound, online counterparts of classical PAC-Bayes terms appear. At time $i$, the measure $Q_i$ (i.e. $Q_{i,S}$ according to remark 3.2.1) has a tradeoff to achieve between an overfitted prediction of $z_i$ (the case $Q_i = \delta_{z_i}$ where $\delta$ is a Dirac measure) and a too weak impact of the new data with regards to our prior knowledge (the case $Q_i = P_i$). The quantity $\lambda > 0$ can be seen as a regulariser to adjust the relative impact of both terms.

**Influence of $\lambda$.** The quantity $\lambda$ also plays a crucial role on the bound as it is involved in an explicit tradeoff between the KL terms, the confidence term $\log(1/\delta)$ and the residual term $mK^2/2$. This idea of seeing $\lambda$ as a trading parameter is not new (Germain *et al.*, 2016; Thiemann *et al.*, 2017). However, the results from Thiemann *et al.* (2017) stand w.p. $1-\delta$ for any $\lambda$ while ours and the ones from Germain *et al.*

(2016) hold for any $\lambda$ w.p. $1-\delta$ which is weaker and implies to discretise $\mathbb{R}^+$ onto a grid to estimate the optimal $\lambda$.
We now move on to the design of online PAC-Bayesian algorithms.

## 3.3 An online PAC-Bayesian procedure

OL algorithms (we refer to HAZAN, 2016 an introduction to the field) are producing sequences of predictors by progressively updating the considered predictor (see **??** for an example). Recall that, in the OL framework, an algorithm outputs at time $i$ a predictor which is $\mathcal{F}_{i-1}$-measurable. Here, our goal is to design an online procedure derived from Th. 3.2.1 which outputs an online predictive sequence (which is assimilated, according to remark 3.2.1, to a sequence of distributions).
**Online PAC-Bayesian (OPB) training bound.** We state a corollary of our main result which paves the way to an online algorithm. This constructive procedure motivates the name *Online PAC-Bayesian training bound* (OPBTRAIN in short).

**Corollary 3.3.1** (OPBTRAIN)**.** For any distribution $\mu$ over $\mathcal{Z}^m$, any $\lambda > 0$ and any online predictive sequences $\hat{Q}, P$, the following holds with probability $1-\delta$ over the sample $S \sim \mu$ :

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_{i+1}} \left[ \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \right] \leq \sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_{i+1}} \left[ \ell(h_i, z_i) \right] + \frac{\mathrm{KL}(\hat{Q}_{i+1} \| P_i)}{\lambda} + \frac{\lambda m K^2}{2} + \frac{\log(1/\delta)}{\lambda}.$$

Here, $\lambda$ is seen as a scale parameter as precised below. The proof consists in applying Th. 3.2.1 with for all $i$, $Q_i = \hat{Q}_{i+1}$ and $P_i$. Note that in this case, our posterior sequence is an online predictive sequence in order to fit with the OL framework.
Cor. 3.3.1 suggests to design $\hat{Q}$ as follows, assuming we have drawn a dataset $S = \{z_1, ..., z_m\}$, fixed a scale parameter $\lambda > 0$ and an online predictive sequence $P_i$:

$$\hat{Q}_1 = P_1, \quad \forall i \geq 1 \; \hat{Q}_{i+1} = \underset{Q \in \mathcal{M}_1(\mathcal{H})}{\operatorname{argmin}} \, \mathbb{E}_{h_i \sim Q} \left[ \ell(h_i, z_i) \right] + \frac{\mathrm{KL}(Q \| P_i)}{\lambda} \tag{3.1}$$

which leads to the explicit formulation

$$\frac{d\hat{Q}_{i+1}}{dP_i}(h) = \frac{\exp\left(-\lambda \ell(h, z_i)\right)}{\mathbb{E}_{h \sim P_i}\left[\exp\left(-\lambda \ell(h, z_i)\right)\right]}. \tag{3.2}$$

Thus, the formulation of Eq. (3.2), which has been highlighted by CATONI (2003, Sec. 5.1) shows that our online procedure produces Gibbs posteriors. So, PAC-Bayesian theory provides sound justification for the somewhat intuitive online procedure in Eq. (3.1):

at time $i$, we adjust our new measure $\hat{Q}_{i+1}$ by optimising a tradeoff between the impact of the newly arrived data $z_i$ and the one of prior knowledge $\hat{Q}_i$.
Notice that $\hat{Q}$ is an online predictive sequence: $\hat{Q}_i$ is $\mathcal{F}_{i-1}$-measurable for all $i$ as it depends only on $\hat{Q}_{i-1}$ and $z_{i-1}$. Furthermore, one has $\hat{Q}_i \gg \hat{Q}_{i-1}$ for all $i$ as $\hat{Q}_i$ is defined as an argmin and the KL term is finite if and only it is absolutely continuous w.r.t. $\hat{Q}_{i-1}$.

**Remark 3.3.1.** In Cor. 3.3.1, while the right hand-side is the reason we considered Eq. (3.1), the left hand side still needs to be analysed. It expresses how the posterior $\hat{Q}_{i+1}$ (designed from $\hat{Q}_i, z_i$) generalises well on average to any new draw of $z_i$. More precisely, this term measures how much the training of $\hat{Q}_{i+1}$ is overfitting on $z_i$. A low value of it ensures our online predictive sequence, which is obtained from a single dataset, is robust to the randomness of $S$, hence the interest of optimising the right hand side of the bound. This is a supplementary reason we refer to Cor. 3.3.1 as an $\mathrm{OPBTrain}$ bound as it provide robustness guarantees for our training.

**Online PAC-Bayesian (OPB) test bound.** However, Cor. 3.3.1 does not say if $\hat{Q}_{i+1}$ will produce good predictors to minimise $\ell(., z_{i+1})$, which is the objective of $\hat{Q}_{i+1}$ in the OL framework (we only have access to the past to predict the future). We then need to provide an *Online PAC-Bayesian (OPB) test bound* ($\mathrm{OPBTest}$ bound) to quantify our prediction's accuracy. We now derive an $\mathrm{OPBTest}$ bound from Th. 3.2.1.

**Corollary 3.3.2** ($\mathrm{OPBTest}$)**.** . For any distribution $\mu$ over $\mathcal{Z}^m$, any $\lambda > 0$, and any online predictive sequence $(\hat{Q}_i)$, the following holds with probability $1-\delta$ over the sample $S \sim \mu$:

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_i} \left[ \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \right] \leq \sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_i} \left[ \ell(h_i, z_i) \right] + \frac{\lambda m K^2}{2} + \frac{\log(1/\delta)}{\lambda}.$$

Optimising in $\lambda$ gives $\lambda = \sqrt{\frac{2\log(1/\delta)}{mK^2}}$ and ensure that:

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_i} \left[ \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \right] \leq \sum_{i=1}^{m} \mathbb{E}_{h_i \sim \hat{Q}_i} \left[ \ell(h_i, z_i) \right] + O\left( \sqrt{\log(1/\delta) K^2 m} \right).$$

The proof consists in applying Th. 3.2.1 with for all $i$, $Q_i = \hat{Q}_i = P_i$.
Cor. 3.3.2 quantifies how efficient will our predictions be. Indeed, the left hand side of this bound relates for all $i$, how good $\hat{Q}_i$ is to predict $z_i$ (on average) which is what $\hat{Q}_i$ is designed for. Note that here, the involved $\lambda$ can differ from the scale parameter of Eq. (3.1), it is now a way to compensate for the tradeoff between the

two last terms of the bound. The strength of this bound is that since $\hat{Q}$ is an online predictive sequence, the Kullback-Leibler terms vanished, leaving terms depending only on hyperparameters.

## Links with previous approaches

We now present a specific case of Cor. 3.3.1 where we choose as priors the online predictive sequence $\hat{Q}$ (*i.e.* in Th. 3.2.1, we choose $Q_i = \hat{Q}_{i+1}, P_i = \hat{Q}_i$). The reason we focus on this specific case is that it enables to build strong links between PAC-Bayes and OL.
We then adapt our $\mathrm{OPBTrain}$ bound (Cor. 3.3.1). The online procedure becomes:

$$\hat{Q}_1 = P, \quad \forall i \geq 1 \; \hat{Q}_{i+1} = \mathrm{argmin}_Q \, \mathbb{E}_{h_i \sim Q} \left[\ell(h_i, z_i)\right] + \frac{\mathrm{KL}(Q \| \hat{Q}_i)}{\lambda}, \tag{3.3}$$

which leads to the explicit formulation

$$\frac{d\hat{Q}_{i+1}}{d\hat{Q}_i}(h) = \frac{\exp\left(-\lambda \ell(h, z_i)\right)}{\mathbb{E}_{h \sim \hat{Q}_i}\left[\exp\left(-\lambda \ell(h, z_i)\right)\right]}.$$

**Links with classical PAC-Bayesian bounds.** We denote that the optimal predictor in this case is such that at any time $i$, $d\hat{Q}_{i+1}(h) \propto \exp(-\lambda \ell(h, z_i)) d\hat{Q}_i(h)$ hence $d\hat{Q}_{m+1}(h) \propto \exp\left(-\lambda \sum_{i=1}^m \ell(h, z_i)\right) d\hat{Q}_1(h)$. One recognises, up to a multiplicative constant, the optimised predictor of Catoni (2007, Th 1.2.6) which solves $\mathrm{argmin}_Q \, \mathbb{E}_{h \sim Q} \left[\frac{1}{m} \sum_{i=1}^m \ell(h, z_i)\right] + \frac{\mathrm{KL}(Q \| \hat{Q}_1)}{\lambda}$, thus one sees that in this case, the output of our online procedure after $m$ steps coincides with Catoni's output. This shows consistency of our general procedure which recovers classical result within an online framework: when too many data are available, treating data sequentially until time $m$ leads to the same Gibbs posterior than if we were treating the whole dataset as a batch.
**Analogy with Online Gradient Descent (OGD).** We propose an analogy between the procedure Eq. (3.3) and the celebrated OGD algorithm (see **??** for a recap). First we remark that our minimisation problem is equivalent to $\mathrm{argmin}_Q \, \lambda \mathbb{E}_{h_i \sim Q} \left[\ell(h_i, z_i)\right] + \mathrm{KL}(Q \| \hat{Q}_i)$. Then we assume that for any $i, \hat{Q}_i = \mathcal{N}(\hat{m}_i, I_d)$ with $\hat{m}_i \in \mathbb{R}^d$ and we set $\mathcal{L}_i(\hat{m}_i) = \mathbb{E}_{h_i \sim \hat{Q}_i} \left[\ell(h_i, z_i)\right]$ . The minimisation problem becomes: $\mathrm{argmin}_{\hat{m}} \, \lambda \mathcal{L}_i(\hat{m}) + \frac{1}{2} \|\hat{m} - \hat{m}_i\|^2$. And so using the first order Taylor expansion, we use the approximation $\mathcal{L}_i(\hat{m}) \approx \mathcal{L}_i(\hat{m}_i) + \langle \hat{m} - \hat{m}_i, \nabla \mathcal{L}_i(\hat{m}_i) \rangle$ which finally transform our argmin into the following optimisation process: $\hat{m}_{i+1} = \hat{m}_i - \lambda \nabla \mathcal{L}_i(\hat{m}_i)$ which is exactly OGD on the loss sequence $\mathcal{L}_i$. We draw an analogy between the scale parameter $\lambda$ and the step size $\eta$ in OGD. the KL term translates the influence of the previous point and the expected loss gives the gradient. This analogy has been already exploited in Shalev-Shwartz

(2012) where they approximated $\mathbb{E}_{h_i \sim q_\mu}[\ell(h_i, z_i)] := \bar{L}_i(\mu) \approx \mu^T \nabla \bar{L}_i(\mu_i)$ where $\mu$ is their considered online predictive sequence.

