Using Region Testing to Evaluate PAC Bounds

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Abstract

The theory of Probably Approximately Correct (PAC) generalization bounds for neural networks has been around since the work of [1]. Initially, they were a theoretical construct that elucidated the details of the learning process and gave probabilistic guarantees on the performance of machine learning models on unseen data. However, their utility in practice was only first realised by [7] who managed to contextualize the bounds practically for neural networks in a non-vacuous manner. Since then there have been other successful implementations [9][10][12]. Each of these optimizes different components of the bounds to ensure their tightness. They are evaluated using finite training sets of discrete points. Although we cannot train networks on regions of points, we can sometimes verify the network's performance in these regions. In this work, we want to understand how knowing the network's performance on a region of the input space can be used to condition PAC bounds.

1 Introduction

Generalization of neural networks refers to the ability to perform well on data that lies outside the training set. For a neural network, this means that it can learn a function that captures information that extends to the underlying data distribution from which the training set is drawn. A network with a capacity to generalize is observed to translate good performance in training to good performance on an unseen test set. During training the network is only exposed to a finite set of samples from which the network is trying to learn a representation of the underlying distribution from which the sample was drawn. The network's quality is estimated using a loss function, which tries to quantify the discrepancy between the current network outputs and the intended output. Therefore, we ideally would like a network that incurs a low loss. As we do not have access to the distribution that the network is trying to learn, we evaluate the loss of the network on the training set. Modern neural networks typically have a far greater number of parameters than samples in the training set which means that there are many possible ways that the network can be tuned to obtain a low loss on the training set. It is not clear that optimizing for good performance on this set will encode the intended behaviour into the network. The network could simply memorize the training set by overfitting to the loss function defined on this set, however, we do not observe networks learning such interpolatory functions. Neural networks portray a remarkable capacity to learn representations that extend reasonably well beyond the training set. There have been many efforts to try and understand this phenomenon either from a theoretical or empirical perspective.

Probably Approximately Correct (PAC) bounds are a theoretical tool that has been developed to provide quantitative guarantees on the generalization property of neural networks. With high probability, they bound the difference in network performance on training data and the underlying distribution. Different types of PAC bounds appeal to different components of the learning process. For example, PAC-Bayes bounds are those developed under the Bayesian machine learning framework and it was these bounds that [7] could implement non-vacuously. Then, [8] introduced compression bounds derived from compression algorithms that were designed to reduce the number of parameters needed to represent a given neural network whilst guaranteeing a certain level of performance. Using these algorithms they were able to derive bounds on the generalization error, however, these particular bounds were not meaningful in practice. It did motivate

the subsequent work of [9] that combines this paradigm with the Bayesian framework by utilizing the notion of a compression scheme to develop priors that tightened PAC-Bayes bounds sufficiently for practical implementation. Then, [12] extended this line of reasoning to further improve the tightness of the bounds. With this work, we intend to introduce a different strategy for evaluating these bounds. The current strategy only considers discrete samples, where here we capitalize on our ability to determine network performance in a region of the input space. The intuition is that operating with a region allows us to infer more information on the true behaviour of the network on the underlying distribution. As we can only train neural networks on discrete finite sets, these updates will have to occur after training which will introduce some added constraints to when our updated bounds will hold.

2 Problem Formalization

2.1 Notation

We will only focus on the PAC generalization bounds that apply to neural networks. We define our data space to be $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ where $\mathcal{X}$ is the feature space and $\mathcal{Y}$ is the output space. We suppose that there is an unknown distribution $\mathcal{D}$ defined on this space and so the training process aims to learn a network $h : \mathcal{X} \to \mathcal{Y}$ that produces outputs in accordance with the distribution $\mathcal{D}$. This will involve employing a learning algorithm on a training set $S = \{z_i\}_{i=1}^m = \{(x_i, y_i)\}_{i=1}^m$ which we assume consists of m i.i.d samples from $\mathcal{D}$. Our neural network will be parameterized by a weight vector $\mathbf{w} \in \mathcal{W}$ with the corresponding network denoted $h_{\mathbf{w}} \in \mathcal{H}$. The sets $\mathcal{W}$ and $\mathcal{H}$ will be referred to as the parameter space and the hypothesis set respectively. To assess the quality of a particular network we use a loss function $l : \mathcal{Y} \times \mathcal{Y} \to [0, C]$ which we will require to be bounded. The loss function quantifies the difference between a network's output and the desired output according to the distribution $\mathcal{D}$. That is for $z = (x, y) \in \mathcal{Z}$ we identify the quantity $l_z(\mathbf{w}) := l(h_{\mathbf{w}}(x), y)$ as the error of this particular example. Using this we can define the risk of our network to be

$$R(\mathbf{w}) = \mathbb{E}_{z \sim \mathcal{D}}(l_z(\mathbf{w}))$$

which is dependent on the unknown distribution $\mathcal{D}$ and hence is also unknown. Instead, we work with the empirical risk of the network

$$\hat{R}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} l_{z_i}$$

which is implicitly dependent on a training set and is such that $\mathbb{E}_{S \sim \mathcal{D}^m}\left(\hat{R}(\mathbf{w})\right)$. It will be useful to introduce the notation $[k] = 1, \ldots, k$ and $[[k]]_m = k, \ldots, m$ for $k, m \in \mathbb{N}$.

2.2 Problem Statement

We will formulate the problem by considering a relatively simple PAC bound.

Theorem 2.1 ([13]). *Let $|\mathcal{W}| = M < \infty$, $\delta \in (0, 1)$ and $\mathbf{w} \in \mathcal{W}$ then it follows that*

$$\mathbb{P}_{S \sim \mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{M}{\delta}\right)}{2m}}\right) \geq 1 - \delta.$$

As is the case with most machine learning problems, we can obtain zero training error on the training set, that is $\hat{R}(\mathbf{w}) = 0$ for some $\mathbf{w} \in \mathcal{W}$. Assuming this we see that Theorem 2.1 gives us a bound on the risk of the network that holds with a confidence of $1 - \delta$. More importantly, it tells us how this bound changes as we add points to the training set. The bound gets tighter to the true risk of the network as we increase the number of points on which we train the network. Adding an extra data point and training the network to zero training error reduces the bound of Theorem 2.1 by

$$C\sqrt{\frac{\log\left(\frac{M}{\delta}\right)}{2}}\left(\frac{1}{\sqrt{m}} - \frac{1}{\sqrt{m+1}}\right).$$

Or we can say that the original bound holds with an increased confidence of

$$1-\delta' = 1 - \frac{M}{\left(\frac{M}{\delta}\right)^{\frac{m+1}{m}}} \geq 1-\delta.$$

Note that the bound of Theorem 2.1 holds for all $\mathbf{w} \in \mathcal{W}$, which is why the factor of M appears. It is necessary to do this because we cannot guarantee that the added data point has a zero training error under the current parameter value. It may be possible to ensure that the updated parameter value is within some subset of the parameter space, perhaps through a stochastic gradient descent argument. However, this will not be discussed in this work. We are going to update our bounds in a slightly different way. Suppose that we have trained to a network $h_{\mathbf{w}}$ for which we can guarantee a zero training error on some region $\Delta \subset \mathcal{Z}$, we will denote this assumption by $l_{\Delta}(\mathbf{w}) = 0$. Note how this is different from the previous case in two different ways. The main difference is that we are now considering a region of points rather than a single point. The more subtle difference is that there is no change in parameter value, we are assuming that for the network trained on the initial m points, there exists such a region Δ. In the previous scenario, we retrained the network so the parameter value is different. If we did not retrain the network and instead supposed that it achieved zero training error on a point, then we cannot update our bounds in the same way as knowing the performance at a (deterministic) point provides no information (when working on a continuous data space). Henceforth, we only discuss the update of bounds in the scenario where we can guarantee performance on a region of the data space. Therefore, when we update our bounds we are going to lose the property that it holds over the entire parameter space. Despite this, we want to understand how this affects bounds such as those given in Theorem 2.1. One of the major implications of our assumptions is that they provide information for the distribution $\mathcal{D}$. From the assumptions, we can understand the shape of $\mathcal{D}$ in the region Δ, however, we are not able to explicitly calculate

$$p_{\Delta} = \mathbb{P}_{z\sim\mathcal{D}}(z \in \Delta) = \int_{z\in\Delta} \mathcal{D}(z)dz.$$

To utilize our knowledge of the shape of $\mathcal{D}$ in this region we need to know p_{Δ} such that we can understand the significance of our region to the overall problem. For now, however, we will suppose that we have access to this quantity and later we will address how we may calculate it. It is important to understand that our assumptions will not affect the quantity $R(\mathbf{w})$ as this value is calculated under the stronger assumption that we know fully the distribution $\mathcal{D}$.

