A PAC-Bayesian Tutorial with A Dropout Bound

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Abstract

This tutorial gives a concise overview of existing PAC-Bayesian theory focusing on three generalization bounds. The first is an Occam bound which handles rules with finite precision parameters and which states that generalization loss is near training loss when the number of bits needed to write the rule is small compared to the sample size. The second is a PAC-Bayesian bound providing a generalization guarantee for posterior distributions rather than for individual rules. The PAC-Bayesian bound naturally handles infinite precision rule parameters, $L_2$ regularization, provides a bound for dropout training, and defines a natural notion of a single distinguished PAC-Bayesian posterior distribution. The third bound is a training-variance bound — a kind of bias-variance analysis but with bias replaced by expected training loss. The training-variance bound dominates the other bounds but is more difficult to interpret. It seems to suggest variance reduction methods such as bagging and may ultimately provide a more meaningful analysis of dropouts.

1 Introduction

PAC-Bayesian theory blends Bayesian and frequentist approaches to the theory of machine learning. PAC-Bayesian theory assumes a probability distribution on “situations” occurring in nature and a prior weighting on “rules” expressing a learner’s preference for some rules over others. There is no assumed relationship between the learner’s bias on rules and nature’s distribution on situations. This is different from Bayesian inference where the starting point is a (perhaps subjective) joint distribution on rules and situations inducing a conditional distribution on rules given situations. The acronym PAC stands for Probably Approximately Correct and is borrowed from Valiant’s notion of PAC learnability [13]. PAC-Bayesian generalization bounds [11, 12, 10, 7, 4, 6] govern the performance (loss) when stochastically selecting rules from a “posterior” distribution. The performance guarantee involves the learner’s bias and an (unrelated) sample of situations.

This tutorial provides a concise overview of existing PAC-Bayesian theory focusing on three bounds. The first is an Occam bound. An Occam bound assumes a discrete (countable) set of rules and bounds the loss of an individual rule. The Occam bound immediately yields guarantees for rules
with sparse finite precision parameters. The second is a PAC-Bayesian bound governing the loss of a stochastic process which draws rules from a PAC-Bayesian rule posterior. The PAC-Bayesian bound easily handles $L_2$ regularization of infinite-precision parameters producing bounds closely related to support vector machines. It also provides bounds for a form of dropout learning [5].

The third bound is a training-variance bound similar to a bias-variance analysis but with bias replaced by expected training loss. This bound assumes a given learning algorithm and provides an upper bound on the expected generalization loss in terms of the expected training loss and a measure of the variance of the output of the learning algorithm. While the training-variance bound is clearly tighter than the PAC-Bayesian bound, the training-variance bound is difficult to interpret. The training-variance bounds seems to suggest variance-reduction methods such as bagging [3].

Unbounded loss functions, such as square loss or log loss, can lead to unstable learning algorithms. Learning algorithms that minimize training loss for an unbounded loss function tend to be overly sensitive to outliers — training points of very high loss. Learning algorithms based on bounded loss functions tend to be more robust (stable). An unbounded loss function can be converted to a bounded loss by selecting an “outlier threshold” $L_{\text{max}}$ and replacing the unbounded loss $L$ by $\min(L, L_{\text{max}})$.\footnote{We should assume that the loss function $L$ is measurable with respect to $D$ and $P$. Here we will avoid this level of rigor.}

PAC-Bayesian bounds apply only to bounded loss functions. We assume the loss is bounded to the interval $[0, L_{\text{max}}]$. It is of course possible to rescale any bounded loss function into the interval $[0, 1]$. However, this obscures the significance of the choice of $L_{\text{max}}$ in the design of a robust versions of square loss or log loss. For this reason we leave $L_{\text{max}}$ explicit in the statement of the bounds.

This tutorial also discusses two improvements or clarifications of the three bounds mentioned above. The first applies the training-variance bound to the learning algorithm defined by the PAC-Bayesian posterior. Unfortunately the results suffer from looseness in the analysis and remain difficult to interpret. The second tightens the Occam bound by incorporating the loss variance into the bound. We show that the improvements achievable in this way a fundamentally limited.

## 2 An Occam Bound

Let $\mathcal{H}$ be a set of “rules”, $S$ be a set of “situations”, $L_{\text{max}} > 0$ be a real number, and $L$ be a loss function such that for a rule $h \in \mathcal{H}$ and a situation $s \in S$ we have that $L(h, s) \in [0, L_{\text{max}}]$. We let $D$ be a probability distribution (measure) on $S$ and let $P$ be a distribution (measure) on $\mathcal{H}$. We think of $D$ as a distribution on situations occurring in nature and $P$ as learner bias on rules. There is no assumed relationship between $D$ and $P$.\footnote{We should assume that the loss function $L$ is measurable with respect to $D$ and $P$. Here we will avoid this level of rigor.} We are interested in drawing a sequence $S$ of $N$ situations IID from $D$ ($S \sim D^N$) and then selecting $h$ based on $S$ so as to minimize the “generalization loss” $L(h) = \mathbb{E}_{s \sim D} [L(h, s)]$. When the sample $S$ is clear from context we will write $\hat{L}(h)$ for $\frac{1}{N} \sum_{s \in S} L(h, s)$.\footnote{We should assume that the loss function $L$ is measurable with respect to $D$ and $P$. Here we will avoid this level of rigor.}
For Occam bounds we consider the case where $\mathcal{H}$ is discrete (countable). An Occam bound states that with probability at least $1 - \delta$ over the draw of the sample $S \sim D^N$ we have $L(h) \leq B(P(h), S, \delta)$ simultaneously for all $h$ where $B(P(h), S, \delta)$ is different in different bounds. While various Occam bounds have appeared in the literature, here we will consider only the following.

