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A Primer on PAC-Bayesian Learning

Benjamin Guedj John Shawe-Taylor

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Inria



What to expect

We will...

- Provide an **overview** of what PAC-Bayes is
- Illustrate its **flexibility** and relevance to tackle modern machine learning tasks, and **rethink generalization**
- Cover **main existing results** and **key ideas**, and briefly sketch some proofs

We won't...

- Cover **all of Statistical Learning Theory**: see the NeurIPS 2018 tutorial "Statistical Learning Theory: A Hitchhiker's guide" (Shawe-Taylor and Rivasplata)
- Provide an **encyclopaedic coverage** of the PAC-Bayes literature (apologies!)

In a nutshell

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.

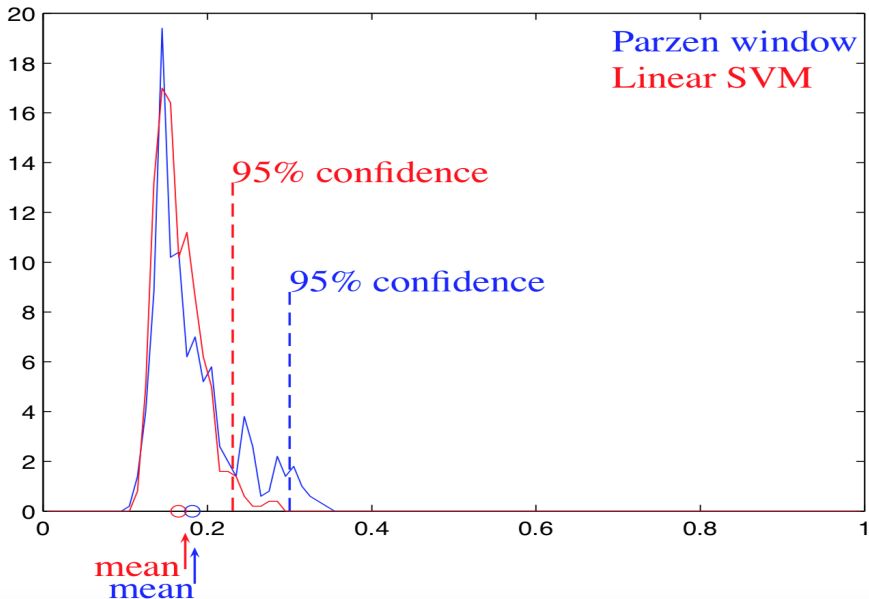
The plan

- 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

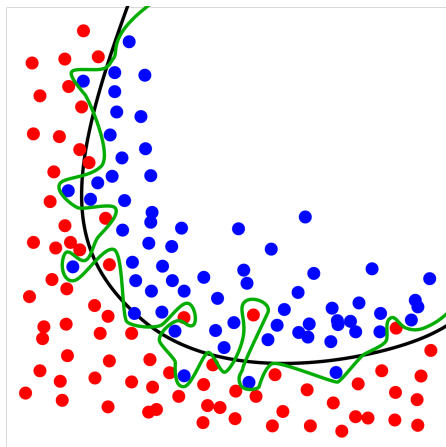
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Error distribution



Learning is to be able to generalize



[Figure from Wikipedia]

From **examples**, what can a system **learn** about the **underlying phenomenon**?

Memorizing the already seen data is usually bad → **overfitting**

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

Statistical Learning Theory is about high confidence

For a fixed algorithm, function class and sample size, generating random samples \rightarrow distribution of test errors

- Focusing on the mean of the error distribution?
 - ▷ can be misleading: learner only has **one** sample
- **Statistical Learning Theory**: tail of the distribution
 - ▷ finding bounds which hold with high probability over random samples of size m
- Compare to a statistical test – at **99%** confidence level
 - ▷ chances of the conclusion not being true are less than **1%**
- **PAC**: probably approximately correct (Valiant, 1984)
Use a ‘confidence parameter’ δ : $\mathbb{P}^m[\text{large error}] \leq \delta$
 δ is the probability of being misled by the training set
- Hence **high confidence**: $\mathbb{P}^m[\text{approximately correct}] \geq 1 - \delta$

Mathematical formalization

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

- $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
 - \mathcal{X} = set of inputs
 - \mathcal{Y} = set of outputs (e.g. labels)
- \mathcal{H} = hypothesis class = set of **predictors** (e.g. classifiers) functions $\mathcal{X} \rightarrow \mathcal{Y}$

Training set (aka **sample**): $S_m = ((X_1, Y_1), \dots, (X_m, Y_m))$
a finite sequence of **input-output examples**.