3 Improving PAC Bounds

3.1 Improving the Tightness of Bounds

As we saw, there are two ways in which we could improve bounds. We can either make the bound smaller or ensure that the existing bound holds with greater confidence. Following the steps of the proof of Theorem 2.1 we can determine an updated bound under our assumptions.

Theorem 3.1. *For $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0,1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + CB(m, p_{\Delta}, \delta) \middle| l_{\Delta}(\mathbf{w}) = 0\right) \geq 1-\delta$$

for

$$B(m, p_{\Delta}, \delta) = \sqrt{\frac{\log\left(\frac{(1-p_{\Delta})+\sqrt{(1-p_{\Delta})^2+4\delta^{\frac{1}{m}}p_{\Delta}}}{2\delta^{\frac{1}{m}}}\right)}{2}}.$$

Remark 3.2. *The region Δ must be independent from the sample set S for this result to hold. This is something that will implicitly be present in all the results that follow.*

Note that by letting $p_\Delta = 0$ we just get the statement of the Theorem 2.1 without the factor of M. That is because we have not included a union bound argument as we are only interested in a single parameter value. The union bound argument is required in the setting of Theorem 2.1 as the result holds for all parameter values. The reason such bounds are derived to hold across all parameter values is that no one parameter value has information that can be leveraged, whereas, in our case, that is exactly what we have. With $p_\Delta = 1$ we see that $B(m, p_\Delta, \delta) > 0$ which is not ideal as in such a scenario we would know that $R(\mathbf{w}) = 0$. The issue arises due to a step in the proof of the theorem.

3.2 Improving the Confidence of Bounds

We can also look at improving the confidence with which bounds hold by conditioning on the event that $l_\Delta(\mathbf{w}) = 0$, which is essentially equivalent to improving the tightness of a bound. It is potentially more desirable to improve the tightness of bounds as this improvement manifests more readily in practical applications. However, we proceed with improving the confidence of bounds as often the explicit results are easier to derive. Furthermore, it provides a standardised metric to quantify the improvement imposed by conditioning on the event $l_\Delta(\mathbf{w}) = 0$.

Theorem 3.3. *For $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0, 1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}}\middle| l_\Delta(\mathbf{w}) = 0\right) \geq 1 - \left(\sum_{k=1}^{m}\binom{m}{k}\delta_k p_\Delta^{m-k}(1-p_\Delta)^k\right)$$

where

$$\delta_k = \frac{1}{\left(\frac{1}{\delta}\right)^{\frac{m^2}{k^2}}}.$$

We note that $\delta_k \leq \delta$ so that we do get an improvement in the confidence of the bound. Again we see that with $p_\Delta = 0$ we recover the bounds and the confidence of Theorem 2.1. However, what we notice now is that when we let $p_\Delta = 1$ we get full confidence in our bound as we expect, which we do not get with the result of Theorem 3.1.

We will now work with a PAC bound that was derived to hold for all parameters in a countable parameter space on which a prior distribution $\pi(\mathbf{w})$ is defined. The requirement that the parameter space is countable is not as restrictive as it may seem, as computers necessarily need to work with floating point numbers and so the values of the parameters will be from a countable set even if we set out the problem over an uncountable parameter space. Furthermore, the requirement of a prior is also not restrictive as networks are often randomly initialized and so one can simply take the prior to be the distribution of the initialization on the parameter space.

Theorem 3.4 ([5])**.** *Simultaneously for all $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0, 1)$ the following holds,*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \inf_{\lambda>\frac{1}{2}} \frac{1}{1-\frac{1}{2\lambda}}\left(\hat{R}(\mathbf{w}) + \frac{\lambda C}{m}\left(\log\left(\frac{1}{\pi(\mathbf{w})}\right) + \log\left(\frac{1}{\delta}\right)\right)\right)\right) \geq 1 - \delta.$$

However, at the moment we are only interested in bounds that hold for a single parameter value. We can re-derive this bound to hold for a single parameter value, which will allow us to drop the assumption that the parameter space is countable and the prior distribution will no longer influence the bound.

Theorem 3.5. *For $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0, 1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \inf_{\lambda>\frac{1}{2}} \frac{1}{1-\frac{1}{2\lambda}}\left(\hat{R}(\mathbf{w}) + \frac{\lambda C}{m}\left(\log\left(\frac{1}{\delta}\right)\right)\right)\right) \geq 1 - \delta.$$

In a similar way to before we can condition this probability on the event that $l_\Delta(\mathbf{w}) = 0$ to improve the confidence with which the bound holds.

Theorem 3.6. *For $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0,1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \inf_{\lambda>\frac{1}{2}} \frac{1}{1-\frac{1}{2\lambda}}\left(\hat{R}(\mathbf{w}) + \frac{\lambda C}{m}\left(\log\left(\frac{1}{\delta}\right)\right)\right) \middle| l_\Delta(\mathbf{w}) = 0\right) \geq 1 - \left(\sum_{k=1}^{m}\binom{m}{k}\exp\left(-\frac{m^2\epsilon(\mathbf{w})^2}{2kR(\mathbf{w})}\right)p_\Delta^{m-k}(1-p_\Delta)^k\right),$$

where

$$\epsilon(\mathbf{w}) = \sqrt{\frac{2R(\mathbf{w})\log\left(\frac{1}{\delta}\right)}{m}}.$$

This is indeed an improvement in confidence as

$$\exp\left(-\frac{m^2\epsilon(\mathbf{w})^2}{2kR(\mathbf{w})}\right) \leq \exp\left(-\frac{m\epsilon(\mathbf{w})^2}{2R(\mathbf{w})}\right) = \delta.$$

Again with $p_\Delta = 0$ and $p_\Delta = 1$ we get the same conclusions we made from our investigation of improving the confidence of Theorem 2.1.

4 Impact on PAC-Bayes Bounds

4.1 Bounding Expected Empirical Error

We now want to operate in the Bayesian machine learning paradigm and investigate PAC Bayes bounds. For this, we make a slightly stronger, but reasonable, assumption that there is a subset $\Omega \subset \mathcal{W}$ in which the weights correspond to networks that achieve zero training error on the region $\Delta \subset \mathcal{Z}$. This seems reasonable if one considers linear classifiers as for a dataset which has a non-zero margin between the clusters of classes then there exists a set of parameters that would achieve zero training error. These sets of parameters would correspond to the subset Ω.

Recall the research on this topic is because neural networks are over-parameterized and can learn functions that overfit to training data. The overfitting arises as there are multiple representations of the data, of which some are more desirable. Hence, it is justified to presume that a subset of our parameter space is capable of achieving zero training error on a particular region of the data space. We must make it clear that we are not considering parameters that achieve zero error on some region, all the parameters in Ω must achieve zero error on the same region. This added assumption will allow us to work with expected risk, as the parameters for which $l_\Delta(\mathbf{w}) = 0$ need to have a non-zero probability mass to have any influence on this value. We will work with Theorem 4.1 and see how we can improve the confidence with which it holds using the assumptions.

Theorem 4.1. *[2] For all $\rho \in \mathcal{M}(\mathcal{W})$ and $\delta \in (0,1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) \leq \hat{R}(\rho) + \sqrt{\frac{\mathrm{KL}(\rho,\pi) + \log\left(\frac{1}{\delta}\right) + \frac{5}{2}\log(m) + 8}{2m-1}}\right) \geq 1-\delta.$$

In the following let

$$p_\Omega = \int_\Omega \rho(\mathbf{w})d\mathbf{w}$$

and $l_\Delta(\Omega) = 0$ be the event that for all $\mathbf{w} \in \Omega$ we have $l_\Delta(\mathbf{w}) = 0$.

