# PAC-Bayesian Bounds and Aggregation: Introduction, and Algorithmic Issues

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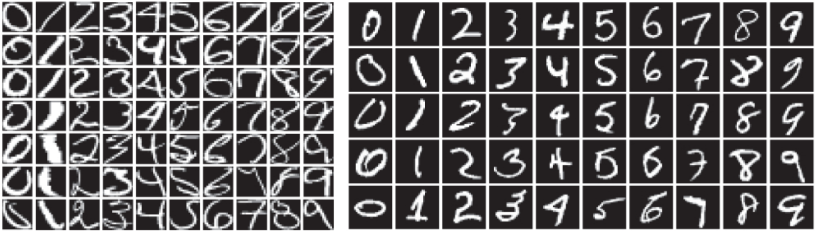

(a) USPS (b) MNIST

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The PAC-Bayesian approach usually provides a "posterior distribution" $\hat{\rho}_\lambda$ and a theoretical guarantee :

$$\int R(\theta)\hat{\rho}_\lambda(\mathrm{d}\theta) \leq \inf_\rho \left[ \int R(\theta)\rho(\mathrm{d}\theta) + \frac{1}{\lambda}\mathcal{K}(\rho,\pi) \right] + o(1).$$

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Usually $o(1)$ is explicit, $\lambda$ is some tuning-parameter to be calibrated (constrained to some range by theory), and

$$\hat{\rho}_\lambda(\mathrm{d}\theta) \propto \exp\left[-\lambda r(\theta)\right]\pi(\mathrm{d}\theta).$$

# 1st example : fixed design regression

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- $X_1, \ldots, X_n$ deterministic ; $Y_i = f(X_i) + \varepsilon_i$ and $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ (say).

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# Dalalyan and Tsybakov's bound for EWA

## Theorem

Dalalyan, A. & Tsybakov, A. (2008). Aggregation by Exponential Weighting, Sharp PAC-Bayesian Bounds and Sparsity. *Machine Learning*.

$$\forall \lambda \leq \frac{n}{4\sigma^2}: \quad \mathbb{E}\left\{ R\left[\int \theta \hat{\rho}_\lambda(\mathrm{d}\theta)\right]\right\} \leq \inf_{\rho}\left[\int R(\theta)\rho(\mathrm{d}\theta) + \frac{1}{\lambda}\mathcal{K}(\rho,\pi)\right]$$

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Based on previous work :

Leung, G. and Barron, A. (2006). Information Theory and Mixing Least-Square Regressions. *IEEE Trans. on Information Theory*.

# Application : finite set of predictors $\theta_1, \dots, \theta_M$

With $\pi$ the uniform distribution on $\{\theta_1, \dots, \theta_M\}$ we get

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&= \inf_{1\leq i\leq M}\left[R(\theta_i) + 4\sigma^2\log(M)\right].
\end{aligned}$$

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With $\pi = \mathcal{N}(0, S^2 I_M)$,

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As $\mathcal{K}(\rho,\pi) = \frac{1}{2}\left[M\left(\frac{s^2}{S^2} - 1 + \log\left(\frac{S^2}{s^2}\right)\right) + \frac{\|\theta_0\|^2}{S^2}\right]$ and (rough) calculations lead to $\int R(\theta)\rho(\mathrm{d}\theta) \leq R(\theta_0) + M^2\|g\|_\infty^2 s^2$,

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## Theorem

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$$\forall \lambda > 0, \quad \mathbb{P}\left\{ \int R(\theta)\hat{\rho}_{\lambda}(\mathrm{d}\theta) \right.$$

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improving on seminal work :

Shawe-Taylor, J. & Williamson, R. C. (1997). A PAC Analysis of a Bayesian Estimator. *COLT'97*.

McAllester, D. A. (1998). Some PAC-Bayesian Theorems. *COLT'98*.