Classical assumptions:

- A **data-generating distribution** \mathbb{P} over \mathcal{Z} .
 - Learner doesn't know \mathbb{P} , only sees the training set.
 - The training set **examples are *i.i.d.*** from \mathbb{P} : $S_m \sim \mathbb{P}^m$
- ▷ these can be relaxed (mostly beyond the scope of this tutorial)

What to achieve from the sample?

Use the available sample to:

- 1 learn a predictor
- 2 certify the predictor's performance

Learning a predictor:

- algorithm driven by some learning principle
- informed by prior knowledge resulting in inductive bias

Certifying performance:

- what happens beyond the training set
- generalization bounds

Actually these two goals interact with each other!

Risk (aka error) measures

A **loss function** $\ell(h(X), Y)$ is used to measure the discrepancy between a predicted output $h(X)$ and the true output Y .

Empirical risk: $R_{\text{in}}(h) = \frac{1}{m} \sum_{i=1}^m \ell(h(X_i), Y_i)$
(in-sample)

Theoretical risk: $R_{\text{out}}(h) = \mathbb{E}[\ell(h(X), Y)]$
(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)

Generalization

If predictor h does well on the in-sample (X, Y) pairs...

...will it still do well on out-of-sample pairs?

Generalization gap: $\Delta(h) = R_{\text{out}}(h) - R_{\text{in}}(h)$

Upper bounds: w.h.p. $\Delta(h) \leq \epsilon(m, \delta)$

$$\blacktriangleright R_{\text{out}}(h) \leq R_{\text{in}}(h) + \epsilon(m, \delta)$$

Lower bounds: w.h.p. $\Delta(h) \geq \tilde{\epsilon}(m, \delta)$

Flavours:

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

Why you should care about generalization bounds

Generalization bounds are a **safety check**: give a **theoretical guarantee** on the **performance** of a learning algorithm on **any unseen data**.

Generalization bounds:

- may be computed with the **training sample only**, do not depend on any test sample
- provide a **computable** control on the error on **any unseen data** with prespecified confidence
- explain **why** specific learning algorithms **actually work**
- and even lead to **designing new algorithm** which scale to more complex settings

Building block: one single hypothesis

For one fixed (non data-dependent) h :

$$\mathbb{E}[R_{\text{in}}(h)] = \mathbb{E}\left[\frac{1}{m} \sum_{i=1}^m \ell(h(X_i), Y_i)\right] = R_{\text{out}}(h)$$

- ▶ $\mathbb{P}^m[\Delta(h) > \epsilon] = \mathbb{P}^m[\mathbb{E}[R_{\text{in}}(h)] - R_{\text{in}}(h) > \epsilon]$ deviation ineq.
- ▶ $\ell(h(X_i), Y_i)$ are independent r.v.'s
- ▶ If $0 \leq \ell(h(X), Y) \leq 1$, using **Hoeffding's inequality**:

$$\mathbb{P}^m[\Delta(h) > \epsilon] \leq \exp\{-2m\epsilon^2\} = \delta$$

- ▶ Given $\delta \in (0, 1)$, equate RHS to δ , solve equation for ϵ , get

$$\mathbb{P}^m\left[\Delta(h) > \sqrt{(1/2m) \log(1/\delta)}\right] \leq \delta$$

- ▶ **with probability** $\geq 1 - \delta$, $R_{\text{out}}(h) \leq R_{\text{in}}(h) + \sqrt{\frac{1}{2m} \log\left(\frac{1}{\delta}\right)}$

Finite function class

Algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{H}$

Function class \mathcal{H} with $|\mathcal{H}| < \infty$

Aim for a uniform bound: $\mathbb{P}^m[\forall f \in \mathcal{H}, \Delta(f) \leq \epsilon] \geq 1 - \delta$

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

known as the **union bound** (aka **countable sub-additivity**)

$$\begin{aligned}\mathbb{P}^m[\exists f \in \mathcal{H}, \Delta(f) > \epsilon] &\leq \sum_{f \in \mathcal{H}} \mathbb{P}^m[\Delta(f) > \epsilon] \\ &\leq |\mathcal{H}| \exp\{-2m\epsilon^2\} = \delta\end{aligned}$$