Finally, we remark that the optimum rate in Cor. 3.3.2 is a $O(\sqrt{m})$ which is comparable to the best rate of Shalev-Shwartz (2012, Eq (2.5)) (see **??**).

**Comparison with previous work.** We acknowledge that the procedure of Eq. (3.3) already appeared in literature. Li *et al.* (n.d., Alg. 1) propose a Gibbs procedure somewhat similar to ours, the main difference being the addition of a surrogate of the true loss at each time step. Within the OL literature, the idea of updating measures online has been recently studied for instance in Chérief-Abdellatif *et al.* (2019). More precisely, our procedure is similar to their Streaming Variational Bayes (SVB) algorithm. A slight difference is that they approximated the expected loss similarly to Shalev-Shwartz (2012). The guarantees Chérief-Abdellatif *et al.* (2019) provided for SVB hold for Gaussian priors and comes at the cost of additional constraints that do not allow to consider any aggregation strategies contrary to what Cor. 3.3.1 propose. Their bounds are deterministic and are using tools and assumptions from convex optimisation (such that convex expected losses) while ours are probabilistic and are using measure theory tools which allow to relax these assumptions.

**Strength of our result.** We emphasize two points. First, to the best of our knowledge, Cor. 3.3.1 is the first bound which theoretically suggests Eq. (3.3) as a learning algorithm. Second, we stress that Eq. (3.3) is a particular case of Cor. 3.3.1 and our result can lead to other fruitful routes. For instance, we consider the idea of adding noise to our measures at each time step to avoid overfitting (this idea has been used *e.g.* in Neelakantan *et al.*, 2015 in the context of deep neural networks): if our online predicitve sequence $(\hat{Q}_i)$ can be defined through a sequence of parameter vectors $\hat{\mu}$, then we can define $P_i$ by adding a small noise on $\hat{\mu}_i$ and thus giving more freedom through stochasticity.

Thus, we see that our procedure led us to the use of the Gibbs posteriors of Catoni. However, in practice, Gaussian distributions are preferred (*e.g.* Dziugaite and Roy, 2017; Rivasplata *et al.*, 2019; Perez-Ortiz *et al.*, 2021a,b,c)). That is why we focus next on new online PAC-Bayesian algorithms involving Gaussian distributions.

## 3.4 Disintegrated online algorithms for Gaussian distributions.

We dig deeper in the field of disintegrated PAC-Bayesian bounds, originally explored by Blanchard and Fleuret (2007) and Catoni (2007), further studied by Alquier and Biau (2013) and Guedj and Alquier (2013) and recently developed by Rivasplata *et al.* (2020) and Viallard *et al.* (2023a) (see **??** for a short presentation of the bound we adapted and used). The strength of the disintegrated approach is that

we have directly guarantees on the random draw of a single predictor, which avoids to consider expectations over the predictor space. This fact is particularly significant in our work as the procedure precised in Eq. (3.2), require the estimation of an exponential moment to be efficient, which may be costful. We then show that disintegrated PAC-Bayesian bounds can be adapted to the OL framework, and that they have the potential to generate proper online algorithms with weak computational cost and sound efficiency guarantees.

**Online PAC-Bayesian disintegrated (OPBD) training bounds.** We present a general form for *online PAC-Bayes disintegrated (OPBD) training bounds*. The terminology comes from the way we craft those bounds: from PAC-Bayesian disintegrated bounds we use the same tools as in Th. 3.2.1 to create the first online PAC-Bayesian disintegrated bounds. OPBD training bounds have the following form.

For any online predictive sequences $\hat{Q}, P$, any $\lambda > 0$ w.p. $1-\delta$ over $S \sim \mu$ and $(h_1, ..., h_m) \sim \hat{Q}_2 \otimes ... \otimes \hat{Q}_{m+1}$:

$$\sum_{i=1}^{m} \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \leq \sum_{i=1}^{m} \ell(h_i, z_i) + \Psi(h_i, \hat{Q}_{i+1}, P_i) \ + \Phi(m), \tag{3.4}$$

with $\Psi, \Phi$ being real-valued functions. $\Psi$ controls the global behaviour of $Q_{i+1}$ w.r.t. the $\mathcal{F}_{i-1}$-measurable prior $P_i$. If one has no dependency on $h_i$ this behaviour is global, otherwise it is local. Note that those functions may depend on $\lambda, \delta$. However, since they are fixed parameters, we do not make these dependencies explicit. Similarly to Cor. 3.3.1, this kind of bound allows to derive a learning algorithm (cf Algorithm 1) which outputs an online predicitve sequence $\hat{Q}$. Finally we draw $(h_1, ..., h_m) \sim \hat{Q}_2 \otimes ... \otimes \hat{Q}_{m+1}$ (and not $\hat{Q}_1 \otimes ... \otimes \hat{Q}_m$) since an OPBD bound is designed to justify theoretically an OPBD procedure in the same way Cor. 3.3.1 allowed to justify Eq. (3.1).

**Why focus on Gaussian measures?** The reason is that a Gaussian variable $h \sim \mathcal{N}(w, \sigma^2 \mathbf{I}_d)$ can be written as $h = w + \varepsilon$ with $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_d)$, and this expression totally defines $h$ ($\mathbf{I}_d$ being the identity matrix).

**A general OPBD algorithm for Gaussian measure with fixed variance** We use an idea presented in Viallard *et al.* (2023a) which restrict the measure set to Gaussian on $\mathbb{R}^d$ **with known and fixed covariance matrix** $\sigma^2 \mathbf{I}_d$. Then we present in Algorithm 1 a general algorithm (derived from an OPBD training bound) for Gaussian measures with fixed variance which outputs a sequence of gaussian $\hat{Q}_i = \mathcal{N}(\hat{w}_i, \sigma^2 \mathbf{I}_d)$ from a prior sequence $P_i = \mathcal{N}(w_i^0, \sigma^2 \mathbf{I}_d)$ where for each $i$, $w_i^0$ is $\mathcal{F}_{i-1}$- measurable. Because the variance is fixed, the distribution is uniquely defined by its mean, thus we identify $\hat{Q}_i$ and $\hat{w}_i$, $P_i$ and $w_i^0$.

At each time $i$, Algorithm 1 requires the draw of $\varepsilon_i \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_d)$. Doing so, we generated the randomness for our $h_i$ (because our bound holds for a single draw of $(h_1, .., h_m) \sim \hat{Q}_2 \otimes ... \otimes \hat{Q}_{m+1}$), we then write $h_i = w + \varepsilon_i$ and we optimise w.r.t. $\Psi$ to find $\hat{w}_{i+1}$.

**Algorithm 1:** A general OPBD algorithm for Gaussian measures with fixed variance.

**Parameters :** Time m, scale parameter $\lambda$
**Initialisation:** Variance $\sigma^2$, Initial mean $\hat{w}_1 \in \mathbb{R}^d$, epoch $m$
**for** *each iteration* $i$ *in* $1..m$ **do**
  Observe $z_i, w_i^0$ and draw $\varepsilon_i \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_d)$
  Update:

$$\hat{w}_{i+1} := \operatorname{argmin}_{w \in \mathbb{R}^d} \ell(w + \varepsilon_i, z_i) + \Psi(w + \varepsilon_i, w, w_i^0)$$

**end**
**Return** $(\hat{w}_i)_{i=1..m+1}$

**Bounds of interest.** We present two possible choices of pairs $(\Psi, \Phi)$ derived from the disintegrated results presented in **??**. Doing so, we explicit two ready-to-use declinations of Algorithm 1.

**Corollary 3.4.1.** For any distribution $\mu$ over $\mathcal{Z}^m$, any online predictive sequences of Gaussian measures with fixed variance $\hat{Q}_i = \mathcal{N}(\hat{w}_i, \sigma^2 \mathbf{I}_d)$ and $P_i = \mathcal{N}(w_i^0, \sigma^2 \mathbf{I}_d)$, any $\lambda > 0$, w.p. $1 - \delta$ over $S \sim \mu$ and $(h_i = \hat{w}_{i+1} + \varepsilon_i)_{i=1..m} \sim \hat{Q}_2 \otimes ... \otimes \hat{Q}_{m+1}$, the bound of Eq. (3.4) holds for the two following pairs $\Psi, \Phi$:

$$\Psi_1(h_i, \hat{w}_{i+1}, w_i^0) = \frac{1}{\lambda}\left(\frac{||\hat{w}_{i+1} + \varepsilon_i - w_i^0||^2 - ||\varepsilon||^2}{2\sigma^2}\right) \quad \Phi_1(m) = \frac{\lambda m K^2}{2} + \frac{\log(1/\delta)}{\lambda}, \tag{3.5}$$

$$\Psi_2(h_i, \hat{w}_{i+1}, w_i^0)) = \frac{1}{\lambda}\frac{||\hat{w}_{i+1} - w_i^0||^2}{2\sigma^2} \quad \Psi_2(m) = \lambda m K^2 + \frac{3\log(1/\delta)}{2\lambda}. \tag{3.6}$$

Where the notation $1, 2$ denote whether the functions have been derived from adapted theorems of Rivasplata *et al.*, 2020; Viallard *et al.*, 2023a recalled in **??** We then can use Algo. 1 with Eq. (3.5), Eq. (3.6).

Proof is deferred to **??**. Note that in Cor. 3.4.1, we identified $\hat{Q}_i$ to $\hat{w}_i$ and for the last formula, $\Psi$ has no dependency on $h_i$.

