A Primer on PAC-Bayesian Learning

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- Provide an encyclopaedic coverage of the PAC-Bayes literature (apologies!)

In a nutshell

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PAC-Bayes is a generic framework to efficiently rethink generalization for numerous machine learning algorithms. It leverages the flexibility of Bayesian learning and allows to derive new learning algorithms.

The plan

1. Elements of Statistical Learning

2. The PAC-Bayesian Theory

3. State-of-the-art PAC-Bayes results: a case study
   - Localized PAC-Bayes: data- or distribution-dependent priors
   - Stability and PAC-Bayes
   - PAC-Bayes analysis of deep neural networks

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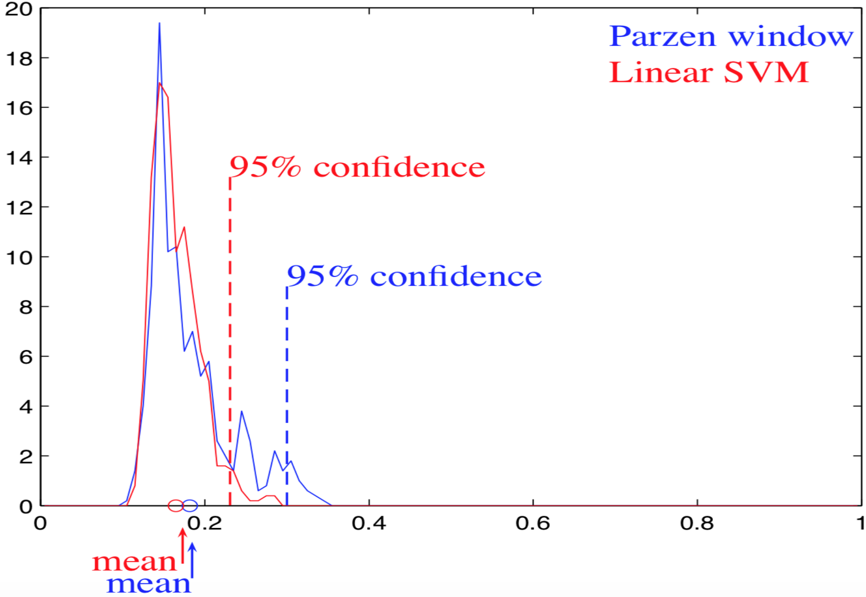
Error distribution



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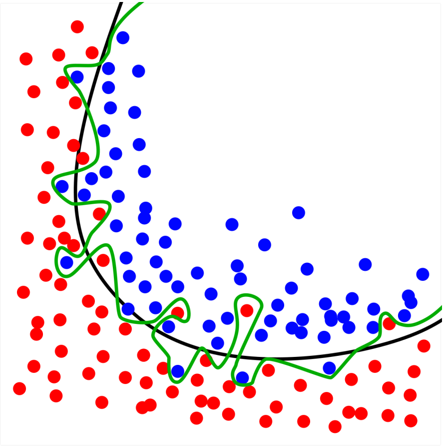

[Figure from Wikipedia]

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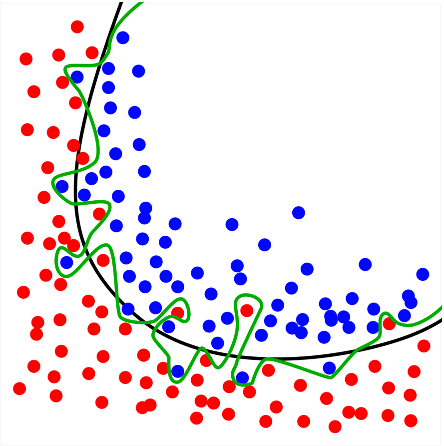

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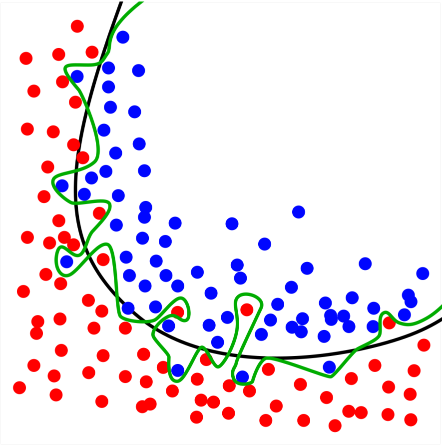

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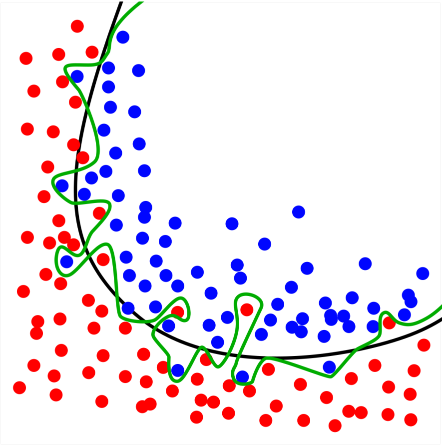

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Generalization is the ability to 'perform' well on unseen data.