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

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

Towards non-uniform learnability

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

$$\text{w.p.} \geq 1 - \delta, \quad \forall h_i \in \mathcal{H}, \quad R_{\text{out}}(h_i) \leq R_{\text{in}}(h_i) + \sqrt{\frac{1}{2m} \log \left(\frac{1}{p_i \delta} \right)}$$

Note that we can also write

$$\text{w.p.} \geq 1 - \delta, \quad \forall h_i \in \mathcal{H}, \\ R_{\text{out}}(h_i) \leq R_{\text{in}}(h_i) + \sqrt{\frac{1}{2m} \left(\text{KL}(\text{Dirac}(h_i) \| P) + \log \left(\frac{1}{\delta} \right) \right)}$$

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

$$\text{return } \arg \min_{h_i \in \mathcal{H}} \left\{ R_{\text{in}}(h_i) + \sqrt{\frac{1}{2m} \log \left(\frac{1}{p_i \delta} \right)} \right\}$$

Uncountably infinite function class?

Algorithm $A : \mathcal{Z}^m \rightarrow \mathcal{H}$

Function class \mathcal{H} with $|\mathcal{H}| \geq |\mathbb{N}|$

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

$$\text{w.p.} \geq 1 - \delta, \quad \forall h \in \mathcal{H}, \quad \Delta(h) \leq \sqrt{\frac{8d}{m} \log\left(\frac{2em}{d}\right) + \frac{8}{m} \log\left(\frac{4}{\delta}\right)}$$

The bound holds for all functions in the class (**uniform over \mathcal{H}**) and for all distributions (**uniform over \mathbb{P}**)

- **Rademacher complexity** (measures how well a function can align with randomly perturbed labels – can be used to take advantage of margin assumptions)

These approaches are suited to analyse the performance of individual functions, and take some account of correlations

→ Extension: PAC-Bayes allows to consider **distributions** over hypotheses.

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The PAC-Bayes framework

- Before data, fix a distribution $P \in M_1(\mathcal{H})$ ▷ ‘prior’
- Based on data, learn a distribution $Q \in M_1(\mathcal{H})$ ▷ ‘posterior’
- Predictions:
 - draw $h \sim Q$ and predict with the chosen h .
 - each prediction with a fresh random draw.

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

$$R_{\text{in}}(Q) \equiv \int_{\mathcal{H}} R_{\text{in}}(h) dQ(h) \quad R_{\text{out}}(Q) \equiv \int_{\mathcal{H}} R_{\text{out}}(h) dQ(h)$$

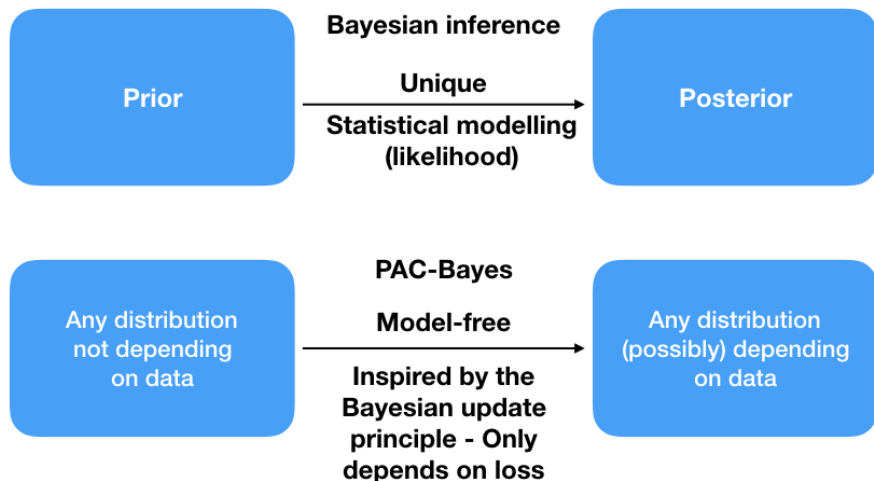
$\text{KL}(Q\|P) = \mathbf{E}_{h \sim Q} \ln \frac{Q(h)}{P(h)}$ is the Kullback-Leibler divergence.

