

# PAC-Bayes bounds

Pierre Alquier



Machine Learning Summer School  
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This lecture will be based on :



Alquier, P. (2024). User-friendly Introduction to PAC-Bayes bounds. *Foundations and Trends in Machine Learning*.

(link to preliminary arXiv version + slides on my webpage).

Many thanks to Richard Cariño III who helped with the drawings !

## 1 PAC-Bayes bounds : introduction

- Generalization bounds and PAC-Bayes
- Minimization of the PAC-Bayes bound
- A zoo of PAC-Bayes bounds

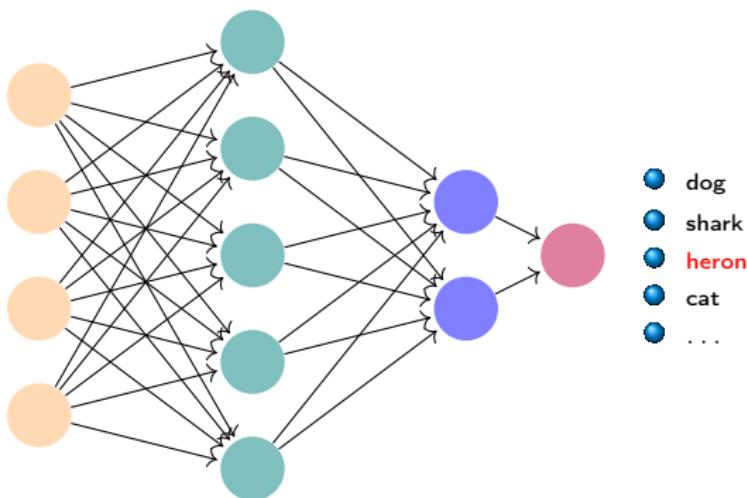
## 2 PAC-Bayes and Mutual Information bounds

- Excess risk bounds
- Fast rates
- Mutual information bounds

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- Data  $(X_1, Y_1), \dots, (X_n, Y_n)$  i.i.d. from  $P$ . Empirical risk :

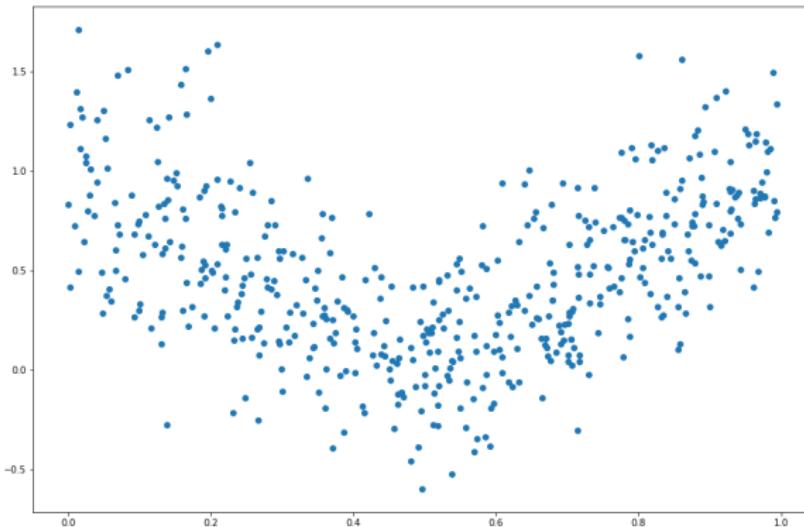
$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell\left(Y_i, f_{\theta}(X_i)\right).$$

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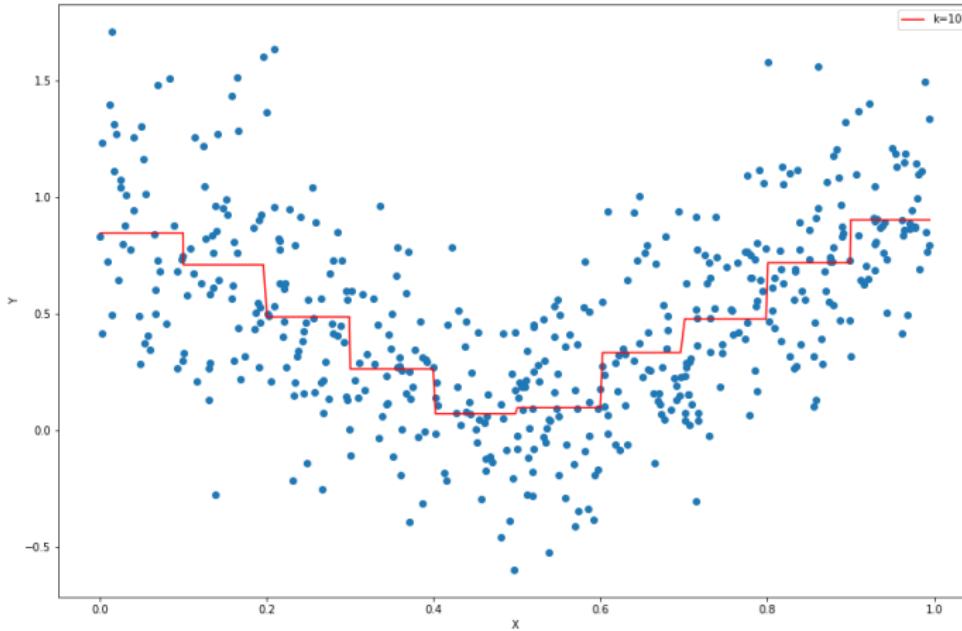
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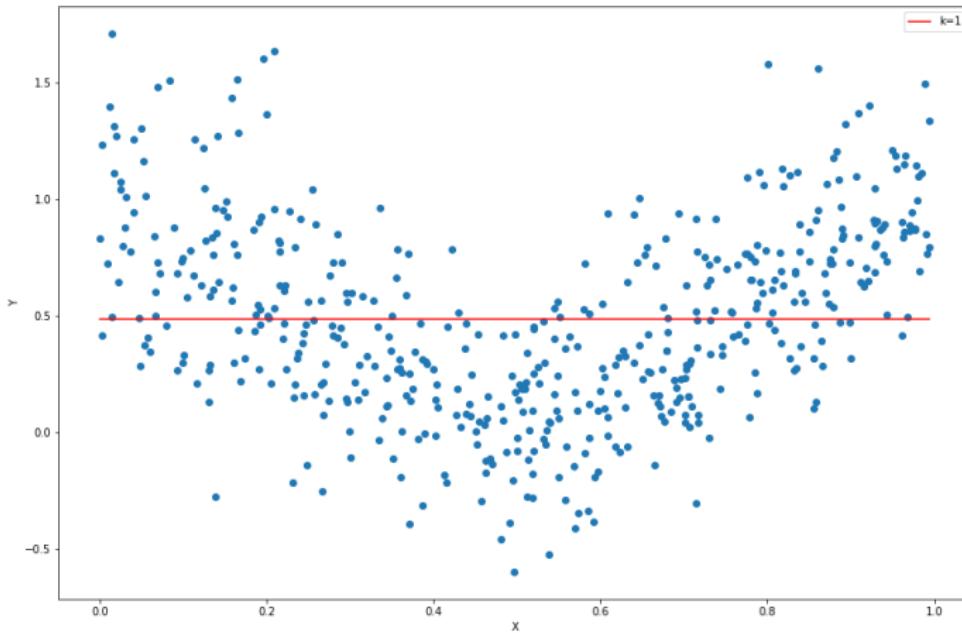
That is,

$$f_\theta(x) = \begin{cases} \theta_1 & \text{if } x \in [0, 1/k), \\ \theta_2 & \text{if } x \in [1/k, 2/k), \\ \vdots & \\ \theta_k & \text{if } x \in [(k-1)/k, 1]. \end{cases}$$

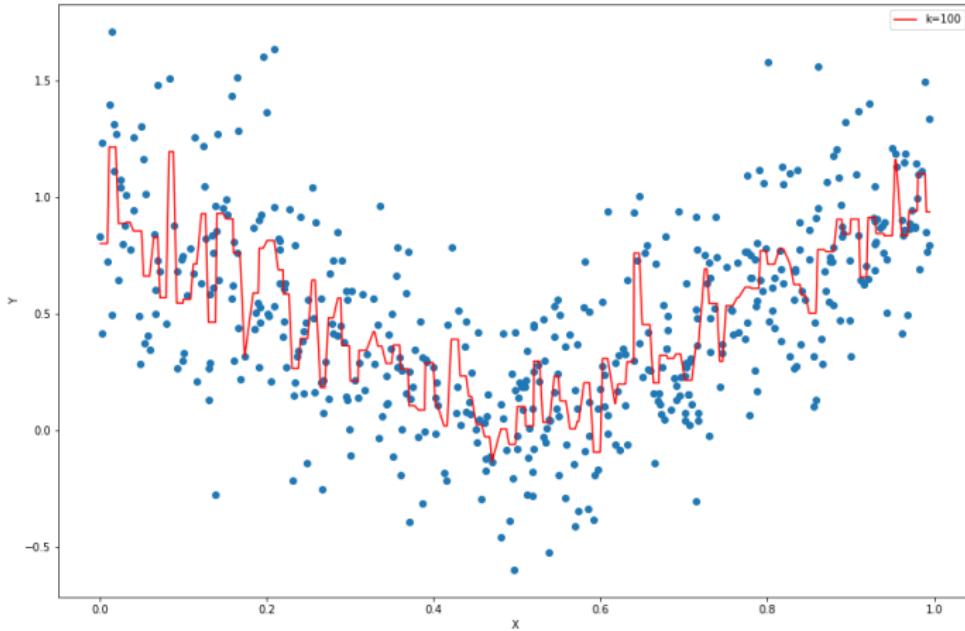
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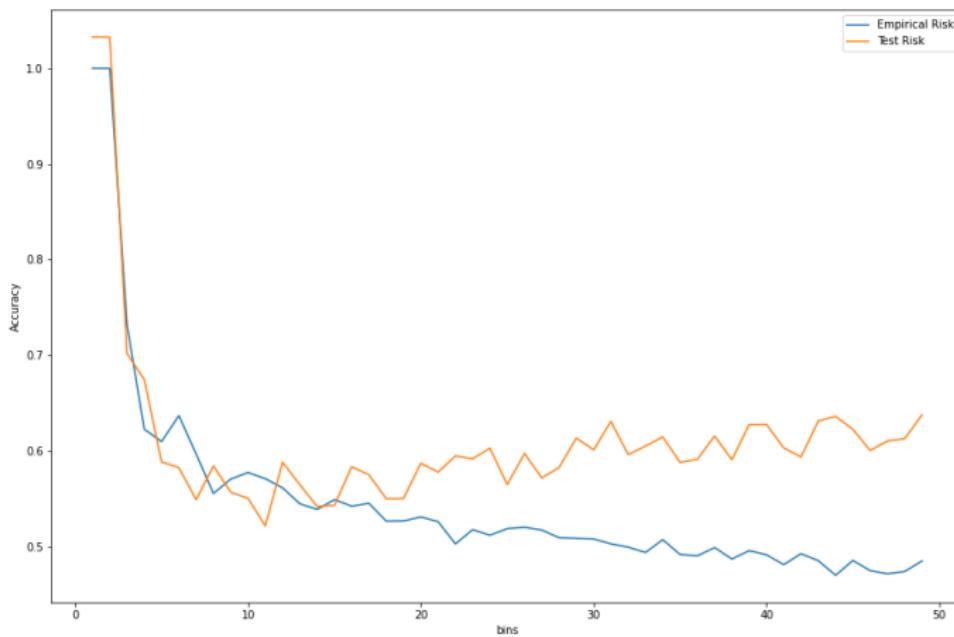


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- algorithmic stability,
- information bounds : MDL, PAC-Bayes, etc.

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$$R(\hat{\theta}) \leq R_n(\hat{\theta}) + \text{data-dependent terms.}$$

- 2 “excess risk bound”

$$R(\hat{\theta}) \leq R^* + \text{rate of convergence.}$$

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Unless specified otherwise,  $0 \leq \ell \leq 1$  and data is i.i.d. from  $P$ .

