Risk Bounds for the Majority Vote (Part II)

From a PAC-Bayesian Analysis to a Learning Algorithm

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This poster presents a recently accepted JMLR paper. Go to http://graal.ift.ulaval.ca/majorityvote/ for a preliminary version, source code, and more!

Setting and Motivation

⇐ **Previously on Part I:** Pascal introduces the $\mathcal{C}$-bound and PAC-Bayesian theorems that bound the risk of the majority vote classifier.

Theorem ($\mathcal{C}$-bound) *For any distribution Q on a set of voters and any distribution D on $\mathcal{X}\times\{-1,1\}$, if $\mu_1(M_Q^{D'}) > 0$, we have*

$$R_D(B_Q) \leq \mathcal{C}_Q^D \stackrel{\text{def}}{=} 1 - \frac{\left(\mu_1(M_Q^D)\right)^2}{\mu_2(M_Q^D)}\,.$$

Minimizing the $\mathcal{C}$-bound favors majority votes for which the voters are maximally uncorrelated. We want an algorithm that minimizes the related PAC-Bayesian upper bounds (see Part I). However, empirical experiments shown that $\mathrm{KL}(Q\|P)$ is a poor regularizer in this case, as its empirical value tends to be overweighted in comparison with the empirical value of the $\mathcal{C}$-bound (*i.e.*, $\mathcal{C}_Q^S$). Let's get rid of it!

Aligned Distributions

Self-complemented set of voters A set of voters $\mathcal{H}$ is said to be *self-complemented* if there exists a bijection $c : \mathcal{H} \to \mathcal{H}$ such that for any $f \in \mathcal{H}$, $c(f) = -f$. In other words, *each voter $f \in \mathcal{H}$ has a complement $-f \in \mathcal{H}$.*

Aligned posterior Given a self-complemented set $\mathcal{H}$, a posterior distribution Q is *aligned* on a prior distribution P if

$$Q(f) + Q(c(f)) \;=\; P(f) + P(c(f))\,, \quad \forall f \in \mathcal{H}\,.$$

Quasi-uniform distribution If P is a uniform prior distribution and Q is aligned on P, we say that Q is a *quasi-uniform* distribution.

L_∞-norm regularization For a self-complemented set $\mathcal{H}$ of $2n$ voters and a quasi-uniform distribution Q on $\mathcal{H}$, the weight of any voter is lower-bounded by 0 and upper-bounded by $\frac{1}{n}$, as for any $i \in \mathcal{H}$, $Q(f_i) + Q(f_{i+n}) = \frac{1}{n}$.

A New Change of Measure Inequality

A key step of PAC-Bayesian proofs is the *change of measure inequality* (Banerjee [2006], Seldin and Tishby [2010]):

Lemma (Change of measure inequality) *For any set $\mathcal{H}$, for any distribution P and Q on $\mathcal{H}$, and for any measurable function $\phi : \mathcal{H} \to \mathbb{R}$, we have*

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

Using aligned posteriors and a suitable ϕ function, the KL term does not appear.

Theorem (Change of measure inequality for aligned posteriors) *For any self-complemented set $\mathcal{H}$, for any distribution P on $\mathcal{H}$, any distribution Q aligned on P, and for any measurable function $\phi : \mathcal{H} \to \mathbb{R}$ such that $\phi(f) = \phi(c(f))$ for all $f \in \mathcal{H}$, we have*

$$\mathop{\mathbf{E}}_{f\sim Q} \phi(f) \leq \ln\left(\mathop{\mathbf{E}}_{f\sim P} e^{\phi(f)}\right)\,.$$

Proof.

$$\begin{aligned}
2\cdot\mathop{\mathbf{E}}_{f\sim Q}\phi(f) &= \int_{\mathcal{H}} df\; Q(f)\,\phi(f) + \int_{\mathcal{H}} df\; Q(c(f))\,\phi(c(f)) \\
&= \int_{\mathcal{H}} df\; Q(f)\,\phi(f) + \int_{\mathcal{H}} df\; Q(c(f))\,\phi(f) \\
&= \int_{\mathcal{H}} df\; \Big(Q(f) + Q(c(f)\Big)\,\phi(f) \\
&= \int_{\mathcal{H}} df\; \Big(P(f) + P(c(f)\Big)\,\phi(f) = \;\ldots\; = 2\cdot\mathop{\mathbf{E}}_{f\sim P}\phi(f)\,.
\end{aligned}$$