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

w.p. $\geq 1 - \delta$, $\forall h_i \in \mathcal{H}$,

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

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

■ Prior

- **PAC-Bayes bounds**: bounds hold even if prior incorrect
- **Bayesian**: inference must assume prior is correct

■ Posterior

- **PAC-Bayes bounds**: bound holds for all posteriors
- **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

Pre-history: PAC analysis of Bayesian estimators

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

Birth: PAC-Bayesian bound

McAllester (1998, 1999)

McAllester Bound

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

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

A history of PAC-Bayes

Introduction of the kl form

Langford and Seeger (2001); Seeger (2002, 2003); Langford (2005)

Langford and Seeger Bound

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

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

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

A General PAC-Bayesian Theorem

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

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

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 $S_m \sim \mathbb{P}^m$,

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

where

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

General theorem

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

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 $\phi : \mathcal{H} \rightarrow \mathbb{R}$, we have

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

Markov's inequality

$$\mathbb{P}(X \geq a) \leq \frac{\mathbf{E}X}{a} \quad \iff \quad \mathbb{P}(X \leq \frac{\mathbf{E}X}{\delta}) \geq 1 - \delta.$$

Probability of observing k misclassifications among m examples

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

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

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

Proof

Jensen's Inequality

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

Change of measure

$$\leq \text{KL}(Q \| P) + \ln \mathbf{E}_{h \sim P} e^{m \Delta \left(R_{\text{in}}(h), R_{\text{out}}(h) \right)}$$

Markov's Inequality

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

Expectation swap

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

Binomial law

$$= \text{KL}(Q \| P) + \ln \frac{1}{\delta} \mathbf{E}_{h \sim P} \sum_{k=0}^m \text{Bin}(k; m, R_{\text{out}}(h)) e^{m \cdot \Delta \left(\frac{k}{m}, R_{\text{out}}(h) \right)}$$

Supremum over risk

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

$$= \text{KL}(Q \| P) + \ln \frac{1}{\delta} J_{\Delta}(m).$$

□

General theorem

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

Corollary

[...] with probability at least $1 - \delta$ over the choice of $S_m \sim \mathbb{P}^m$, for all Q on \mathcal{H} :

(a) $\text{kl} \left(R_{\text{in}}(Q), R_{\text{out}}(Q) \right) \leq \frac{1}{m} \left[\text{KL}(Q \| P) + \ln \frac{2\sqrt{m}}{\delta} \right]$ Langford and Seeger (2001)

(b) $R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + \sqrt{\frac{1}{2m} \left[\text{KL}(Q \| P) + \ln \frac{2\sqrt{m}}{\delta} \right]}$, McAllester (1999, 2003a)

(c) $R_{\text{out}}(Q) \leq \frac{1}{1 - e^{-c}} \left(c \cdot R_{\text{in}}(Q) + \frac{1}{m} \left[\text{KL}(Q \| P) + \ln \frac{1}{\delta} \right] \right)$, Catoni (2007)

(d) $R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + \frac{1}{\lambda} \left[\text{KL}(Q \| P) + \ln \frac{1}{\delta} + f(\lambda, m) \right]$. Alquier et al. (2016)

$$\text{kl}(q, p) \stackrel{\text{def}}{=} q \ln \frac{q}{p} + (1 - q) \ln \frac{1 - q}{1 - p} \geq 2(q - p)^2,$$

$$\Delta_c(q, p) \stackrel{\text{def}}{=} -\ln[1 - (1 - e^{-c}) \cdot p] - c \cdot q,$$

$$\Delta_\lambda(q, p) \stackrel{\text{def}}{=} \frac{\lambda}{m} (p - q).$$

Recap

What we've seen so far

- Statistical learning theory is about **high confidence control of generalization**
- PAC-Bayes is a **generic, powerful tool** to derive generalization bounds

What is coming next

- PAC-Bayes application to **large classes** of algorithms
- PAC-Bayesian-inspired algorithms
- Case studies

A flexible framework

Since 1997, PAC-Bayes has been successfully used in **many** machine learning settings.