**Comparison with Eq. (3.1).** The main difference with Eq. (3.1) provided by the disintegrated framework is that the optimisation route does not include an expected term within the optimisation objective. The main advantage is a weaker computational cost when we restrict to Gaussian distributions. The main weakness is a lack of stability as our algorithm now depends at time $i$ on $\ell(h + \varepsilon_i, z_i)$ so on $\varepsilon_i$ directly. We denote that Eq. (3.5) is less stable than Eq. (3.6) as it involves another dependency on $\varepsilon_i$

through $\Psi$. The reason is that RIVASPLATA *et al.*, 2020 proposed a bound involving a disintegrated KL divergence while VIALLARD *et al.*, 2023a proposed a result involving a Rényi divergence avoiding a dependency on $\varepsilon_i$. We refer to **??** for a detailed statement of those properties.

**Comparison with Hoeven *et al.*, 2018.** Theorem 3 of HOEVEN *et al.* (2018) recovers OGD from the exponential weights algorithm by taking a sequence of moving distributions being Gaussians with fixed variance which is exactly what we consider here. From these, they retrieve the classical OGD algorithm as well as its classical convergence rate. Let us compare our results with theirs.

First, if we fix a single step $\eta$ in their bound and assume two traditional assumptions for OGD (a finite diameter $D$ of the convex set and an uniform bound $G$ on the loss gradients), we recover for the OGD (greedy GD in HOEVEN *et al.*, 2018) a rate of $\frac{D^2}{2\sigma^2\eta} + \frac{\eta\sigma^2 TG^2}{2}$. This is, up to constants and notation changes, exactly our $\Psi_i$ ($i \in \{1, 2\}$). Also, we notice a difference in the way to use Gaussian distributions: Theorem 3 of HOEVEN *et al.* (2018) is based on their Lemma 1 which provides guarantees for the expected regret. This is a clear incentive to consider as predictors the mean of the sucessive Gaussians of interest. On the contrary, Cor. 3.4.1 involves a supplementary level of randomness by considering predictors $h_i$ drawn from our Gaussians. This additional randomness appears in our optimisation process (Algo. 1). Finally, notice that HOEVEN *et al.* (2018) based their whole work on the use of a KL divergence while Cor. 3.4.1 not only exploit a disintegrated KL ($\Psi_1$) but also a Rényi $\alpha$-divergence ($\Psi_2$). Note that we propose a result only for $\alpha = 2$ for the sake of space constraints but any other value of $\alpha$ leads to another optimisation objective to explore.

**OPBD test bounds.** Similarly to what we did in section 3.3, we also provide *OPBD test bounds* to provide efficiency guarantees for online predicitve sequences (e.g. the output of Algo. 1). Our proposed bounds have the following general form.

For any online predictive sequence $\hat{Q}$, any $\lambda > 0$ w.p. $1 - \delta$ over $S$ and $(h_1, ..., h_m) \sim \hat{Q}_1 \otimes ... \otimes \hat{Q}_m$:

$$\sum_{i=1}^{m} \mathbb{E}[\ell(h_i, z_i) \mid \mathcal{F}_{i-1}] \leq \sum_{i=1}^{m} \ell(h_i, z_i) + \Phi(m), \tag{3.7}$$

with $\Phi$ being a real-valued function(possibly dependent on $\lambda, \delta$ though it is not explicited here).

Note that our predictors $(h_1, ..., h_m)$ are now drawn from $\hat{Q}_1 \otimes ... \otimes \hat{Q}_m$. Thus, the left-hand side of the bound considers a $h_i$ drawn from an $\mathcal{F}_{i-1}$-measurable distribution evaluated on $\ell(., z_i)$: this is effectively a measure of the prediction performance.

We now state a corollary which gives disintegrated guarantees for any online predicitve sequence.

**Corollary 3.4.2.** For any distribution $\mu$ over $\mathcal{Z}^m$, any $\lambda > 0$, and any online predictive sequence $(\hat{Q}_i)$, the following holds with probability $1-\delta$ over the sample $S \sim \mu$ and the predictors $(h_1, ..., h_m) \sim \hat{Q}_1 \otimes ... \otimes \hat{Q}_m$, the bound of Eq. (3.7) holds with :

$$\Phi_1(m) = \frac{\lambda m K^2}{2} + \frac{\log(1/\delta)}{\lambda}, \quad \Phi_2(m) = 2\lambda m K^2 + \frac{\log(1/\delta)}{\lambda}.$$

Where the notation $1, 2$ denote whether the functions have been derived from adapted theorems of RIVASPLATA *et al.*, 2020; VIALLARD *et al.*, 2023a recalled in **??**. The optimised $\lambda$ gives in both cases a $O(\sqrt{m \log(1/\delta)}$.

Proof is deferred to **??**.

## 3.5 Experiments

We adapt the experimental framework introduced in CHÉRIEF-ABDELLATIF *et al.* (2019, Sec.5) to our algorithms (anonymised code available here). We conduct experiments on several real-life datasets, in classification and linear regression. Our objective is twofold: check the convergence of our learning methods and compare their efficiencies with classical algorithms. We first introduce our experimental setup.

**Algorithms.** We consider four online methods of interest: the OPB algorithm of Eq. (3.3) which update through time a Gibbs posterior. We instantiate it with two different priors $\hat{Q}_1$: a Gaussian distribution and a Laplace one. We also implement Algorithm 1 with the functions $\Psi_1, \Psi_2$ from Cor. 3.4.1. To assess efficiency, we implement the classical OGD (as described in Alg. 1 of ZINKEVICH, 2003) and the SVB method of CHÉRIEF-ABDELLATIF *et al.* (2019).

**Binary Classification.** At each round $i$ the learner receives a data point $x_i \in \mathbb{R}^d$ and predicts its label $y_i \in \{-1, +1\}$ using $\langle x_i, h_i \rangle$, with $h_i = \mathbb{E}_{h \sim \hat{Q}_i}[h]$ for OPB methods or $h_i$ being drawn under $\hat{Q}_i$ for OPBD methods. The adversary reveals the true value $y_i$, then the learner suffers the loss $\ell(h_i, z_i) = \left(1 - y_i h_i^T x_i\right)_+$ with $z_i = (x_i, y_i)$ and $a_+ = a$ if $a > 0$ and $a_+ = 0$ otherwise. This loss is unbounded but can be thresholded.

**Linear Regression.** At each round $i$, the learner receives a set of features $x_i \in \mathbb{R}^d$ and predicts $y_i \in \mathbb{R}$ using $\langle x_i, h_i \rangle$ with $h_i = \mathbb{E}_{h \sim \hat{Q}_i}[h]$ for SVB and OPB methods or $h_i$ being drawn under $\hat{Q}_i$ for OPBD methods. Then the adversary reveals the true value $y_t$ and the learner suffers the loss $\ell(h_i, z_i) = \left(y_i - h_i^T x_i\right)^2$ with $z_i = (x_i, y_i)$. This loss is unbounded but can be thresholded.

**Datasets.** We consider four real world dataset: two for classification (Breast Cancer and Pima Indians), and two for regression (Boston Housing and California Housing).

All datasets except the Pima Indians have been directly extracted from `sklearn` (Pedregosa *et al.*, 2011). Breast Cancer dataset (Street *et al.*, 1993) is available here and comes from the UCI ML repository as well as the Boston Housing dataset (Belsley *et al.*, 2005) which can be obtained here. California Housing dataset (Pace and Barry, 1997) comes from the StatLib repository and is available here. Finally, Pima Indians dataset (Smith *et al.*, 1988) has been recovered from this Kaggle repository. Note that we randomly permuted the observations to avoid to learn irrelevant human ordering of data (such that date or label).

**Parameter settings.** We ran our experiments on a 2021 MacBookPro with an M1 chip and 16 Gb RAM. For OGD, the initialisation point is $\mathbf{0}_{\mathbb{R}^d}$ and the values of the learning rates are set to $\eta = 1/\sqrt{m}$. For SVB, mean is initialised to $\mathbf{0}_{\mathbb{R}^d}$ and covariance matrix to Diag$(1)$. Step at time $i$ is $\eta_i = 0.1/\sqrt{i}$. For both of the OPB algorithms with Gibbs posterior, we chose $\lambda = 1/m$. As priors, we took respectively a centered Gaussian vector with the covariance matrix Diag$(\sigma^2)$ ($\sigma = 1.5$) and an iid vector following the standard Laplace distribution. For the OPBD algorithm with $\Psi_1$, we chose $\lambda = 10^{-4}/m$, the initial mean is $\mathbf{0}_{\mathbb{R}^d}$ and our fixed covariance matrix is Diag$(\sigma^2)$ with $\sigma = 3.10^{-3}$. For the OPBD algorithm with $\Psi_1$, we chose $\lambda = 2.10^{-3}/m$, the initial mean is $\mathbf{0}_{\mathbb{R}^d}$ and our covariance matrix is Diag$(\sigma^2)$ with $\sigma = 10^{-2}$. The reason of those higher scale parameters and variance is that $\Psi$ from Rivasplata *et al.* (2020) is more stochastic (yet unstable) than the one Viallard *et al.* (2023a).

**Experimental results.** For each dataset, we plot the evolution of the average cumulative loss $\sum_{i=1}^{t} \ell\left(h_i, z_i\right)/t$ as a function of the step $t = 1, \ldots, m$, where $m$ is the dataset size and $h_i$ is the decision made by the learner $h_i$ at step $i$. The results are gathered in fig. 3.1

**Empirical findings.** OPB with Gaussian prior ('Gibbs Gauss') outperforms OGD on all datasets except California Housing (on which this method is not implemented ) while OPB with Laplace prior ('Gibbs Laplace') always fail w.r.t. OGD. OPB methods fail to compete with SVB on the Boston Housing dataset. OPBD methods compete with SVB on regression problems and clearly outperforms OGD on classification tasks. OPBD with $\Psi_2$ (labeled as 'OPBD Via' in fig. 3.1) performs better on the California Housing dataset while OPBD with $\Psi_1$ (labeled as 'OPBD Riva') is more efficient on the Boston Housing dataset. Both methods performs roughly equivalently on classification tasks. This brief experimental validation shows the consistency of all our online procedures as we observe a visible decrease of the cumulative losses through time. It particularly shows that OPBD procedures improve on OGD on these dataset. We refer to **??** for additional table gathering the error bars of our OPBD methods.