**Theorem 1.** With probability at least $1 - \delta$ over the draw of $S \sim D^N$ we have that the following holds simultaneously for all $h$.

$$L(h) \leq \inf_{\lambda > \frac{1}{2}} \frac{1}{1 - \frac{1}{2\lambda}} \left( \hat{L}(h) + \frac{\lambda L_{\max}}{N} \left( \ln \frac{1}{P(h)} + \ln \frac{1}{\delta} \right) \right)$$  \hspace{0.5cm} (1)

**Proof.** We consider the case of $L_{\max} = 1$, the case for general $L_{\max}$ follows by rescaling the loss function. Define $\epsilon(h)$ by

$$\epsilon(h) = \sqrt{\frac{2L(h)}{N} \left( \ln \frac{1}{P(h)} + \ln \frac{1}{\delta} \right)}.$$

For a given $h \in \mathcal{H}$ the relative Chernoff bound \cite{1} states that

$$P_{S \sim D^N} \left( \hat{L}(h) \leq L(h) - \epsilon(h) \right) \leq e^{-\frac{\epsilon(h)^2}{2L(h)}} = \delta P(h).$$

Hence, for a fixed $h$ the probability of $L(h) > \hat{L}(h) + \epsilon(h)$ is at most $P(h)\delta$. By the union bound the probability that there exists an $h$ with $L(h) > \hat{L}(h) + \epsilon(h)$ is at most the sum over $h$ of $P(h)\delta$ which equals $\delta$. Hence we get that with probability at least $1 - \delta$ over the draw of the sample the following holds simultaneously for all $h$.

$$L(h) \leq \hat{L}(h) + \sqrt{\frac{2L(h)}{N} \left( \ln \frac{1}{P(h)} + \ln \frac{1}{\delta} \right)}$$

Using

$$\sqrt{ab} = \inf_{\lambda > 0} \frac{a}{2\lambda} + \frac{\lambda b}{2}$$

we get

$$L(h) \leq \hat{L}(h) + \frac{L(h)}{2\lambda} + \frac{\lambda \left( \ln \frac{1}{P(h)} + \ln \frac{1}{\delta} \right)}{N}$$

Solving for $L(h)$ yields the result. \hfill \Box

An important observation for (1) is that there is no point in taking $\lambda$ to be large. Restricting $\lambda$ to be less than $\lambda_{\max}$ increases the bound by a factor of at most $1/(1 - 1/2\lambda_{\max})$. For example, restricting $\lambda$ to be less than 10 increases the bound by a factor of at most 20/10. So for practical purposes we can assume that $\lambda$ is no larger than 10.
2.1 Finite Precision Bounds

As an example application of (1) we can consider rules of the form $h_\Theta$ for some parameter vector $\Theta \in \mathbb{R}^d$ where each component of the vector $\Theta$ is represented with a $b$-bit finite precision representation. In this case we can take the prior $P$ to be uniform on the $2^{bd}$ possible rules and (1) then gives that with probability at least $1 - \delta$ over the draw of the sample we have that the following holds simultaneously for all such $\Theta$.

$$L(h_\Theta) \leq \inf_{\lambda > \frac{1}{2}} \frac{1}{1 - \frac{1}{2^\lambda}} \left( \bar{L}(h_\Theta) + \frac{\lambda L_{\text{max}}}{N} \left( \ln(2)bd + \ln\frac{1}{\delta} \right) \right)$$

We can also consider sparse representations. For $\Theta \in \mathbb{R}^d$ we say that $\Theta$ has sparsity level $s$ if at most $s$ components of $\Theta$ are non-zero. We can then represent a sparse vector by first specifying the sparsity $s$ and then listing $s$ pairs each of which specifies a non-zero component and its value. Intuitively we can write a rule by first using $\log_2 d$ bits to specify $s$ plus $(\log_2 d)b$ bits for each pair of a component index and $b$-bit parameter value representation. The probability of a rule $h$ can always be taken to be $2^{-|h|}$ where $h$ is the number of bits needed to name $h$. Formally we avoid coding and instead defining a probability distribution where we first select $s$ uniformly from $1$ to $d$ and then select $s$ pairs with indices drawn uniformly from $1$ to $d$ and a parameter representation drawn uniformly from all $2^b$ bit strings. In this case we get that with probability at least $1 - \delta$ over the draw of the sample of situations we have the following holds simultaneously for all sparsity levels $s$ and $\Theta$ with sparsity $s$ and with $b$-bit representations for the non-zero components of $\Theta$.

$$L(h_\Theta) \leq \inf_{\lambda > \frac{1}{2}} \frac{1}{1 - \frac{1}{2^\lambda}} \left( \bar{L}(h_\Theta) + \frac{\lambda L_{\text{max}}}{N} \left( \ln d + s(\ln d + (\ln 2)b) + \ln\frac{1}{\delta} \right) \right)$$

More sophisticated codings of classifiers are possible. For example, variable precision codes for real numbers can be useful when the error rate is insensitive to the precision. However, the PAC-Bayesian theorem stated in section 3 handles infinite precision parameters and seems generally preferable. The Occam bound is included here primarily because of its conceptual simplicity and the intuitive value of its proof.

3 A PAC-Bayesian Bound

Let $\mathcal{H}$, $S$, $L_{\text{max}}$, $L$, $D$ and $P$ be defined as in section 2. We now allow the rule set $\mathcal{H}$ to be continuous (uncountable). Let $Q$ be a variable ranging over distributions (measures) on the rule space $\mathcal{H}$. For $s \in S$ we define the loss $L(Q, s)$ to be $E_{h \sim Q}[L(h, s)]$. We have that $L(Q, s)$ is the loss of a stochastic process that selects the hypothesis $h$ according to distribution $Q$. We define $L(Q)$ to be $E_{h \sim D}[L(Q, s)]$. Given a sample $S = \{s_1, \ldots, s_N\}$ we define $\hat{L}(Q)$ to be $\frac{1}{N} \sum_{s \in S} L(Q, s)$. Finally we will write $\mathcal{D}(Q, P)$ for the Kullback-Leibler divergence from $Q$ to $P$.

$$\mathcal{D}(Q, P) = E_{h \sim Q} \left[ \ln \frac{Q(h)}{P(h)} \right]$$
A PAC-Bayesian theorem uniformly bounds $L(Q)$ in terms of $\hat{L}(Q)$ and $D(Q, P)$. The first PAC-Bayesian theorem was given in [11]. Tighter PAC-Bayesian theorems have been given by various authors [12, 10, 7, 4, 6]. Here we will focus on the following PAC-Bayesian version of the Occam bound (1) which can be derived as a corollary of statements by Catoni [4]. A proof is included here in appendix A.