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## Vapnik-Chervonenkis – classification ( $\mathcal{Y} = \{0, 1\}$ )

With probability at least  $1 - \delta$  on the data, for any  $\hat{\theta}$  learnt from the data,

$$R(\hat{\theta}) \leq R_n(\hat{\theta}) + \sqrt{\frac{8d \log\left(\frac{2en}{d}\right) + 8 \log\left(\frac{4}{\delta}\right)}{n}}$$

where  $d$  : the VC-dimension of the set of classifiers ( $f_\theta, \theta \in \Theta$ ).

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$$(\mathcal{X} \times \mathcal{Y})^n \longrightarrow \mathcal{M}(\Theta) \dashrightarrow \Theta$$

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- For each new pair object-label  $(x, y) \sim P$ , we can draw a predictor  $\theta \sim \hat{\rho}$ . We incur a loss  $\ell(y, f_\theta(x))$ .
- If we repeat this for each new object to classify, our average loss will converge to

$$\mathbb{E}_{\theta \sim \hat{\rho}} \mathbb{E}_{(x,y) \sim P} \ell(y, f_\theta(x)) = \textcolor{red}{\mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta)]}.$$

## McAllester's PAC-Bayes bound

Fix a prior distribution  $\pi \in \mathcal{M}(\Theta)$ . With probability at least  $1 - \delta$  on the data  $\mathcal{S}$ , for any probability distribution  $\rho$  learnt on the data,

$$\mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[R_n(\theta)] + \sqrt{\frac{\text{KL}(\rho \| \pi) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}}.$$

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- we will see later that the bound is helpful to define good randomized estimators  $\hat{\rho}$ .

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- discrete case :

$$\text{KL}(\rho\|\pi) = \sum_{\theta \in \Theta} \rho(\theta) \log \frac{\rho(\theta)}{\pi(\theta)}$$

and  $\text{KL}(\rho\|\pi) = \infty$  if for some  $\theta$ ,  $\pi(\theta) = 0$  and  $\rho(\theta) > 0$ .

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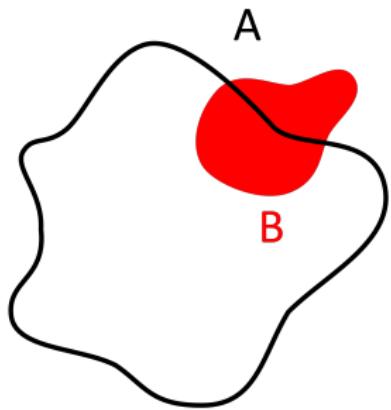
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$\text{KL}(\rho\|\pi) \geq 0$  and  $\text{KL}(\rho\|\pi) = 0 \Leftrightarrow \rho = \pi$ .

## Intuition on KL :



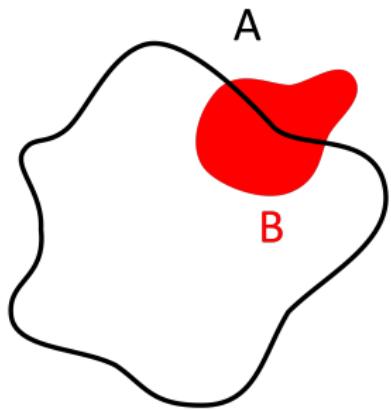
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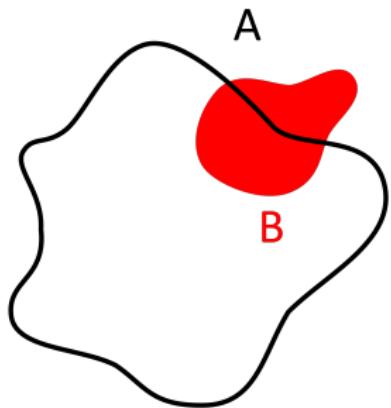
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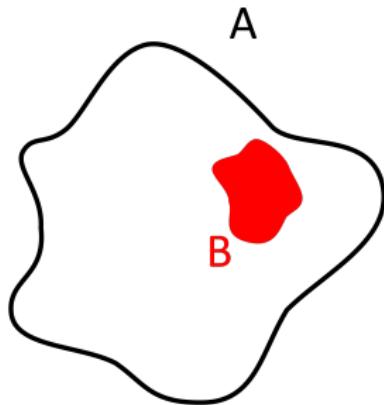
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$B \not\subseteq A \Rightarrow \text{KL}(\rho\|\pi) = +\infty.$

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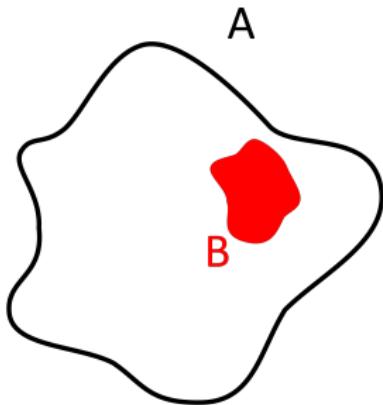
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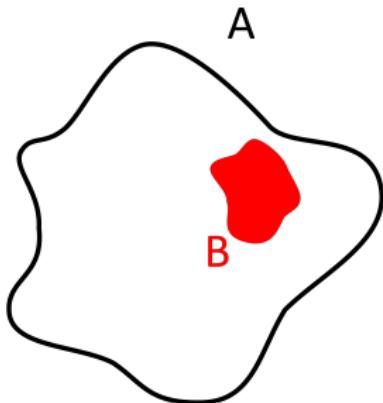
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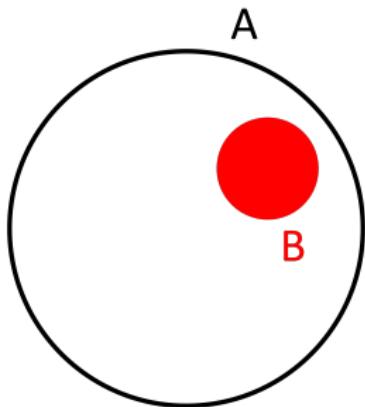
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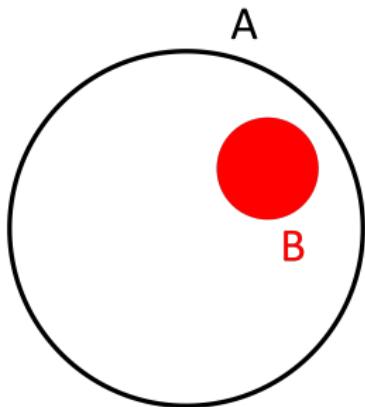


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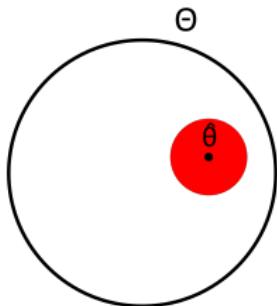
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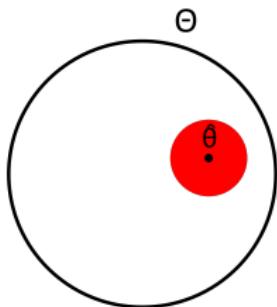
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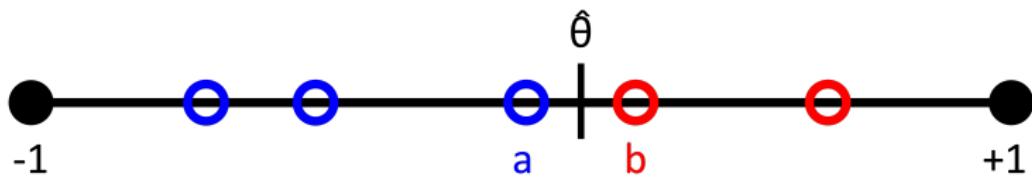
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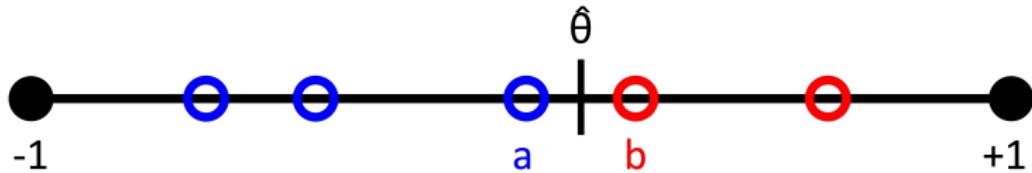
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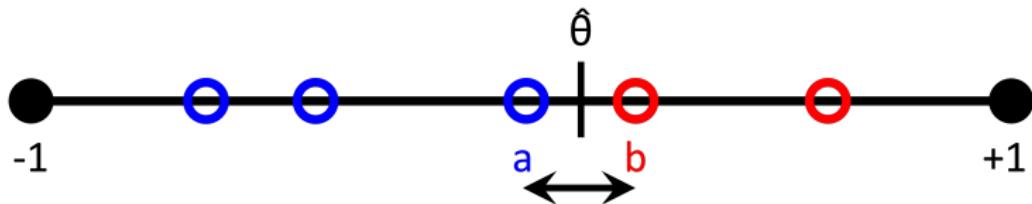


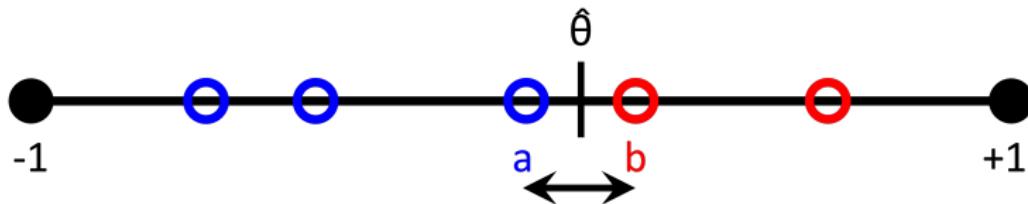




Vapnik-type bound :

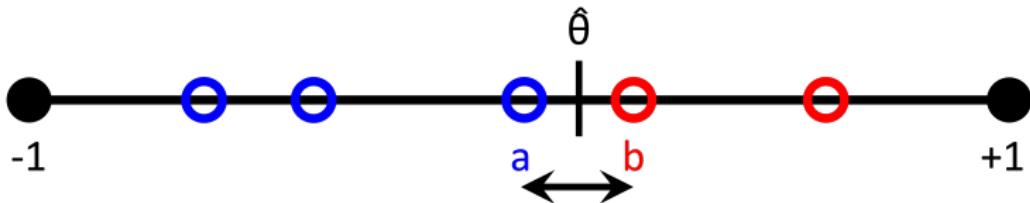
$$R(\hat{\theta}) \leq \sqrt{\frac{8 \log(2en) + 8 \log\left(\frac{4}{\delta}\right)}{n}}$$





PAC-Bayes :

- $\pi$  uniform on  $[-1, 1]$ ,
- $\hat{\rho}$  uniform on  $[a, b]$ .