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  δ is the probability of being misled by the training set
- Hence high confidence: $\mathbb{P}^m[\text{approximately correct}] \geqslant 1 - \delta$

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Learning algorithm $A : \mathcal{Z}^m \to \mathcal{H}$

- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
  $\mathcal{X}$ = set of inputs
  $\mathcal{Y}$ = set of outputs (e.g. labels)

- $\mathcal{H}$ = hypothesis class
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▷ these can be relaxed (mostly beyond the scope of this tutorial)

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Actually these two goals interact with each other!

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(out-of-sample)

Examples:

- $\ell(h(X), Y) = \mathbf{1}[h(X) \neq Y]$: 0-1 loss (classification)
- $\ell(h(X), Y) = (Y - h(X))^2$: square loss (regression)
- $\ell(h(X), Y) = (1 - Yh(X))_+$: hinge loss
- $\ell(h(X), 1) = -\log(h(X))$: log loss (density estimation)

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Flavours:

- distribution-free
- algorithm-free
- distribution-dependent
- algorithm-dependent

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- explain why specific learning algorithms actually work
- and even lead to designing new algorithm which scale to more complex settings

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- with probability $\geqslant 1 - \delta$, $\quad R_{\mathrm{out}}(h) \leqslant R_{\mathrm{in}}(h) + \sqrt{\frac{1}{2m}\log\left(\frac{1}{\delta}\right)}$

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Basic tool: $\mathbb{P}^m(E_1 \text{ or } E_2 \text{ or } \cdots) \leqslant \mathbb{P}^m(E_1) + \mathbb{P}^m(E_2) + \cdots$

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w.p. $\geqslant 1 - \delta$, $\quad \forall h \in \mathcal{H},\ R_{\mathrm{out}}(h) \leqslant R_{\mathrm{in}}(h) + \sqrt{\frac{1}{2m} \log\left(\frac{|\mathcal{H}|}{\delta}\right)}$

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This is a worst-case approach, as it considers uniformly all hypotheses.

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A route to improve this is to consider data-dependent hypotheses h_i, associated with prior distribution $P = (p_i)_i$ (structural risk minimization):

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- First attempt to introduce hypothesis-dependence
  (i.e. complexity depends on the chosen function)

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$$R_{\mathrm{out}}(h_i) \leqslant R_{\mathrm{in}}(h_i) + \sqrt{\frac{1}{2m}\left(\mathrm{KL}(\mathrm{Dirac}(h_i) \| P) + \log\left(\frac{1}{\delta}\right)\right)}$$

- First attempt to introduce hypothesis-dependence (i.e. complexity depends on the chosen function)
- This leads to a bound-minimizing algorithm:

$$\text{return} \quad \operatorname*{arg\,min}_{h_i \in \mathcal{H}} \left\{ R_{\mathrm{in}}(h_i) + \sqrt{\frac{1}{2m} \log\left(\frac{1}{p_i \delta}\right)} \right\}$$

Uncountably infinite function class?

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- Vapnik & Chervonenkis dimension: for $\mathcal{H}$ with $d = VC(\mathcal{H})$ finite, for any m, for any $\delta \in (0, 1)$,

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  These approaches are suited to analyse the performance of individual functions, and take some account of correlations
  $\longrightarrow$ Extension: PAC-Bayes allows to consider *distributions* over hypotheses.

The plan

1. Elements of Statistical Learning

2. The PAC-Bayesian Theory

3. State-of-the-art PAC-Bayes results: a case study
   - Localized PAC-Bayes: data- or distribution-dependent priors
   - Stability and PAC-Bayes
   - PAC-Bayes analysis of deep neural networks

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The risk measures $R_{\mathrm{in}}(h)$ and $R_{\mathrm{out}}(h)$ are extended by averaging:

$$R_{\mathrm{in}}(Q) \equiv \int_{\mathcal{H}} R_{\mathrm{in}}(h)\, dQ(h) \qquad R_{\mathrm{out}}(Q) \equiv \int_{\mathcal{H}} R_{\mathrm{out}}(h)\, dQ(h)$$

$\mathrm{KL}(Q \| P) = \underset{h \sim Q}{\mathbf{E}} \ln \frac{Q(h)}{P(h)}$ is the Kullback-Leibler divergence.