**Theorem 2.** For $\lambda > \frac{1}{2}$ selected before the draw of the sample (for any fixed $\lambda > \frac{1}{2}$) we have that, with probability at least $1 - \delta$ over the draw of the sample, the following holds simultaneously for all distributions $Q$ on $H$.

$$L(Q) \leq \frac{1}{1 - \frac{1}{2\lambda}} \left( \hat{L}(Q) + \frac{\lambda L_{\max}}{N} \left( D(Q, P) + \ln \frac{1}{\delta} \right) \right)$$

(2)

As with (1), there is no point in taking $\lambda$ in (2) to be large — we can in practice assume that $\lambda$ is no larger than 10. Second, although (2) is not uniform in $\lambda$ we can select $k$ different values $\lambda_1, \ldots, \lambda_k$ (all of which are selected before the draw of the sample) and by a simple union bound over these values derive that with probability at least $1 - \delta$ over the draw of the sample the following holds simultaneously for all $Q$.

$$L(Q) \leq \min_{1 \leq i \leq k} \frac{1}{1 - \frac{1}{2\lambda_i}} \left( \hat{L}(Q) + \frac{\lambda_i L_{\max}}{N} \left( D(Q, P) + \ln \frac{k}{\delta} \right) \right)$$

(3)

For minimizing the bound we can assume $1/2 \leq \lambda \leq 10$ and a small number of values of $\lambda$ should suffice. While it is possible to give a version of this theorem that is uniform over all $\lambda > 1/2$, achieving this uniformity increases the complexity of the proof.

### 3.1 An Infinite Precision $L_2$ Bound

As in section 2.1, we consider rules $h_\omega$ with $\omega \in \mathbb{R}^d$. Here we also assume that the rule is scale-invariant — that the rule $h_\omega$ depends only on the direction of the vector $\omega$. For example linear predictors of the form

$$h_\omega(x) = \arg\max_y \omega^T \Phi(x, y)$$

are scale-invariant. For scale-invariant rules it is natural to consider the uniform distribution over the directions of $\omega$. This uniform distribution can be formalized as an isotropic unit-variance prior $P = \mathcal{N}(0, 1)^d$ where $\mathcal{N}(0, 1)$ is the zero mean unit-variance Gaussian distribution. For $\Theta \in \mathbb{R}^d$ we define the distribution $Q_\Theta$ to be the isotropic unit-variance Gaussian centered on $\Theta$. Since only the direction of $\omega$ matters, we should think of $P$ as the uniform distribution over directions and think of $Q_\Theta$ as a non-uniform distribution over directions. We then have the following.

$$L(Q_\Theta) = \mathbb{E}_{\epsilon \sim \mathcal{N}(0,1)^d} [L(f_{\Theta + \epsilon})]$$

$$\hat{L}(Q_\Theta) = \mathbb{E}_{\epsilon \sim \mathcal{N}(0,1)^d} [\hat{L}(f_{\Theta + \epsilon})]$$

$$D(Q_\Theta, P) = \frac{1}{2}||\Theta||^2$$

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The PAC-Bayesian bound (2) then gives that with probability at least $1 - \delta$ over the draw of the sample the following holds simultaneously for all $\Theta$.

$$L(Q_\Theta) \leq \frac{1}{1 - \frac{1}{2\lambda}} \left( \hat{L}(Q_\Theta) + \frac{\lambda \max N}{N} \left( \frac{1}{2} ||\Theta||^2 + \ln \frac{1}{\delta} \right) \right)$$ (4)

### 3.2 Binary and Multi-Class classification

As an example we can consider linear binary classification. In this case we have that each situation is a pair $(x, y)$ with $y \in \{-1, 1\}$ and we have

$$h_\omega(x) = \text{sign}(\omega^T \Phi(x))$$

where $\Phi$ is a feature map such that $\Phi(x) \in \mathbb{R}^d$. We also use 0-1 loss

$$L(h, (x, y)) = 1_{h(x) \neq y}.$$  

We then have

$$L(Q_\Theta, (x, y)) = P_{\omega \sim Q_\Theta}[h_\omega(x) \neq y] = P_{\epsilon \sim N(0,1)}(\epsilon > y\Theta^T \Phi(x)/||\Phi(x)||).$$

In this case we have that (4) is very similar to the objective defining a support vector machine but where the hinge loss is replaced by a (non-convex) sigmoidal loss function (the cumulative of a Gaussian). In practice the rule $h_\theta$ is used at test time noting that $\Theta$ is the mean of the distribution $Q_\Theta$.

As another example we can consider expected loss for multi-class classification. In this case each situation is a pair $(x, y)$ with $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ and where $\mathcal{Y}$ is small enough to be feasibly enumerated. We assume a feature map $\Phi$ with $\Phi(x, y) \in \mathbb{R}^d$ and a loss function $\tilde{L}$ with $\tilde{L}(\hat{y}, y) \in [0, L_{\max}]$. For $\beta > 0$ we then have the following definitions.

$$h_\omega(x, y) = \frac{\omega^T \Phi(x, y)}{||\omega|| \ ||\Phi(x, y)||}$$

$$P_{\beta, \omega}(\hat{y}|x) = \frac{1}{Z_{\beta, \omega, x}} e^{\beta h_\omega(x, \hat{y})}$$

$$Z_{\beta, \omega, x} = \sum_{\hat{y} \in \mathcal{Y}} e^{\beta h_\omega(x, \hat{y})}$$

$$L_\beta(h_\omega, (x, y)) = E_{\hat{y} \sim P_{\beta, \omega}(\cdot|x)}[\tilde{L}(\hat{y}, y)]$$

This particular formulation has the property that $h_\omega$ is scale invariant (depends only on the direction of $\omega$) and $\beta$ is a parameter of the loss function. This formulation also has the property that $L_\beta(h_\omega, (x, y))$ is differentiable in $\omega$. We can then optimize the right hand side of (4) by stochastic gradient descent using

$$\nabla_\Theta \hat{L}(Q_\Theta) = \frac{1}{N} \sum_{i=1}^{N} E_{\epsilon \sim N(0,1)}[\nabla_\Theta L(h_{\Theta + \epsilon}, s_i)].$$
3.3 Dropouts

We now present a dropout bound inspired by the recent success of dropout training in deep neural networks [5]. This dropout bound is the only original contribution of this tutorial.