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$$\mathcal{R} = \sum_{t=1}^{T} (Y_t - \hat{Y}_t)^2 - \inf_\theta \sum_{t=1}^{T} (Y_t - f_\theta(X_t))^2.$$

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Fix $\lambda \leq \frac{1}{8B^2}$ and define, at each time $t$ :

$$\hat{\rho}_{\lambda,t}(\mathrm{d}\theta) \propto \exp[-\lambda r_{t-1}(\theta)]\pi(\mathrm{d}\theta) \text{ and } \hat{Y}_t = \int f_\theta(X_t)\hat{\rho}_{\lambda,t}(\mathrm{d}\theta).$$

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Based on a result with general loss to be found in

Audibert, J.-Y. (2009). Fast learning Rates in Statistical Inference through Aggregation. *Annals of Statistics*.

# Bibliographical remarks (1/2)

**"Catoni's type bound"** : under the name "PAC-Bayesian bounds", many authors including Langford, Seeger, Meir, Cesa-Bianchi, Li, Jiang, Tanner, Laviolette, Guedj, sorry for not being exhaustive, see the papers for more references !

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**Related to other works on aggregation :** Vovk, Rissanen, Abramovitch, Nemirovski, Yang, Rigollet, Lecué, Bellec, Michel, Gaïffas...

# Bibliographical remarks (2/2)

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Bayesian interpretation : $\exp\left[-\lambda r(\theta)\right] =$ "pseudo-likelihood".

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**Asymptotic study of Bayesian estimators** : Ghosh, Ghoshal, van der Vaart, Gassiat, Rousseau, Castillo... different from PAC-Bayes but most calculations are similar !

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$$\hat{\rho}_\lambda(\mathrm{d}\theta) \propto \exp\left[-\lambda r(\theta)\right]\pi(\mathrm{d}\theta).$$

Depending on the setting, we have to

- sample from $\hat{\rho}_\lambda$,
- compute $\int \theta \hat{\rho}_\lambda(\mathrm{d}\theta)$.

# A natural idea : MCMC methods

Langevin Monte-Carlo :

Dalalyan, A. and Tsybakov, A. (2011). Sparse regression learning by aggregation and Langevin Monte-Carlo. *Journal of Computer and System Science*.

Markov Chain Monte-Carlo :

Alquier, P. & Biau, G. (2013). Sparse Single-Index Model. *Journal of Machine Learning Reseach*.

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However : very hard to prove the convergence of the algorithm. Usually not possible to provide guarantees after a finite number of steps. See however

Joulin, A. & Ollivier, Y. (2010). Curvature, Concentration, and Error Estimates for Markov Chain Monte Carlo. *The Annals of Probability*.

Dalalyan, A. (2014). Theoretical Guarantees for Approximate Sampling from a Smooth and Log-Concave Density. *Preprint*.

# Variational Bayes methods

Idea from Bayesian statistics : approximate the posterior distribution $\pi(\theta|x)$. We fix a convenient family of probability distributions $\mathcal{F}$ and approximate the posterior by $\tilde{\pi}(\theta)$ :

$$\tilde{\pi} = \arg\min_{\rho\in\mathcal{F}} \mathcal{K}(\rho, \pi(\cdot|x)).$$

Jordan, M. *et al* (1999). An Introduction to Variational Methods for Graphical Models. *Machine Learning*.

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$\mathcal{F}$ is either parametric or non-parametric. In the parametric case, the problem boils down to an optimization problem :

$$\mathcal{F} = \{\rho_a, a \in \mathcal{A} \subset \mathbb{R}^d\} \dashrightarrow \min_{a \in \mathcal{A}} \mathcal{K}(\rho_a, \pi(\cdot|x)).$$

# Variational Bayes methods

Idea from Bayesian statistics : approximate the posterior distribution $\pi(\theta|x)$. We fix a convenient family of probability distributions $\mathcal{F}$ and approximate the posterior by $\tilde{\pi}(\theta)$ :

$$\tilde{\pi} = \arg\min_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \pi(\cdot|x)).$$

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Theoretical guarantees on the approximation ?