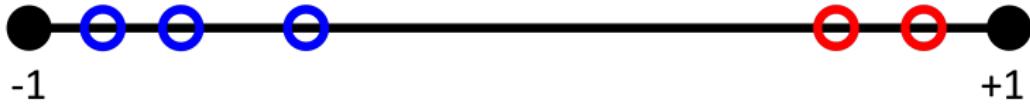


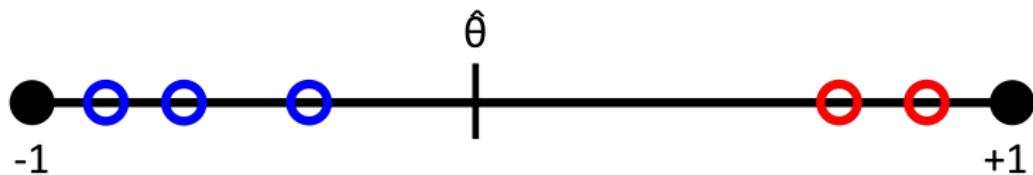
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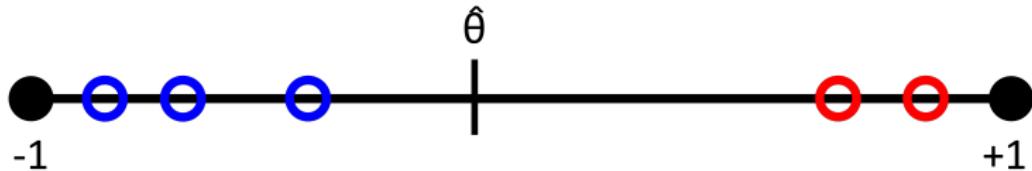
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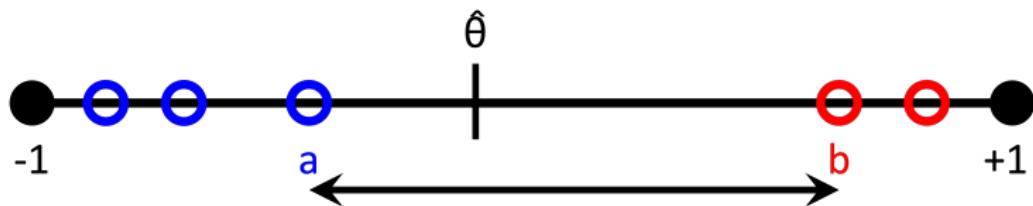


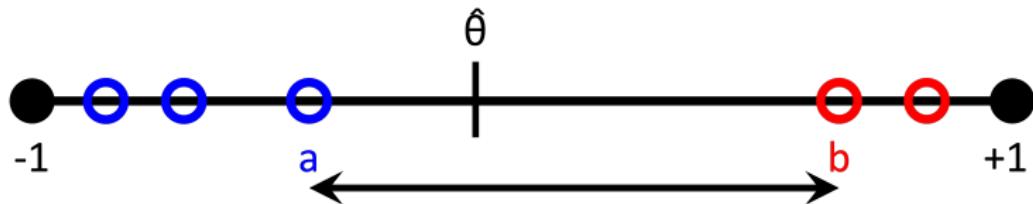




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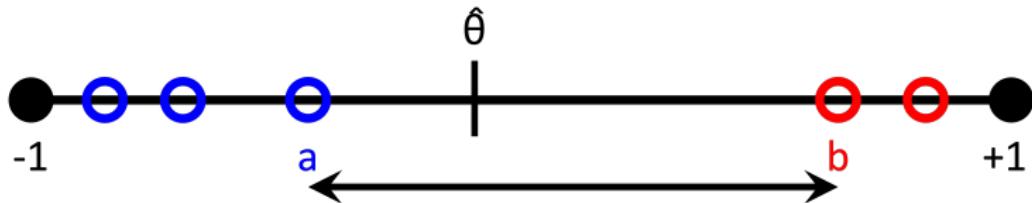
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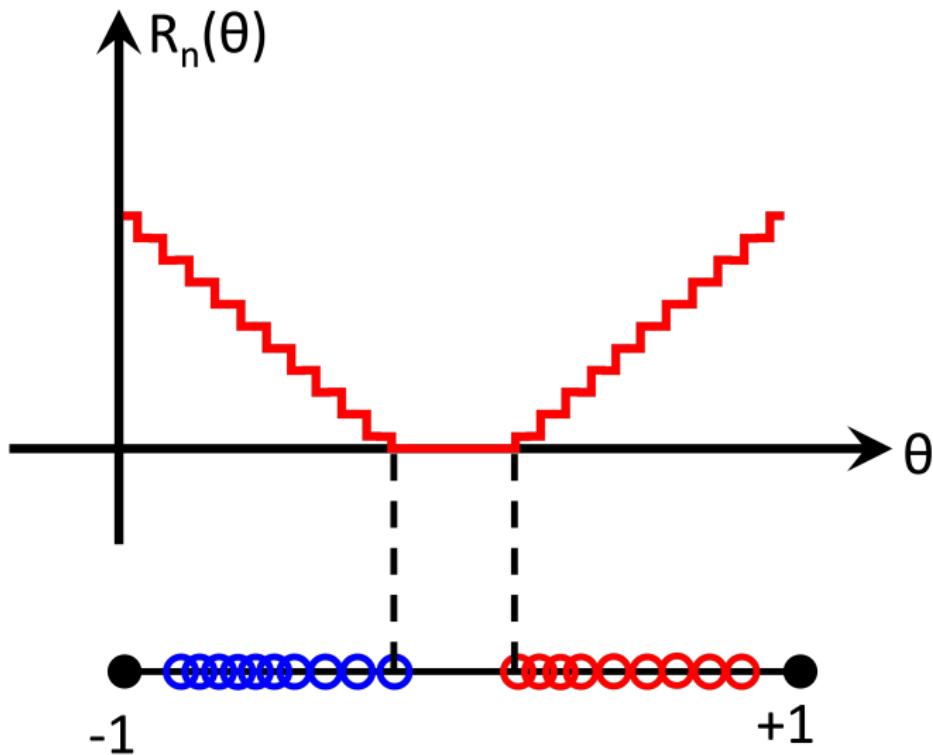
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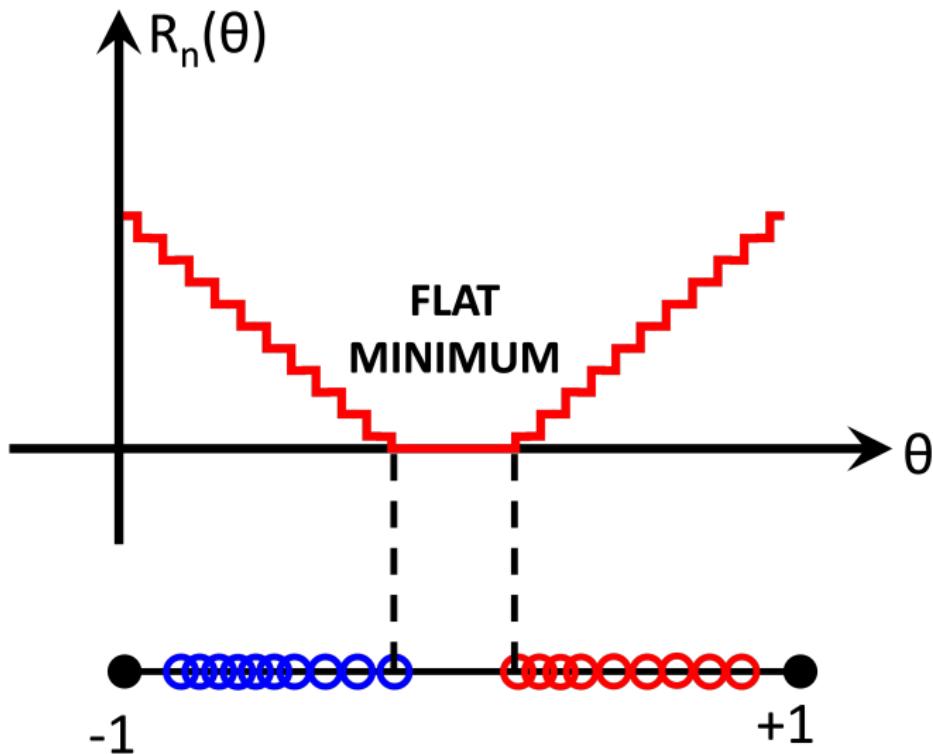


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## 2 PAC-Bayes and Mutual Information bounds

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## McAllester's PAC-Bayes bound

Fix prior  $\pi \in \mathcal{M}(\Theta)$ . With proba. at least  $1 - \delta$ ,  $\forall \rho \in \mathcal{M}(\Theta)$ ,

$$\mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[R_n(\theta)] + \sqrt{\frac{\text{KL}(\rho \| \pi) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}}.$$

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## Definition - Gibbs posterior

$$\hat{\pi}_\lambda(d\theta) = \frac{\exp(-\lambda R_n(\theta))}{\mathbb{E}_{\vartheta \sim \pi}[\exp(-\lambda R_n(\vartheta))]} \pi(d\theta).$$

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## Theorem

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

Proof :

$$\begin{aligned}
 0 &\leq \text{KL}(\rho \parallel \hat{\pi}_\lambda) \\
 &= \mathbb{E}_{\theta \sim \rho} \left[ \log \frac{d\rho}{d\hat{\pi}_\lambda}(\theta) \right] \\
 &= \mathbb{E}_{\theta \sim \rho} \left[ \log \frac{d\rho}{d\pi}(\theta) - \log \frac{d\hat{\pi}_\lambda}{d\pi}(\theta) \right] \\
 &= \mathbb{E}_{\theta \sim \rho} \left[ \log \frac{d\rho}{d\pi}(\theta) + \lambda R_n(\theta) + \log \mathbb{E}_{\vartheta \sim \pi} [\exp(-\lambda R_n(\vartheta))] \right] \\
 &= \text{KL}(\rho \parallel \pi) + \lambda \mathbb{E}_{\theta \sim \rho} [R_n(\theta)] + \log \mathbb{E}_{\vartheta \sim \pi} [\exp(-\lambda R_n(\vartheta))].
 \end{aligned}$$

## Consequence of the PAC-Bayes bound

Fix prior  $\pi \in \mathcal{M}(\Theta)$ . With proba. at least  $1 - \delta$ ,  $\forall \lambda > 0$ ,

$$\mathbb{E}_{\theta \sim \hat{\pi}_\lambda}[R(\theta)] \leq \frac{-\log \mathbb{E}_{\vartheta \sim \pi}[\exp(-\lambda R_n(\vartheta))] + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{\lambda} + \frac{\lambda}{8n}.$$

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- in simple cases, we can sample from  $\hat{\pi}_\lambda$  by standard Monte Carlo / MCMC techniques,
- the minimization in  $\lambda$  can be tricky.

Approximate minimization of the PAC-Bayes bound.

$$\forall \lambda > 0, \mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[R_n(\theta)]$$

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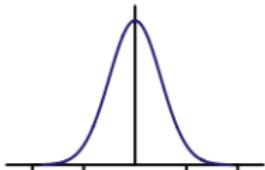
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Example :  $\rho = \mathcal{N}(\mu, \Sigma)$ , optimize  $(\mu, \Sigma)$ .

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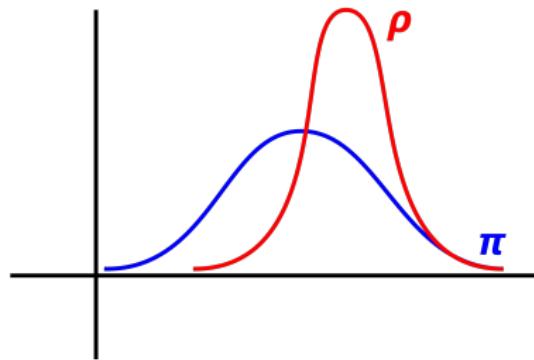
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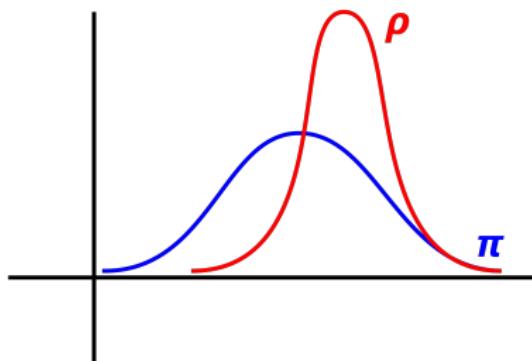
$$\pi = \mathcal{N}(\mu_0, \Sigma_0) \text{ and } \rho = \mathcal{N}(\mu_1, \Sigma_1) \text{ in } \mathbb{R}^d.$$

$$\begin{aligned} \text{KL}(\rho\|\pi) &= \frac{1}{2} \left[ \text{tr}(\Sigma_1 \Sigma_0^{-1}) - d \right. \\ &\quad \left. + (\mu_1 - \mu_0)^T \Sigma_0^{-1} (\mu_1 - \mu_0) + \log \frac{\det \Sigma_0}{\det \Sigma_1} \right]. \end{aligned}$$