**Why do we perform better than OGD?** As stated in section 3.4, OGD can be recovered as a Gaussian approximation of the exponential weights algorithm (EWA). Thus, a legitimate question is why do we perform better than OGD as our OPBD methods are also based on a Gaussian surrogate of EWA? Hoeven *et al.*, 2018 only

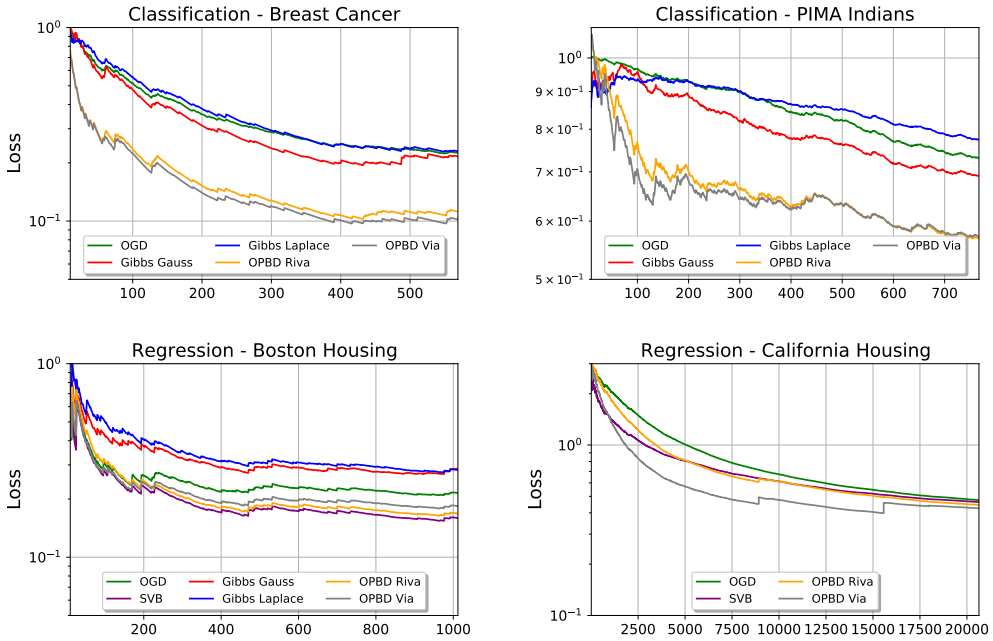


***Figure 3.1.*** *Averaged cumulative losses for all four considered datasets. 'Gibbs Gauss' denotes OPB with Gaussian Prior, 'Gibbs Laplace' denotes OPB with Laplace prior. 'OPBD Riva' denotes OPBD with $\Psi_1$, 'OPBD Via' denotes OPBD with $\Psi_2$.*

used Gaussians distributions with fixed variance as a technical tool when the considered predictors are the Gaussian means. In our work, we exploited a richer characteristic of our distributions in the sense our predictors are points sampled from our Gaussians and not only the means. This also has consequences in our learning algorithm as at time $i$ of our Algo. 1, our optimisation step involves a noise $\varepsilon_i \sim \mathcal{N}(0, \sigma^2\mathbf{I})$. Thus, we believe that OPBD methods should perform at least as well as OGD. We write 'at least' as we think that the higher flexibility due to this additional level of randomness might result in slightly better empirical performances, as seen on the few datasets in fig. 3.1.

## 3.6 Conclusion

We establish links between Online Learning and PAC-Bayes. We show that PAC-bayesian bounds are useful to derive new OL algorithms. We also prove sound theoretical guarantees for such algorithms. We emphasise that all of our results stand for any general bounded loss, especially no convexity assumption is needed. Having no convexity assumption on the loss paves the way to exciting future practical studies, starting with *Spiking Neural Network* which is investigated in an online fashion (see

LOBO *et al.*, 2020 for a recent survey). A follow-up question on the theoretical part is whether we can relax the bounded loss assumption: we leave this for future work.

## 3.7 Online PAC-Bayes learning beyond bounded losses.

Recently, an online learning framework has been designed in HADDOUCHE and GUEDJ (2022). This allowed the design of Online PAC-Bayes (OPB) algorithms which involved the use of history-dependent priors evolving at each time step of the learning procedure. The main contribution of this section is an OPB bound valid for unbounded losses.

**Framework** We consider the same framework as in Section 2.2.3 except we do not make any assumption on the data distribution. Our goal is now to define a posterior sequence $(\mathrm{Q}_i)_{i\geq 1}$ from a prior sequence $(\mathrm{P}_i)_{i\geq 1}$. We also define a filtration $(\mathcal{F}_i)_{i\geq 1}$ adapted to $(z_i)_{i\geq 1}$. We reuse the following definitions extracted from HADDOUCHE and GUEDJ, 2022.

**Definitions** For all $i$, we denote by $\mathbb{E}_i[.]$ the conditional expectation $\mathbb{E}[. \mid \mathcal{F}_i]$.
A *stochastic kernel* from $\cup_{m=1}^{\infty}\mathcal{Z}^m$ to $\mathcal{H}$ is defined as a mapping $Q : \cup_{m=1}^{\infty}\mathcal{Z}^m \times \Sigma_{\mathcal{H}} \to [0,1]$ where (i) For any $B \in \Sigma_{\mathcal{H}}$, the function $S \mapsto Q(S,B)$ is measurable, (ii) For any $\mathcal{S}$, the function $B \mapsto Q(S,B)$ is a probability measure over $\mathcal{H}$.
We also say that a sequence of stochastic kernels $(P_i)_{i\geq 1}$ is an *online predictive sequence* if (i) for all $i \geq 1, S \in \cup_{m=1}^{\infty}\mathcal{Z}^m, P_i(S,.)$ is $\mathcal{F}_{i-1}$ measurable and (ii) for all $i \geq 2$, $P_i(S,.) \gg P_1(S,.)$.
**Main result.** We now state the main theorem of this section, which extends the remits of the Online PAC-Bayes framework to the case of unbounded losses.

**Theorem 3.7.1.** For any distribution over the (countable) dataset $\mathcal{S}$, any $\lambda > 0$ and any online predictive sequence (used as priors) $(P_i)_{i\geq 1}$, we have with probability at least $1-\delta$ over the sample $S \sim \mu$, the following, holding for the data-dependent measures $P_{i,S} := P_i(S,.)$ any posterior sequence $(Q_i)_{i\geq 1}$ and any $m \geq 1$:

$$\sum_{i=1}^{m} \mathbb{E}_{h_i\sim Q_i}\left[\mathbb{E}[\ell(h_i,z_i) \mid \mathcal{F}_{i-1}]\right] \leq \sum_{i=1}^{m} \mathbb{E}_{h_i\sim Q_i}\left[\ell(h_i,z_i)\right] + \frac{\lambda}{2}\sum_{i=1}^{m} \mathbb{E}_{h_i\sim Q_i}\left[\hat{V}_i(h_i,z_i) + V_i(h_i)\right] + \sum_{i=1}^{m} \frac{\mathrm{KL}(Q_i\|P_{i,S})}{\lambda} + \frac{\log(1/\delta)}{\lambda}.$$

With for all $i$, $\hat{V}_i(h_i,z_i) = (\ell(h_i,z_i) - \mathbb{E}_{i-1}[\ell(h_i,z_i)])^2$ is the empirical variance at time $i$ and $V_i(h_i) = \mathbb{E}_{i-1}[\hat{V}(h_i,z_i)]$ is the true conditional variance.

Proof lies in Section 3.7.1.

**Analysis of the bound.** This bound is, to our knowledge, the first Online PAC-Bayes bound in literature holding for unbounded losses. It is semi-empirical as the variance and empirical variance terms have theoretical components. However, these terms can be controlled with assumptions on conditional second-order moments and not on exponential ones (as made in HADDOUCHE and GUEDJ, 2022 where the bounded loss assumption was used to obtain conditional subgaussianity). To emphasise our point, we consider as in Section 2.2.3 the case of the quadratic loss $\ell(h,z) = (h-z)^2$. Here, we only need to assume that our data have a finite variance if we restrict our posteriors to have both bounded means and variance. Also the meaning of the online predictive sequence $P_i$ is that we must be able to design properly a sequence of priors before drawing our data, this can be for instance an online algorithm whihc generate a prior distribution from past data at each time step.

Finally, we note that if we assume being able to bound simultaneaously all condtional means and variance (which is strictly less restrictive than bounding the loss),then Th. 3.7.1 suggests a new online learning objective which is an online counterpart to Equation (2.4).

$$\forall i \geq 1 \; \hat{Q}_{i+1} = \underset{Q \in \mathcal{M}_1^+(\mathcal{H})}{\operatorname{argmin}} \; \mathbb{E}_{h_i \sim Q} \left[ \ell(h_i, z_i) + \frac{\lambda}{2} \ell(h_i, z_i)^2 \right] + \frac{\mathrm{KL}(Q \| P_{i,S})}{\lambda} \tag{3.8}$$

**Comparison with literature.** Our most natural comparison point is Theorem 2.3 of HADDOUCHE and GUEDJ, 2022 (re-stated in appendix C.1). We claim that Theorem 3.7.1 is a strict improvement of their result on various sides described below.

- If we assume our loss to be bounded, then we can upper bound our empirical/theoretical variance terms to recover exactly HADDOUCHE and GUEDJ (2022, Theorem 2.3). Our bound can then be seen as a strict extension of theirs and shows that bounding order two moments is a sufficient condition to perform online PAC-Bayes: subgaussianity induced by boundedness is not necessary even when our data are non iid.

- Another crucial point lies on the range of our result which holds with high probability for any countable posterior sequence $(Q_i)_{i\geq 1}$, any time $m$ and the priors $(P_{i,S})_{i\geq 1}$. This is far much general than HADDOUCHE and GUEDJ (2022, Theorem 2.3) which holds only for a single $m$ and a single posterior sequence $(Q_{i,S})_{i=1..m}$. This happens because in HADDOUCHE and GUEDJ (2022), the change of measure inequality has not been exploited: they used a preliminary theorem from RIVASPLATA *et al.* (2020) which holds for a single (data-dependent) prior/posterior couple. This preliminary theorem already involved Markov's inequality which forced the authors to assume conditionnal subgaussianity to deal

with an exponential moment. On the contrary, we exploited the fact that our online predictive sequence was history-dependent to use the change of measure inequality at any time step and control an exponential supermartingale through Ville's inequality.

- In HADDOUCHE and GUEDJ (2022, Eq. 1), an OPB algorithm is given by their upper bound. This works because their associated learning objective admits a close form (Gibbs posterior) which matches the fact their bound hold for a single posterior sequence. Because our bound holds uniformly on all posteriors, it is now legitimate to restrict their algorithms to any parametric class of distributions and perform any optimisation algorithm to obtain a surrogate of the best candidate.