Theorem 4.2. *For all $\rho \in \mathcal{M}(\mathcal{W})$ and $\delta \in (0,1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) \leq \hat{R}(\rho)+\sqrt{\frac{\mathrm{KL}(\rho,\pi)\log\left(\frac{1}{\delta}\right)+\frac{5}{2}\log(m)+8}{2m-1}}\middle| l_\Delta(\Omega)=0\right) \geq 1-\left(\sum_{k=1}^{m}\binom{m}{k}\left(\delta_k p_\Omega+\delta(1-p_\Omega)\right)p_\Delta^{m-k}(1-p_\Delta)^k\right),$$

where δ_k is such that

$$\frac{m}{k}\sqrt{\frac{\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta}\right)+\frac{5}{2}\log(m)+8}{2m-1}} = \sqrt{\frac{\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta_k}\right)+\frac{5}{2}\log(m)+8}{2m-1}}.$$

Again we observe that is indeed an improvement in confidence as

$$\sqrt{\frac{\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta}\right)+\frac{5}{2}\log(m)+8}{2m-1}}$$

is a decreasing function in δ. So that

$$\sqrt{\frac{\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta}\right)+\frac{5}{2}\log(m)+8}{2m-1}} \leq \sqrt{\frac{\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta_k}\right)+\frac{5}{2}\log(m)+8}{2m-1}}$$

implies that $\delta_k \leq \delta$.

4.2 Data-Dependent Probability Measure

In machine learning, we form the posterior distribution by the application of a learning algorithm on our training sample. For the case of neural networks we often choose our network parameter by drawing a realisation from the posterior distribution defined by stochastic gradient descent (SGD). As SGD is a random process, it does define some probabilistic distribution on the parameter space.

Definition 4.3 ([13])**.** *Let $\mathcal{M}(\mathcal{W})$ be a set of probability distributions defined over $\mathcal{W}$. A data-dependent probability measure is a function*

$$\tilde{\rho} : \bigcup_{m=1}^{\infty}(\mathcal{X}\times\mathcal{Y})^m \to \mathcal{M}(\mathcal{W}).$$

Theorem 4.4 ([13])**.** *For all $\lambda > 0$, and data-dependent probability measure $\tilde{\rho}$, we have that*

$$\mathbb{E}_{S\sim\mathcal{D}^m}(R(\tilde{\rho})) \leq \mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})+\frac{\lambda C^2}{8m}+\frac{\mathrm{KL}(\tilde{\rho},\pi)}{\lambda}\right).$$

Suppose that we find that the network $h_{\tilde{\mathbf{w}}}$ is such that $l_\Delta(\tilde{\mathbf{w}})=0$. Then we could simply let our data-dependent probability measure be $\tilde{\rho}(\mathbf{w}) = \mathbb{I}(\mathbf{w})_{\{\mathbf{w}=\tilde{\mathbf{w}}\}}$. So that

$$\mathrm{KL}(\tilde{\rho},\pi) = \log\left(\frac{1}{\pi(\tilde{\mathbf{w}})}\right)$$

and

$$\begin{aligned}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})\middle| l_\Delta(\tilde{\mathbf{w}})=0\right) &= \sum_{k=0}^{m}\binom{m}{k}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\middle| z_{[k]}\notin\Delta, z_{[[k]]_m}\in\Delta\right)p_\Delta^{m-k}(1-p_\Delta)^k\\ &= \sum_{k=0}^{m}\binom{m}{k}\frac{k}{m}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right)p_\Delta^{m-k}(1-p_\Delta)^k\\ &= (1-p_\Delta)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right).\end{aligned}$$

Corollary 4.5. *For all $\lambda > 0$, with the data-dependent probability measure $\tilde{\rho}(\mathbf{w}) = \mathbb{I}(\mathbf{w})_{\{\mathbf{w}=\tilde{\mathbf{w}}\}}$, we have that*

$$\mathbb{E}_{S\sim\mathcal{D}^m}(R(\tilde{\rho})) \leq (1-p_\Delta)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) + \frac{\lambda C^2}{8m} + \frac{1}{\lambda}\log\left(\frac{1}{\pi(\tilde{\mathbf{w}})}\right).$$

On the other hand, we could assume that we have optimized to some posterior distribution $\rho \in \mathcal{W}$ which we can augment using the information that $l_\Delta(\tilde{\mathbf{w}}) = 0$ by defining the data-dependent probability measure

$$\tilde{\rho} = \gamma\mathbb{I}(\mathbf{w})_{\{\mathbf{w}=\tilde{\mathbf{w}}\}} + (1-\gamma)\rho(\mathbf{w})\mathbb{I}(\mathbf{w})_{\{\mathbf{w}\neq\tilde{\mathbf{w}}\}},$$

for $\gamma \in (0,1)$.

Corollary 4.6. *For all $\lambda > 0$, with the data dependent probability measure*

$$\tilde{\rho} = \gamma\mathbb{I}(\mathbf{w})_{\{\mathbf{w}=\tilde{\mathbf{w}}\}} + (1-\gamma)\rho(\mathbf{w})\mathbb{I}(\mathbf{w})_{\{\mathbf{w}\neq\tilde{\mathbf{w}}\}},$$

for $\gamma \in (0,1)$ we have that

$$\begin{aligned}\mathbb{E}_{S\sim\mathcal{D}^m}(R(\tilde{\rho})) \leq &(1-\gamma)\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})\right) + \frac{\mathrm{KL}(\tilde{\rho},\pi)}{\lambda} + \frac{\lambda C^2}{8m}\right)\\ &+\gamma\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) + \frac{1}{\lambda}\log\left(\frac{1}{\pi(\tilde{\mathbf{w}})}\right) + \frac{\lambda C^2}{8m}\right) - \gamma p_\Delta\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) + \frac{1-\gamma}{\lambda}\log(1-\gamma).\end{aligned}$$

Reassuringly, we see that for $\gamma = 0$ we recover the original bound of Theorem 4.4 and with $\gamma = 1$ we get the bounded we deduced previously. The general expression is minimized by,

$$\gamma = 1 - \exp\left(\lambda(1-p_\Delta)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) - \lambda\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\rho)\right) - \mathrm{KL}(\rho,\pi) + \log\left(\frac{1}{\pi(\tilde{\mathbf{w}})}\right) - 1\right).$$

The reason we do not minimize the bound for $\gamma = 1$ is because we have no control on the behaviour of $h_{\tilde{\mathbf{w}}}$ on $\mathcal{Z}\setminus\Delta$. It may be the case that another parameter exists that achieves zero error on Δ and performs better on $\mathcal{Z}\setminus\Delta$ than $h_{\tilde{\mathbf{w}}}$. Similarly, if p_Δ is small then optimizing for performance on this region will probably not be a good proxy for optimizing performance on the $\mathcal{Z}$ which is what the bound is aiming to do. We can also work with the probabilistic version of Theorem 4.4 which takes the form of Theorem 4.7.

Theorem 4.7 ([4])**.** *For all $\lambda > 0$, for all $\rho \in \mathcal{M}(\mathcal{W})$, and $\delta \in (0,1)$ it follows that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) \leq \hat{R}(\rho) + \frac{\lambda C^2}{8m} + \frac{\mathrm{KL}(\rho,\pi) + \log\left(\frac{1}{\delta}\right)}{\lambda}\right) \geq 1-\delta.$$

For our next results, we resume the assumption that $l_\Delta(\Omega) = 0$ for some $\Omega \subset \mathcal{W}$.