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Recall the bound for data-dependent hypotheses h_i associated with prior weights p_i:

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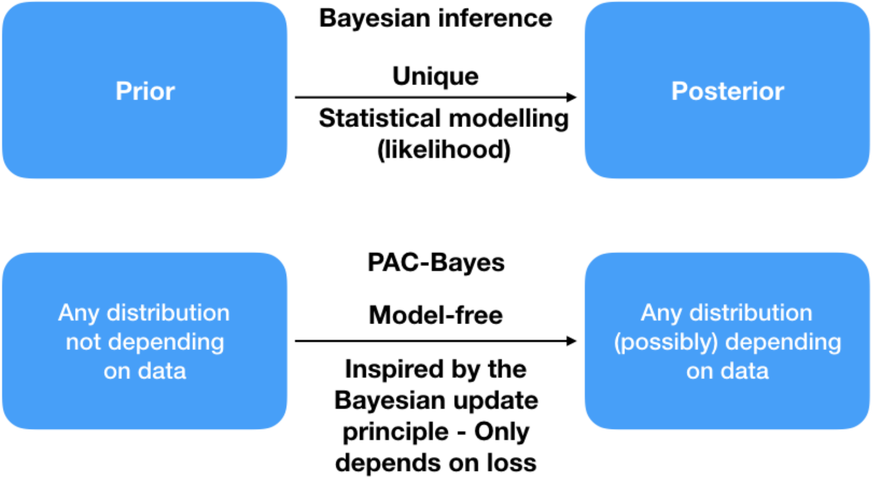

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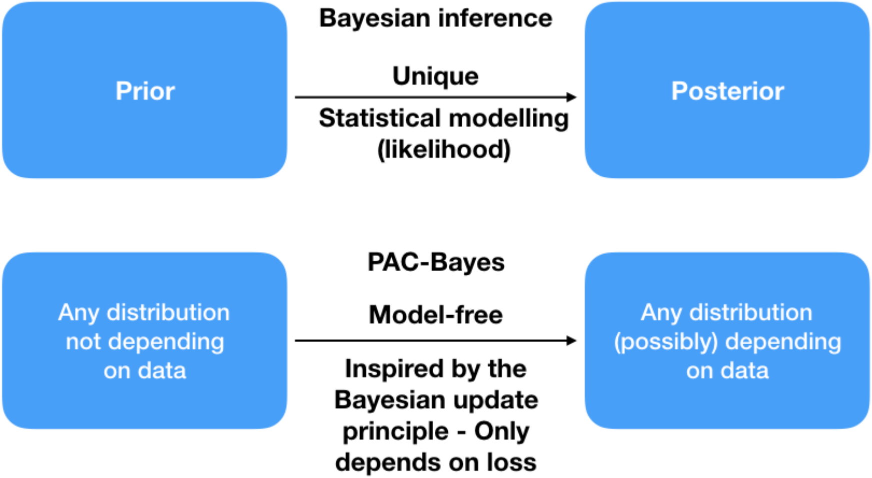
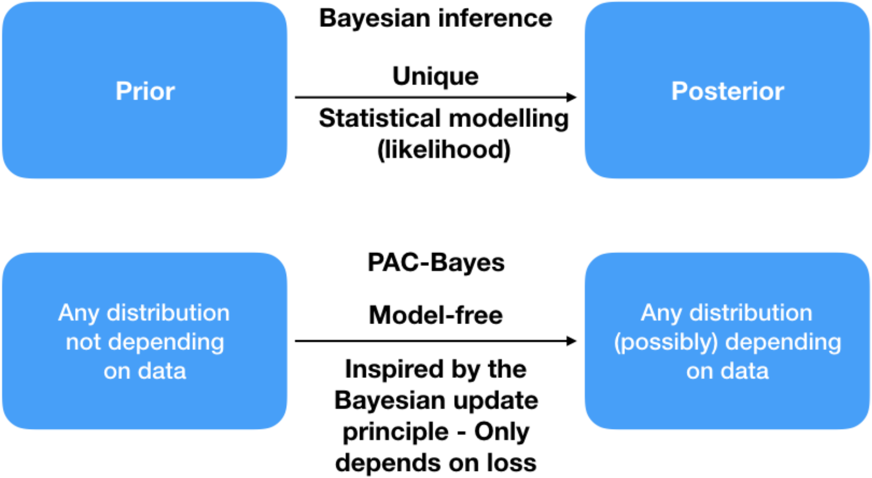