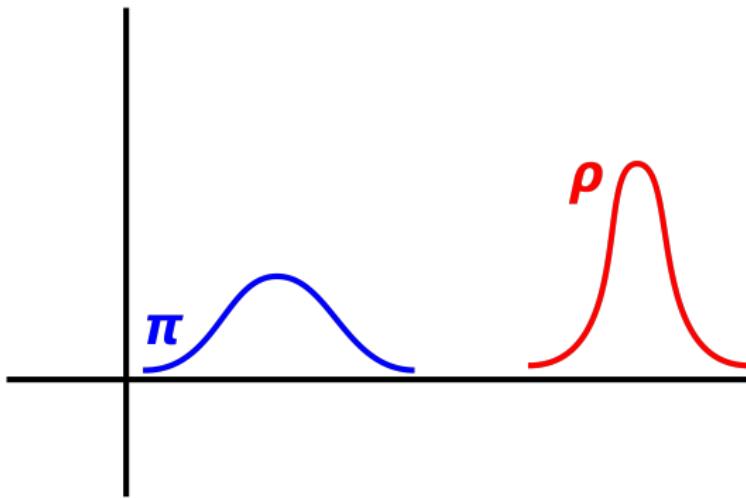
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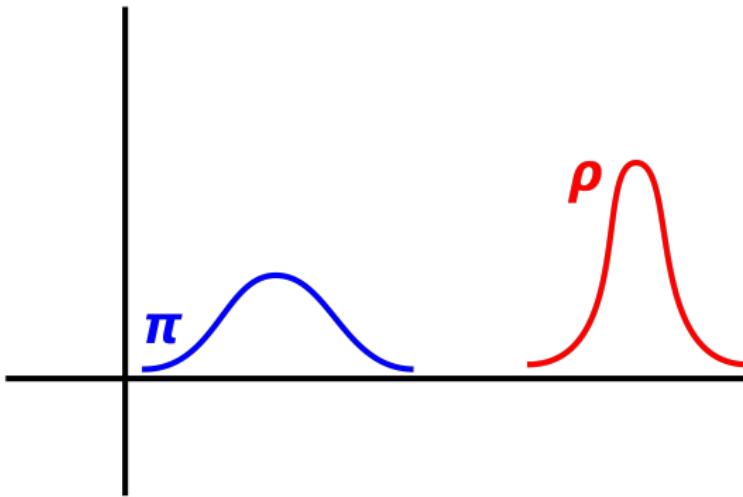


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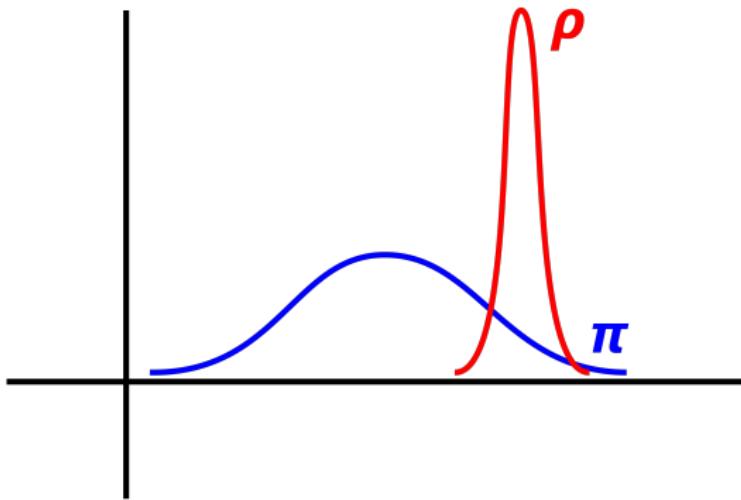
$$\text{KL}(\rho\|\pi) = \frac{1}{2} \left[ \frac{\Sigma_1}{\Sigma_0} - 1 + \frac{(\mu_0 - \mu_1)^2}{\Sigma_0} + \log \frac{\Sigma_0}{\Sigma_1} \right].$$

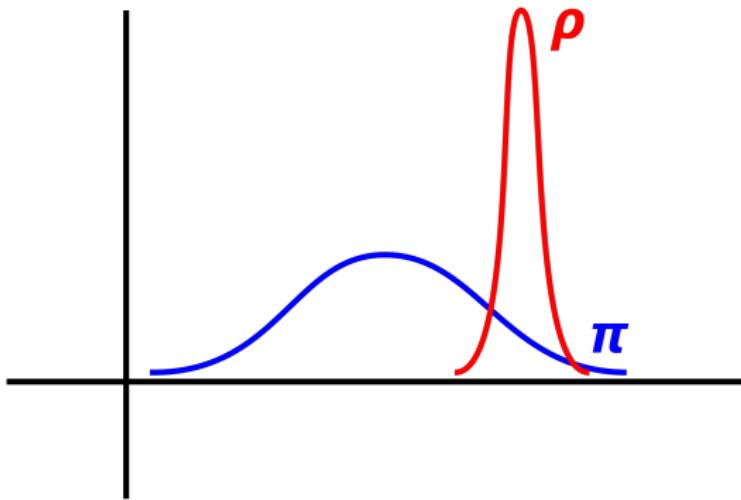




If  $\mu_1$  goes far away from  $\mu_0$  to  $\infty$ ,

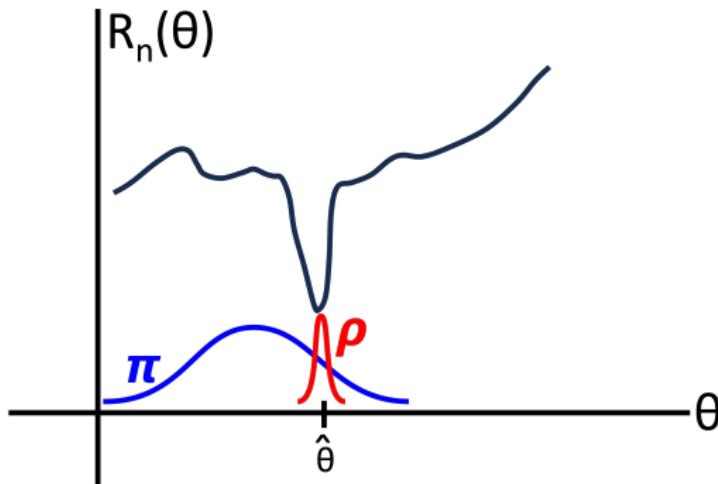
$$\text{KL}(\rho\|\pi) \sim \frac{(\mu_0 - \mu_1)^2}{2\Sigma_0} \rightarrow \infty.$$





If  $\Sigma_1 \rightarrow 0$ ,

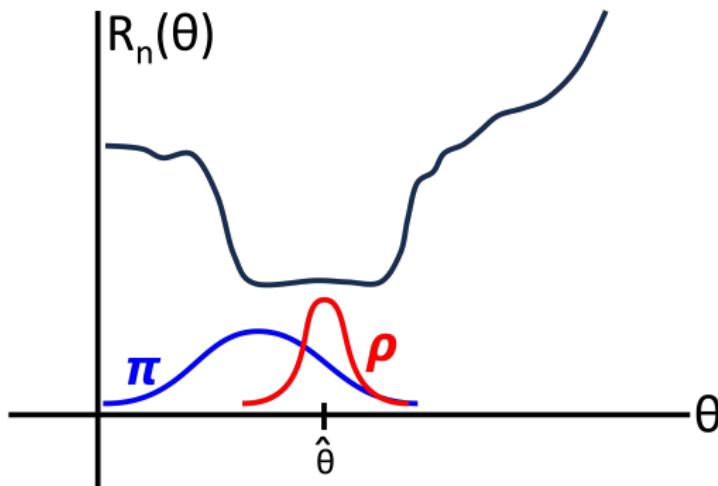
$$\text{KL}(\rho \parallel \pi) \sim \frac{1}{2} \log \frac{\Sigma_0}{\Sigma_1} \rightarrow \infty.$$



With a sharp minimum, to keep

$$\mathbb{E}_{\theta \sim \mathcal{N}(\hat{\theta}, \Sigma_1)} [R_n(\theta)] \sim R_n(\hat{\theta}),$$

$\Sigma_1$  should be small, and thus  $\text{KL}(\rho \parallel \pi)$  will be large.



With a flat minimum,

$$\mathbb{E}_{\theta \sim \mathcal{N}(\hat{\theta}, \Sigma_1)} [R_n(\theta)] \sim R_n(\hat{\theta})$$

for  $\Sigma_1$  “not so small”, thus  $\text{KL}(\rho \| \pi)$  does not have to be large.

$$\rho = \rho_{\mu_1, \Sigma_1} = \mathcal{N}(\mu_1, \Sigma_1) = \mathcal{N}(\mu_1, UU^T).$$

$$\min_{\mu_1, U} \left\{ \mathbb{E}_{\theta \sim \mathcal{N}(\mu_1, UU^T)} [R_n(\theta)] + \frac{\text{KL}(\rho \parallel \pi)}{\lambda} \right\}.$$

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## Stochastic Gradient Algorithm

Random initialization of  $\mu_1$  and  $U$ , then iterate :

- sample  $\xi \sim \mathcal{N}(0, I)$ ,
- update

$$\begin{cases} \mu_1 \leftarrow \mu_1 - \eta \frac{\partial}{\partial \mu_1} [R_n(\mu_1 + U\xi) + \text{KL}(\rho_{\mu_1, \Sigma_1} \| \pi)] \\ U \leftarrow U - \eta \frac{\partial}{\partial U} [R_n(\mu_1 + U\xi) + \text{KL}(\rho_{\mu_1, \Sigma_1} \| \pi)] \end{cases}$$

Application : generalization bounds for deep learning.

Train a neural network for  
classification (0-1 loss).

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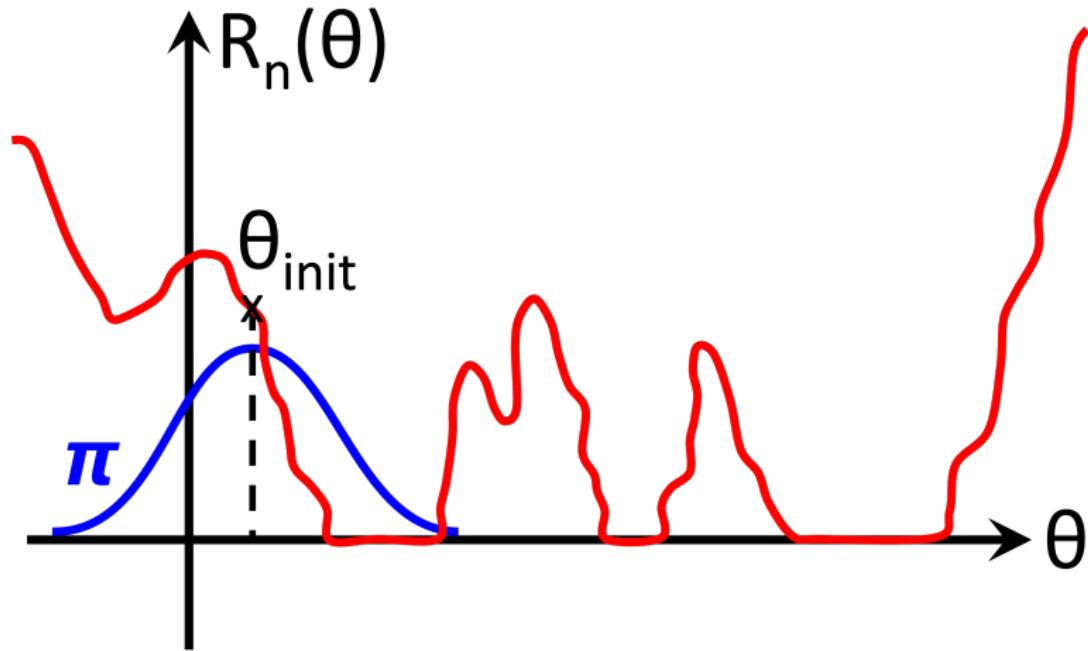
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- replace  $R_n(\theta)$  by convex surrogate.
- ...