Statistical learning theory *Shawe-Taylor and Williamson (1997); McAllester (1998, 1999, 2003a,b); Seeger (2002, 2003); Maurer (2004); Catoni (2004, 2007); Audibert and Bousquet (2007); Thiemann et al. (2017)*

SVMs & linear classifiers *Langford and Shawe-Taylor (2002); McAllester (2003a); Germain et al. (2009a)*

Supervised learning algorithms reinterpreted as bound minimizers
Ambroladze et al. (2007); Shawe-Taylor and Hardoon (2009); Germain et al. (2009b)

High-dimensional regression *Alquier and Lounici (2011); Alquier and Biau (2013); Guedj and Alquier (2013); Li et al. (2013); Guedj and Robbiano (2018)*

Classification *Langford and Shawe-Taylor (2002); Catoni (2004, 2007); Lacasse et al. (2007); Parrado-Hernández et al. (2012)*

A flexible framework

Transductive learning, domain adaptation *Derbeko et al. (2004); Bégin et al. (2014); Germain et al. (2016)*

Non-iid or heavy-tailed data *Lever et al. (2010); Seldin et al. (2011, 2012); Alquier and Guedj (2018)*

Density estimation *Seldin and Tishby (2010); Higgs and Shawe-Taylor (2010)*

Reinforcement learning *Fard and Pineau (2010); Fard et al. (2011); Seldin et al. (2011, 2012); Ghavamzadeh et al. (2015)*

Sequential learning *Gerchinovitz (2011); Li et al. (2018)*

Algorithmic stability, differential privacy *London et al. (2014); London (2017); Dziugaite and Roy (2018a,b); Rivasplata et al. (2018)*

Deep neural networks *Dziugaite and Roy (2017); Neyshabur et al. (2017)*

PAC-Bayes-inspired learning algorithms

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

Error on unseen data \leq Error on sample + complexity term

$$R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + F(Q, \cdot)$$

This defines a principled strategy to obtain new learning algorithms:

$$h \sim Q^*$$

$$Q^* \in \arg \inf_{Q \ll P} \left\{ R_{\text{in}}(Q) + F(Q, \cdot) \right\}$$

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

PAC-Bayes interpretation of celebrated algorithms

SVM with a sigmoid loss and KL-regularized Adaboost have been reinterpreted as **minimizers of PAC-Bayesian bounds**.

Ambroladze et al. (2007), Shawe-Taylor and Hadoon (2009), Germain et al. (2009b)

For any $\lambda > 0$, the minimizer of

$$\left\{ R_{\text{in}}(Q) + \frac{\text{KL}(Q, P)}{\lambda} \right\}$$

is the celebrated **Gibbs posterior**

$$Q_{\lambda}(h) \propto \exp(-\lambda R_{\text{in}}(h)) P(h), \quad \forall h \in \mathcal{H}.$$

Extreme cases: $\lambda \rightarrow 0$ (flat posterior) and $\lambda \rightarrow \infty$ (Dirac mass on ERM). Note: continuous version of the **exponentially weighted aggregate** (EWA).

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

Let (A, \mathcal{A}) be a measurable space.

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

$$\log \int (\exp \circ \phi) dP = \sup_{Q \ll P} \left\{ \int \phi dQ - \text{KL}(Q, P) \right\}.$$

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

$$\frac{dG}{dP}(a) = \frac{\exp \circ \phi(a)}{\int (\exp \circ \phi) dP}, \quad a \in A.$$

$$\log \int (\exp \circ \phi) dP = \sup_{Q \ll P} \left\{ \int \phi dQ - \text{KL}(Q, P) \right\}, \quad \frac{dG}{dP} = \frac{\exp \circ \phi}{\int (\exp \circ \phi) dP}.$$

Proof: let $Q \ll P$.

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

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

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

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

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

PAC-Bayes for non-iid or heavy-tailed data

We drop the iid and bounded loss assumptions. For any integer p ,

$$\mathfrak{M}_p := \int \mathbb{E} (|R_{\text{in}}(h) - R_{\text{out}}(h)|^p) dP(h).$$

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

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

when $Q \ll P$ and $D_f(Q, P) = +\infty$ otherwise.

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

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

Let $\phi_p: x \mapsto x^p$. 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

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

The bound decouples

- **the moment** \mathcal{M}_q (which depends on the distribution of the data)
- and **the divergence** $D_{\phi_{p-1}}(Q, P)$ (measure of complexity).

Corollary: with probability at least $1 - \delta$, for any Q ,

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

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

Proof

Let $\Delta(h) := |R_{\text{in}}(h) - R_{\text{out}}(h)|$.