"Prior": exploration mechanism of $\mathcal{H}$

PAC-Bayes aka Generalized Bayes



"Prior": exploration mechanism of $\mathcal{H}$

"Posterior" is the twisted prior after confronting with data

PAC-Bayes bounds vs. Bayesian learning

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  - Bayesian: posterior computed by Bayesian inference, depends on statistical modeling
- Data distribution
  - PAC-Bayes bounds: can be used to define prior, hence no need to be known explicitly
  - Bayesian: input effectively excluded from the analysis, randomness lies in the noise model generating the output

A history of PAC-Bayes

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Pre-history: PAC analysis of Bayesian estimators

Shawe-Taylor and Williamson (1997); Shawe-Taylor et al. (1998)

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Birth: PAC-Bayesian bound

McAllester (1998, 1999)

McAllester Bound

For any prior P, any $\delta \in (0,1]$, we have

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\;\; R_{\mathrm{out}}(Q) \leqslant\; R_{\mathrm{in}}(Q) + \sqrt{\frac{\mathrm{KL}(Q\|P) + \ln\frac{2\sqrt{m}}{\delta}}{2m}} \right) \;\geqslant\; 1 - \delta\,,$$

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Langford and Seeger Bound

For any prior P, any $\delta \in (0, 1]$, we have

$$\mathbb{P}^m \left(\begin{array}{l} \forall\, Q \text{ on } \mathcal{H}: \\ \mathrm{kl}(R_{\mathrm{in}}(Q) \| R_{\mathrm{out}}(Q)) \leqslant \frac{1}{m} \left[\mathrm{KL}(Q \| P) + \ln \frac{2\sqrt{m}}{\delta} \right] \end{array} \right) \geqslant 1 - \delta \,,$$

where $\quad \mathrm{kl}(q \| p) \stackrel{\text{def}}{=} q \ln \frac{q}{p} + (1-q) \ln \frac{1-q}{1-p} \geqslant 2(q-p)^2.$

A General PAC-Bayesian Theorem

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Δ-function: "distance" between $R_{\text{in}}(Q)$ and $R_{\text{out}}(Q)$

Convex function $\Delta : [0,1] \times [0,1] \to \mathbb{R}$.

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Convex function $\Delta : [0,1] \times [0,1] \to \mathbb{R}$.

General theorem

Bégin et al. (2014, 2016); Germain (2015)

For any prior P on $\mathcal{H}$, for any $\delta \in (0,1]$, and for any Δ-function, we have, with probability at least $1-\delta$ over the choice of $S_m \sim \mathbb{P}^m$,

$$\forall\, Q \text{ on } \mathcal{H} : \quad \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \;\leqslant\; \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln \frac{\mathcal{I}_\Delta(m)}{\delta}\right],$$

where

$$\mathcal{I}_\Delta(m) \;=\; \sup_{r\in[0,1]} \left[\; \sum_{k=0}^{m} \underbrace{\binom{m}{k} r^k (1-r)^{m-k}}_{\mathbf{Bin}\left(k;m,r\right)} e^{m\Delta\left(\frac{k}{m},\, r\right)} \right].$$

General theorem

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \leq \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

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Proof ideas.

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Proof ideas.

Change of Measure Inequality (Csiszár, 1975; Donsker and Varadhan, 1975)

For any P and Q on $\mathcal{H}$, and for any measurable function $\phi : \mathcal{H} \to \mathbb{R}$, we have

$$\mathop{\mathbf{E}}_{h\sim Q} \phi(h) \ \leqslant\ \mathrm{KL}(Q\|P) + \ln\left(\mathop{\mathbf{E}}_{h\sim P} e^{\phi(h)}\right).$$

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Markov's inequality

$$\mathbb{P}\,(X \geqslant a) \leq \frac{\mathbf{E}\,X}{a} \qquad \Longleftrightarrow \qquad \mathbb{P}\left(X \leqslant \frac{\mathbf{E}\,X}{\delta}\right) \geq 1{-}\delta\,.$$

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Probability of observing k misclassifications among m examples

Given a voter h, consider a **binomial variable** of m trials with **success** $R_{\rm out}(h)$:

$$\mathbb{P}^m\left(R_{\rm in}(h) = \tfrac{k}{m}\right) = \binom{m}{k}\Big(R_{\rm out}(h)\Big)^k\Big(1 - R_{\rm out}(h)\Big)^{m-k} = \mathbf{Bin}\Big(k; m, R_{\rm out}(h)\Big)$$

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\text{in}}(Q), R_{\text{out}}(Q)\Big) \le \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