Experiment	T-600	T-1200	T-300 <sup>2</sup>	T-600 <sup>2</sup>	T-1200 <sup>2</sup>	T-600 <sup>3</sup>	R-600
Train error	0.001	0.002	0.000	0.000	0.000	0.000	0.007
Test error	0.018	0.018	0.015	0.016	0.015	0.013	0.508
SNN train error	0.028	0.027	0.027	0.028	0.029	0.027	0.112
SNN test error	0.034	0.035	0.034	0.033	0.035	0.032	0.503
PAC-Bayes bound	0.161	0.179	0.170	0.186	0.223	0.201	1.352
KL divergence	5144	5977	5791	6534	8558	7861	201131
# parameters	471k	943k	326k	832k	2384k	1193k	472k
VC dimension	26m	56m	26m	66m	187m	121m	26m

Table 1: Results for experiments on binary class variant of MNIST. SGD is either trained on (T) true labels or (R) random labels. The network architecture is expressed as  $N^L$ , indicating  $L$  hidden layers with  $N$  nodes each. Errors are classification error. The reported VC dimension is the best known upper bound (in millions) for ReLU networks. The SNN error rates are tight upper bounds (see text for details). The PAC-Bayes bounds upper bound the test error with probability 0.965.

## Results taken from :



Dzuigaite, G. K. and Roy, D. M. (2017). Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data. *UAI*.

More recent results (among others !) :



Pérez-Ortiz, M., Rivasplata, O., Shawe-Taylor, J. and Szepesvári, C. (2021). Tighter risk certificates for neural networks. *Journal of Machine Learning Research*.



Clerico, E., Farghly, T., Deligiannidis, G., Guedj, B. and Doucet, A. (2022). Generalisation under gradient descent via deterministic PAC-Bayes. ArXiv preprint arXiv :2209.02525.

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### PAC-Bayesian Model Averaging

David A. McAllester  
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180 Park Avenue  
Florham Park, NJ 07932-0971  
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#### Abstract

PAC-Bayesian learning methods combine the informative power of Bayesian methods with distribution-free PAC guarantees. Building on earlier methods for PAC-Bayesian model selection, this paper presents a method for PAC-Bayesian model averaging. The method constructs an optimized weighted mixture of concepts that minimizes the expected error of prediction. Although the main result is aimed for bounded loss, a preliminary analysis for unbounded loss is also given.

#### 1 INTRODUCTION

A PAC-Bayesian approach to machine learning attempts to combine the advantages of both PAC and Bayesian approaches [12, 8]. The Bayesian approach has the advantage of having arbitrary domain knowledge in the form of a Bayesian prior. The PAC approach has the advantage that one can prove guarantees for generalization error based on the training set. The PAC and Bayesian approaches combine the features of the PAC and Bayesian approaches – it bases the bias of the learning algorithm on an arbitrary prior distribution, thus allowing the incorporation of domain knowledge, and yet provides a guarantee on generalization error that depends only on the training set size.

PAC-Bayesian approaches are related to structural risk minimization (SRM) [6]. Here we interpret this broadly as describing any learning algorithm optimizing a trade-off between “complexity”, “structure”, or “prior probability” of the concepts in the model and the “goodness of fit”, “description length”, or “likelihood” of the training data. Under this interpretation of SRM, Bayesian algorithms which select a concept of maximum posterior probability (MAP algorithms) are viewed as a kind of SRM algorithms. Various approaches to SRM

are compared both theoretically and experimentally by Kearns et al. in [6]. They give experimental evidence that Bayesian and MDL algorithms tend to over-fit in experiments involving noisy Bayesian networks. A PAC-Bayesian approach uses a prior distribution analogous to that used in MAP or MDL but provides a theoretical guarantee against over-fitting independent of the truth of the prior.

Earlier work on PAC-Bayesian algorithms has focused on model selection, either a single concept or a uniformly weighted set of concepts. Here we consider nonuniform model averaging, i.e., selecting a weighted mixture of the concepts.

Model averaging is empirically important in certain applications. For example, in statistical language modeling or speech recognition, “smooth” a trigram model with a bigram model and smooth the bigram model with a unigram model. This smoothing is essential for minimizing the cross entropy between, say, the model and a set of corpus of newspaper sentences. It turns out that smoothing in statistical language modeling is most naturally formulated as model averaging rather than as model selection. A smoothed language model is very large – it contains a full trigram model, a full bigram model and a full unigram model as parts. If one uses MDL to select a single model, a language model, after all model parameters with maximum likelihood, the resulting structure is much smaller than that of a smoothed trigram model. Furthermore, the MDL model performs quite badly. However, a smoothed trigram model can be theoretically derived as a compact representation of a Bayesian mixture of an exponential number of (smaller) suffix tree models [10].

Model averaging can also be applied to decision trees. A common method of constructing decision trees is to first build an overly large tree which over-fits the training data. Then some tree pruning is done to get a smaller tree that does not over-fit the data [11, 5]. An alternative to pruning is to construct a weighted mixture of the subtrees of the original over-fit tree. It is possible to construct a concise representation of a weighting over exponentially many different trees [3, 9, 4].

This paper proves a new PAC-Bayesian bound giving a bound on the generalization error of weighted mixtures. A weighted mixture which gives too much weight to models with low prior probability will over-fit the

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Seminal paper, that contains the bound stated earlier today.

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#### Abstract

PAC-Bayesian learning methods combine the informative priors of Bayesian methods with distribution-free PAC guarantees. Building on earlier methods for PAC-Bayesian model selection, this paper presents a method for PAC-Bayesian model averaging. The method constructs an optimized weighted mixture of competing models that minimizes the generalization error. Although the main result is aimed for bounded loss, a preliminary analysis for unbounded loss is also given.

#### 1 INTRODUCTION

A PAC-Bayesian approach to machine learning attempts to combine the advantages of both PAC and Bayesian approaches [12, 8]. The Bayesian approach has the advantage of using arbitrary domain knowledge in the form of a Bayesian prior. The PAC approach has the advantage that one can prove guarantees for generalization error based on the training set. The PAC and Bayesian approaches combine the features of the PAC and Bayesian approaches: it bases the bias of the learning algorithm on an arbitrary prior distribution, thus allowing the incorporation of domain knowledge, and yet provides a guarantee on generalization error that is based on the training set.

PAC-Bayesian approaches are related to structural risk minimization (SRM) [6]. Here we interpret this broadly as describing any learning algorithm optimizing a trade-off between “complexity”, “structure”, “prior probability” of the concepts in mind, and the “goodness of fit”, “description length”, or “likelihood” of the training data. Under this interpretation of SRM, Bayesian algorithms which select a concept of maximum posterior probability (MAP algorithms) are viewed as a kind of SRM algorithm. Various approaches to SRM

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are compared both theoretically and experimentally by Kearns et al. in [6]. They give experimental evidence that Bayesian and MDL algorithms tend to over-fit in experiments involving noisy Bayesian networks. A PAC-Bayesian approach uses a prior distribution analogous to that used in MAP or MDL but provides a theoretical guarantee against over-fitting independent of the truth of the prior.

Earlier work on PAC-Bayesian algorithms has focused on model selection [12, 8] and either a single concept or a uniformly weighted set of concepts. Here we consider nonuniform model averaging, i.e., selecting a weighted mixture of the concepts.

Model averaging is empirically important in certain applications. For example, in statistical language modeling or speech recognition, one “smooths” a trigram model with a bigram model and smooths the bigram model with a unigram model. This smoothing is essential for minimizing the cross entropy between, say, the model and a set of corpus of newspaper sentences. It turns out that smoothing in statistical language modeling is more naturally formulated as model averaging than as model selection. A smoothed language model is very large – it contains a full trigram model, a full bigram model and a full unigram model as parts. If one uses MDL to select a model from a language model, after a model is selected with maximum likelihood, the resulting structure is much smaller than that of a smoothed trigram model. Furthermore, the MDL model performs quite badly. However, a smoothed trigram model is theoretically derived as a compact representation of a Bayesian mixture of an exponential number of (smaller) suffix tree models [10].

Model averaging can also be applied to decision trees. A common method of constructing decision trees is to first build an overly large tree which over-fits the training data. Then one prunes the tree in such a way as to get a smaller tree that does not over-fit the data [11, 5]. An alternative to pruning is to construct a weighted mixture of the subtrees of the original over-fit tree. It is possible to construct a concise representation of a weighting over exponentially many different subtrees [3, 9, 4].

This paper proves a new PAC-Bayesian bound giving a bound on the generalization error of weighted mixtures. A weighted mixture which gives too much weight to models with low prior probability will over-fit the

Seminal paper, that contains the bound stated earlier today.

Since then, various bounds published :

- tighter,
- with less assumptions (i.i.d, bounded loss),
- easier to optimize,

● ...

## Catoni's PAC-Bayes bound, 2003

Fix  $\lambda > 0$  and  $\pi$ . With proba. at least  $1 - \delta$  on  $\mathcal{S}$ , for any  $\hat{\rho}$ ,

$$\mathbb{E}_{\theta \sim \hat{\rho}}[R(\theta)] \leq \mathbb{E}_{\theta \sim \hat{\rho}}[R_n(\theta)] + \frac{\text{KL}(\hat{\rho} \parallel \pi) + \log \frac{1}{\delta}}{\lambda} + \frac{\lambda}{8n}.$$

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## "De-randomized" PAC-Bayes bound, 2003

- Fix  $\lambda > 0$ ,  $\pi$  and a randomized estimator  $\hat{\rho}$ .
- Sample  $\hat{\theta} \sim \hat{\rho}(\mathcal{S})$ .

With probability at least  $1 - \delta$  on  $(\mathcal{S}, \hat{\theta})$ ,

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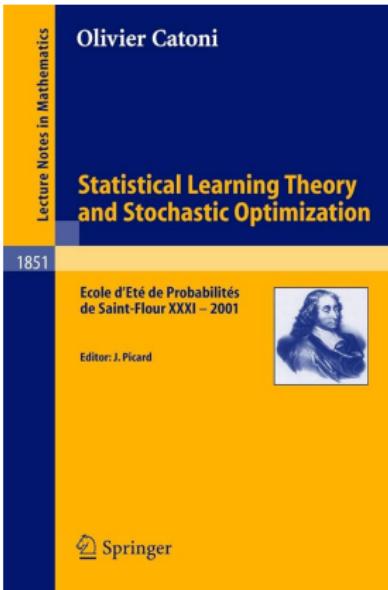
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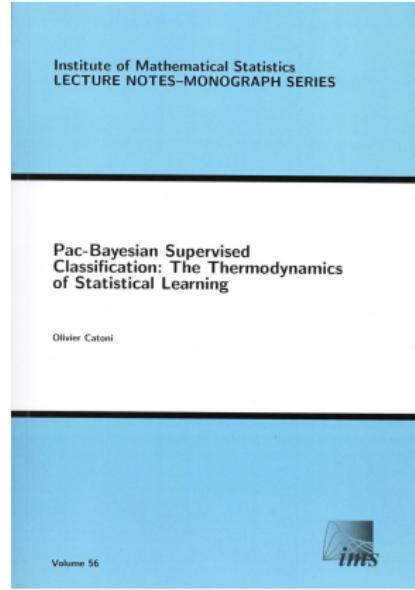


Catoni, O. (2003). A PAC-Bayesian approach to adaptive classification. Preprint LPMA 840.

## Classical references :



Connections with information theory  
and MDL.



Very tight bounds, applications to  
Support Vector Machines.



Seeger, M. (2002). PAC-Bayesian generalisation error bounds for Gaussian process classification. *Journal of Machine Learning Research*.



Maurer, A. (2004). *A note on the PAC-Bayesian theorem*. Arxiv preprint arXiv :cs/0411099.



Tolstikhin, I. and Seldin, Y. (2013). PAC-Bayes-empirical-Bernstein inequality. *NeurIPS*.