# VB in PAC-Bayesian framework

$$\hat{\rho}_\lambda(\mathrm{d}\theta) \propto \exp\left[-\lambda r(\theta)\right]\pi(\mathrm{d}\theta).$$

Then :

$$\begin{aligned}\mathcal{K}(\rho_a, \hat{\rho}_\lambda) &= \int \log\left[\frac{\mathrm{d}\rho_a}{\mathrm{d}\pi}\frac{\mathrm{d}\pi}{\mathrm{d}\hat{\rho}_\lambda}\right]\mathrm{d}\rho_a \\ &= \lambda \int r(\theta)\rho_a(\mathrm{d}\theta) + \mathcal{K}(\rho_a, \pi) + \log\int \exp[-\lambda r]\mathrm{d}\pi.\end{aligned}$$

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We put

$$\tilde{a}_\lambda = \arg\min_{a\in\mathcal{A}}\left[\lambda\int r(\theta)\rho_a(\mathrm{d}\theta) + \mathcal{K}(\rho_a,\pi)\right] \text{ and } \tilde{\rho}_\lambda = \rho_{\hat{a}_\lambda}.$$

# A PAC-Bound for VB Approximation

## Theorem

Alquier, P., Ridgway, J. & Chopin, N. (2015). On the Properties of Variational Approximations of Gibbs Posteriors. *Preprint*.

$$\forall \lambda > 0, \quad \mathbb{P}\Biggl\{ \int R(\theta) \tilde{\rho}_\lambda(\mathrm{d}\theta)$$

$$\leq \inf_{a \in \mathcal{A}} \left[ \int R(\theta) \rho_a(\mathrm{d}\theta) + \frac{\lambda}{n} + \frac{2}{\lambda} \left[ \mathcal{K}(\rho_a, \pi) + \log\left(\frac{2}{\varepsilon}\right) \right] \right] \Biggr\}$$

$$\geq 1 - \varepsilon.$$

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$$\geq 1-\varepsilon.$$

$\dashrightarrow$ if we can derive a tight oracle inequality from this bound, we know that the VB approximation is sensible !

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Optimization criterion :

$$\frac{\lambda}{n} \sum_{i=1}^n \Phi \left( \frac{-Y_i \langle X_i, \mu \rangle}{\sqrt{\langle X_i, \Sigma X_i \rangle}} \right) + \frac{\|\mu\|^2}{2\vartheta} + \frac{1}{2} \left( \frac{1}{\vartheta} \mathrm{tr}(\Sigma) - \log |\Sigma| \right)$$

using deterministic annealing and gradient descent.

# Application of the main theorem

## Corollary

Assume that, for $\|\theta\| = \|\theta'\| = 1$, $\mathbb{P}(\langle\theta, X\rangle \langle\theta', X\rangle) \leq c\|\theta - \theta'\|$ and take $\lambda = \sqrt{nd}$ and $\vartheta = 1/\sqrt{d}$. Then

$$\mathbb{P}\left\{ \int R(\theta)\tilde{\rho}_\lambda(\mathrm{d}\theta) \leq \inf_\theta R(\theta) + \sqrt{\frac{d}{n}}\left[\log(4n\mathrm{e}^2) + c\right] + \frac{2\log\left(\frac{2}{\varepsilon}\right)}{\sqrt{nd}} \right\} \geq 1 - \varepsilon.$$

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N.B : under margin assumption, possible to obtain $d/n$ rates...

# Test on real data

| Dataset | Covariates | VB | SMC | SVM |
|---|---|---|---|---|
| Pima | 7 | 21.3 | 22.3 | 30.4 |
| Credit | 60 | 33.6 | 32.0 | 32.0 |
| DNA | 180 | 23.6 | 23.6 | 20.4 |
| SPECTF | 22 | 06.9 | 08.5 | 10.1 |
| Glass | 10 | 19.6 | 23.3 | 4.7 |
| Indian | 11 | 25.5 | 26.2 | 26.8 |
| Breast | 10 | 1.1 | 1.1 | 1.7 |

Table: Comparison of misclassification rates (%). Last column : kernel-SVM with radial kernel. The hyper-parameters $\lambda$ and $\vartheta$ are chosen by cross-validation.