Proof

$$m \cdot \Delta\Big(\mathop{\mathbf{E}}_{h\sim Q} R_{\text{in}}(h), \mathop{\mathbf{E}}_{h\sim Q} R_{\text{out}}(h)\Big)$$

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \le \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln \frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

Proof

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Jensen's Inequality

$$\leqslant \quad \mathop{\mathbf{E}}_{h\sim Q} m \cdot \Delta\Big(R_{\mathrm{in}}(h), R_{\mathrm{out}}(h)\Big)$$

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Change of measure $\leqslant \mathrm{KL}(Q\|P) + \ln \mathop{\mathbf{E}}_{h\sim P} e^{m\Delta\left(R_{\mathrm{in}}(h), R_{\mathrm{out}}(h)\right)}$

Markov's Inequality $\leq_{1-\delta} \mathrm{KL}(Q\|P) + \ln\frac{1}{\delta} \mathop{\mathbf{E}}_{S'_m\sim\mathbb{P}^m} \mathop{\mathbf{E}}_{h\sim P} e^{m\cdot\Delta(R_{\mathrm{in}}(h), R_{\mathrm{out}}(h))}$

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Expectation swap

$$= \quad \mathrm{KL}(Q\|P) + \ln\frac{1}{\delta}\mathop{\mathbf{E}}_{h\sim P}\ \mathop{\mathbf{E}}_{S'_m\sim\mathbb{P}^m} e^{m\cdot\Delta(R_{\text{in}}(h), R_{\text{out}}(h))}$$

$$\mathbb{P}^m\left(\forall Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\text{in}}(Q), R_{\text{out}}(Q)\Big) \leq \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

Proof

$$
\begin{array}{lll}
 & & m\cdot\Delta\Big(\mathop{\mathbf{E}}_{h\sim Q} R_{\text{in}}(h), \mathop{\mathbf{E}}_{h\sim Q} R_{\text{out}}(h)\Big) \\
\textbf{Jensen's Inequality} & \leqslant & \mathop{\mathbf{E}}_{h\sim Q} m\cdot\Delta\Big(R_{\text{in}}(h), R_{\text{out}}(h)\Big) \\
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\textbf{Expectation swap} & = & \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta} \mathop{\mathbf{E}}_{h\sim P} \mathop{\mathbf{E}}_{S'_m\sim\mathbb{P}^m} e^{m\cdot\Delta(R_{\text{in}}(h), R_{\text{out}}(h))} \\
\textbf{Binomial law} & = & \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta} \mathop{\mathbf{E}}_{h\sim P} \sum_{k=0}^{m} \mathbf{Bin}\Big(k; m, R_{\text{out}}(h)\Big)\, e^{m\cdot\Delta(\frac{k}{m}, R_{\text{out}}(h))}
\end{array}
$$

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\textbf{Supremum over risk} & \leqslant & \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta} \sup_{r\in[0,1]} \left[\sum_{k=0}^{m} \mathbf{Bin}\Big(k;\, m,\, r\Big)\, e^{m\Delta(\frac{k}{m}, r)}\right]
\end{array}
$$

$$\mathbb{P}^m\left(\forall\, Q \text{ on } \mathcal{H}:\ \Delta\Big(R_{\mathrm{in}}(Q), R_{\mathrm{out}}(Q)\Big) \leq \frac{1}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{\mathcal{I}_\Delta(m)}{\delta}\right]\right) \geqslant 1-\delta\,.$$

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Binomial law

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Supremum over risk

$$\leqslant \quad \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta} \sup_{r\in[0,1]} \left[\sum_{k=0}^{m} \mathbf{Bin}\Big(k; m, r\Big)\, e^{m\Delta(\frac{k}{m}, r)}\right]$$

$$= \quad \mathrm{KL}(Q\|P) + \ln \frac{1}{\delta}\, \mathcal{I}_\Delta(m)\,. \qquad \square$$

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In all the previous bounds, with an arbitrarily high probability and for any posterior distribution Q,

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(optimization problem which can be solved or approximated by [stochastic] gradient descent-flavored methods, Monte Carlo Markov Chain, Variational Bayes...)

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Variational definition of KL-divergence (Csiszár, 1975; Donsker and Varadhan, 1975; Catoni, 2004).