Online PAC-Bayes as presented in HADDOUCHE and GUEDJ (2022) relies on a conditional subgaussiannity assumption to control an exponential moment. They did not exploit a martingale-type structure to do so. Our supermartingale approach has proven to be well suited to Online PAC-Bayes as we provided atheorem valid for unbounded losses holding simultaneously on all posteriors: two points which have not been reached in HADDOUCHE and GUEDJ (2022).

### 3.7.1 Proof of Theorem 3.7.1

*Proof.* We fix $m \geq 1$, $\mathcal{S}$ a countable dataset and $(P_i)_{i\geq 1}$ an online predictive sequence. We aim to design a $m$-tuple of probabilities. Thus, our predictor set of interest is $\mathcal{H}_m := \mathcal{H}^{\otimes m}$ and then, our predictor $h$ is a tuple $(h_1, .., h_m) \in \mathcal{H}$.
Our goal is to apply the change of measure inequality on $\mathcal{H}_m$ to a specific function $f_m$ inspired from Lemma 2.1.2. We define this function below, for any sample $\mathcal{S}$ and any predictor $h^m = (h_1, ..., h_m)$

$$f_m(S, h^m) := \sum_{i=1}^{m} \lambda X_i(h_i, z_i) - \frac{\lambda^2}{2} \sum_{i=1}^{m} (\hat{V}_i(h_i, z_i) + V_i(h_i)),$$

where $X_i(h_i, z_i) = \mathbb{E}_{i-1}[\ell(h_i, z_i)] - \ell(h_i, z_i)$. Notice that for fixed $h$, the sequence $(f_m(\mathcal{S}, h))_{m\geq 1}$ is a supermartingale according to Lemma 2.1.2.
Now for a given posterior tuple $Q_1, ...Q_m$ we define $Q = Q_1 \otimes ... \otimes Q_m$ and also $P_S^m = P_{1,S} \otimes ... \otimes P_{m,S}$. We can now properly apply the change of measure

inequality for any $m$:

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim Q_i}[\lambda X_i(h_i, z_i) - \frac{\lambda^2}{2}(\hat{V}_i(h_i, z_i) + V_i(h_i))] = \mathbb{E}_{h^m \sim Q}\left[f_m(S, h^m)\right] \\ \leq \mathrm{KL}(Q, P_S^m) + \log\left(\mathbb{E}_{h^m \sim P_S^m} \exp(f_m(S, h^m))\right).$$

Noticing that $\mathrm{KL}(Q, P_S^m) = \sum_{i=1}^m \mathrm{KL}(Q_i, P_{i,S})$, the only remaining term to deal with is the exponential rv.
To do so we prove the following lemma:

**Lemma 3.7.1.** The sequence $(M_m := \mathbb{E}_{h^m \sim P_S^m} \exp(f_m(S, h^m))_{m \geq 1}$ is a non-negative supermartingale.

*Proof.* We fix $m \geq 1$ and we recall that for any $i$, $P_{i,S}$ is $\mathcal{F}_{i-1}$-measurable. We show that $\mathbb{E}_{m-1}[M_m] \leq M_{m-1}$. We first recover $M_{m-1}$ from $\mathbb{E}_{m-1}[M_m]$.

$$\begin{aligned}
\mathbb{E}_{m-1}[M_m] &= \mathbb{E}_{m-1}\left[\mathbb{E}_{h^m\sim P_S^m} \exp(f_m(S,h^m)\right] \\
&= \mathbb{E}_{m-1}\left[\mathbb{E}_{h_1,..,h_m\sim P_{1,S}\otimes...\otimes P_{m,S}} \exp(f_m(S,h^m)\right] \\
&= \mathbb{E}_{m-1}\left[\mathbb{E}_{h_1,..,h_m\sim P_{1,S}\otimes...\otimes P_{m,S}}\left[\Pi_{i=1}^m \exp\left(\lambda X_i(h_i,z_i) - \frac{\lambda^2}{2}(\hat{V}_i(h_i,z_i)+V_i(h_i))\right)\right]\right] \\
&= M_{m-1}\mathbb{E}_{m-1}\left[\mathbb{E}_{h_m\sim P_{m,S}}\left[\exp\left(\lambda X_m(h_m,z_m) - \frac{\lambda^2}{2}(\hat{V}_m(h_m,z_m)+V_m(h_m))\right)\right]\right].
\end{aligned}$$

The last line holding because $P_S^{m-1} = P_{1,S}\otimes...\otimes P_{m-1,S}$ is $\mathcal{F}_{m-1}$ measurable. Now we exploit the fact that $P_{m,S}$ is $\mathcal{F}_{m-1}$ measurable to apply a conditional Fubini lemma stated in Haddouche and Guedj (2022, Lemma D.3). We have:

$$\begin{aligned}
&\mathbb{E}_{m-1}\left[\mathbb{E}_{h_m\sim P_{m,S}}\left[\exp\left(\lambda X_m(h_m,z_m) - \frac{\lambda^2}{2}(\hat{V}_m(h_m,z_m)+V_m(h_m))\right)\right]\right] \\
&= \mathbb{E}_{h_m\sim P_{m,S}}\left[\mathbb{E}_{m-1}\left[\exp\left(\lambda X_m(h_m,z_m) - \frac{\lambda^2}{2}(\hat{V}_m(h_m,z_m)+V_m(h_m))\right)\right]\right].
\end{aligned}$$

Now we can apply Lemma 2.1.2 for any $h_m \in \mathcal{H}$ with $\Delta M_m = X_m(h_m,z_m), \Delta[M]_m = \hat{V}(h_m,z_m)$ and $\Delta\langle M\rangle_m = V_m(h_m)$. We then have for all $h_m \in \mathcal{H}$:

$$\mathbb{E}_{m-1}\left[\exp\left(\lambda X_m(h_m,z_m) - \frac{\lambda^2}{2}(\hat{V}_m(h_m,z_m)+V_m(h_m))\right)\right] \leq 1.$$

Thus $\mathbb{E}_{m-1}[M_m] \leq M_{m-1}$, this concludes the lemma's proof. ■

Now we can apply Ville's inequality which implies that with probability at least $1-\delta$, for any $m \geq 1$:

$$\mathbb{E}_{h^m\sim P_S^m} \exp(f_m(S,h^m)) \leq \frac{1}{\delta}.$$

Thus we have with probability at least $1-\delta$, for any posterior sequence $(Q_i)_{i\geq 1}$, the data-dependent measures $P_{1,S},...,P_{m,S}$ and any $m \geq 1$:

$$\sum_{i=1}^{m} \mathbb{E}_{h_i \sim Q_i} \left[ \lambda X_i(h_i, z_i) - \frac{\lambda^2}{2} (\hat{V}_i(h_i, z_i) + V_i(h_i)) \right] \leq \sum_{i=1}^{m} \mathrm{KL}(Q_i, P_{i,S}) + \log\left(\frac{1}{\delta}\right).$$

Re-organising the terms in this bound and dividing by $\lambda$ concludes the proof.

■

# 4 Mitigating Initialisation Impact through Flat Minima: Fast Rates for Small Gradients

**This chapter is based on the following paper**

TODO

## Contents



**Abstract**

This is the PLS paper, precise that the supermartingales bounds are richer than simply recovering classical batch guarantees: we can incorporate gradient norms, which explains generalisation when a flat minima is reached.

## 4.1 Introduction

# 5 Wasserstein PAC-Bayes Learning: Exploiting Optimisation Guarantees to Explain Generalisation

**This chapter is based on the following papers**

Maxime Haddouche and Benjamin Guedj. Wasserstein PAC-Bayes Learning: A Bridge Between Generalisation and Optimisation. *arXiv*. abs/2304.07048. (2023)
Paul Viallard, Maxime Haddouche, Umut Simsekli, and Benjamin Guedj. Learning via Wasserstein-Based High Probability Generalisation Bounds. *Advances in Neural Information Processing Systems (NeurIPS)*. (2023b)

## Contents



**Abstract**

Put WPB here, precise that, when the prior is seen as the learning goal, it is possible for a certain optimisation algorithm to directly incorporate sound geometric optimisation guarantee into a generalisation bound, trading the hope to reach a flat minima with a sound convergence guarantees. However, this comes at the cost of the explicit impact of the dimension. Also put the paper with Paul(batch bounds) as a supplementary content.

## 5.1 Introduction

# 6 Wasserstein PAC-Bayes in practice: Learning Algorithms with Guarantees for Deterministic Predictors

**This chapter is based on the following paper**

TODO

## Contents



**Abstract**

This is the Wasserstein paper with Paul: practical transition to PAC-Bayes with both batch and online approach. Pb: the batch approach use data-dependent priors: does not fit the story as it is an information theoretic wiw and should be precised.

## 6.1 Introduction

# Some Mathematical Tools

# A

## A.1 Jensen's Inequality

**Theorem A.1.1** (Jensen's Inequality)**.** Let $X$ a random variable following a probability distribution $\nu$ with $f$ a real-valued measurable convex function, we have

$$f\left(\mathop{\mathbb{E}}_{X\sim\nu}[X]\right) \leq \mathop{\mathbb{E}}_{X\sim\nu}\Big[f\left(X\right)\Big].$$

*Proof.* Since $f()$ is a convex function, the following inequality holds, *i.e.*, we have

$$\forall X', \quad a\left(X' - \mathop{\mathbb{E}}_{X\sim\nu}[X]\right) \leq f(X') - f\left(\mathop{\mathbb{E}}_{X\sim\nu}[X]\right),$$

where $a$ is the tangent's slope. By taking the expectation to both sides of the inequality, we have

$$\underbrace{a\left(\mathop{\mathbb{E}}_{X\sim\nu}[X] - \mathop{\mathbb{E}}_{X\sim\nu}[X]\right)}_{=0} \leq \mathop{\mathbb{E}}_{X\sim\nu}[f(X)] - f\left(\mathop{\mathbb{E}}_{X\sim\nu}[X]\right).$$

Hence, by rearranging the terms, we prove the claimed result. ■

## A.2 Markov's Inequality

**Theorem A.2.1** (Markov's Inequality)**.** Let $X$ a non-negative random variable following a probability distribution $\nu$ and $\delta > 0$, we have

$$\mathop{\mathbb{P}}_{X\sim\nu}[X \geq \delta] \leq \frac{\mathbb{E}_{X\sim\nu}[X]}{\delta}.$$

*Proof.* First of all, remark that we have the following inequality for any $X$

$$\delta \mathbb{1}[X \geq \delta] \;\leq\; X \mathbb{1}[X \geq \delta] \;\leq\; X. \tag{A.1}$$