For a given dropout rate $\alpha \in [0, 1]$ and vector $\Theta \in \mathbb{R}^d$ we can stochastically generate a vector $w \in \mathbb{R}^d$ by selecting, for each coordinate $w_i$, the value 0 with probability $\alpha$ (dropping the coordinate $\omega_i$) or with probability $1 - \alpha$ setting $\omega_i = \Theta_i + \epsilon$ with $\epsilon \sim \mathcal{N}(0, 1)$. We let $Q_{\alpha, \Theta}$ denote the distribution on vectors defined by this generation process. To apply the PAC-Bayesian bound we will take $Q_{\alpha, 0}$ as the prior distribution and $Q_{\alpha, \Theta}$ as the posterior distribution. The PAC-Bayesian theorem then implies that for a dropout rate $\alpha$ selected before the draw of the sample we have that with probability at least $1 - \delta$ over the draw of the sample the following holds simultaneously for all $\Theta$.

$$L(Q_{\alpha, \Theta}) \leq \frac{1}{1 - \frac{\alpha}{2}} \left( \hat{L}(Q_{\alpha, \Theta}) + \frac{\lambda L_{\max}}{N} \left( D(Q_{\alpha, \Theta}, Q_{\alpha, 0}) + \ln \frac{1}{\delta} \right) \right)$$

To clarify formal notation we first consider the Boolean $d$-cube $B$ which is the set of vectors $s \in \mathbb{R}^d$ such that $s_i \in \{0, 1\}$ for all $1 \leq i \leq d$. We will call vectors $s \in B$ “sparsity patterns”. We let $S_{\alpha}$ be the distribution on the $d$-cube $B$ (the distribution on sparsity patterns) generated by selecting each $s_i$ independently with the probability of $s_i = 0$ being $\alpha$. For a sparsity pattern $s$ and for $\omega \in \mathbb{R}^d$ we will write $s \circ \omega$ for the Hadamard product defined by $(s \circ \omega)_i = s_i \omega_i$. We then have that a draw from $Q_{\alpha, \Theta}$ can be made by first drawing a sparsity pattern $s \sim S_{\alpha}$ and a noise vector $\epsilon \sim \mathcal{N}(0, 1)^d$ and then constructing $s \circ (\Theta + \epsilon)$. More formally we have the following.

$$E_{\omega \sim Q_{\alpha, \Theta}} [f(\omega)] = E_{s \sim S_{\alpha}, \epsilon \sim \mathcal{N}(0, 1)^d} [f(s \circ (\Theta + \epsilon))]$$

We then have

$$D(Q_{\alpha, \Theta}, Q_{\alpha, 0}) = E_{s \sim S_{\alpha}, \epsilon \sim \mathcal{N}(0, 1)^d} \left[ \ln \frac{S_{\alpha}(s) e^{-\frac{1}{2} ||s \circ \epsilon||^2}}{S_{\alpha}(s) e^{-\frac{1}{2} ||s \circ (\Theta + \epsilon)||^2}} \right]$$

$$= E_{s \sim S_{\alpha}} \left[ \frac{1}{2} ||s \circ \Theta||^2 \right]$$

$$= \frac{1 - \alpha}{2} ||\Theta||^2$$

The PAC-Bayesian bound then gives that, for a dropout rate $\alpha$ selected before the draw of the sample, with probability at least $1 - \delta$ over the draw of the sample the following holds simultaneously for all $\Theta$.

$$L(Q_{\alpha, \Theta}) \leq \frac{1}{1 - \frac{\alpha}{2}} \left( \hat{L}(Q_{\alpha, \Theta}) + \frac{\lambda L_{\max}}{N} \left( \frac{1 - \alpha}{2} ||\Theta||^2 + \ln \frac{1}{\delta} \right) \right)$$

Comparing (5) with (4) we see that a dropout rate of $\alpha$ reduces the complexity cost by a factor of $1 - \alpha$. However, for $\alpha$ very small we expect
\( \hat{L}(Q, \Theta) \) to be large. We can optimize the right hand side of this bound by stochastic gradient descent using the following.

\[
\nabla_{\Theta} \hat{L}(Q, \Theta) = \frac{1}{N} \sum_{i=1}^{N} E_{s \sim S, \epsilon \sim N(0,1)} d \left[ \nabla_{\Theta} L(h_{s \Theta+\epsilon}(\Theta), s_i) \right]
\]

### 3.4 The PAC-Bayesian Posterior

It is important to note that (2) has a closed-form solution for the distribution \( Q \) minimizing the bound.

\[
Q^* = \arg\min_{Q} \hat{L}(Q) + \frac{\lambda L_{\max}}{N} \mathcal{D}(Q, P)
\]

In the case where the rule space \( \mathcal{H} \) is finite we have the constraint that \( \sum_{h \in \mathcal{H}} Q(h) = 1 \) and a straightforward application of the KKT conditions yields the following.

\[
Q^*(h) = Q_\lambda(h) = \frac{1}{Z_\lambda} P(h) e^{-\frac{N \hat{L}(h)}{\lambda L_{\max}}} \quad \quad Z_\lambda = E_{h \sim P} \left[ e^{-\frac{N \hat{L}(h)}{\lambda L_{\max}}} \right]
\]

Here we can think of \( Q_\lambda \) as “the” PAC-Bayesian posterior distribution for regularization parameter \( \lambda \). It is important to note that the choice of \( L_{\max} \) strongly influences the posterior distribution. In the case of (3) we can optimize over \( \lambda \) as follows.

\[
Q^* = Q_{\lambda^*}, \quad \lambda^* = \arg\min_{1 \leq i \leq k} \hat{L}(Q_{\lambda_i}) + \frac{\lambda_i L_{\max}}{N} \mathcal{D}(Q_{\lambda_i}, P)
\]

\[
L(Q^*) \leq \min_{1 \leq i \leq k} \frac{1}{1 - \frac{1}{\lambda_i^2}} \left( \hat{L}(Q_{\lambda_i}) + \frac{\lambda_i L_{\max}}{N} \left( \mathcal{D}(Q_{\lambda_i}, P) + \ln \frac{k}{\delta} \right) \right)
\]

### 4 A Training-Variance Bound

We now consider a fixed learning algorithm \( A \) which takes as input a sample \( S \sim \mathcal{D}^N \) and returns a rule distribution \( Q_A(S) \). For a given learning algorithm \( A \) we now consider the expected loss \( E_{S \sim \mathcal{D}^N} [L(Q_A(S))] \) and the expected posterior

\[
Q_A(h) = E_{S \sim \mathcal{D}^N} [Q_A(S)(h)]
\]

The training-variance bound is the following where we will write \( E_{S} [f(S)] \) for \( E_{S \sim \mathcal{D}^N} [f(S)] \).