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(i) For any probability P on $(A, \mathcal{A})$ and any measurable function $\phi : A \to \mathbb{R}$ such that $\int (\exp \circ \phi) \mathrm{d}P < \infty$,

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(ii) If ϕ is upper-bounded on the support of P, the supremum is reached for the Gibbs distribution G given by

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$\mathrm{KL}(\cdot, \cdot)$ is non-negative, $Q \mapsto -\mathrm{KL}(Q, G)$ reaches its max. in $Q = G$:

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\end{aligned}$$

$\mathrm{KL}(\cdot,\cdot)$ is non-negative, $Q \mapsto -\mathrm{KL}(Q,G)$ reaches its max. in $Q = G$:

$$0 = \sup_{Q\ll P}\left\{\int \phi \mathrm{d}Q - \mathrm{KL}(Q,P)\right\} - \log\int(\exp\circ\phi)\,\mathrm{d}P.$$

$$\log \int (\exp \circ \phi) \mathrm{d}P = \sup_{Q \ll P} \left\{ \int \phi \mathrm{d}Q - \mathrm{KL}(Q, P) \right\}, \quad \frac{\mathrm{d}G}{\mathrm{d}P} = \frac{\exp \circ \phi}{\int (\exp \circ \phi) \mathrm{d}P}.$$

Proof: let $Q \ll P$.

$$\begin{aligned} -\mathrm{KL}(Q, G) &= -\int \log \left(\frac{\mathrm{d}Q}{\mathrm{d}P} \frac{\mathrm{d}P}{\mathrm{d}G} \right) \mathrm{d}Q \\ &= -\int \log \left(\frac{\mathrm{d}Q}{\mathrm{d}P} \right) \mathrm{d}Q + \int \log \left(\frac{\mathrm{d}G}{\mathrm{d}P} \right) \mathrm{d}Q \\ &= -\mathrm{KL}(Q, P) + \int \phi \mathrm{d}\rho - \log \int (\exp \circ \phi) \, \mathrm{d}P. \end{aligned}$$

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Take $\phi = -\lambda R_{\mathrm{in}}$,

$$Q_\lambda \propto \exp\left(-\lambda R_{\mathrm{in}}\right) P = \arg\inf_{Q \ll P} \left\{ R_{\mathrm{in}}(Q) + \frac{\mathrm{KL}(Q, P)}{\lambda} \right\}.$$

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Csiszár f-divergence: let f be a convex function with $f(1) = 0$,

$$D_f(Q, P) = \int f\left(\frac{\mathrm{d}Q}{\mathrm{d}P}\right) \mathrm{d}P$$

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The KL is given by the special case $\mathrm{KL}(Q\|P) = D_{x\log(x)}(Q, P)$.

PAC-Bayes with f-divergences *Alquier and Guedj (2018)*

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Let $\phi_p \colon x \mapsto x^p$. Fix $p > 1$, $q = \frac{p}{p-1}$ and $\delta \in (0, 1)$. With probability at least $1 - \delta$ we have for any distribution Q

$$|R_{\text{out}}(Q) - R_{\text{in}}(Q)| \leqslant \left(\frac{\mathcal{M}_q}{\delta}\right)^{\frac{1}{q}} \left(D_{\phi_p - 1}(Q, P) + 1\right)^{\frac{1}{p}} .$$

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- the moment $\mathcal{M}_q$ (which depends on the distribution of the data)
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Corolloray: with probability at least $1 - \delta$, for any Q,

$$R_{\mathrm{out}}(Q) \leqslant R_{\mathrm{in}}(Q) + \left(\frac{\mathcal{M}_q}{\delta}\right)^{\frac{1}{q}} \left(D_{\phi_p - 1}(Q, P) + 1\right)^{\frac{1}{p}}.$$

Again, strong incitement to define the posterior as the minimizer of the right-hand side!

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Assume that the loss is upper-bounded by B, for any $\lambda > 0$, with probability greater that $1 - \delta$

$$R_{\text{out}}(Q_\lambda) \leqslant \inf_{Q \ll P} \left\{ R_{\text{out}}(Q) + \frac{\lambda B}{m} + \frac{2}{\lambda}\left(\mathrm{KL}(Q, P) + \log \frac{2}{\delta}\right)\right\}$$

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Pros: Q_λ now enjoys stronger guarantees as its performance is comparable to the (forever unknown) oracle.
Cons: the right-hand side is no longer computable.

The plan

1. Elements of Statistical Learning

2. The PAC-Bayesian Theory

3. State-of-the-art PAC-Bayes results: a case study
   - Localized PAC-Bayes: data- or distribution-dependent priors
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- An important component in the PAC-Bayes analysis is the choice of the **prior distribution**
- The results hold whatever the choice of prior, provided that it is chosen *before* seeing the data sample
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  - defining the prior in terms of the *data generating distribution* *(aka localised PAC-Bayes)*.

SVM Application

- Prior and posterior distributions are spherical Gaussians:

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- Generalization of deterministic classifier can be bounded by *twice* stochastic error

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- We present some results to show the bounds and their use in model selection (regularisation and band-width of kernel).