Indeed, on the one hand, if $X < \delta$, $\mathbb{1}[X \geq \delta] = 0$, the inequality holds trivially. On the other hand, if $X \geq \delta$, $\mathbb{1}[X \geq \delta] = 1$ and the inequality becomes $\delta \leq X$, which is true. By taking the expectation of Equation (A.1), we have

$$\mathop{\mathbb{E}}_{X \sim \nu}\Big[\delta \mathbb{1}[X \geq \delta]\Big] \leq \mathop{\mathbb{E}}_{X \sim \nu}\Big[X\Big].$$

From the fact that the expectation of a constant is the constant and by definition of the probability, we have

$$\delta \mathop{\mathbb{P}}_{X \sim \nu}[X \geq \delta] \leq \mathop{\mathbb{E}}_{X \sim \nu}\Big[X\Big] \quad \iff \quad \mathop{\mathbb{P}}_{X \sim \nu}[X \geq \delta] \leq \frac{\mathbb{E}_{X \sim \nu}[X]}{\delta},$$

which is the desired result. ■

## A.3 Ville's Inequality

**Lemma A.3.1** (Ville's maximal inequality for supermartingales)**.** Let $(\mathcal{F}_t)$ be a filtration and $(Z_t)$ a non-negative super-martingale satisfying $Z_0 = 1$ a.s. If $Z_t$ is adapted to $\mathcal{F}_t$ and $\mathbb{E}[Z_t \mid \mathcal{F}_{t-1}] \leq Z_{t-1}$ a.s., $t \geq 1$, then, for any $0 < \delta < 1$, it holds

$$\mathbb{P}\left(\exists T \geq 1 : Z_T > \delta^{-1}\right) \leq \delta.$$

*Proof.* We apply the optional stopping theorem (Durrett, 2019, Thm 4.8.4) with Markov's inequality defining the stopping time $i = \inf\{t > 1 :\; Z_t > \delta^{-1}\}$ so that

$$\mathbb{P}\left(\exists t \geq 1 : Z_t > \delta^{-1}\right) = \mathbb{P}\left(Z_i > \delta^{-1}\right) \leq \mathbb{E}[Z_i]\,\delta \leq \mathbb{E}[Z_0]\,\delta \leq \delta.$$

■

# Additional Background

# B

## B.1 Online Learning

## B.2 Wasserstein distances and optimisation on distributions spaces

## B.3 Differential privacy

## B.4 Log-Sobolev and Poincaré Inequalities

# Appendix of Chapter 2

C

## C.1 Some PAC-Bayesian background

We present below an immediate corollary of Seldin *et al.* (2012a, Thm 2.1) where we upper bounded the cumulative by an empirical quantity (the sum of squared upper bound of the martingale difference sequence).

**Theorem C.1.1** (Seldin *et al.*, 2012a, Theorem 2.1)**.** Let $\{C_1, C_2, \ldots\}$ be an increasing sequence set in advance, such that $|X_i(S_i, h)| \leq C_i$ for all $S_i, h$ with probability 1. Let $\{P_1, P_2, \ldots\}$ be a sequence of data-free prior distributions over $\mathcal{H}$. Let $(\lambda_i)_{i\geq 1}$ be a sequence of positive numbers such that

$$\lambda_m \leq \frac{1}{C_m}.$$

Then with probability $1-\delta$ over $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1}$, for all $m \geq 1$, any posterior $\mathrm{Q}$ over $\mathcal{H}$,

$$|M_m(Q)| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}_m) + 2\log(m+1) + \log\frac{2}{\delta}}{\lambda_m} + (e-2)\lambda_m V_m(\mathrm{Q}),$$

where $V_m(\mathrm{Q})$ is defined in appendix C.2.1.
Furthermore, if we bound the variance term, we would have:

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}_m) + 2\log(m+1) + \log\frac{2}{\delta}}{\lambda_m} + (e-2)\lambda_m \sum_{i=1}^{m} C_i^2.$$

Below, we use the definitions introduced in Section 2.2.3. We study here a particular case of Alquier *et al.*, 2016 for bounded losses which are especially subgaussian thanks to Hoeffding's lemma.

**Theorem C.1.2** (Adapted from Alquier *et al.*, 2016, Theorem 4.1)**.** Let $m > 0$,$\mathcal{S}_m = (\mathbf{z}_1, ..., \mathbf{z}_m)$ be an *i.i.d.* sample from the same law $\mu$. For any data-free prior $\mathrm{P}$, for any loss function $\ell$ bounded by $K$, any $\lambda > 0, \delta \in ]0;1[$, one has with probability $1-\delta$ for any posterior $Q \in \mathcal{M}_1(\mathcal{H})$

$$\mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}(h)] \leq \mathbb{E}_{h\sim\mathrm{Q}}[\hat{\mathsf{R}}_{\mathcal{S}_m}(h)] + \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(1/\delta)}{\lambda} + \frac{\lambda K^2}{2m}.$$

**Theorem C.1.3** (Haddouche *et al.*, 2021, Theorem 3)**.** Let the loss $\ell$ be $\mathrm{HYPE}(K)$ compliant. For any $\mathrm{P} \in \mathcal{M}(\mathcal{H})$ with no data dependency, for any $\alpha \in \mathbb{R}$ and for any $\delta \in [0,1]$, we have with probability at least $1-\delta$ over size-$m$ samples S, for any Q

$$\mathbb{E}_{h\sim \mathrm{Q}}\left[\mathsf{R}(h)\right] \leq \mathbb{E}_{h\sim \mathrm{Q}}\left[\hat{\mathsf{R}}_{\mathcal{S}_m}(h)\right] + \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log\left(\frac{1}{\delta}\right)}{m^{\alpha}} + \frac{1}{m^{\alpha}}\log\left(\mathbb{E}_{h\sim \mathrm{P}}\left[\exp\left(\frac{K(h)^2}{2m^{1-2\alpha}}\right)\right]\right).$$

## C.2 Extensions of previous results

Here we gather several corollaries of our main result in order to show how our Theorem 2.2.1 extends the validity of some classical results in the literature. More precisely we show that our result extends (up to numerical factors) the PAC-Bayes Bernstein inequality of Seldin *et al.* (2012a). Then, going back to the bounded case, we generalise a result from Catoni (2007) reformulated in Alquier *et al.* (2016) and we also show how our work strictly improves on the bound of Haddouche *et al.* (2021).

### C.2.1 Extension of the PAC-Bayes Bernstein inequality

Here we rename two terms for consistency with Theorem 2.1 of Seldin *et al.* (2012a) (see Theorem C.1.1). For a martingale $M_m(h) = \sum_{i=1}^m X_i(\mathcal{S}_i, h)$, we define, at time $m$, *empirical cumulative variance* to be $\hat{V}_m(h) = [M]_m(h) = \sum_{i=1}^m X_i(\mathcal{S}_i,h)^2$ and the *cumulative variance* as $V_m(h) = \langle M\rangle_m(h) = \sum_{i=1}^m \mathbb{E}_{i-1}[X_i(\mathcal{S}_i,h)^2]$.
We provide below a corollary containing two bounds: the first one being a straightforward corollary of Th. 2.2.1, the second being valid for bounded martingales and formally close to Theorem 2.1 of Seldin *et al.* (2012a).

**Corollary C.2.1.** Let $\{\mathrm{P}_1, \mathrm{P}_2, \ldots\}$ be a sequence of data-free prior distributions over $\mathcal{H}$. Let $(\lambda_i)_{i\geq 1}$ be a sequence of positive numbers. Then the following holds with probability $1-\delta$ over $\mathcal{S} = (\mathbf{z}_i)_{i\geq 1}$: for any tuple $(m, \lambda_k, \mathrm{P}_k)$ with $m, k \geq 1$, any posterior Q over $\mathcal{H}$,

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}_k) + 2\log(k+1) + \log(2/\delta)}{\lambda_k} + \frac{\lambda_k}{2}\left(\hat{V}_m(\mathrm{Q}) + V_m(\mathrm{Q})\right), \tag{C.1}$$

with $\hat{V}_m(\mathrm{Q}) = \mathbb{E}_{h\sim\mathrm{Q}}[\hat{V}_m(h)], V_m(\mathrm{Q}) = \mathbb{E}_{h\sim\mathrm{Q}}[V_m(h)]$. Furthermore, if we assume that for any $i$, there exists $C_i > 0$ such that $|X_i(\mathcal{S}_i,h)| \leq C_i$ for all $\mathcal{S}_i, h$ then we

have the following corollary: with probability $1-\delta$ over $S$, for any tuple $(m, \lambda_m, \mathrm{P}_m)$ $m \geq 1$, any posterior $\mathrm{Q}$,

$$|M_m(Q)| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}_m) + 2\log(m+1) + \log(2/\delta)}{\lambda_m} + \lambda_m \sum_{i=1}^{m} C_i^2. \tag{C.2}$$

The proof is deferred to appendix C.3. Note that Eq. (C.1) holds uniformly on all tuples $\{(\lambda_k, \mathrm{P}_k, m) \mid k \geq 1, m \geq 1\}$ while Eq. (C.2), as well as Theorem 2.1 of Seldin *et al.* (2012a) holds uniformly on the tuples $\{(\lambda_m, \mathrm{P}_m, m) \mid m \geq 1\}$ which is a strictly smaller collection. Hence our approach gives guarantees for a larger event with the same confidence level.
Furthermore, Theorem 2.1 of Seldin *et al.* (2012a) involves the cumulative variance $V_m(\mathrm{Q})$ (and not its empirical counterpart). Because this term is theoretical, we bound it in Th. C.1.1 by $\sum_{i=1}^{m} C_i^2$ which is supposedly empirical. In this context, Eq. (C.2), recovers nearly exactly the bound of Seldin *et al.*, 2012a with the transformation of a factor $(e-2)$ into $1$. Notice also that Eq. (C.2) stands with no assumption on the range of the $\lambda_i$, which is not the case in Th. C.1.1.
Finally, we stress two fundamental differences between our work and the one of Seldin *et al.* (2012a). First, we replace Markov's inequality by Ville's inequality; second, we exploited the exponential inequality of Lemma 2.1.2 instead of the Bernstein inequality. These allow for results for unbounded martingales for all $m$ simultaneously.

## C.2.2 Extensions of learning theory results

### C.2.2.1 A general result for bounded losses

We use definitions from Section 2.2.3 and provide a corollary of our main result when the loss is bounded by a positive constant $K > 0$. We assume our data are iid.