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## Tolstikhin and Seldin's PAC-Bayes bound, 2013

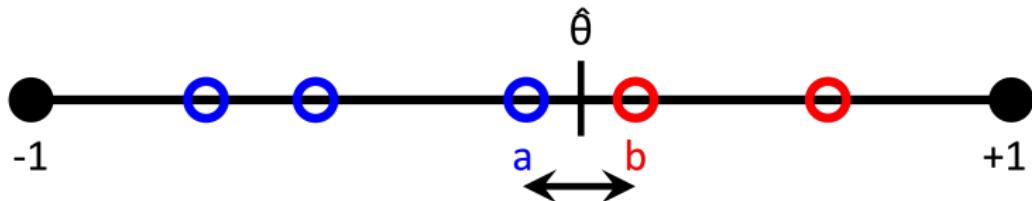
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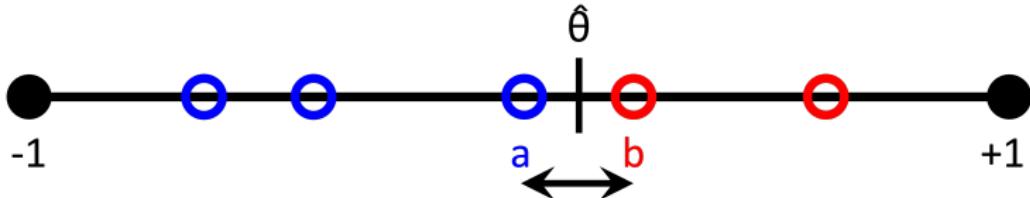
$$\begin{aligned} \mathbb{E}_{\theta \sim \rho}[R(\theta)] &\leq \mathbb{E}_{\theta \sim \rho}[R_n(\theta)] \\ &+ \sqrt{2\mathbb{E}_{\theta \sim \rho}[R_n(\theta)] \frac{\text{KL}(\rho\|\pi) + \log \frac{2\sqrt{n}}{\delta}}{n}} \\ &+ 2\frac{\text{KL}(\rho\|\pi) + \log \frac{2\sqrt{n}}{\delta}}{n}. \end{aligned}$$

Consequence : if  $\mathbb{E}_{\theta \sim \rho}[R_n(\theta)]$ ,

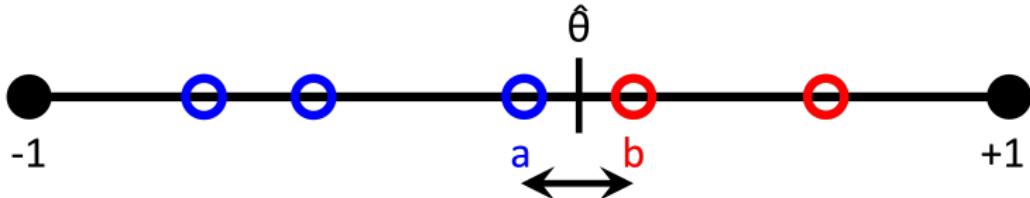
$$\mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \underline{\mathbb{E}_{\theta \sim \rho}[R_n(\theta)]}$$

$$+ \sqrt{2\mathbb{E}_{\theta \sim \rho}[R_n(\theta)]} \frac{\text{KL}(\rho \parallel \pi) + \log \frac{2\sqrt{n}}{\delta}}{n} + 2 \frac{\text{KL}(\rho \parallel \pi) + \log \frac{2\sqrt{n}}{\delta}}{n}.$$





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Bound in expectation → bound on the weighted majority vote :



Germain, P., Lacasse, A., Laviolette, F., Marchand, M. and Roy, J.-F. (2015). Risk bounds for the majority vote : from a PAC-Bayesian analysis to a learning algorithm *Journal of Machine Learning Research*.

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François Laviolette (1962-2021).

## Tutorials :

-  McAllester, D. (2013). *A PAC-Bayesian tutorial with a dropout bound*. ArXiv preprint arXiv :1307.2118.
-  Van Erven, T. (2014). *PAC-Bayes mini-tutorial : a continuous union bound*. ArXiv preprint arXiv :1405.1580.
-  Guedj, B. (2019). *A primer on PAC-Bayesian learning*. ArXiv preprint arXiv :1901.05353.

## 1 PAC-Bayes bounds : introduction

- Generalization bounds and PAC-Bayes
- Minimization of the PAC-Bayes bound
- A zoo of PAC-Bayes bounds

## 2 PAC-Bayes and Mutual Information bounds

- Excess risk bounds
- Fast rates
- Mutual information bounds

Recap :

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Today, we study “excess-risk bounds”, that is :

$$\mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta)] \leq R^* + \dots \text{ (rate of convergence).}$$

## Catoni's PAC-Bayes bound, 2003

Fix  $\lambda > 0$  and  $\pi$ . With proba. at least  $1 - \delta$  on  $\mathcal{S}$ , for any  $\hat{\rho}$ ,

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Zhang, T. (2006). Information-theoretic upper and lower bounds for statistical estimation *IEEE Transactions on Information Theory*.

Note : sometimes referred to as “MAC-Bayes” for “Mean Approximately Correct”...

## Reminder – Gibbs posterior

$$\hat{\pi}_\lambda = \arg \min_{\rho \in \mathcal{M}(\Theta)} \left\{ \mathbb{E}_{\theta \sim \rho} [R_n(\theta)] + \frac{\text{KL}(\rho \| \pi)}{\lambda} \right\}$$
$$\hat{\pi}_\lambda(d\theta) = \frac{\exp(-\lambda R_n(\theta))}{\mathbb{E}_{\vartheta \sim \pi} [\exp(-\lambda R_n(\vartheta))]} \pi(d\theta).$$

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Consequence of PAC-Bayes bound in expectation :

$$\begin{aligned}\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] \right] &\leq \mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R_n(\theta)] + \frac{\text{KL}(\hat{\pi}_\lambda \| \pi)}{\lambda} + \frac{\lambda}{8n} \right] \\ &= \mathbb{E}_{\mathcal{S}} \inf_{\rho} \left[ \mathbb{E}_{\rho} [R_n(\theta)] + \frac{\text{KL}(\rho \| \pi)}{\lambda} + \frac{\lambda}{8n} \right] \\ &\leq \inf_{\rho} \mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\rho} [R_n(\theta)] + \frac{\text{KL}(\rho \| \pi)}{\lambda} + \frac{\lambda}{8n} \right].\end{aligned}$$

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- In this result, we use  $\hat{\pi}_\lambda$  as our randomized estimator.

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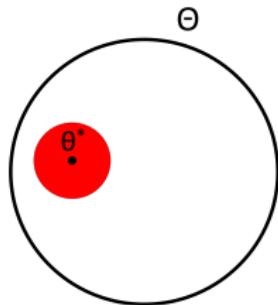
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- But to explicit the right-hand side, we can substitute anything to  $\rho$  in the infimum...

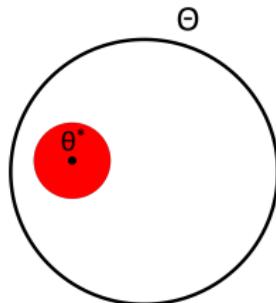
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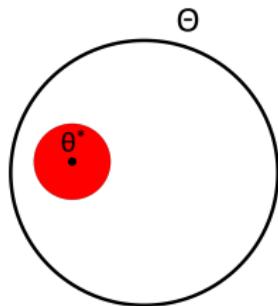
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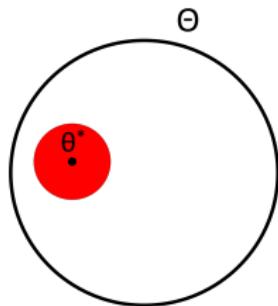
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Assume  $\theta \mapsto \ell(y, f_\theta(x))$  is  $L$ -Lipschitz around  $\theta^*$ , that is :

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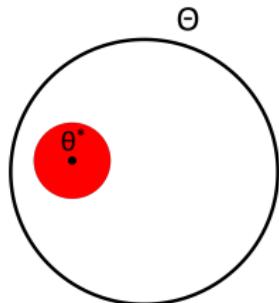
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Thus  $\mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq R^* + L\epsilon$ .

$$\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] \right] \leq \inf_{\epsilon > 0} \left[ R^* + \epsilon + \frac{d \log \frac{C}{\epsilon}}{\lambda} + \frac{\lambda}{8n} \right].$$

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The bound is exactly minimized for  $\epsilon = d/\lambda$  :

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In this case, we can calibrate the Gibbs posterior with  $\lambda = \sqrt{n/d}$  which leads to

$$\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] \right] \leq R^* + \mathcal{O} \left( \sqrt{\frac{d}{n}} \log \frac{n}{d} \right).$$

## Reminder : Catoni's PAC-Bayes oracle bound

$$\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] \right] \leq \inf_{\rho \in \mathcal{M}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [R(\theta)] + \frac{\text{KL}(\rho \| \pi)}{\lambda} + \frac{\lambda}{8n} \right].$$

Recap on the previous example :

- $\pi$  uniform on  $B_d(0, C)$ ,
- $\rho$  uniform on  $B_d(\theta^*, \epsilon)$ ,
- $L$ -Lipschitz loss function.

$$\Rightarrow \mathbb{E}_{\theta \sim \rho} [R(\theta)] \leq R^* + L\epsilon.$$

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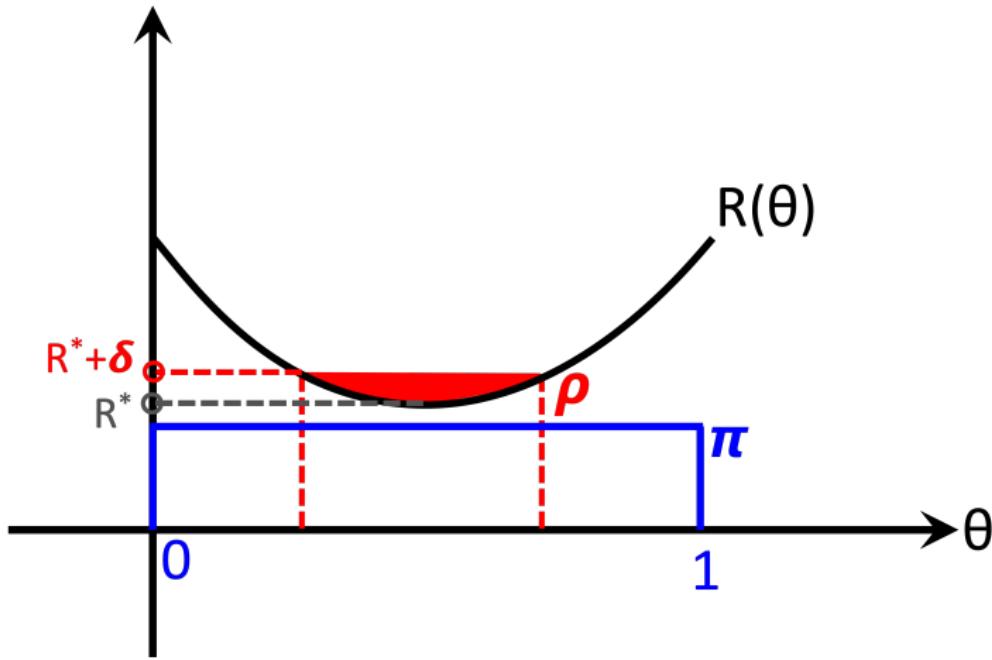
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More generally, we can consider in the PAC-Bayes oracle bound :

$$\rho = \pi_\delta := \text{restriction of } \pi \text{ to } \{\theta : R(\theta) \leq R^* + \delta\}.$$

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In the previous example,

$$\log \frac{1}{\pi\{\theta : R(\theta) \leq R^* + \delta\}} \leq d \log \frac{C}{\delta}$$

and we obtained a bound in  $\sqrt{d/n} \log(n/d)$ .