Results

		Classifier					
		SVM				ηPrior SVM	
Problem		2FCV	10FCV	PAC	PrPAC	PrPAC	τ-PrPAC
digits	Bound	–	–	0.175	0.107	0.050	**0.047**
	TE	**0.007**	**0.007**	**0.007**	0.014	0.010	0.009
waveform	Bound	–	–	0.203	0.185	0.178	**0.176**
	TE	0.090	0.086	**0.084**	0.088	0.087	0.086
pima	Bound	–	–	0.424	0.420	0.428	**0.416**
	TE	0.244	0.245	**0.229**	**0.229**	0.233	0.233
ringnorm	Bound	–	–	0.203	0.110	0.053	**0.050**
	TE	**0.016**	**0.016**	0.018	0.018	**0.016**	**0.016**
spam	Bound	–	–	0.254	0.198	0.186	**0.178**
	TE	0.066	**0.063**	0.067	0.077	0.070	0.072

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- Model selection from the bounds is as good as 10FCV: in fact all but one of the PAC-Bayes model selections give better averages for TE.

- The better bounds do not appear to give better model selection - best model selection is from the simplest bound.
  Ambroladze et al. (2007), *Germain et al. (2009a)*

Distribution-defined priors

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- Consider P and Q are Gibbs-Boltzmann distributions

$$P_\gamma(h) := \frac{1}{Z'} e^{-\gamma R_{\mathrm{out}}(h)} \qquad Q_\gamma(h) := \frac{1}{Z} e^{-\gamma R_{\mathrm{in}}(h)}$$

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- These distributions are hard to work with since we cannot apply the bound to a single weight vector, but the bounds can be very tight:

$$\mathrm{kl}(R_{\text{in}}(Q_\gamma)\|R_{\text{out}}(Q_\gamma)) \leqslant \frac{1}{m}\left(\frac{\gamma}{\sqrt{m}}\sqrt{\ln\frac{8\sqrt{m}}{\delta}} + \frac{\gamma^2}{4m} + \ln\frac{4\sqrt{m}}{\delta}\right)$$

with the only uncertainty the dependence on γ.

Catoni (2003), *Catoni (2007)*, *Lever et al. (2010)*

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- The Gibbs distributions are hard to sample from so not easy to work with this bound.

Other distribution defined priors

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- An alternative distribution defined prior for an SVM is to place symmetrical Gaussian at the weight vector: $\mathbf{w}_p = \mathbb{E}_{(\mathbf{x},y)\sim D}(y\,\boldsymbol{\phi}(\mathbf{x}))$ to give distributions that are easier to work with, but results not impressive...

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- This is connected to stability...

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Stability

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Uniform hypothesis sensitivity β at sample size m:

$$\| \mathsf{A}(z_{1:m}) - \mathsf{A}(z'_{1:m}) \| \leqslant \beta \sum_{i=1}^{m} \mathbf{1}[z_i \neq z'_i]$$

$(z_1, \dots, z_m)$

- $\mathsf{A}(z_{1:m}) \in \mathcal{H}$ normed space
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- worst-case
- data-insensitive
- distribution-insensitive
- Open: data-dependent?

Generalization from Stability

If A has sensitivity β at sample size m, then for any $\delta \in (0, 1)$,

w.p. $\geqslant 1 - \delta$, $\quad R_{\mathrm{out}}(h) \leqslant R_{\mathrm{in}}(h) + \epsilon(\beta, m, \delta)$

Bousquet and Elisseeff (2002)

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- can be applied to kernel methods where β is related to the regularisation constant, but bounds are quite weak
- question: algorithm output is highly concentrated
  $\Longrightarrow$ stronger results?

Stability + PAC-Bayes

If A has uniform hypothesis stability β at sample size m, then for any $\delta \in (0,1)$, w.p. $\geqslant 1-2\delta$,

$$\mathrm{kl}\big(R_{\mathrm{in}}(Q) \| R_{\mathrm{out}}(Q)\big) \leqslant \frac{\frac{m\beta^2}{2\sigma^2}\left(1+\sqrt{\frac{1}{2}\log\left(\frac{1}{\delta}\right)}\right)^2 + \log\left(\frac{m+1}{\delta}\right)}{m}$$

Gaussian randomization

- $P = \mathcal{N}(\mathbb{E}[W_m], \sigma^2 I)$
- $Q = \mathcal{N}(W_m, \sigma^2 I)$
- $\mathrm{KL}(Q\|P) = \frac{1}{2\sigma^2}\|W_m - \mathbb{E}[W_n]\|^2$