Theorem 4.8. *For all $\lambda > 0$, for all $\rho \in \mathcal{M}(\mathcal{W})$ and $\delta \in (0,1)$ it follows that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) \leq \hat{R}(\rho) + \frac{\log\left(B(\lambda,m,p_\Delta,p_\Omega)\right) + \mathrm{KL}(\rho,\pi) + \log\left(\frac{1}{\delta}\right)}{\lambda}\middle| l_\Delta(\Omega) = 0\right) \geq 1-\delta,$$

where

$$B(\lambda,m,p_\Delta,p_\Omega) = p_\Omega\left(p_\Delta + (1-p_\Delta)\exp\left(\frac{\lambda^2C^2}{8m^2}\right)\right)^m + (1-p_\Omega)\exp\left(\frac{\lambda^2C^2}{8m}\right).$$

Remark 4.9. *When $p_\Delta = 0$ we recover the result of Theorem 4.7.*

Corollary 4.10. *If we let ρ be the point mass at $\tilde{\mathbf{w}} \in \Omega$ then for all $\lambda > 0$ and $\delta \in (0,1)$ we have that*

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\tilde{\mathbf{w}}) \leq \hat{R}(\tilde{\mathbf{w}}) + \frac{m\log\left(p_\Delta + (1-p_\Delta)\exp\left(\frac{\lambda^2C^2}{8m^2}\right)\right) + \log\left(\frac{1}{\pi(\tilde{\mathbf{w}})}\right) + \log\left(\frac{1}{\delta}\right)}{\lambda}\middle| l_\Delta(\tilde{\mathbf{w}}) = 0\right) \geq 1-\delta.$$

5 Approximation p_Δ

So far, we have operated under the assumption that we know the value of p_Δ. We used p_Δ as a theoretical device to explore its interaction with the bounds. For our results to be practically justified we need to get an explicit grip on this quantity. Knowing the value of p_Δ exactly would just amount to the notion that we know the shape and the value of $\mathcal{D}$ in the region Δ, which is theoretically possible but realistically unlikely. Instead, we will determine a confidence region for the value of p_Δ. However, we have to proceed with caution here as in most machine learning settings the Δ we determine is not independent of our training sample. For example, if we use SGD to train to the parameter $\mathbf{w}$ which we find has the property that $l_\Delta(\mathbf{w}) = 0$ then there is an implicit connection between our training set S an Δ. To mitigate this issue we generate a different sample, S_A, of size m_A to estimate p_Δ.

For $(x_i, y_i) \in S_A$, it is either in Δ or in $\mathcal{Z}\backslash\Delta$. Therefore, we can define the random variable $Z_i \sim \text{Bern}(p_\Delta)$ which is 1 when our data point is in Δ and 0 otherwise. An estimate of p_Δ is given by

$$\hat{p}_\Delta = \frac{1}{m_A}\sum_{i=1}^{m_A} Z_i,$$

which we can use to derive confidence intervals for p_Δ and update our results accordingly. Due to the often large sample sizes we deal with in the machine learning setting we should be able to infer relatively small confidence intervals. Ideally, we would like to find the shortest confidence interval such that the variability of the bound using this approximation is minimized. A common method for forming these intervals is by using the normal approximation, which asymptotically provides the shortest confidence interval. However, we would like to generate exact results so that we can provide a concrete comparison to the bound before we condition on this information. Hence, we use the $1-\alpha$ Clopper-Pearson confidence interval that is exact and is given by

$$\left[q_B\left(\frac{\alpha}{2}, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1\right), q_B\left(1-\frac{\alpha}{2}, m_A\hat{p}_\Delta + 1, m_A - m_A\hat{p}_\Delta\right)\right],$$

where $q_B(\cdot, \beta_1, \beta_2)$ is the quantile function for the beta distribution with shape parameters β_1 and β_2 [11]. As our bounds are decreasing functions in δ we will instead work with the $1-\alpha$ one-sided confidence interval

$$\left[q_B\left(\alpha, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1\right), 1\right].$$

Recall that we have determined a region Δ for which we know the shape of the unknown distribution $\mathcal{D}$. We can say that with probability $1-\alpha$ the probability mass of the region Δ under $\mathcal{D}$ is greater than $p_L := q_B\left(\alpha, m_A\hat{p}_\Delta, m_A - m_A\hat{p}_\Delta + 1\right)$. Suppose we have a bound $B(p_\Delta)$ that is a decreasing function of p_Δ such that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + B(p_\Delta)\right) \leq \delta.$$

Then $B(p_L) \geq B(p')$ for all $p' \geq p_L$ so that,

$$\begin{aligned}
\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + B(p_L)\right) =& \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + B(p_L)\middle| p_\Delta \geq p_L\right)\mathbb{P}_{S\sim\mathcal{D}^m}(p_\Delta \geq p_L) \\
&+ \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + B(p_L)\middle| p_\Delta < p_L\right)\mathbb{P}_{S\sim\mathcal{D}^m}(p_\Delta < p_L) \\
\leq& \delta(1-\alpha) + (1)(\alpha) \\
=& \delta + \alpha(1-\delta).
\end{aligned}$$

The intention is choose to α sufficiently small so that the added $\alpha(1-\delta)$ term is small. Decreasing α will always decrease p_L and hence increase $B(p_L)$ and so to maintain a tight bound we must supplement the decreasing of α with an increase in m_A, as this will increase p_L and subsequently decrease $B(p_L)$. In the machine learning paradigm, this may involve holding out some data from the training set to approximate p_Δ. We will explore this trade-off in our experiments.

6 Experiment

6.1 Details

Our experiment will involve a ReLU neural network classifier trained on the MNIST dataset. To explicitly analyse the performance of our bound we will need access to some underlying distribution from which we can evaluate the true error of our neural network, and establish the quality of our approximation of the value p_Δ. To do this we will use the entire dataset of 60000 points to define a discrete underlying distribution. Recall that we have some independence conditions to satisfy and so we sample from this distribution and partition this sample to maintain these.

1. One segment will be used to train the network.
2. One segment will be used to approximate the value of p_Δ.
3. One segment will be used to obtain an empirical error which will then be used to form the bound on the true error.

As we partition our points into three segments we can introduce two hyper-parameters, η and ζ say. Let η define the fraction of our entire sample that we will hold out to approximate the value of p_Δ and let ζ define the fraction of the rest of our sample that will be used to obtain the empirical error. Therefore, if we take a sample of size m from the underlying distribution we have that

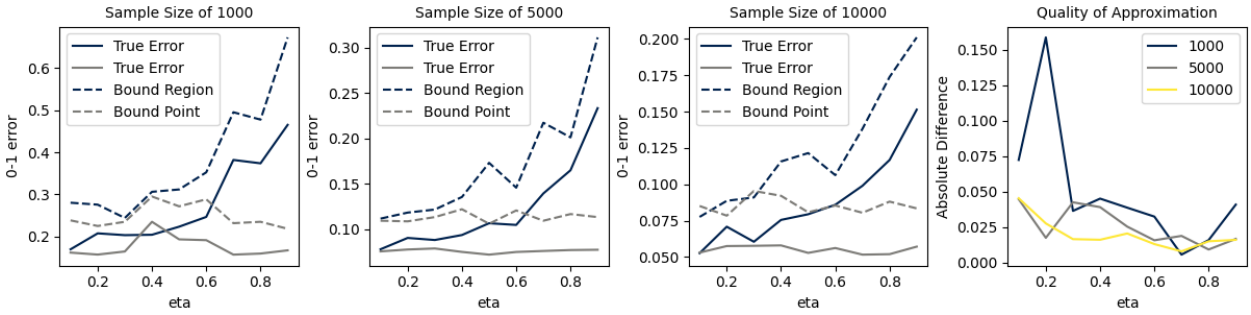
1. $m_A = \eta m$ points will be used to approximate p_Δ,
2. $m_E = \zeta(1-\eta)m$ points will be used to determine an empirical error, and
3. the remaining $m_T = (1-\zeta)(1-\eta)m$ points will be used to train the network.
4. We would like to compare the performance of our bound with its unconditioned version. To test this bound we have to do a similar partitioning, except we do not require a segment to approximate p_Δ. We will split the original sample into two segments of size $m_{T'} = (1-\zeta)$ and $m_{E'} = \zeta m$ for training and evaluating the empirical error respectively.