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Definition : the **prior mass condition** is satisfied if there are  $C, D > 0$  such that, for any  $\delta > 0$  small enough,

$$\log \frac{1}{\pi\{\theta : R(\theta) \leq R^* + \delta\}} \leq D \log \frac{C}{\delta}.$$

## Theorem - excess risk bound

- Assume the prior mass condition with  $C, D > 0$ .
- Fix  $\lambda = \sqrt{n/D} \log(D/n)$ , and let  $\hat{\pi}_\lambda$  be the Gibbs posterior.

$$\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] \right] \leq R^* + \mathcal{O} \left( \sqrt{\frac{D}{n}} \log \frac{n}{D} \right).$$

## 1 PAC-Bayes bounds : introduction

- Generalization bounds and PAC-Bayes
- Minimization of the PAC-Bayes bound
- A zoo of PAC-Bayes bounds

## 2 PAC-Bayes and Mutual Information bounds

- Excess risk bounds
- Fast rates
- Mutual information bounds

## Reminder – Tolstikhin and Seldin’s PAC-Bayes bound, 2013

With proba. at least  $1 - \delta$ , for any  $\rho$ ,

$$\mathbb{E}_{\theta \sim \rho}[R(\theta)] \leq \mathbb{E}_{\theta \sim \rho}[R_n(\theta)]$$

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→ if there is a perfect predictor  $\theta^*$ ,  $R_n(\theta^*) = R(\theta^*) = 0$ , then using the previous approach (prior mass condition) :

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This can happen beyond the case  $R_n(\theta^*) = R(\theta^*) = 0$  !

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Recall :

- $\eta(x) = \mathbb{P}(Y = 1 | X = x)$ ,
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- $\mathbb{P}(|\eta(X) - 1/2| < \tau) = 0$  for some small enough  $\tau > 0$ .
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Mammen, E. and Tsybakov, A. B. (1999). Smooth discrimination analysis. *The Annals of Statistics*.



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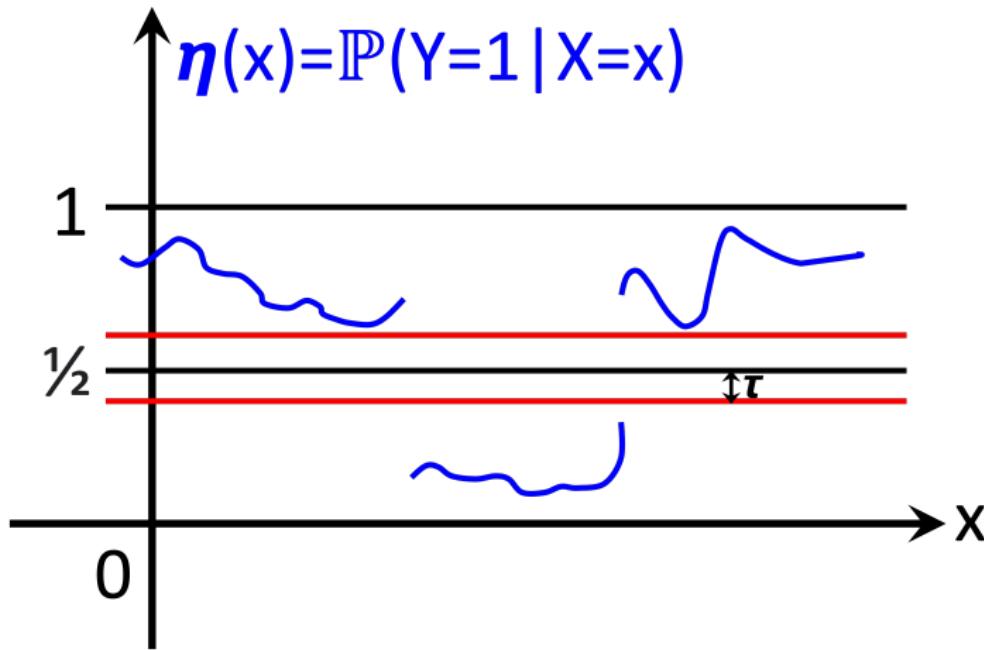


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Under the margin assumption, they prove fast rates in  $\frac{1}{n}$  for various predictors.

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$$\forall \theta, \frac{g(\theta) + g(\theta^*)}{2} - g\left(\frac{\theta + \theta^*}{2}\right) \geq \frac{1}{2\alpha} \delta(\theta, \theta^*),$$

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Bartlett, P. L., Jordan, M. I. and McAuliffe, J. D. (2003). Convexity, classification, and risk bounds. *Journal of the American Statistical Association*.

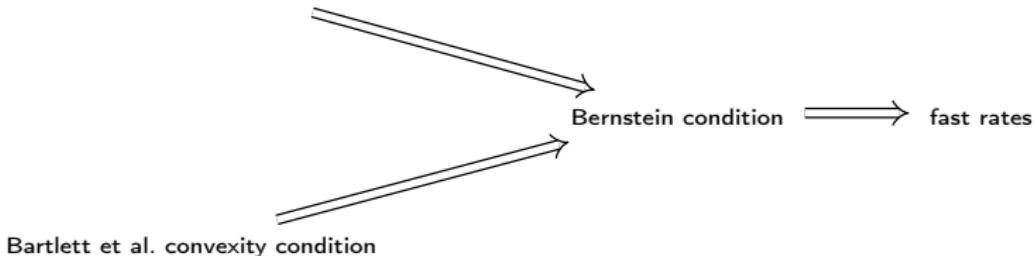
→ fast rates also in this case.

## Definition – Bernstein condition

Bernstein condition is satisfied with constant  $K$  if

$$\begin{aligned} \mathbb{E}\left[\left(\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X))\right)^2\right] \\ \leq K \underbrace{\mathbb{E}\left[\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X))\right]}_{=R(\theta) - R^*}. \end{aligned}$$

Mammen & Tsybakov margin assumption



Intuition : for a fixed  $\theta \in \Theta$  we have

$$\begin{aligned}\mathbb{E} \left[ \left( R_n(\theta) - R(\theta) \right)^2 \right] &= \text{Var} \left( \frac{1}{n} \sum_{i=1}^n \ell(Y_i, f_\theta(X_i)) \right) \\ &= \frac{1}{n^2} \sum_{i=1}^n \underbrace{\text{Var} \left( \ell(Y_i, f_\theta(X_i)) \right)}_{=: v(\theta)}.\end{aligned}$$

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If  $\theta$  and  $\theta'$  have the same empirical risk  $R_n(\theta) = R_n(\theta')$ , their risks might differ by  $1/\sqrt{n}$  !

$$\begin{aligned} & \mathbb{E} \left[ \left( R_n(\theta) - R_n(\theta^*) - (R(\theta) - R^*) \right)^2 \right] \\ &= \text{Var} \left( \frac{1}{n} \sum_{i=1}^n \left[ \ell(Y_i, f_\theta(X_i)) - \ell(Y_i, f_{\theta^*}(X_i)) \right] \right) \\ &= \frac{1}{n^2} \sum_{i=1}^n \text{Var} \left( \ell(Y_i, f_\theta(X_i)) - \ell(Y_i, f_{\theta^*}(X_i)) \right) \\ &\leq \frac{1}{n} \mathbb{E} \left[ (\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X)))^2 \right] \\ &\leq \frac{K}{n} [R(\theta) - R^*] \quad (\text{using Bernstein condition}). \end{aligned}$$

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If  $\theta$  and  $\theta^*$  have the same empirical risk  $R_n(\theta) = R_n(\theta^*)$ ,

$$\left( R(\theta) - R^* \right)^2 \leq \frac{K}{n} [R(\theta) - R^*] \Rightarrow R(\theta) - R^* \leq \frac{K}{n}.$$

## PAC-Bayes oracle inequality under Bernstein condition

- Assume Bernstein condition is satisfied with constant  $K$ .

Put  $\lambda = n / \max(2K, 1)$ ,

$$\begin{aligned} & \mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] - R^* \right] \\ & \leq 2 \inf_{\rho \in \mathcal{M}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [R(\theta)] - R^* + \frac{\max(2K, 1) \text{KL}(\rho \| \pi)}{n} \right]. \end{aligned}$$

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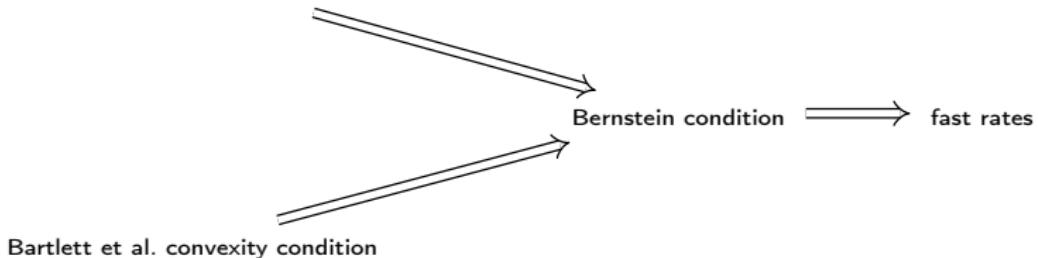
- Assume moreover the prior mass condition with  $C, D > 0$ .

$$\mathbb{E}_{\mathcal{S}} \left[ \mathbb{E}_{\theta \sim \hat{\pi}_\lambda} [R(\theta)] - R^* \right] \leq \frac{2 \max(2K, 1) D}{n} \log \left( \frac{e C n}{D} \right).$$

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Mammen & Tsybakov margin assumption



Bartlett et al. convexity condition

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If we assume that there is a “uniformly best”  $\theta^*$ , that is, with probability 1 on  $(X, Y)$ ,

$$\ell(Y, f_{\theta^*}(X)) \leq \ell(Y, f_\theta(X))$$

then we obtain

$$\begin{aligned} & \mathbb{E} \left[ (\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X)))^2 \right] \\ &\leq \mathbb{E} \left[ (\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X))) \right] = R(\theta) - R^*. \end{aligned}$$

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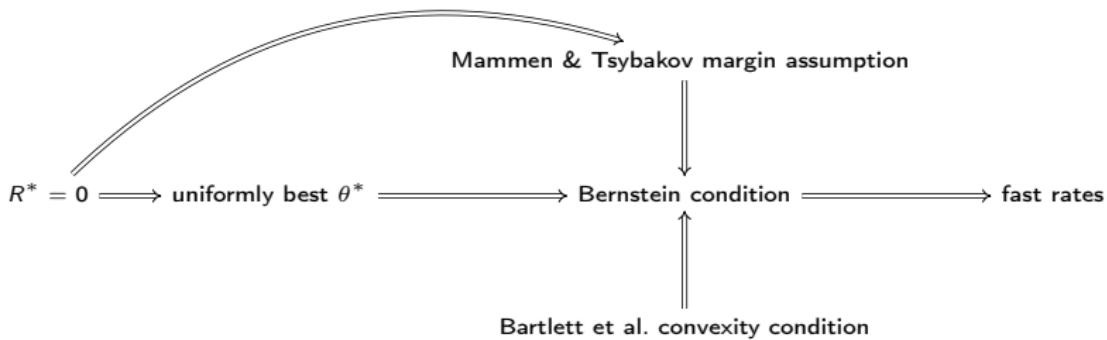
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This is the case if  $R^* = 0 \Rightarrow \ell(Y, f_{\theta^*}(X)) = 0$  with proba. 1.