Main proof components:

- w.p. $\geqslant 1-\delta$, $\quad \mathrm{kl}\big(R_{\mathrm{in}}(Q) \| R_{\mathrm{out}}(Q)\big) \leqslant \frac{\mathrm{KL}(Q\|Q_0) + \log\left(\frac{m+1}{\delta}\right)}{m}$
- w.p. $\geqslant 1-\delta$, $\quad \|W_m - \mathbb{E}[W_m]\| \leqslant \sqrt{m}\,\beta\left(1+\sqrt{\frac{1}{2}\log\left(\frac{1}{\delta}\right)}\right)$

Dziugaite and Roy (2018a), *Rivasplata et al. (2018)*

The plan

1. Elements of Statistical Learning

2. The PAC-Bayesian Theory

3. State-of-the-art PAC-Bayes results: a case study
   - Localized PAC-Bayes: data- or distribution-dependent priors
   - Stability and PAC-Bayes
   - PAC-Bayes analysis of deep neural networks

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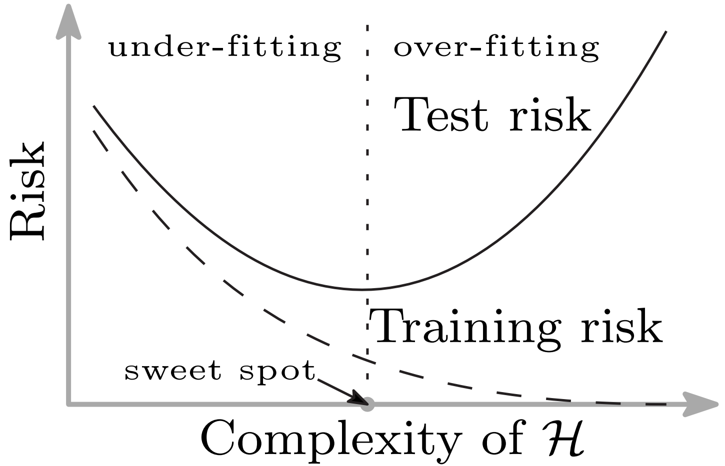
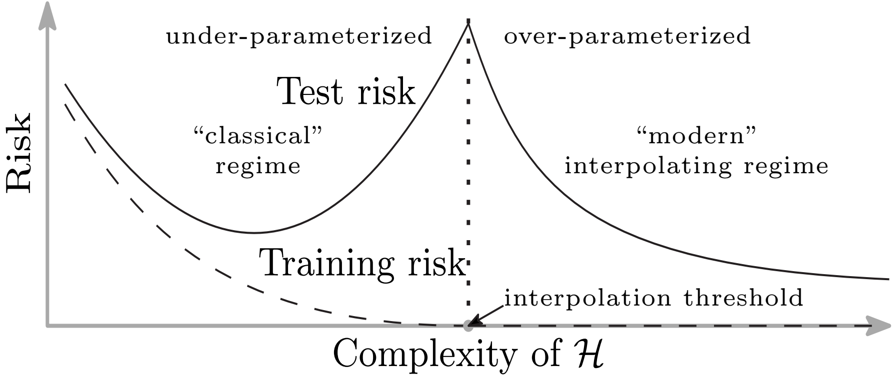
PAC-Bayes is a solid candidate to better understand how deep nets generalize.

The celebrated bias-variance tradeoff



Belkin et al. (2018)

Towards a better understanding of deep nets



Belkin et al. (2018)

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- For SVMs we can think of the margin as capturing an accuracy with which we need to estimate the weights

- If we have a deep network solution with a wide basin of good performance we can take a similar approach using PAC-Bayes with a broad posterior around the solution

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- There have also been suggestions that stability of SGD is important in obtaining good generalization *(see Dziugaite and Roy (2018b))*
- We presented stability approach combining with PAC-Bayes: this results in a new learning principle linked to recent analysis of information stored in weights

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- Potential for algorithms that optimize the bound

Conclusion

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Conclusion

- PAC-Bayes arises from two fields:
    - Statistical learning theory
    - Bayesian learning
- As such, it generalizes both in interesting and promising directions.
- We believe PAC-Bayes can be an inspiration towards
    - new theoretical analyses
    - but also drive novel algorithms design, especially in settings where theory has proven difficult.

Acknowledgments

We warmly thank our many co-authors on PAC-Bayes, with a special mention to Omar Rivasplata, François Laviolette and Pascal Germain who helped shape this tutorial.

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Thank you!

Slides available on
`https://bguedj.github.io/icml2019/index.html`

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