**Theorem 3.** For any fixed learning algorithm \( A \) and for \( \lambda > \frac{1}{2} \) we have

\[
E_{S} [L(Q_A(S))] \leq \frac{1}{1 - \frac{1}{2\lambda}} \left( E_{S} \left[ \hat{L}(Q_A(S)) \right] + \frac{\lambda L_{\max}}{N} E_{S} \left[ \mathcal{D}(Q_A(S), \tilde{Q}_A) \right] \right).
\] (6)
We can think of $E_S [D(Q_A(S), \bar{Q}_A)]$ as a measure of the variation of $Q_A(S)$ over the draw of $S$. For the PAC-Bayesian bound \(^2\) we have a closed form solution for the optimal posterior. But for the training-variance bound \(^6\) we do not have a solution for the optimal algorithm. The training-variance bound seems to motivate variance-reduction methods such as bagging \(^3\).

The training-variance bound is an immediate corollary of the following more general theorem which is implicit in Catoni \(^4\) and which is proved in appendix \[^3\] 

**Theorem 4.** For any rule distribution $P$, learning algorithm $A$, and for $\lambda > \frac{1}{2}$, we have

$$E_S [L(Q_A(S))] \leq \frac{1}{1 - \frac{1}{2}} \left( E_S \left[ \hat{L}(Q_A(S)) \right] + \frac{\lambda L_{\text{max}}}{N} E_S [D(Q_A(S), P)] \right). \quad (7)$$

It was observed by Langford \[^8\] that the rule distribution $P$ minimizing $E_S [D(Q_A(S), P)]$ is $\bar{Q}_A$. This can be shown as follows.

$$E_S [D(Q_A(S), P)] = E_{S, h \sim Q_A(S)} \left[ \ln \frac{Q_A(S)(h)}{P(h)} \right]$$

$$= E_{S, h \sim Q_A(S)} \left[ \ln \frac{Q_A(S)(h)}{Q_A(h)} \right] + E_{h \sim \bar{Q}_A} \left[ \ln \frac{\bar{Q}(h)}{P(h)} \right]$$

$$= E_S [D(Q_A(S), \bar{Q}_A)] + D(\bar{Q}_A, P)$$

This shows that \[^6\] dominates \[^7\] and is much better when $D(\bar{Q}_A, P)$ is large.

For a given learning algorithm $A$ we can insert $\bar{Q}_A$ for $P$ in the PAC-Bayesian bound \(^2\) yielding the following high confidence version of \[^6\].

**Theorem 5.** For any given learning algorithm $A$ and $\lambda > \frac{1}{2}$ we have the following with probability at least $1 - \delta$ over the draw of the sample.

$$L(Q_A(S)) \leq \frac{1}{1 - \frac{1}{2}} \left( \hat{L}(Q_A(S)) + \frac{\lambda L_{\text{max}}}{N} (D(Q_A(S), \bar{Q}_A) + \ln \frac{1}{\delta}) \right) \quad (8)$$

5 Applying the Training-Variance Bound to the PAC-Bayesian Posterior

We now consider the learning algorithm that maps a sample $S$ to the PAC-Bayesian posterior $Q_\lambda(S)$. Here $\lambda$ is a parameter of the learning algorithm. We should note that, although $Q_\lambda$ is the posterior optimizing the PAC-Bayesian bound \(^2\), it seems unlikely that $Q_\lambda$ is the algorithm optimizing the training-variance bound \[^6\]. Also, as we will see below, the analysis given here is somewhat loose.

Following Catoni \[^1\] and Lever et al. \[^9\] we approximate $\bar{Q}_\lambda$ with the following.

$$\bar{Q}_\lambda(h) = \frac{1}{Z_\lambda} P(h) e^{-\frac{N L(h)}{\lambda L_{\text{max}}}}$$

$$\bar{Z}_\lambda = E_{h \sim P} \left[ e^{-\frac{N L(h)}{\lambda L_{\text{max}}}} \right]$$
Inserting $\bar{Q}_\lambda$ for $P$ in (7) gives that for $\gamma > \frac{1}{2}$ we have the following.

$$
E_S \left[ L(Q_\lambda(S)) \right] \leq \frac{1}{1 - \frac{\gamma}{2}} \left( E_S \left[ \hat{L}(Q_\lambda(S)) \right] + \frac{\gamma L_{\text{max}}}{N} E_S \left[ D(Q_\lambda(S), \bar{Q}_\lambda) \right] \right) + \frac{\gamma L_{\text{max}}}{N} \ln \frac{1}{\delta}.
$$

(9)

Note that we allow $\gamma$ to be different from $\lambda$. We now have the following bound from Catoni [4] and whose proof is given in appendix C.

$$
E_S \left[ D(Q_\lambda(S), \bar{Q}_\lambda) \right] \leq \frac{N}{\lambda L_{\text{max}}} \left( E_S \left[ L(Q_\lambda(S)) \right] - E_S \left[ \hat{L}(Q_\lambda(S)) \right] \right) \quad (10)
$$

By inserting (10) into (9), setting $\gamma = \frac{1}{2} \lambda$ and solving for $E_S \left[ L(Q_\lambda(S)) \right]$ one can derive the following for $\lambda > 2$.

$$
E_S \left[ L(Q_\lambda(S)) \right] \leq \frac{1}{1 - \frac{\lambda}{2}} E_S \left[ \hat{L}(Q_\lambda(S)) \right] + \frac{\lambda L_{\text{max}}}{N} \ln \frac{1}{\delta}.
$$

(11)

Note that $\frac{1}{2} \lambda$ in the Occam and PAC-Bayesian bound has been replaced with $\frac{1}{2} \lambda$. Also note that $L_{\text{max}}$ appears in the definition of $Q_\lambda(S)$.

To get a corresponding high-confidence bound we first note that by inserting $\bar{Q}_\lambda$ for $P$ in the PAC-Bayesian bound (2) we get that, for $\gamma > \frac{1}{2}$, with probability at least $1 - \delta$ over the draw of the sample we have

$$
L(Q_\lambda(S)) \leq \frac{1}{1 - \frac{\gamma}{2}} \left( \hat{L}(Q_\lambda(S)) + \frac{\gamma L_{\text{max}}}{N} \left( D(Q_\lambda(S), \bar{Q}_\lambda) + \ln \frac{1}{\delta} \right) \right).
$$

(12)

This can be combined with the following whose proof is given in appendix C.