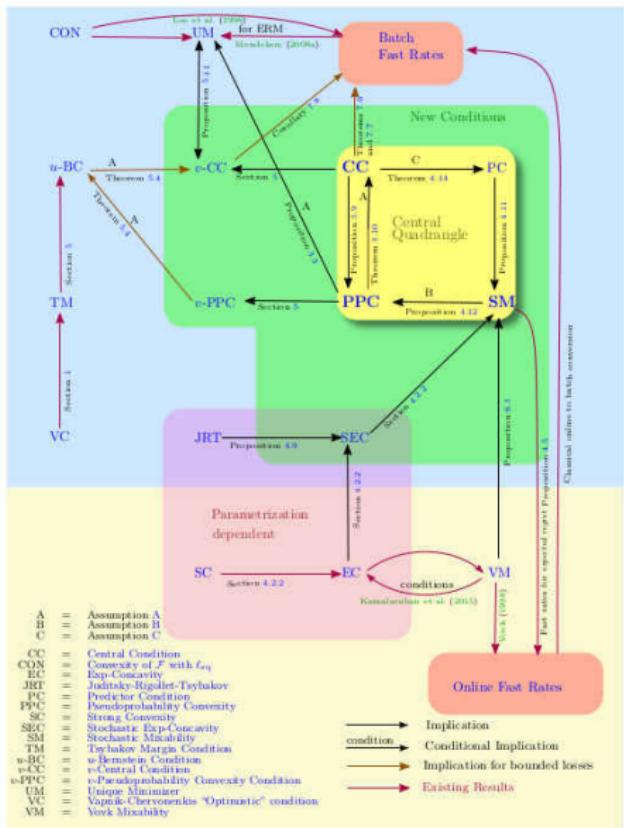
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## PAC-Bayes bounds : introduction PAC-Bayes and Mutual Information bounds

Excess risk bounds  
Fast rates  
Mutual information bounds



Van Erven, T., Grünwald, P.,  
Mehta, N., Reid, M. and  
Williamson, R. (2015). Fast  
Rates in Statistical and  
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Example : linear regression with quadratic loss,

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- We have to impose boundedness conditions on  $\mathcal{Y} \subset \mathbb{R}$  and  $\mathcal{X}, \Theta \subset \mathbb{R}^d$  to get  $0 \leq \ell \leq 1$ .
- We can check Bartlett *et al* condition with  $\delta(\theta, \theta^*) = \langle x, \theta - \theta^* \rangle$ .

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- Note that it is actually possible to get rid of some boundedness conditions, as well as to get rid of the log terms.



Catoni, O. (2004). *Statistical learning theory and Stochastic optimization*. Saint-Flour summer school on Probability Theory, Springer Lecture Notes in Mathematics.

Example : high-dimensional sparse linear regression with quadratic loss. That is,  $d > n$  but  $\theta^*$  has  $d_0 \ll d$  non-zero components.

Example : high-dimensional **sparse** linear regression with quadratic loss. That is,  $d > n$  but  $\theta^*$  has  $d_0 \ll d$  non-zero components.

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Dalalyan, A. and Tsybakov, A. B. (2008). Aggregation by exponential weighting, sharp PAC-Bayesian bounds and sparsity. *Machine Learning*.



Alquier, P. and Lounici, K. (2011). PAC-Bayesian bounds for sparse regression estimation with exponential weights. *Electronic Journal of Statistics*.

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- quantum tomography (reconstructing the quantum state of a system from measurements) :



Mai, T. T. and Alquier, P. (2017). Pseudo-Bayesian quantum tomography with rank-adaptation. *Journal of Statistical Planning and Inference*.

- ...

## (General) Bernstein condition

For  $K > 0$  and  $\gamma \in [0, 1]$ ,

$$\mathbb{E} \left[ (\ell(Y, f_\theta(X)) - \ell(Y, f_{\theta^*}(X)))^2 \right] \leq K[R(\theta) - R^*]^\gamma.$$

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- Mammen and Tsybakov proved a sufficient margin condition for  $0 < \gamma < 1$  :

$$\mathbb{P}(|\eta(X) - 1/2| < \tau) = \mathcal{O} \left( \tau^{\frac{1}{1-\gamma}} \right) \text{ for } \tau \rightarrow 0.$$

## 1 PAC-Bayes bounds : introduction

- Generalization bounds and PAC-Bayes
- Minimization of the PAC-Bayes bound
- A zoo of PAC-Bayes bounds

## 2 PAC-Bayes and Mutual Information bounds

- Excess risk bounds
- Fast rates
- Mutual information bounds

## Reminder – Catoni's PAC-Bayes bound, 2003

Fix  $\lambda > 0$  and  $\pi$ . With proba. at least  $1 - \delta$  on  $\mathcal{S}$ , for any randomized estimator  $\hat{\rho}$ ,

$$\mathbb{E}_{\theta \sim \hat{\rho}}[R(\theta)] \leq \mathbb{E}_{\theta \sim \hat{\rho}}[R_n(\theta)] + \frac{\text{KL}(\hat{\rho} \parallel \pi) + \log \frac{1}{\delta}}{\lambda} + \frac{\lambda}{8n}.$$

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But... why did we keep the same  $\lambda$  and  $\pi$  ?

## PAC-Bayes bound in expectation – v2.0

- Fix  $\Lambda > 0$ ,  $\Pi$  and the randomized estimator  $\hat{\rho}$  (for example  $\hat{\rho} = \hat{\pi}_\lambda$ ).

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- the first term in the r.h.s. has a nice interpretation...

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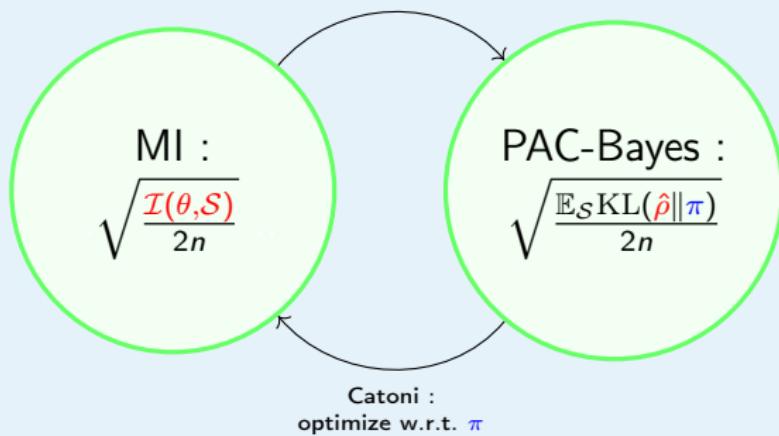


Russo, D. and Zou, J. (2019). How much does your data exploration overfit? controlling bias via information usage. *IEEE Transactions on Information Theory*.

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Let us illustrate the improvements of MI over PAC-Bayes on a simple example :

- finite parameter set  $\Theta = \{\theta_1, \dots, \theta_M\}$ .
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### MI bound for the ERM

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## Reminder – MI bound for the ERM

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PAC-Bayes : let  $\pi$  be uniform on  $\Theta$ ,

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Catoni :  $\pi(\theta) = \frac{\exp(-\alpha\Delta(\theta))}{\sum_{\theta \in \Theta} \exp(-\alpha\Delta(\theta))}$  where  $\Delta(\theta) = R(\theta) - R^*$ ,

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Put  $\zeta = \log \sum_{\theta \in \Theta} \exp(-\alpha\Delta(\theta))$ , we obtain the inequation :

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$$\mathbb{E}_{\mathcal{S}}[\Delta(\hat{\theta})] \leq \frac{\alpha}{4n} + \frac{1}{2} \sqrt{\frac{1}{n} \left[ \frac{\alpha^2}{4n} + 2\zeta \right]}.$$

$$\zeta = \log \sum_{\theta \in \Theta} \exp(-\alpha \Delta(\theta)) \leq \log(M)$$

$$\zeta = \log \left[ 1 + \sum_{\theta \neq \theta^*} \exp(-\alpha \Delta(\theta)) \right] \leq M \exp \left( -\alpha \min_{\theta \neq \theta^*} \Delta(\theta) \right).$$

Take  $\alpha = 2\sqrt{n}$ .

Recap : MI bound for the ERM on a finite  $\Theta$ 

Assume  $\Theta = \{\theta_1, \dots, \theta_M\}$  and put  $\Delta = \min_{\theta \neq \theta^*} [R(\theta) - R^*]$ .  
Then

$$\mathbb{E}_{\mathcal{S}}[R(\hat{\theta})] \leq R^* + \sqrt{\frac{\frac{1}{2} + \min[M \exp(-\Delta\sqrt{2n}), \log(M)]}{2n}} + \frac{1}{2n}.$$

Starting from the PAC-Bayes bound in expectation, we can combine the improvements due to Bernstein assumption to the optimization with respect to the prior.

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### MI bound with Bernstein condition

- Assume Bernstein condition is satisfied with constant  $K$ .

Fix  $\lambda = n / \max(2K, 1)$ , and  $\hat{\rho}$ , then

$$\begin{aligned} & \mathbb{E}_{\mathcal{S}} \mathbb{E}_{\theta \sim \hat{\rho}} [R(\theta) - R^*] \\ & \leq 2 \mathbb{E}_{\mathcal{S}} \mathbb{E}_{\theta \sim \hat{\rho}} [R_n(\theta) - R^*] + \frac{\max(2K, 1) \mathcal{I}(\theta, \mathcal{S})}{n}. \end{aligned}$$

A recent survey/tutorials that covers MI bounds in depth, and their relation to PAC-Bayes bounds :



Hellström, F., Durisi, G., Guedj, B. and Raginsky, M. (2023). *Generalization bounds : Perspectives from information theory and PAC-Bayes*. Arxiv preprint arXiv :2309.04381.

Review of topics not covered in these slides.

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### Unbounded losses :

-  Haddouche, M. and Guedj, B. (2023). *PAC-Bayes Generalisation Bounds for Heavy-Tailed Losses through Supermartingales*. Transactions on Machine Learning Research.
-  Rodríguez-Gálvez, B., Thobaben, R. and Skoglund, M. (2023). *More PAC-Bayes bounds : From bounded losses, to losses with general tail behaviors, to anytime-validity*. ArXiv preprint arXiv :2306.12214

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### Non i.i.d., time series...

-  Alquier, P. and Wintenberger, O. (2012). Model selection for weakly dependent time series forecasting. *Bernoulli*.
-  Alquier, P., Li. X. and Wintenberger, O. (2013). Prediction of time series by statistical learning : general losses and fast rates. *Dependence Modeling*.
-  Banerjee, I., Rao, V. A. and Honnappa, H. (2021). PAC-Bayes bounds on variational tempered posteriors for Markov models. *Entropy*.

Robust estimator (not Bayesian) studied by adding a random perturbation, and then using PAC-Bayes bounds.

-  Catoni, O. (2012). Challenging the empirical mean and empirical variance : a deviation study. *Annales de l'IHP*.
-  Catoni, O. and Giulini, I. (2017). Dimension free PAC-Bayesian bounds for the estimation of the mean of a random vector. *NeurIPS 2017 Workshop : (Almost) 50 Shades of Bayesian Learning : PAC-Bayesian trends and insights*.
-  Zhivotovskiy, N. (2024). Dimension-free bounds for sums of independent matrices and simple tensors via the variational principle. *Electronic Journal of Probability*.

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## Meta-learning.

-  Rothfuss, J., Fortuin, V., Josifoski, M. and Krause, A. (2021). PACOH : Bayes-optimal meta-learning with PAC-guarantees. *ICML*.
-  Riou, C., Alquier, P. and Chérif-Abdellatif, B.-E. (2023). *Bayes meets Bernstein at the Meta Level : an Analysis of Fast Rates in Meta-Learning with PAC-Bayes*. Arxiv preprint arXiv :2302.11709.

PAC-Bayes or MI bounds where  $\text{KL}(\rho\|\pi)$  is replaced by another  $D(\rho, \pi)$ .

-  Alquier, P. and Guedj, B. (2018). Simpler PAC-Bayesian bounds for hostile data. *Machine Learning*.
-  Neu, G. and Lugosi, G. (2022). Generalization Bounds via Convex Analysis. *ICML*.

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In particular, Wasserstein distance studied in :

-  Rodríguez-Gálvez, B., Bassi, G., Thobaben, R. and Skoglund, M. (2021). Tighter expected generalization error bounds via Wasserstein distance *NeurIPS*.
-  Clerico, E., Shidani, A., Deligiannidis, G. and Doucet, A. (2022). Chained Generalisation Bounds. *COLT*.
-  Viallard, P., Haddouche, M., Simsekli, U. and Guedj, B. (2023). Learning via Wasserstein-based high probability generalisation bounds. *NeurIPS*.
-  Neu, G. and Lugosi, G. (2023). *Online-to-PAC Conversions : Generalization Bounds via Regret Analysis*. Arxiv preprint arXiv :2305.19674.

終わり

C'est la fin.

The end.

$t = +\infty$ .

終わり

C'est la fin.

The end.

$t = +\infty$ .

Thank you !

ありがとうございました。