# Convexification of the loss

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- $r_n(\theta) = \frac{1}{n}\sum_{i=1}^n (1 - Y_i f_\theta(X_i))_+$.
- Gaussian approx. : $\mathcal{F} = \left\{\mathcal{N}(\mu, \sigma^2 I), \mu \in \mathbb{R}^d, \sigma > 0\right\}$.

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- Gaussian approx. : $\mathcal{F} = \left\{\mathcal{N}(\mu, \sigma^2 I), \mu \in \mathbb{R}^d, \sigma > 0\right\}$.

$\dashrightarrow$ the following criterion (which turns out to be convex !) :

$$\frac{1}{n}\sum_{i=1}^n (1 - Y_i \langle \mu, X_i \rangle) \Phi\left(\frac{1 - Y_i \langle \mu, X_i \rangle}{\sigma \|X_i\|_2}\right)$$

$$+\frac{1}{n}\sum_{i=1}^n \sigma \|X_i\| \varphi\left(\frac{1 - Y_i \langle \mu, X_i \rangle}{\sigma \|X_i\|_2}\right) + \frac{\|\mu\|_2^2}{2\vartheta} + \frac{d}{2}\left(\frac{\vartheta}{\sigma^2} - \log \sigma^2\right).$$

# Application of the main theorem

Optimization with stochastic gradient descent on a ball of radius $M$. On this ball, the objetive function is $L$-Lipschitz. After $k$ step, we have the approximation $\tilde{\rho}_\lambda^{(k)}$ of the posterior.

## Corollary

Assume $\|X\| \leq c_x$ a.s., take $\lambda = \sqrt{nd}$ and $\vartheta = 1/\sqrt{d}$. Then

$$\mathbb{P}\left\{ \int R(\theta)\tilde{\rho}_\lambda^{(k)}(\mathrm{d}\theta) \leq \inf_\theta R(\theta) + \frac{LM}{\sqrt{1+k}} + \frac{c_x}{2}\sqrt{\frac{d}{n}}\log\left(\frac{n}{d}\right) + \frac{\frac{c_x^2+1}{2c_x} + 2c_x \log\left(\frac{2}{\varepsilon}\right)}{\sqrt{nd}} \right\} \geq 1 - \varepsilon.$$

| Dataset | Convex VB | VB | SMC | SVM |
|---|---|---|---|---|
| Pima | 21.8 | 21.3 | 22.3 | 30.4 |
| Credit | 27.2 | 33.6 | 32.0 | 32.0 |
| DNA | 4.2 | 23.6 | 23.6 | 20.4 |
| SPECTF | 19.2 | 06.9 | 08.5 | 10.1 |
| Glass | 26.1 | 19.6 | 23.3 | 4.7 |
| Indian | 26.2 | 25.5 | 26.2 | 26.8 |
| Breast | 0.5 | 1.1 | 1.1 | 1.7 |

Table: Comparison of misclassification rates (%), including the convexified version of VB.

# Convergence graphs

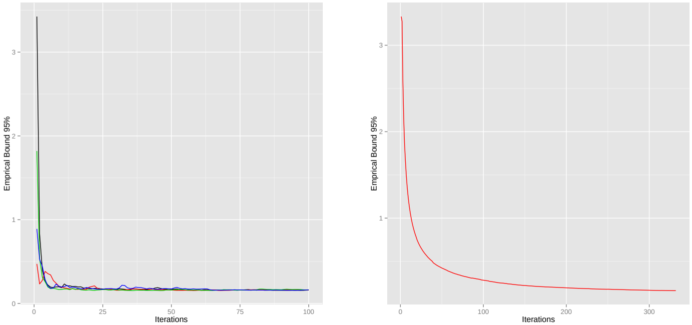


Figure: Stochastic gradient descent, Pima and Adult datasets.

Thanks & best wishes for 2016 !