**Corollary C.2.2.** For any data-free prior $P \in \mathcal{M}(\mathcal{H})$, any $\lambda > 0$ the following holds with probability $1-\delta$ over the sample $S = (z_i)_{i \in \mathbb{N}}$, for all $m \in \mathbb{N}/\{0\}$, $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$

$$\left| \mathbb{E}_{h \sim \mathrm{Q}}[\mathsf{R}(h)] - \mathbb{E}_{h \sim \mathrm{Q}}\left[\hat{\mathsf{R}}_{\mathcal{S}_m}(h)\right] \right| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(2/\delta)}{\lambda m} + \lambda K^2.$$

We also have the local bound: for any $m \geq 1$, with probability $1-\delta$ over $S$, for all $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$

$$\mathbb{E}_{h \sim \mathrm{Q}}[\mathsf{R}(h)] \leq \mathbb{E}_{h \sim \mathrm{Q}}\left[\hat{\mathsf{R}}_{\mathcal{S}_m}(h)\right] + \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(2/\delta)}{\lambda} + \frac{\lambda K^2}{m}.$$

The proof is deferred to appendix C.3. Remark that the second bound of Corollary C.2.2 is exactly the Catoni bound stated in ALQUIER *et al.* (2016) (see Theorem C.1.2 in Appendix C.1) up to a numerical factor of $2$.
The first bound is, to our knowledge, the first PAC-Bayesian bound for bounded losses holding uniformly (for a given parameter $\lambda$) on the choice of $Q, m$ and thus extends the scope of Catoni's bound which holds for a single $m$ with high probability. Indeed, if we want for instance Theorem C.1.2 to hold for any $i \in \{1..m\}$, we then have to take an union bound on $m$ events which turns the term $\log(1/\delta)$ into $\log(m/\delta)$ (but with the benefit of holding for $m$ parameters $\lambda_1, ..., \lambda_m$). This point is common to the most classical PAC-Bayesian bounds (including McAllester and Catoni's ones (1.3), (1.4)) and impeach us to have a bound uniformly on all $m \in \mathbb{N}/\{0\}$ as $\log(m)$ goes to infinity asymptotically.

### C.2.2.2 An extension of Haddouche *et al.* (2021)

We now focus on the work of HADDOUCHE *et al.* (2021) which provides general PAC-Bayesian bounds for unbounded losses. Their theorems hold for iid data and under the so-called *HYPE* (for HYPothesis-dependent rangE) condition. It states that a loss function $\ell$ is *HYPE*$(K)$ compliant if there exists a function $K : \mathcal{H} \to \mathbb{R}^+$ (supposedly accessible) such that $\forall z \in \mathcal{Z}, \ell(h, \mathbf{z}) \leq K(h)$. We provide Corollary C.2.3 to compare ourselves with their main result (stated in Theorem C.1.3 for convenience).

**Corollary C.2.3.** For any data-free prior $\mathrm{P} \in \mathcal{M}(\mathcal{H})$, any loss function $\ell$ being *HYPE*$(K)$ compliant, any $\alpha \in [0, 1], m \geq 1$, the following holds with probability $1 - \delta$ over the sample $\mathcal{S} = (\mathbf{z}_i)_{i \in \mathbb{N}}$, for all $\mathrm{Q} \in \mathcal{M}(\mathcal{H})$

$$\mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}(h)] \leq \mathbb{E}_{h\sim\mathrm{Q}}\left[\frac{1}{m}\sum_{i=1}^{m}\left(\ell(h,\mathbf{z}_i) + \frac{1}{2m^{1-\alpha}}\ell(h,\mathbf{z}_i)^2\right)\right] + \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(1/\delta)}{m^\alpha} + \frac{1}{2m^{1-\alpha}}\mathbb{E}_{h\sim\mathrm{Q}}[K^2(h)].$$

*Proof.* The proof is a straightforward application of Th. 2.2.2 by fixing $m \geq 1$ choosing $\lambda = m^{\alpha-1}$ (thus we localise Theorem 2.2.2 to a single $m$), and bounding $\mathrm{Quad}(h)$ by $K^2(h)$. ■

The main improvement of our bound over Theorem C.1.3 is that we do not have to assume the convergence of an exponential moment to obtain a non-trivial bound. Indeed, we transformed the (implicit) assumption $\mathbb{E}_{h\sim\mathrm{P}}\left[\exp\left(\frac{K(h)^2}{2m^{1-2\alpha}}\right)\right] < +\infty$ onto

$\mathbb{E}_{h\sim \mathrm{Q}}[K(h)^2] < +\infty$, which is significantly less restrictive. Furthermore, Theorem C.1.3 holds for a single choice of $m$ while ours still holds uniformly over all integers $m > 0$. Cor. C.2.3 also sheds new light on the *HYPE* condition. Indeed, in HADDOUCHE *et al.* (2021), $K$ only intervenes in an exponential moment involving the prior $\mathrm{P}$, while ours considers a second-order moment on $K$ implying the posterior $\mathrm{Q}$. The difference is major as $\mathbb{E}_{h\sim \mathrm{Q}}[K(h)^2]$ can be controlled by a wise choice of posterior. Thus it can be incorporated in our optimisation route, acting now as an optimisation constraint instead of an environment constraint.

# C.3 Proofs

## C.3.1 Proof of Th. 2.2.2

*Proof.* Let $\mathrm{P}$ a fixed data-free prior, set $(\mathcal{F}_i)_{i\geq 0}$ such that for all $i$, $\mathbf{z}_i$ is $\mathcal{F}_i$ measurable. We also set for any fixed $h \in \mathcal{H}, M_m(h) := \sum_{i=1}^m \ell(h, \mathbf{z}_i) - \mathsf{R}(h)$. Note that because data are *i.i.d.*, for any fixed $h$, the sequence $(M_m(h))_m$ is indeed a martingale. We set for any $m \geq 1, h \in \mathcal{H}$

$$[M]_m(h) = \sum_{i=1}^m \left(\ell(h, \mathbf{z}_i) - \mathsf{R}(h)\right)^2$$

and

$$\langle M\rangle_m(h) = \sum_{i=1}^m \mathbb{E}_{i-1}[\left(\ell(h, \mathbf{z}_i) - \mathsf{R}(h)\right)^2] = \sum_{i=1}^m \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\left(\ell(h, \mathbf{z}) - \mathsf{R}(h)\right)^2].$$

The last equality holds because data is assumed iid. Thus, we can apply Th. 2.2.1 to obtain with probability $1-\delta$

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(2/\delta)}{\lambda} + \frac{\lambda}{2}\left([M]_m(Q)^2 + \langle M\rangle_m(Q)^2\right).$$

Now, we notice that $|M_m(\mathrm{Q})| = m|\mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}(h) - \hat{\mathsf{R}}_{\mathcal{S}_m}(h)]|$ and that for any $m, h$, because $\ell$ is nonnegative

$$\begin{aligned}[M]_m(h) + \langle M\rangle_m(h) &= \sum_{i=1}^m (\ell(h, \mathbf{z}_i) - \mathsf{R}(h))^2 + \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\left(\ell(h, \mathbf{z}) - \mathsf{R}(h)\right)^2] \\ &\leq \sum_{i=1}^m \ell(h, \mathbf{z}_i)^2 + \mathsf{R}(h)^2 + \mathbb{E}_{\mathbf{z}\sim\mathcal{D}}[\ell(h, \mathbf{z})^2] - \mathsf{R}(h)^2.\end{aligned}$$

Thus integrating over $h$ gives:

$$[M]_m(Q) + \langle M \rangle_m(Q) \leq \sum_{i=1}^{m} \mathbb{E}_{h\sim \mathrm{Q}}[\ell(h, \mathbf{z}_i)^2] + m\mathbb{E}_{h\sim \mathrm{Q}}[\mathrm{Quad}(h)].$$

Then dividing by $m$ and applying the last inequality gives

$$\mathbb{E}_{h\sim \mathrm{Q}}[\mathsf{R}(h)] \leq \mathbb{E}_{h\sim \mathrm{Q}}\left[\frac{1}{m}\sum_{i=1}^{m}\left(\ell(h, \mathbf{z}_i) + \frac{\lambda}{2}\ell(h, \mathbf{z}_i)^2\right)\right] + \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(2/\delta)}{\lambda m} + \frac{\lambda}{2}\mathbb{E}_{h\sim \mathrm{Q}}[\mathrm{Quad}(h)].$$

This concludes the proof. ■

## C.3.2 Proof of Th. 2.3.1

*Proof.* Let $(\lambda_m)_{i\geq 1}$ be a countable sequence of positive scalars. As precised earlier $M_m(a) := m\left(\hat{\Delta}_m(a) - \Delta(a)\right)$ is a martingale. We then apply Theorem 2.2.1 with the uniform prior ($\forall a, P(a) = \frac{1}{K}$) and $\lambda = \lambda_m$ (depending possibly on $m$): with probability $1 - \delta/2$, for any tuple $(m, \lambda_m)$ with $m \geq 1$, any posterior $\mathrm{Q}$,

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}) + 2 + \log(4/\delta)}{\lambda_m} + \frac{\lambda_m}{2}\left(\hat{V}_m(\mathrm{Q}) + V_m(\mathrm{Q})\right).$$

Notice that for any $\mathrm{Q}$, $\mathrm{KL}(\mathrm{Q}, \mathrm{P}) \leq \log(K)$ by concavity of the log. We now fix an horizon $M > 0$, we then have in particular, with probability $1 - \delta/2$: for any posterior $\mathrm{Q}$,

$$|M_m(Q)| \leq \frac{\log(K) + 2\log(k+1) + \log(4/\delta)}{\lambda_k} + \frac{\lambda_m}{2}\left(\hat{V}_m(\mathrm{Q}) + V_m(\mathrm{Q})\right).$$

We now have to deal with $V_k(\mathrm{Q}), \hat{V}_k(\mathrm{Q})$ for all $k \leq m$. To do so, we propose the two following lemmas.

> **Lemma C.3.1.** For all $m \geq 1$, $a \in \mathcal{A}$, $V_m(a) \leq \frac{2Cm}{\varepsilon_m}$. Then, we have for any $m, Q$, $V_m(\mathrm{Q}) \leq \frac{2Cm}{\varepsilon_m}$.