**Lemma 1.** For $\lambda > 0$, with probability at least $1 - \delta$ over the draw of the sample we have

$$
D(Q_\lambda(S), \bar{Q}_\lambda) \leq \frac{N}{\lambda L_{\text{max}}} \left( L(Q_\lambda(S)) - \hat{L}(Q_\lambda(S)) \right) + \frac{N}{\lambda} \sqrt{\ln \frac{1}{2 \delta}}.
$$

(13)

Taking a union bound over (13) and (12) so that both are true simultaneously, then inserting (13) into (12), setting $\gamma = \frac{1}{2} \lambda$, and solving for $L(Q_\lambda(S))$, yields that with probability at least $1 - \delta$ over the draw of the sample we have

$$
L(Q_\lambda(S)) \leq \frac{1}{1 - \frac{\lambda}{2}} \left( \hat{L}(Q_\lambda(S)) + L_{\text{max}} \sqrt{\ln \frac{\lambda}{2 \delta}} + \frac{\lambda L_{\text{max}}}{N} \ln \frac{\lambda}{2 \delta} \right).
$$

(14)

Improvements in these bounds should be possible. To see this consider the PAC-Bayesian bound (2) for which $Q_\lambda(S)$ is the optimal posterior.

$$
L(Q_\lambda(S)) \leq \frac{1}{1 - \frac{\lambda}{N}} \left( \hat{L}(Q_\lambda(S)) + \frac{\lambda L_{\text{max}}}{N} \left( D(Q_\lambda(S), P) + \ln \frac{1}{\delta} \right) \right).
$$

Replacing $P$ by $\bar{Q}_\lambda$ should significantly improve this bound. However, replacing $P$ by $\bar{Q}_\lambda$ and then inserting (13) makes the bound vacuous.
6 Incorporating Empirical Loss Variance

For a given rule $h$ and sample $S = \{s_1, \ldots, s_n\}$ one can measure an empirical loss variance.

$$\hat{\sigma}^2(h) = \frac{1}{N-1} \sum_{i=1}^{N} (L(h, s_i) - \hat{L}(h))^2$$

It is natural to ask whether tighter bounds are possible if we allow the bounds to involve $\hat{\sigma}^2(h)$. Audibert, Munos and Szepesvari [2] give a bound motivated by this question. Consider a random variable $x \in [0, L_{\text{max}}]$ with expectation $\mu$ and an IID sample $\{x_1, \ldots, x_n\}$ with empirical mean $\hat{\mu}$ and empirical variance $\hat{\sigma}^2$. Audibert, Munos and Szepesvari prove that the following holds with probability at least $1 - \delta$ over the draw of the sample.

$$\mu \leq \hat{\mu} + \sqrt{\frac{2\hat{\sigma}^2 \ln \frac{3}{\delta}}{N} + \frac{3L_{\text{max}}}{N}}$$

Taking a union bound over a prior $P$ we get that with probability at least $1 - \delta$ the following holds for all $h \in \mathcal{H}$.

$$L(h) \leq \hat{L}(h) + \sqrt{\frac{2\hat{\sigma}^2(h) \left( \ln \frac{1}{P(h)} + \ln \frac{3}{\delta} \right)}{N} + \frac{3L_{\text{max}}}{N}}$$

To show the limitations of these bounds we consider the best possible case where $\hat{\sigma}^2(h) = 0$. For this case we have the following theorem whose proof is given in appendix D.

**Theorem 6.** With probability at least $1 - \delta$ over the draw of the sample we have that the following holds for all $h$ such that $\hat{\sigma}^2(h) = 0$.

$$L(h) \leq \hat{L}(h) + \frac{L_{\text{max}} \left( \ln \frac{1}{P(h)} + \ln \frac{3}{\delta} \right)}{N - 1}$$

(15)

The inequality (15) is essentially the best that can be done using a union bound over $P(h)$. The basic idea is that even if $\hat{\sigma}^2(h) = 0$ one cannot rule out the possibility of outliers which happened not to occur in the data. The probability of outliers cannot be bounded to be less than $(\ln \frac{1}{P(h)} + \ln \frac{3}{\delta})/N$ and an outlier can have loss $L_{\text{max}}$ so (15) is the best that can be done.

But (15) is not significantly tighter than the general Occam bound (1). In particular, by taking $\lambda = 1$ in (1) we get a bound that is only a factor of 2 worse than (15). If (15) is dominated by $\hat{L}(h)$ then we can take $\lambda$ in the Occam bound (1) to be large and the two bounds are essentially the same.

7 Conclusion

This paper focuses on three generalization bounds — an Occam bound, a PAC-Bayesian bound, and a training-variance bound. The Occam
bound and PAC-Bayesian bound seem to be important primarily because they provide the conceptual foundation required for the proof of the training-variance bound which dominates the other two. While the PAC-Bayesian posterior defines a learning algorithm optimizing the PAC-Bayesian bound, there is no known analogous optimal algorithm for the training-variance bound. The bound seems to suggest variance reduction methods such as boosting. There is clearly room for improved theoretical understanding of the consequences of the training-variance bound.

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A Proof of Theorem 2

All proofs in these appendices are adapted from Catoni [4] except for the proof of theorem 6 which is straightforward.

The theorem states that for \( \lambda > \frac{1}{2} \) selected before the draw of the sample (for any fixed \( \lambda > \frac{1}{2} \)) we have that, with probability at least \( 1 - \delta \) over the draw of the sample, the following holds simultaneously for all distributions \( Q \) on \( \mathcal{H} \).

\[
L(Q) \leq \frac{1}{1 - \frac{1}{2^\lambda}} \left( \hat{L}(Q) + \frac{\lambda L_{\max}}{N} \left( D(Q,P) + \ln \frac{1}{\delta} \right) \right)
\]

We will consider the case of \( L_{\max} = 1 \), the general case follows by rescaling the loss function. For real numbers \( p, q \in [0,1] \) we define \( D(q,p) \) to be the divergence from a Bernoulli variable with bias \( q \) to a Bernoulli variable with bias \( p \).

\[
D(q,p) = q \ln \frac{q}{p} + (1 - q) \ln \frac{1 - p}{1 - q}
\]

For a real number \( \gamma \) we define \( D_{\gamma}(q,p) \) to be

\[
D_{\gamma}(q,p) = \gamma q - \ln (1 - p + pe^{\gamma}).
\]

By a straightforward optimization over \( \gamma \) one can show

\[
\mathcal{D}(q,p) = \sup_{\gamma} D_{\gamma}(q,p).
\]

Now consider a random variable \( x \) with \( x \in [0,1] \) and with mean \( \mu \). Let \( \hat{\mu} \) be the mean of \( N \) independent draws of \( x \). We first show that for any fixed \( \gamma \) we have

\[
E \left[ e^{N D_{\gamma}(\hat{\mu},\mu)} \right] \leq 1. \tag{17}
\]