To train the network we will use stochastic gradient descent with a learning rate of 0.1 and momentum of 0.9. For training, we will use the cross entropy loss function and for evaluating our bound we will use the 0-1 loss, as our results require a bounded loss function and the 0-1 is more interpretable. Once our network is trained we can compute explicitly the empirical 0-1 error on the determined segment of our sample, $\hat{R}(\mathbf{w})$, and the true 0-1 error, $R(\mathbf{w})$. To define the region Δ we determine the points from the underlying distribution that are correctly classified by our network, call this set $\mathcal{C}$, and then sample from these points. We can only do this as we have access to the underlying distribution which of course in reality is not the case. Consequently, we can control the true value of p_Δ in our experiment. Suppose we wanted to investigate our bound when $p_\Delta = \gamma$, then we can define Δ to be a $\min\left(1, \frac{\gamma}{R(\mathbf{w})}\right)$ portion of $\mathcal{C}$. Obviously, if $R(\mathbf{w}) < \gamma$ then we cannot define a Δ such $p_\Delta = \gamma$. This sampling process from $\mathcal{C}$ is where the dependence of Δ on S arises, and is why we required the partitioning of the dataset. Using the determined segment of our sample we can approximate the value of p_Δ with a lower bound, and hence calculate an upper value for our bound.

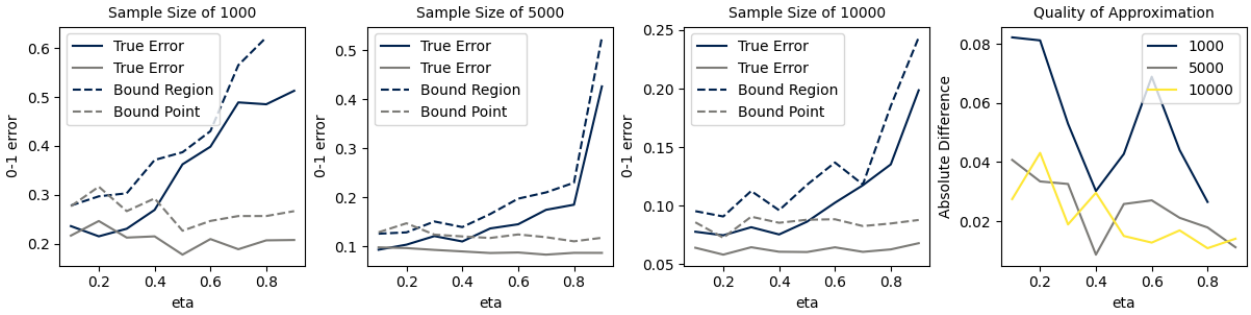
6.2 Bounds on MNIST

With this setup, we investigate the bound we derived in Theorem 3.1. We implement the experiment with $\gamma = 0.5$ and we keep $\delta = \alpha = 0.025$ throughout to give a confidence of ≈ 0.95. We use different values for the sample size, η and ζ.

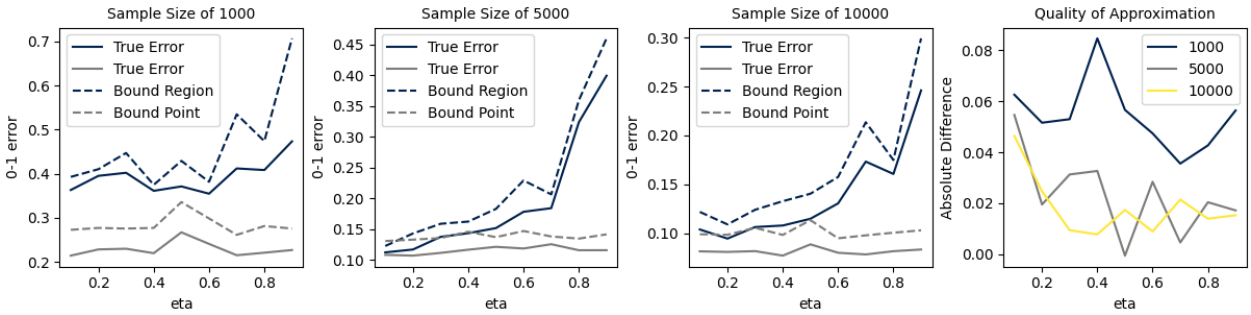
1. $m \in \{1000, 5000, 10000\}$,
2. $\eta \in \{0.1, 0.2, \ldots, 0.9\}$, and
3. $\zeta \in \{0.3, 0.5, 0.7\}$.



(a) $\zeta = 0.3$.



(b) $\zeta = 0.5$.



(c) $\zeta = 0.7$.

Figure 1: The results of our experiment for different values of ζ, the title of each subplot indicates the overall sample size used for the particular experiment.

From Figure 1 we can see that in all cases we get non-vacuous bounds on the true error. When ζ is larger we get bounds that are tighter to the true error, however, when ζ is smaller we get bounds that are smaller in value. This is as expected as with a larger ζ we are using fewer samples to train and so the quality of our neural network classifier is going to be hindered. However, we are using more samples to evaluate our bound which is inversely proportional to the size of the sample. It seems that the improvements gained by decreasing ζ are more significant than any of the negative consequences, and so one would be inclined to choose a lower value for ζ.

Similarly, one is motivated to choose a smaller value of η. As we are dealing with relatively large samples the confidence interval is sufficiently tight for even small values of η. The changes in our bound over the interval $p_\Delta \in [0, 1]$ are insignificant compared to the improved performance gained by increasing the size of our training sample, and so there is little justification for holding out a larger segment to get an improved approximation on p_Δ.

We support these conclusions with a focused investigation of the bound. We conducted the experiment five times for nine values of η in the interval $\eta \in [0.01, 0.1]$, an overall sample size of 10000, $\zeta = 0.4$ and $\gamma = 0.8$. In practice, we saw p_L values of around 0.75 and obtained the results of Figure 2

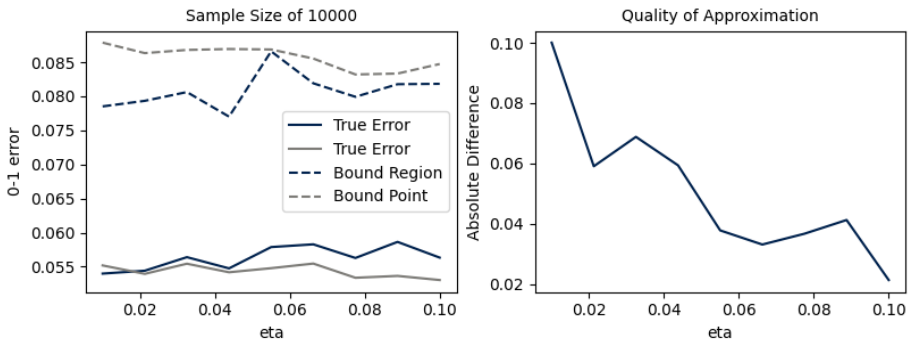


Figure 2: With this more focused investigation, and obtaining averaged results, we can more clearly determine that the conditioned bounds provide as much as a roughly 10% improvement in tightness.

6.3 Comparison to Point Bounds

What we can also see from Figure 1 is that the conditioned bound does not provide any significant improvements in terms of absolute performance. This is due to the fact that this updated bound is not a significant improvement on the point bound. The improvement is accentuated for loss functions with a larger range. As we noted in the previous section the value of η can be taken to be small, a lot smaller than initially expected, as the value of a larger sample size for training has more significant improvements than the drawbacks of choosing a small value of η. When we compare the region and point bounds for low values of eta, we tend to see a slightly better performance in the region bound. This is particularly the case for larger overall sample sizes. Despite the absolute performance of the network being degraded by the compromises introduced by implementing the region-conditioned bound, it seems that the bound we do achieve is tighter to the true error of the network. We repeat our experiment with $\zeta = 0.3$ and $\eta = 0.1$ but with varying values of γ. We then compare the tightness of the region bounds to the tightness of the point bounds.

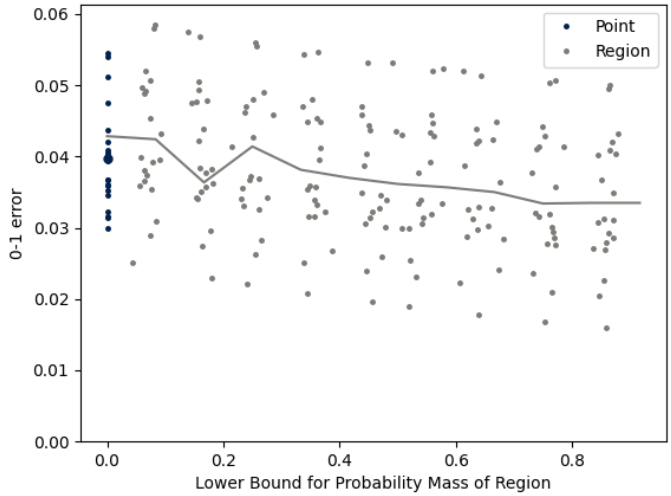


Figure 3: Shows the tightness of the region bounds for different values of the approximated lower bound, p_L, of p_Δ. We also compute the point bound for the same networks and plot their values on the $p_L = 0$ line, with the enlarged dot representing their mean.