*Proof.* We have

$$\begin{aligned}
V_t(a) &= \sum_{i=1}^{m} \mathbb{E}\left[\left(\left[R_i^{a^*} - R_i^a\right] - \Delta(a)\right)^2 \mid \mathcal{F}_{i-1}\right] \\
&= \sum_{i=1}^{m} \mathbb{E}\left[\left(R_i^{a^*} - R_i^a\right)^2 \mid \mathcal{F}_{i-1}\right] - m\Delta(a)^2 \\
&\leq \sum_{i=1}^{m} \mathbb{E}\left[\left(R_i^{a^*} - R_i^a\right)^2 \mid \mathcal{F}_{i-1}\right] \\
&= \sum_{i=1}^{m} \mathbb{E}\left[\mathbb{E}_{A_i\sim\pi_i}\mathbb{E}_{R_i}\left[\frac{1}{\pi_i(a^*)^2}R_i(a^*)^2\mathbb{1}(A_i = a^*) + \frac{1}{\pi_i(a)^2}R_i(a)^2\mathbb{1}(A_i = a)\right] \mid \mathcal{F}_{i-1}\right].
\end{aligned}$$

The last line holding because $R_i$ is independent of $\mathcal{F}_{i-1}$, $A_i$ is independent of $R_i$ and $\pi$ is $\mathcal{F}_{i-1}$ measurable. We now use that for all $i, a$, $\mathbb{E}_{R_i}[R_i(a)^2] \leq C$

$$\begin{aligned}
&= \sum_{i=1}^{m} \mathbb{E}\left[\mathbb{E}_{A_i\sim\pi_i}\left[\frac{1}{\pi_i(a^*)^2}C\mathbb{1}(A_i = a^*) + \frac{1}{\pi_i(a)^2}C\mathbb{1}(A_i = a)\right] \mid \mathcal{F}_{i-1}\right] \\
&= \sum_{i=1}^{m} C\left(\frac{\pi_i(a)}{\pi_i(a)^2} + \frac{\pi_i(a^*)}{\pi_i(a^*)^2}\right) \\
&= \sum_{i=1}^{m} C\left(\frac{1}{\pi_i(a)} + \frac{1}{\pi_i(a^*)}\right) \\
&\leq \frac{2Cm}{\varepsilon_m}.
\end{aligned}$$

■

**Lemma C.3.2.** Let $m \geq 1$, with probability $1 - \delta/2$, for any posterior $\mathrm{Q}$, we have

$$\hat{V}_m(\mathrm{Q}) \leq \frac{4CKm}{\varepsilon_m\delta}.$$

*Proof.* Let $\mathrm{Q}$ a distribution over $\mathcal{A}$. Recall that

$$\begin{aligned}\hat{V}_m(\mathrm{Q}) &= \sum_{i=1}^{m} \left(R_i^{a^*} - R_i^a - [R(a^*) - R(a)]\right)^2 \\ &= \sum_{a\in\mathcal{A}} Q(a)\hat{V}_m(a).\end{aligned}$$

Notice that for any $a$, $(S\hat{M}_m^a)_m$ is a nonnegative random variable. We then apply Markov's inequality for any $a$, with probability $1-\delta/2K$

$$\hat{V}_m(a) \leq \frac{2K\mathbb{E}[\hat{V}_m(a)]}{\delta}.$$

Noticing that $\mathbb{E}[\hat{V}_m(a)] = \mathbb{E}[V_m(a)]$, we can apply lemma C.3.1 to conclude that

$$\mathbb{E}[\hat{V}_m(a)] \leq \frac{2Cm}{\varepsilon_m}.$$

Finally, taking an union bound on thoser events for all $a \in \mathcal{A}$ gives us, with probability $1-\delta/2$, for any posterior $\mathrm{Q}$

$$\begin{aligned}V_m(\mathrm{Q}) &\leq \sum_{a\in\mathcal{A}} Q(a)\hat{V}_m(a) \\ &\leq \sum_{a\in\mathcal{A}} Q(a)\frac{4CKm}{\varepsilon_m\delta} \\ &= \frac{4CKm}{\varepsilon_m\delta}.\end{aligned}$$

This concludes the proof. ■

To conclude, we apply lemmas C.3.1 and C.3.2 to get that with probability $1-\delta$, for any posterior $\mathrm{Q}$

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(4/\delta)}{\lambda_m} + \frac{Cm\lambda_m}{\varepsilon_m}\left(1+\frac{2K}{\delta}\right).$$

Dividing by $m$ and taking

$$\lambda_m = \sqrt{\frac{(\log(K)+\log(4/\delta))\,\varepsilon_m}{Cm\left(1+\frac{2K}{\delta}\right)}}$$

concludes the proof.

■

### C.3.3 Proof of Cor. C.2.1

*Proof.* Fix $\delta > 0$. For any pair $(\lambda_k, P_k), k \geq 1$, we apply Theorem 2.2.1 with

$$\delta_k := \frac{\delta}{k(k+1)} \geq \frac{\delta}{(k+1)^2}.$$

Notice that we have $\sum_{k=1}^{+\infty} \delta_k = \delta$. We then have with probability $1 - \delta_k$ over $S$, for any $m \geq 1$, any posterior $\mathrm{Q}$,

$$|M_m(\mathrm{Q})| \leq \frac{\mathrm{KL}(\mathrm{Q}, \mathrm{P}_k) + 2\log(k+1) + \log(2/\delta)}{\lambda_k} + \frac{\lambda_k}{2}\left(\hat{V}_m(\mathrm{Q}) + V_m(\mathrm{Q})\right).$$

Taking an union bound on all those event, gives the final result, valid with probability $1 - \delta$ over the sample $S$, for any any tuple $(m, \lambda_k, P_k)$ with $m, k \geq 1$, any posterior $\mathrm{Q}$ over $\mathcal{H}$. This gives Equation (C.1).
To obtain Eq. (C.2), we restrict the range of Eq. (C.1) to the tuples $(m, \lambda_m, P_m), m \geq 1$ (the restricted set of tuples where $k = m$) and we bound both $\hat{V}_m(\mathrm{Q}), V_m(\mathrm{Q})$ by $\sum_{i=1}^m C_i^2$ to conclude. ■

### C.3.4 Proof of Cor. C.2.2

*Proof.* For the first bound we start from the intermediary result Eq. (2.3) of Th. 2.2.1. Using the same marrtingale as in Th. 2.2.2 gives, for any $\eta \in \mathbb{R}$, holding with probability $1 - \delta$ for any $m > 0, Q \in \mathcal{M}(\mathcal{H})$

$$\eta\left(\sum_{i=1}^m \mathbb{E}_{h\sim\mathrm{Q}}[\ell(h, \mathbf{z}_i)] - m\mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}(h)]\right)$$
$$\leq \mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(1/\delta) + \frac{\eta^2}{2}\sum_{i=1}^m \mathbb{E}_{h\sim\mathrm{Q}}[\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)].$$

Taking $\eta = \pm\lambda$ with $\lambda > 0$ gives

$$\lambda m\left|\mathbb{E}_{h\sim\mathrm{Q}}[\mathsf{R}(h) - \hat{\mathsf{R}}_{\mathcal{S}_m}(h)]\right| \leq \mathrm{KL}(\mathrm{Q}, \mathrm{P}) + \log(1/\delta) \tag{C.3}$$
$$+ \frac{\lambda^2}{2}\sum_{i=1}^m \mathbb{E}_{h\sim\mathrm{Q}}[\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)]. \tag{C.4}$$

Finally, divide by $\lambda m$ and bound $\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)$ by $2K^2$ to conclude.
For the second bound, we start from Equation (C.3) again and for a fixed $m$, we now apply our result with $\lambda' = \lambda/m$. We then have for any $m$, with probability

$1-\delta$, for any $\mathrm{Q}$

$$\lambda \left| \mathbb{E}_{h\sim \mathrm{Q}}[\mathsf{R}(h) - \hat{\mathsf{R}}_{\mathcal{S}_m}(h)] \right| \leq \mathrm{KL}(\mathrm{Q},\mathrm{P}) + \log(1/\delta) + \frac{\lambda^2}{2m^2} \sum_{i=1}^{m} \mathbb{E}_{h\sim \mathrm{Q}}[\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)].$$

Finally, dividing by $\lambda$, bounding $\Delta[M]_i(h) + \Delta\langle M\rangle_i(h)$ by $2K^2$ and rearranging the terms concludes the proof. ■

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**Abstract.** In machine learning, a model is learned from data to solve a task automatically. In the supervised classification setting, the model aims to predict the label associated with an input. The model is learned using a limited number of examples, each consisting of an input and its associated label. However, the model's performance on the examples, computed by the empirical risk, does not necessarily reflect the performance on the task, which is represented by the true risk. Moreover, since it is not computable, the true risk is upper-bounded by a generalization bound that mainly depends on two quantities: the empirical risk and a complexity measure. One way to learn a model is to minimize a bound by a type of algorithm called self-bounding. PAC-Bayesian bounds are well suited to the derivation of this type of algorithm. In this context, the first contribution consists in developing self-bounding algorithms that minimize PAC-Bayesian bounds to learn majority votes. If these bounds are well adapted to majority votes, their use for other models becomes less natural. To overcome this difficulty, a second contribution focuses on the disintegrated PAC-Bayesian bounds that are natural for more general models. In this framework, we provide the first empirical study of these bounds. In a third contribution, we derive bounds that allow us to incorporate complexity measures defined by the user.

**Keywords.** Machine Learning, Generalization, PAC-Bayesian Bound, Disintegrated PAC-Bayesian Bound, Self-Bounding Algorithm, Majority Vote, Neural Network, Complexity Measure.

**Résumé.** En apprentissage automatique, un modèle est appris à partir de données pour résoudre une tâche de manière automatique. Dans le cadre de la classification supervisée, le modèle vise à prédire la classe associée à une entrée. Le modèle est appris à l'aide d'un nombre limité d'exemples, chacun étant constitué d'une entrée et de sa classe associée. Cependant, la performance du modèle sur les exemples, calculée par le risque empirique, ne reflète pas nécessairement la performance sur la tâche qui est représentée par le risque réel. De plus, n'étant pas calculable, le risque réel est majoré pour obtenir une borne en généralisation qui dépend principalement de deux quantités : le risque empirique et une mesure de complexité. Une façon d'apprendre un modèle est de minimiser une borne par un type d'algorithme appelé auto-certifié (ou auto-limitatif). Les bornes PAC-Bayésiennes sont bien adaptées à la dérivation de ce type d'algorithmes. Dans ce contexte, la première contribution consiste à développer des algorithmes auto-certifiés qui minimisent des bornes PAC-Bayésiennes pour apprendre des votes de majorité. Si ces bornes sont bien adaptées aux votes de majorité, leur utilisation pour d'autres modèles devient moins naturelle. Pour pallier cette difficulté, une seconde contribution se concentre sur les bornes PAC-Bayésiennes désintégrées qui sont naturelles pour des modèles plus généraux. Dans ce cadre, nous apportons la première étude empirique de ces bornes. Dans une troisième contribution, nous dérivons des bornes permettant d'incorporer des mesures de complexité pouvant être définies par l'utilisateur.

**Mot-clés.** Apprentissage Automatique, Généralisation, Borne PAC-Bayésienne, Borne PAC-Bayésienne Désintégrée, Algorithme Auto-certifié, Algorithme Auto-limitatif, Vote de Majorité, Réseau de Neurones, Mesure de Complexité.