To see this note that \( E \left[ e^{N \gamma \hat{\mu}} \right] = (E[e^{\gamma x}])^N \). For \( x \in [0,1] \) we note that the convexity of the exponential function implies \( e^{\gamma x} \leq 1 - x + xe^{\gamma} \). This gives \( E \left[ e^{N \gamma \hat{\mu}} \right] \leq (1 - \mu + \mu e^{\gamma})^N \). Dividing by the right hand side gives \( E \left[ e^{N (\gamma \hat{\mu} - \ln(1 - \mu + \mu e^{\gamma}))} \right] \leq 1 \) which is the same as (17). It is interesting to note that

\[
E_{S \sim D_N} \left[ e^{N D_{\gamma}(\hat{\mu},\mu)} \right] = E_{S \sim D_N} \left[ \sup_{\gamma} e^{N D_{\gamma}(\hat{\mu},\mu)} \right] \geq \sup_{\gamma} E_{S \sim D_N} \left[ e^{N D_{\gamma}(\hat{\mu},\mu)} \right] \leq 1
\]

For \( h \) fixed (17) implies the following.

\[
E_{S \sim D_N} \left[ e^{N D_{\gamma}(\hat{L}(h),L(h))} \right] \leq 1
\]

\[
E_{h \sim P} E_{S \sim D_N} \left[ e^{N D_{\gamma}(\hat{L}(h),L(h))} \right] \leq 1
\]

\[
E_{S \sim D_N} \left[ E_{h \sim P} \left[ e^{N D_{\gamma}(\hat{L}(h),L(h))} \right] \right] \leq 1 \tag{18}
\]
Applying Markov’s inequality to (18) we get that with probability at least \(1 - \delta\) over the draw of \(S\) we have
\[
E_{h \sim P} \left[ e^{\gamma \mathcal{D}_\gamma(\hat{L}(h), L(h, P))} \right] \leq \frac{1}{\delta}.
\] (19)

Next we observe the shift of measure lemma
\[
E_{h \sim Q} [f(h)] \leq \mathcal{D}(Q, P) + \ln E_{h \sim P} \left[ e^{f(h)} \right]
\] (20)
which can be derived as follows.
\[
E_{h \sim Q} [f(h)] = E_{h \sim Q} \left[ \ln e^{f(h)} \right] = E_{h \sim Q} \left[ \ln \frac{P(h)}{Q(h)} e^{f(h)} \right] + \mathcal{D}(Q, P)
\]
\[
\leq \ln E_{h \sim Q} \left[ \frac{P(h)}{Q(h)} e^{f(h)} \right] + \mathcal{D}(Q, P).
\]

Setting \(f(h) = \mathcal{N}D_\gamma(\hat{L}(h), L(h))\) in (20) and using (19) we get
\[
E_{h \sim Q} \left[ \mathcal{N}D_\gamma(\hat{L}(h), L(h)) \right] \leq \mathcal{D}(Q, P) + \ln \frac{1}{\delta}.
\]

Noting that \(\mathcal{D}(q, p)\) is jointly convex in \(q\) and \(p\) we get
\[
\mathcal{D}(\hat{L}(Q), L(Q)) \leq \frac{1}{\mathcal{N}} \left( \mathcal{D}(Q, P) + \ln \frac{1}{\delta} \right).
\] (21)

Theorem 2 is now implied by the following lemma.

**Lemma 2.** For \(\lambda > \frac{1}{2}\), if \(\mathcal{D}_{-\frac{1}{\lambda}}(p, q) \leq c\) then \(p \leq \frac{1}{1 - e^c} (q + \lambda c)\).

**Proof.** Let \(\gamma\) abbreviate \(-\frac{1}{\lambda}\). We are given \(q\gamma - \ln (1 - p + pe^\gamma) \leq c\). Since \(\lambda > \frac{1}{2}\) we have \(\gamma \in (-2, 0)\). We then get
\[
p \leq \frac{1 - e^{q\gamma + c}}{1 - e^\gamma}.
\]

Applying \(e^\gamma \geq 1 + \gamma\) in the numerator and \(e^\gamma \leq 1 + \gamma + \frac{1}{2} \gamma^2 \) \leq 1 for \(\gamma \in (-2, 0)\) in the denominator we get
\[
p \leq \frac{-\gamma q + c}{-\gamma - \frac{1}{2} \gamma^2} = \frac{q - \frac{c}{\gamma}}{1 + \frac{1}{2} \gamma^2}.
\]
Replacing \(\gamma\) by \(-1/\lambda\) proves the lemma. \(\square\)
B Proof of Theorem 4

The theorem states that for distribution $P$ on rules, any algorithm $A$, and for $\lambda > \frac{1}{2}$, we have

$$E_S [L(Q_A(S))] \leq \frac{1}{1-\lambda} \left( E_S \left[ \hat{L}(Q_A(S)) \right] + \frac{M_{\text{max}}}{N} E_S \left[ D(Q_A(S), P) \right] \right).$$

**Proof.** The proof is a slight modification of the proof of theorem 2 given in section A. By the shift of measure lemma (20) we have the following for any fixed sample $S$.

$$E_{h \sim Q_A(S)} \left[ N \mathcal{D}_\gamma(\hat{L}(h), L(h)) \right] \leq \mathcal{D}(Q_A(S), P) + \ln E_{h \sim P} \left[ e^{N \mathcal{D}_\gamma(\hat{L}(h), L(h))} \right].$$

By the joint convexity of $\mathcal{D}_\gamma$ we then have

$$\mathcal{D}_\gamma(\hat{L}(Q_A(S)), L(Q_A(S))) \leq \frac{1}{N} \left( \mathcal{D}(Q_A(S), P) + \ln E_{h \sim P, S \sim D_N} \left[ e^{N \mathcal{D}_\gamma(\hat{L}(h), L(h))} \right] \right).$$

Taking the expectation of both sides with respect to $S$ and using the convexity of $\mathcal{D}_\gamma$ and the concavity of $\ln$ we get

$$E_S \left[ \mathcal{D}_\gamma(\hat{L}(Q_A(S)), L(Q_A(S))) \right] \leq \frac{1}{N} \left( E_S \left[ \mathcal{D}(Q_A(S), P) \right] + \ln E_{h \sim P, S \sim D_N} \left[ e^{N \mathcal{D}_\gamma(\hat{L}(h), L(h))} \right] \right).$$