We see is that the region bound is only insignificantly tighter than the point bound on average. However, there is a lot more variability in the region bound, and in some cases, we have significantly tighter bounds.

This variability is probably due in larger part to the training sample being smaller, and hence are network is giving less opportunity to converge during training. We only get slight improvements as the conditioned bound is sub-optimal, and we know this because when $p_\Delta = 1$ we get a strictly positive bound. An optimal bound would be 0 in this case as we know the underlying distribution and can therefore compute the true error exactly.

6.4 Performance of the PAC-Bayes Bound

Recall, the conditioned PAC-Bayes bound we derived in Theorem 4.8 from Theorem 4.7. To understand the improvement gained by our updated bound we only need to compare the $\frac{\lambda C^2}{8m}$ term of Theorem 4.7 and $\frac{\log(B(\lambda,m,p_\Delta,p_\Omega))}{\lambda}$ term of Theorem 4.8. Note that λ is a hyper-parameter that is optimized non-trivially and so, for the purposes of our discussion, we can ignore it (i.e. let $\lambda = 1$). Hence, we simply need to compare the performance of the quantities $\frac{C^2}{8m}$ and $\log(B(\lambda, m, p_\Delta, p_\Omega))$. Let us assume that we are in the context of Corollary 4.10 so that

$$\log(B(\lambda, m, p_\Delta, p_\Omega)) = m \log\left(p_\Delta + (1 - p_\Delta) \exp\left(\frac{\lambda^2 C^2}{8m^2}\right)\right).$$

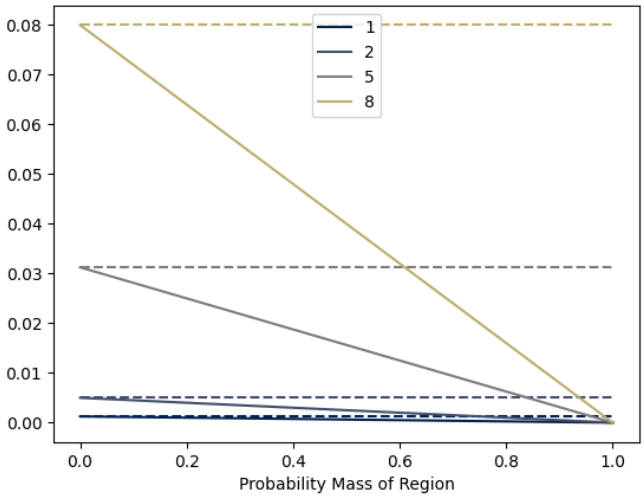


Figure 4: A plot showing the performance of the identified quantities from Theorem 4.7 (dashed) and Theorem 4.8 (solid) for $C \in \{1, 2, 5, 8\}$.

What we see from Figure 4 is a roughly linear improvement in the performance of these quantities as p_Δ increases. However, note that the absolute value of this improvement is small, especially for the smaller values of C. Therefore, if we want to bound the 0-1 error of a network, we will likely see little improvement by using our conditioned bound. The reason for this is that the KL divergence term plays a more significant role in this bound, and the PAC-Bayes framework as a whole. A lot of the work to optimize these bounds for the neural network setting has focused on minimizing this term of the bounds.

7 Conclusion

We have seen how the knowledge that a network operates as intended on a region of the data space can tighten PAC bounds. Through experimentation, we saw that the conditioned bounds' improvements were insignificant. The conditioned bounds were only slightly tighter as any improvements they provided were

masked by the added computation required to implement them. However, we only tested one bound in our experiments and we noted that this bound was not optimal. It may be the case that updating other bounds would see a more significant improvement. Furthermore, it may be possible to mitigate some of the added computation we incurred by using our particular method of implementing the conditioned bounds. In the PAC-Bayes setting, we draw similar conclusions. In this framework, the more prominent term of the bound is the KL divergence which is not affected by our method of conditioning on our assumptions. It would be interesting to explore how our assumptions can optimize the prior, similar to much of the work we mentioned in optimizing PAC-Bayes bounds.

References

[1] David A. McAllester. "Some PAC-Bayesian Theorems". In: *Machine Learning* 37 (1998), pp. 355–363.

[2] David A. McAllester. "PAC-Bayesian model averaging". In: *Annual Conference Computational Learning Theory*. 1999.

[3] Michael Mitzenmacher and Eli Upfal. *Probability and Computing: Randomized Algorithms and Probabilistic Analysis*. Cambridge University Press, 2005.

[4] Olivier Catoni. "A PAC-Bayesian approach to adaptive classification". In: (Jan. 2009).

[5] David A. McAllester. "A PAC-Bayesian Tutorial with A Dropout Bound". In: *CoRR* (2013).

[6] Clayton Scott. *Hoeffding's Inequality*. 2014.

[7] Gintare Karolina Dziugaite and Daniel M. Roy. "Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data". In: *CoRR* (2017).

[8] S. Arora, R. Ge, B. Neyshabur, and Y. Zhang. "Stronger generalization bounds for deep nets via a compression approach". In: *CoRR* (2018).

[9] Wenda Zhou, Victor Veitch, Morgane Austern, Ryan P. Adams, and Peter Orbanz. *Non-Vacuous Generalization Bounds at the ImageNet Scale: A PAC-Bayesian Compression Approach*. 2019.

[10] Gintare Karolina Dziugaite, Kyle Hsu, Waseem Gharbieh, and Daniel M. Roy. "On the role of data in PAC-Bayes bounds". In: *CoRR* (2020).

[11] Nathaniel E. Helwig. *Inference for Proportions*. 2020.

[12] Sanae Lotfi, Marc Finzi, Sanyam Kapoor, Andres Potapczynski, Micah Goldblum, and Andrew Gordon Wilson. *PAC-Bayes Compression Bounds So Tight That They Can Explain Generalization*. 2022.

[13] Pierre Alquier. *User-friendly introduction to PAC-Bayes bounds*. 2023.

8 Appendix

8.1 Detailing the Proofs

Lemma 8.1 ([6]). *Let $U_1, \ldots, U_n$ be independent random variables taking values in an interval $[a, b]$. Then for any $t > 0$ we have that*

$$\mathbb{E}\left(\exp\left(t\sum_{i=1}^{n}\left(U_i - \mathbb{E}(U_i)\right)\right)\right) \leq \exp\left(\frac{nt^2(b-a)^2}{8}\right).$$

Proof. For $s > 0$ the function $x \mapsto e^{sx}$ is convex so that

$$e^{sx} \leq \frac{x-a}{b-a}e^{sb} + \frac{b-x}{b-a}e^{sa}.$$

Let $V_i = U_i - \mathbb{E}(U_i)$, then as $\mathbb{E}(V_i) = 0$ it follows that

$$\mathbb{E}\left(\exp(sV_i)\right) \leq \frac{b}{b-a}e^{sa} - \frac{a}{b-a}e^{sb}.$$

With $p = \frac{b}{b-a}$ and $u = (b-a)s$ consider

$$\psi(u) = \log\left(pe^{sa} + (1-p)e^{sb}\right) = (p-1)u + \log\left(p + (1-p)e^{u}\right).$$