Jensen

Change of measure

Holder

Markov

$$\begin{aligned} & \left| \int R_{\text{out}} dQ - \int R_{\text{in}} dQ \right| \\ & \leq \int \Delta dQ \\ & = \int \Delta \frac{dQ}{dP} dP \\ & \leq \left(\int \Delta^q dP \right)^{\frac{1}{q}} \left(\int \left(\frac{dQ}{dP} \right)^p dP \right)^{\frac{1}{p}} \\ & \stackrel{1-\delta}{\leq} \left(\frac{\mathbb{E} \int \Delta^q dP}{\delta} \right)^{\frac{1}{q}} \left(\int \left(\frac{dQ}{dP} \right)^p dP \right)^{\frac{1}{p}} \\ & = \left(\frac{\mathcal{M}_q}{\delta} \right)^{\frac{1}{q}} (D_{\Phi_{p-1}}(Q, P) + 1)^{\frac{1}{p}}. \end{aligned}$$

Oracle bounds

Catoni (2004, 2007) further derived PAC-Bayesian bound for the Gibbs posterior

$$Q_\lambda \propto \exp(-\lambda R_{\text{in}}) P.$$

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

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

(can be optimized with respect to λ)

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.

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Data- or distribution-dependent priors

PAC-Bayesian bounds express a tradeoff between empirical accuracy and a measure of complexity

$$R_{\text{out}}(Q) \leq R_{\text{in}}(Q) + \sqrt{\frac{\text{KL}(Q\|\mathcal{P}) + \ln \frac{\xi(m)}{\delta}}{2m}}.$$

How can this complexity be controlled?

- 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
- Are there ways we can choose a ‘better’ prior?
- Will explore:
 - using part of the data to *learn the prior* for SVMs, but also more interestingly and more generally
 - defining the prior in terms of the *data generating distribution* (aka *localised PAC-Bayes*).

SVM Application

- **Prior** and **posterior** distributions are spherical Gaussians:
 - **Prior** centered at the origin
 - **Posterior** centered at a scaling μ of the unit SVM weight vector
- Implies KL term is $\mu^2/2$
- We can compute the stochastic error of the posterior distribution exactly and it behaves like a *soft margin*; scaling μ trades between margin loss and KL
- Bound holds for all μ , so choose to optimise the bound
- Generalization of deterministic classifier can be bounded by *twice* stochastic error

Learning the prior for SVMs

- Bound depends on the **distance between prior and posterior**
- Better prior (closer to posterior) would lead to **tighter bound**
- **Learn** the prior P with part of the data
- Introduce the learnt prior **in the bound**
- Compute stochastic error with **remaining data: PrPAC**
- We can go a step further:
 - Consider scaling the prior in the chosen direction: **τ -PrPAC**
 - adapt the SVM algorithm to optimise the new bound: **η -Prior SVM**
- We present some results to show the bounds and their use in model selection (regularisation and band-width of kernel).

Results

| | | Classifier | | | | | |
|----------|-------|--------------|--------------|--------------|--------------|------------------|---------------|
| | | SVM | | | | η Prior 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 |

Results

- Bounds are remarkably tight: for final column average factor between bound and TE is under 3.
- 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

- Consider P and Q are Gibbs-Boltzmann distributions

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

- 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:

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

with the only uncertainty the dependence on γ .

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

Observations

- We cannot compute the prior distribution P or even sample from it:
 - Note that this would not be possible to consider in normal Bayesian inference;
 - Trick here is that the error measures only depend on the posterior Q , while the bound depends on KL between posterior and prior: an estimate of this KL is made without knowing the prior explicitly

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

Other distribution defined priors

- 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...
- What if we were to take the expected weight vector returned from a random training set of size m : then the KL between posterior and prior is related to the concentration of weight vectors from different training sets
- This is connected to stability...

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Stability

Uniform **hypothesis sensitivity** β at sample size m :

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

(z_1, \dots, z_m)

■ $A(z_{1:m}) \in \mathcal{H}$ normed space

■ $w_m = A(z_{1:m})$ 'weight vector'

(z'_1, \dots, z'_m)

■ Lipschitz

■ smoothness

Uniform **loss sensitivity** β at sample size m :

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

■ worst-case

■ data-insensitive

■ distribution-insensitive

■ Open: data-dependent?