The result is obtained by changing the expectation over Q to an expectation over P, and then by applying Jensen's inequality:

$$\mathop{\mathbf{E}}_{f\sim Q}\phi(f) \;=\; \mathop{\mathbf{E}}_{f\sim P}\phi(f) \;=\; \mathop{\mathbf{E}}_{f\sim P}\ln e^{\phi(f)} \;\leq\; \ln\left(\mathop{\mathbf{E}}_{f\sim P} e^{\phi(f)}\right)\,. \qquad \square$$

PAC-Bayesian Bounds revisited

Corollary *For any distribution D on $\mathcal{X}\times\{-1,1\}$, for any set $\mathcal{H}$ of voters $\mathcal{X}\to[-1,1]$, for any prior distribution P on $\mathcal{H}$, and any $\delta\in(0,1]$, we have*

$$\Pr_{S\sim D^m}\left(\begin{array}{l}\text{For all posteriors } Q \text{ on } \mathcal{H}: \\ \mu_1(M_Q^D) \geq \mu_1(M_Q^S) - \sqrt{\frac{2}{m}\left[\mathrm{KL}(Q\|P) + \ln\frac{2\sqrt{m}}{\delta}\right]}\end{array}\right) \geq 1-\delta\,.$$

Corollary *If $\mathcal{H}$ is a self-complemented set of voters, we have*

$$\Pr_{S\sim D^m}\left(\begin{array}{l}\text{For all posteriors } Q \text{ aligned on } P: \\ \mu_1(M_Q^D) \geq \mu_1(M_Q^S) - \sqrt{\frac{2}{m}\left[\ln\frac{2\sqrt{m}}{\delta}\right]}\end{array}\right) \geq 1-\delta\,.$$

A PAC-Bayesian Bound without KL

PAC-Bound 3 *For any distribution D on $\mathcal{X}\times\{-1,1\}$, for any self-complemented set $\mathcal{H}$ of voters $\mathcal{X}\to[-1,1]$, for any prior distribution P on $\mathcal{H}$, and any $\delta\in(0,1]$, we have, with probability $1-\delta$ over the choice of $S\sim D^m$*

$$\forall\, Q \text{ aligned on } P: \quad R_D(B_Q) \;\leq\; 1 - \frac{\left(\max\left(0,\, \mu_1(M_Q^S) - \sqrt{\frac{2}{m}\left[\ln\frac{2\sqrt{m}}{\delta/2}\right]}\right)\right)^2}{\min\left(1,\, \mu_2(M_Q^S) + \sqrt{\frac{2}{m}\left[\ln\frac{2\sqrt{m}}{\delta/2}\right]}\right)}\,.$$

Problem 1: Minimizing $\mathcal{C}_Q^S$ tends to overfit

Solution We restrict Q to be quasi-uniform. It does not reduce the set of possible majority votes: different distributions Q that give rise to a same majority vote have the same (real and empirical) C-bound values.

Theorem *Let $\mathcal{H}$ be a self-complemented set. For all distributions Q on $\mathcal{H}$, there exists a quasi-uniform distribution Q' on $\mathcal{H}$ that gives the same majority vote as Q, and that has the same empirical and true $\mathcal{C}$-bound values, i.e.,*

$$B_{Q'} = B_Q\,, \quad \mathcal{C}_{Q'}^S = \mathcal{C}_Q^S \quad \text{and} \quad \mathcal{C}_{Q'}^D = \mathcal{C}_Q^D\,.$$

Problem 2: 0/0 numerical instability

Distribution Q minimizing the $\mathcal{C}$-bound are such that both $\mu_1(M_Q^S)$ and $\mu_2(M_Q^S)$ are very close to zero.