This is a smooth function so that by Taylor's theorem we have that for any $u \in \mathbb{R}$ there exists $\xi = \xi(u) \in \mathbb{R}$ such that

$$\psi(u) = \psi(0) + \psi'(0)u + \frac{1}{2}\psi''(\xi)u^2.$$

As

$$\psi'(u) = (p-1) + 1 - \frac{p}{p + (1-p)e^{u}}$$

we have that $\psi(0) = 0$ and $\psi'(0) = 0$. Furthermore, as

$$\psi''(u) = \frac{p(1-p)e^{u}}{(p + (1-p)e^{u})^2}, \text{ and } \psi^{(3)}(u) = \frac{p(1-p)e^{u}(p + (1-p)e^{u})(p - (1-p)e^{u})}{(p + (1-p)e^{u})^2}$$

we see that $\psi''(u)$ has a stationary point at $u^* = \log\left(\frac{p}{p-1}\right)$. For u slightly less than u^* we have $\psi^{(3)}(u) > 0$ and for u slightly larger than u^* we have $\psi^{(3)}(u) < 0$. Therefore, u^* is a maximum point and so

$$\psi''(u) \leq \psi''(u^*) = \frac{1}{4}.$$

Hence, $\psi(u) \leq \frac{u^2}{8}$ which implies that

$$\log\left(\mathbb{E}\left(\exp(sV_i)\right)\right) \leq \frac{u^2}{8} = \frac{s^2(b-a)^2}{8}.$$

Therefore,

$$\begin{aligned}
\mathbb{E}\left(\exp\left(t\sum_{i=1}^{n}\left(U_i - \mathbb{E}(U_i)\right)\right)\right) &= \prod_{i=1}^{n}\mathbb{E}\left(\exp\left(t(U_i - \mathbb{E}(U_i))\right)\right) \\
&\leq \prod_{i=1}^{n}\exp\left(\frac{t^2(b-a)^2}{8}\right) \\
&\leq \exp\left(\frac{nt^2(b-a)^2}{8}\right)
\end{aligned}$$

which completes the proof. □

Proof. (Theorem 3.1). Using the law of total expectation and Lemma 8.1 we observe that

$$\begin{aligned}
&\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(t\sum_{i=1}^{m}(\mathbb{E}(l_{z_i}(\mathbf{w})) - l_{z_i}(\mathbf{w}))\right)\middle| l_\Delta = 0\right) \\
&\qquad = \sum_{k=0}^{m}\binom{m}{k}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(t\sum_{i=1}^{m}(\mathbb{E}(l_{z_i}(\mathbf{w})) - l_{z_i}(\mathbf{w}))\right)\middle| z_{[i]} \notin \Delta, z_{[[k]]} \in \Delta, l_\Delta = 0\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\qquad \leq \sum_{k=0}^{m}\binom{m}{k}\exp\left(\frac{kt^2C^2}{8}\right) p_\Delta^{m-k}(1-p_\Delta)^k.
\end{aligned}$$

Then applying Markov's inequality we get that

$$\begin{aligned}
\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + s\middle| l_\Delta = 0\right) &\leq \frac{1}{\exp(mts)}\sum_{k=0}^{m}\binom{m}{k}\exp\left(\frac{kt^2C^2}{8}\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&= \frac{1}{\exp(mts)}\left(p_\Delta + (1-p_\Delta)\exp\left(\frac{t^2C^2}{8}\right)\right)^m.
\end{aligned}$$

This holds for all $t \geq 0$, hence, we would like to find the t for which this bound is minimized. For $p_\Delta = 0$ this is done by letting $t = \frac{4s}{C^2}$. However, for $p_\Delta \in (0,1)$ we cannot find explicitly the minimizer of this expression and so we will simply use $t = \frac{4s}{C^2}$ as well. If $p_\Delta = 1$ we know that $R(\mathbf{w}) = 0$ and so the result holds trivially. Proceeding for the case where $p_\Delta \in [0,1)$ we see that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + s \middle| l_\Delta = 0\right) \leq \frac{1}{\exp\left(\frac{4ms^2}{C^2}\right)}\left(p_\Delta + (1-p_\Delta)\exp\left(\frac{2s^2}{C^2}\right)\right)^m.$$

Therefore, letting

$$\delta = \frac{1}{\exp\left(\frac{4ms^2}{C^2}\right)}\left(p_\Delta + (1-p_\Delta)\exp\left(\frac{2s^2}{C^2}\right)\right)^m$$

we can rearrange to get that

$$s = \sqrt{\frac{C^2 \log\left(\frac{(1-p_\Delta)+\sqrt{(1-p_\Delta)^2+4\delta^{\frac{1}{m}}p_\Delta}}{2\delta^{\frac{1}{m}}}\right)}{2}}$$

which completes the proof. □

Proof. Theorem 3.3. Here we will proceed directly with the law of total probability

$$\begin{aligned}
&\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0\right) \\
&\quad = \sum_{k=0}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k+1]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k.
\end{aligned}$$

For each k we have that $l_{z_i} = 0$ for $i \in [[k+1]]_m$, so we can think of each empirical error as $\frac{k}{m}$ of the empirical error of k samples. Therefore,

$$\begin{aligned}
&\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0\right) \\
&\quad = \sum_{k=0}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \frac{k}{m}\hat{R}_k(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k+1]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\quad = \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^k}\left(\frac{m}{k}R(\mathbf{w}) > \hat{R}_k(\mathbf{w}) + \frac{mC}{k}\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k+1]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\qquad + \mathbb{I}\left(R(\mathbf{w}) > C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[m]} \in \Delta\right) p_\Delta^m \\
&\quad = \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^k}\left(\frac{m}{k}R(\mathbf{w}) > \hat{R}_k(\mathbf{w}) + \frac{mC}{k}\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k+1]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k
\end{aligned}$$

where in the last inequality we have used the fact that $R(\mathbf{w}) = 0$ to deduce that

$$\mathbb{I}\left(R(\mathbf{w}) > C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}} \middle| l_\Delta(\mathbf{w}) = 0, z_{[m]} \in \Delta\right) = 0.$$

Letting

$$\delta_k = \frac{1}{\left(\frac{1}{\delta}\right)^{\frac{m^2}{k^2}}} \leq \delta$$

for $k = 1, \ldots, m$ we get that

$$\begin{aligned}
&\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) > \hat{R}(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2m}}\middle| l_\Delta(\mathbf{w}) = 0\right) \\
&\quad = \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^k}\left(R(\mathbf{w}) > \hat{R}_k(\mathbf{w}) + C\sqrt{\frac{\log\left(\frac{1}{\delta_i}\right)}{2k}}\middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k+1]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\quad \leq \sum_{k=1}^{m}\binom{m}{k}\delta_i p_\Delta^{m-k}(1-p_\Delta)^k
\end{aligned}$$

which completes the proof of the theorem. □

Theorem 8.2 ([3])**.** *Suppose $X_1, \ldots, X_n$ are independent random variables with range $\{0,1\}$. Let $\mu = \sum_{i=1}^n X_i$. Then for $\delta \in (0,1)$ we have*

$$\mathbb{P}\left(X \leq (1-\delta)\mu\right) \leq \exp\left(-\frac{\mu\delta^2}{2}\right).$$

Proof. Theorem 3.5. We deal with the case that $C = 1$ for simplicity as we can just rescale the loss function as required. Let

$$\epsilon(\mathbf{w}) = \sqrt{\frac{2R(\mathbf{w})\log\left(\frac{1}{\delta}\right)}{m}},$$

then using Theorem 8.2 we get that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(\hat{R}(\mathbf{w}) \leq R(\mathbf{w}) - \epsilon(\mathbf{w}) - \epsilon(\mathbf{w})\right) \leq \exp\left(-\frac{m\epsilon(\mathbf{w})}{2R(\mathbf{w})}\right) = \delta.$$

Therefore,

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + \sqrt{\frac{2R(\mathbf{w})\log\left(\frac{1}{\delta}\right)}{m}}\right) \geq 1-\delta.$$