Generalization from Stability

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

$$\text{w.p.} \geq 1 - \delta, \quad R_{\text{out}}(h) \leq R_{\text{in}}(h) + \epsilon(\beta, m, \delta)$$

Bousquet and Elisseeff (2002)

- the intuition is that if individual examples do not affect the loss of an algorithm then it will be concentrated
- 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
 \implies 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.** $\geq 1 - 2\delta$,

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

Gaussian randomization

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

Main proof components:

- **w.p.** $\geq 1 - \delta$, $\text{kl}(R_{\text{in}}(Q) \| R_{\text{out}}(Q)) \leq \frac{\text{KL}(Q \| Q_0) + \log\left(\frac{m+1}{\delta}\right)}{m}$
- **w.p.** $\geq 1 - \delta$, $\|W_m - \mathbb{E}[W_m]\| \leq \sqrt{m} \beta \left(1 + \sqrt{\frac{1}{2} \log\left(\frac{1}{\delta}\right)}\right)$

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

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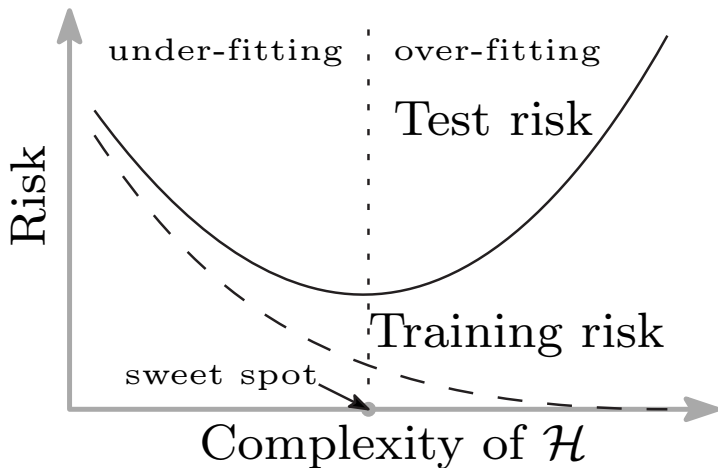
Is deep learning breaking the statistical paradigm we know?

Neural networks architectures trained on massive datasets achieve **zero training error** which does not bode well for their performance...

... yet they also achieve **remarkably low errors** on **test** sets!

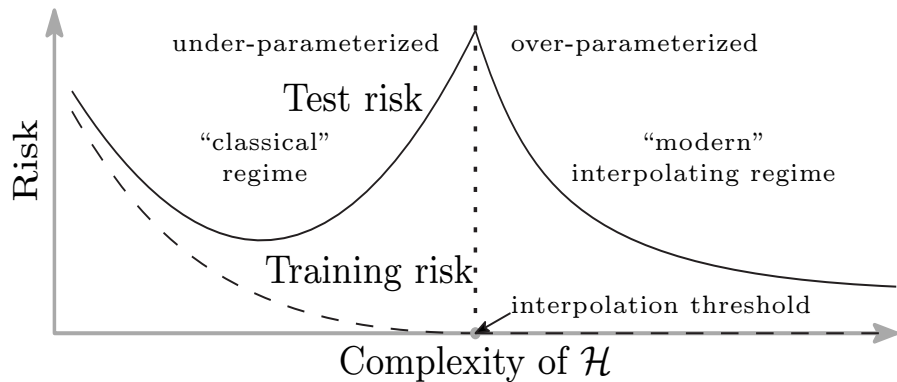
PAC-Bayes is a solid candidate to **better understand how deep nets generalize**.

The celebrated bias-variance tradeoff



Belkin et al. (2018)

Towards a better understanding of deep nets



Belkin et al. (2018)

Performance of deep nets

- Deep learning has thrown down a challenge to Statistical Learning Theory: **outstanding performance** with **overly complex hypothesis classes** (most bounds turn vacuous)
- 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

Performance of deep nets

- *Dziugaite and Roy (2017)*, *Neyshabur et al. (2017)* have derived some of the tightest deep learning bounds in this way
 - by training to expand the basin of attraction
 - hence not measuring good generalisation of normal training
 - *Dziugaite and Roy (2017)* have also tried to apply the *Lever et al. (2013)* bound but observed cannot measure generalisation correctly for deep networks as has no way of distinguishing between successful fitting of true and random labels
- 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

Information contained in training set

- *Achille and Soatto (2018)* studied the amount of information stored in the weights of deep networks
- Overfitting is related to information being stored in the weights that encodes the particular training set, as opposed to the data generating distribution
- This corresponds to reducing the concentration of the distribution of weight vectors output by the algorithm
- They argue that the Information Bottleneck criterion introduced by *Tishby et al. (1999)* can control this information: hence could potentially lead to a tighter PAC-Bayes bound
- Potential for algorithms that optimize the bound

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.

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Thank you!

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

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