Solution We want to constraint $\mu_1(M_Q^S)$ to be higher to some threshold value μ, which is equivalent to constraint the margin to be exactly equal to μ : among all the posteriors Q that minimize the $\mathcal{C}$-bound, there is always one whose empirical margin $\mu_1(M_Q^S)$ is as close to 0 as we want.

Theorem *Let $\mathcal{H}$ be a self-complemented set. For all $\mu\in(0,1]$ and for all quasi-uniform distributions Q on $\mathcal{H}$ having an empirical margin $\mu_1(M_Q^S)\geq\mu$, there exists a quasi-uniform distribution Q' on $\mathcal{H}$, having an empirical margin equal to μ, such that Q and Q' induce the same majority vote and have the same empirical and true $\mathcal{C}$-bound values, i.e.,*

$$\mu_1(M_{Q'}^S) = \mu\,, \quad B_{Q'} = B_Q\,, \quad \mathcal{C}_{Q'}^S = \mathcal{C}_Q^S \quad \text{and} \quad \mathcal{C}_{Q'}^D = \mathcal{C}_Q^D\,.$$

MinCq: The Algorithm Minimizing the $\mathcal{C}$-bound

MinCq Algorithm Given a self-complemented set $\mathcal{H}$ of $2n$ voters, a training set S, and a S-realizable $\mu > 0$, among all quasi-uniform distributions Q of empirical margin $\mu_1(M_Q^S)$ exactly equal to μ, the algorithm MinCq consists in finding one that minimizes $\mu_2(M_Q^S)$.

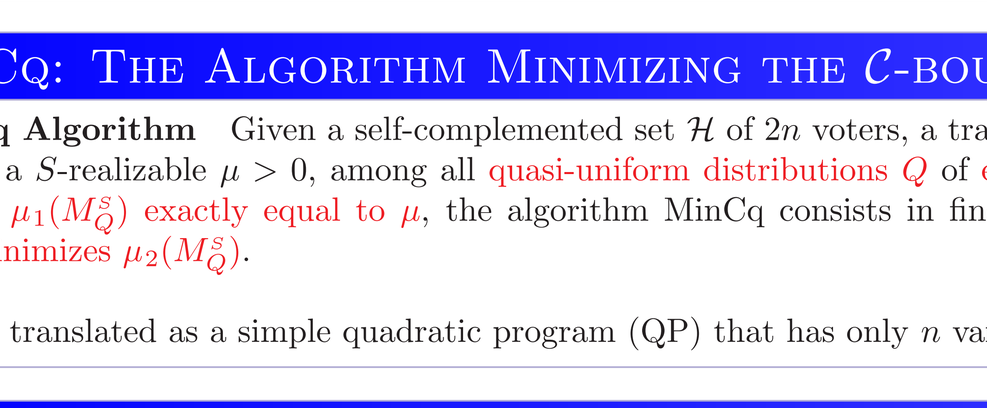
Can be translated as a simple quadratic program (QP) that has only n variables.

Empirical Results

We compare MinCq using decision stumps as voters against AdaBoost, and using *kernel voters* against SVM.

A **kernel voter** is defined as $f_i(\cdot) = y_i k(x_i,\cdot)$ for some example $(x_i,\, y_i)$ and kernel function k. One can interpret its output as a confidence level.

Handwritten Digits Recognition (MNIST)



Sentiment Analysis (Amazon Reviews)

Dataset information			Risk $R_T(B_Q)$ for each algorithm	
Name	$\lvert S\rvert$	$\lvert T\rvert$	LinearMinCq	LinearSVM
Books	2000	4465	**0.158**	**0.158**
DVD	2000	3586	**0.162**	0.163
Kitchen	2000	5945	**0.130**	0.131
Electronics	2000	5681	**0.116**	0.118

Statistical comparison on MNIST, Amazon and 31 UCI datasets.

	MNIST		**Amazon**	**UCI**	
	RBF Kernel	Stumps	Linear Kernel	RBF Kernel	Stumps
Poisson binomial test*	**88%**	**99%**	68%	54%	48%
Sign test (p-value)*	**.01**	**.00**	0.31	0.36	0.35

* For the Poisson binomial test, a higher value is better. For the sign test, a lower value is better.