Theorem 4 now follows from (17) and lemma 2. \qed

C Proof of (10) and (13)

(10) is the following.

$$E_S \left[ \mathcal{D}(Q_\lambda(S), Q_{\hat{\lambda}}) \right] \leq \frac{N}{\lambda L_{\text{max}}} \left( E_S \left[ L(Q_\lambda(S)) \right] - E_S \left[ \hat{L}(Q_\lambda(S)) \right] \right).$$

**Proof.**

$$E_S \left[ \mathcal{D}(Q_\lambda(S), Q_{\hat{\lambda}}) \right] = E_{S, h \sim Q_\lambda(S)} \left[ \ln \frac{Q_\lambda(S)(h)}{Q_{\hat{\lambda}}(h)} \right]$$

$$= E_{S, h \sim Q_\lambda(S)} \left[ \frac{N}{\lambda L_{\text{max}}} \hat{L}(h) - \frac{N}{\lambda L_{\text{max}}} \hat{L}(h) \right]$$

$$- E_S \left[ \ln Z_\lambda(S) \right] + \ln \hat{Z}_\lambda$$

$$= \frac{N}{\lambda L_{\text{max}}} \left( E_S \left[ L(Q_\lambda(S)) \right] - E_S \left[ \hat{L}(Q_\lambda(S)) \right] \right)$$

$$- E_S \left[ \ln Z_\lambda(S) \right] + \ln \hat{Z}_\lambda$$
But the log partition function is convex in energy which gives

$$E_S \ln Z_\lambda(S) = E_S \ln E_{h \sim P} \left[ e^{-\frac{N}{\lambda L_{\max}} L(h)} \right] \geq \ln E_{h \sim P} \left[ e^{-\frac{N}{\lambda L_{\max}}} E_\delta[L(h)] \right] = \ln E_{h \sim P} \left[ e^{-\frac{N}{\lambda L_{\max}}} L(h) \right] = \tilde{Z}_\lambda$$

(13) states that with probability at least $1 - \delta$ we have

$$\mathcal{D}(Q_\lambda(S), \tilde{Q}_\lambda) \leq \frac{N}{\lambda L_{\max}} \left( E_S \left[ L(Q_\lambda(S)) - \hat{L}(Q_\lambda(S)) \right] \right) + \frac{N}{\lambda} \sqrt{\frac{\ln \frac{1}{\delta}}{2N}}.$$

**Proof.**

$$\mathcal{D}(Q_\lambda(S), \tilde{Q}_\lambda) = E_{h \sim Q_\lambda(S)} \left[ \ln \frac{Q_\lambda(S)(h)}{Q_\lambda(h)} \right] = E_{h \sim Q_\lambda(S)} \left[ \frac{N}{\lambda L_{\max}} L(h) - \frac{N}{\lambda L_{\max}} \hat{L}(h) \right] - \ln Z_\lambda + \ln \tilde{Z}_\lambda = \frac{N}{\lambda L_{\max}} \left( L(Q_\lambda(S)) - \hat{L}(Q_\lambda(S)) \right) - \ln Z_\lambda + \ln \tilde{Z}_\lambda$$

$$= \ln E_{h \sim P} \left[ e^{\frac{N}{\lambda L_{\max}}} L(h) \right] = \ln E_{h \sim Q_\lambda} \left[ \frac{P(h)}{Q_\lambda(h)} e^{\frac{N}{\lambda L_{\max}}} L(h) \right] \geq E_{h \sim Q_\lambda} \left[ \ln \frac{P(h)}{Q_\lambda(h)} - \frac{N}{\lambda L_{\max}} \hat{L}(h) \right] = \ln \tilde{Z}_\lambda + \frac{N}{\lambda L_{\max}} \left( L(\tilde{Q}_\lambda) - \hat{L}(\tilde{Q}_\lambda) \right)$$

Since $\lambda$ is selected before the draw of the sample, a Hoeffding bound can be used to bound $L(\tilde{Q}_\lambda) - \hat{L}(\tilde{Q}_\lambda)$ yielding that with probability at least $1 - \delta$ over the draw of the sample we have

$$\ln Z_\lambda(S) \geq \ln \tilde{Z}_\lambda - \frac{N}{\lambda} \sqrt{\frac{\ln \frac{1}{\delta}}{2N}}. \quad (22)$$
D Proof of Theorem 6

The theorem states that with probability at least $1 - \delta$ over the draw of the sample we have that the following holds for all $h$ such that $\hat{\sigma}^2(h) = 0$.

$$L(h) \leq \hat{L}(h) + \frac{L_{\text{max}} \left( \ln \frac{1}{P(h)} + \ln \frac{1}{\delta} \right)}{N - 1}$$

**Proof.** Consider a sample $S = \{s_1, \ldots, s_n\}$. We let the sample $s_1$ define a target loss value for each rule. We consider a sample $s_i$ for $i > 1$ to be an “outlier” for rule $h$ if $L(h, s_i) \neq L(h, s_1)$. We can then use the standard “realizable” analysis over the sample $\{s_2, \ldots, s_N\}$ to bound the outlier rate. More specifically, let $\mu(h)$ be the probability that a new draw of a situation from $D$ is an outlier for $h$.

$$\mu(h) = P_{s \sim D}(L(h, s) \neq L(h, s_1))$$

We will first show that with probability at least $1 - \delta$ over the draw of $\{s_2, \ldots, s_N\}$ we have that the following holds simultaneously for all $h$ such that $\hat{\sigma}^2(h) = 0$.

$$\mu(h) \leq \frac{\ln \frac{1}{P(h)} + \ln \frac{1}{\delta}}{N - 1}$$

(23)

The probability over the draw of $\{s_2, \ldots, s_N\} \sim D^{N-1}$ that $\hat{\sigma}^2(h) = 0$ equals $(1 - \mu(h))^{N-1} \leq e^{-(N-1)\mu(h)}$. So if $h$ violates (23) then the probability that $\sigma^2(h) = 0$ is at most $P(h)\delta$. By the union bound the probability that there exists an $h$ with $\sigma^2(h) = 0$ and violating (23) is at most $\sum_h P(h)\delta = \delta$ and thus with high probability (23) holds for all $h$. The theorem then follows from the observation that if $\sigma^2(h) = 0$ then $\hat{L}(h) = L(h, s_1)$ and $L(h) \leq L(h, s_1) + L_{\text{max}}\mu(h)$.

$\square$