Using $\sqrt{ab} = \inf_{\lambda>0}\left(\frac{a}{2\lambda} + \frac{\lambda b}{2}\right)$ we get that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\mathbf{w}) \leq \hat{R}(\mathbf{w}) + \frac{R(\mathbf{w})}{2\lambda} + \frac{\lambda\left(\log\left(\frac{1}{\delta}\right)\right)}{m}\right) \geq 1-\delta$$

which upon re-arrangement completes the proof of the theorem. □

Proof. Theorem 3.6. We proceed by applying the law of total probability and the reasoning we explained in the proof of Theorem 3.3 to get that

$$\begin{aligned}
&\mathbb{P}_{S\sim\mathcal{D}^m}\Big(\hat{R}(\mathbf{w}) \leq R(\mathbf{w}) - \epsilon(\mathbf{w})\Big| l_\Delta(\mathbf{w}) = 0\Big) \\
&\quad = \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^m}\left(\frac{k}{m}\hat{R}_k(\mathbf{w}) \leq R(\mathbf{w}) - \epsilon(\mathbf{w})\middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\quad\quad + \mathbb{I}\left(\epsilon(\mathbf{w}) \leq R(\mathbf{w}) | l_\Delta(\mathbf{w}) = 0, z_{[m]} \in \Delta\right) p_\Delta^m \\
&\quad = \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^k}\left(\hat{R}_k(\mathbf{w}) \leq R(\mathbf{w}) + \frac{m-k}{k}R(\mathbf{w}) - \frac{m}{k}\epsilon(\mathbf{w})\middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k \\
&\quad \leq \sum_{k=1}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^k}\left(\hat{R}_k(\mathbf{w}) \leq R(\mathbf{w}) - \frac{m}{k}\epsilon(\mathbf{w})\middle| l_\Delta(\mathbf{w}) = 0, z_{[k]} \notin \Delta, z_{[[k]]_m} \in \Delta\right) p_\Delta^{m-k}(1-p_\Delta)^k.
\end{aligned}$$

Applying Theorem 8.2 to this we can deduce that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(\hat{R}(\mathbf{w}) \leq R(\mathbf{w}) - \epsilon(\mathbf{w})\middle| l_\Delta(\mathbf{w}) = 0\right) \leq \sum_{k=1}^{m}\binom{m}{k}\exp\left(-\frac{kR(\mathbf{w})\left(\frac{m\epsilon(\mathbf{w})}{kR(\mathbf{w})}\right)^2}{2}\right)p_\Delta^{m-k}(1-p_\Delta)^k$$
$$= \sum_{k=1}^{m}\binom{m}{k}\exp\left(-\frac{m^2\epsilon(\mathbf{w})^2}{2kR(\mathbf{w})}\right)p_\Delta^{m-k}(1-p_\Delta)^k.$$

With this one can proceed in the same way as we do in the proof of Theorem 3.5 to complete the proof of this theorem. □

Proof. Theorem 4.2. For ease of notation let

$$B(\rho,\pi,\delta,m) = \sqrt{\frac{\mathrm{KL}(\rho,\pi) + \log\left(\frac{1}{\delta}\right) + \frac{5}{2}\log(m) + 8}{2m-1}}.$$

We first observe that for a sample S if we have $z_{[k]} \notin \Delta$ and $z_{[[k+1]]_m} \in \Delta$, for $k \neq 0$, then

$$\begin{aligned}\hat{R}(\rho|\mathbf{w}\in\Omega) &= \mathbb{E}_{\mathbf{w}\sim\rho}\left(\hat{R}(\mathbf{w})\middle|\mathbf{w}\in\Omega\right)\\ &= \frac{k}{m}\mathbb{E}_{\mathbf{w}\sim\rho}\left(\hat{R}(\mathbf{w})\right)\\ &= \frac{k}{m}\hat{R}(\rho).\end{aligned}$$

So for $k \neq 0$,

$$\begin{aligned}&\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)\\ &\quad= \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho|\mathbf{w}\in\Omega) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)p_\Omega\\ &\qquad+ \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho|\mathbf{w}\notin\Omega) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)(1-p_\Omega)\\ &\quad= \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \frac{k}{m}\hat{R}(\rho) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)p_\Omega\\ &\qquad+ \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)(1-p_\Omega)\\ &\quad\leq \mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho) + \frac{m}{k}B(\rho,\pi,\delta,m)\right)p_\Omega + \delta(1-p_\Omega)\\ &\quad= \delta_k p_\Omega + \delta(1-p_\Omega)\end{aligned}$$

If $k = 0$ then the inequality clearly doesn't hold so that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho) + B(\rho,\pi,\delta,m)|l_\Delta(\Omega))=0, z_{[m]}\in\Delta\right) = 0$$

Therefore,

$$\begin{aligned}&\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) > \hat{R}(\rho) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0\right)\\ &\quad= \sum_{k=0}^{m}\binom{m}{k}\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho) \leq \hat{R}(\rho) + B(\rho,\pi,\delta,m)\middle| l_\Delta(\Omega) = 0, z_{[k]}\notin\Delta, z_{[[k+1]]_m}\in\Delta\right)p_\Delta^{m-k}(1-p_\Delta)^k\\ &\quad\leq \sum_{k=1}^{m}\binom{m}{k}\left(\delta_k p_\Omega + \delta(1-p_\Omega)\right)p_\Delta^{m-k}(1-p_\Delta)^k.\end{aligned}$$

Taking the complement completes the proof of the theorem. □

Proof. Corollary 4.6. We first observe that

$$\begin{aligned}\mathrm{KL}\left(\tilde{\rho},\pi\right) &= \int_{\mathcal{W}} \tilde{\rho}(\mathbf{w}) \log\left(\frac{\tilde{\rho}(\mathbf{w})}{\pi(\mathbf{w})}\right) d\mathbf{w} \\ &= \int_{\mathcal{W}\setminus\{\tilde{\mathbf{w}}\}} (1-\gamma)\rho(\mathbf{w}) \log\left(\frac{(1-\gamma)\rho(\mathbf{w})}{\pi(\mathbf{w})}\right) d\mathbf{w} + \gamma \log\left(\frac{\gamma}{\pi(\tilde{\mathbf{w}})}\right) \\ &= (1-\gamma)(\mathrm{KL}(\rho,\pi) + \log(1-\gamma)) + \gamma \log\left(\frac{\gamma}{\pi(\tilde{\mathbf{w}})}\right).\end{aligned}$$

Next we see that

$$\begin{aligned}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})\middle| l_\Delta(\tilde{\mathbf{w}})=0\right) &= \gamma\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})\middle| l_\Delta(\tilde{\mathbf{w}})=0, \mathbf{w}=\tilde{\mathbf{w}}\right) + (1-\gamma)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\rho})\middle| l_\Delta(\tilde{\mathbf{w}})=0, \mathbf{w}\neq\tilde{\mathbf{w}}\right) \\ &= \gamma(1-p_\Delta)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) + (1-\gamma)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\rho)\right).\end{aligned}$$

Now using Theorem 4.4 we get that

$$\begin{aligned}\mathbb{E}_{S\sim\mathcal{D}^m}\left(R(\tilde{\rho})\right) \leq& \gamma(1-p_\Delta)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\tilde{\mathbf{w}})\right) + (1-\gamma)\mathbb{E}_{S\sim\mathcal{D}^m}\left(\hat{R}(\rho)\right) \\ &+ \frac{1-\gamma}{\lambda}\left(\mathrm{KL}(\rho,\pi) + \log(1-\gamma)\right) + \frac{\gamma}{\lambda}\log\left(\frac{\gamma}{\pi(\tilde{\mathbf{w}})}\right) + \frac{\lambda C^2}{8m},\end{aligned}$$

which upon re-arrangement completes the proof of the corollary. □

Lemma 8.3. *For any measurable, bounded function $f : \mathcal{W} \to \mathbb{R}$ we have,*

$$\log\left(\mathbb{E}_{\mathbf{w}\sim\pi}\left(e^{f(\mathbf{w})}\right)\right) = \sup_{\rho\in\mathcal{M}(\mathcal{W})}\left(\mathbb{E}_{\mathbf{w}\sim\rho}\left(f(\mathbf{w})\right) - \mathrm{KL}(\rho,\pi)\right).$$

Proof. Theorem 4.8. Using the law of total expectation we have that

$$\begin{aligned}&\mathbb{E}_{\mathbf{w}\sim\pi}\Big(\mathbb{E}_{S\sim\mathcal{D}^m}\Big(\exp\Big(tm\Big(R(\mathbf{w})-\hat{R}(\mathbf{w})\Big)\Big)\Big)\Big| l_\Delta(\Omega)=0\Big) \\ &\quad= \mathbb{E}_{\mathbf{w}\sim\pi}\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\right)\middle| l_\Delta(\tilde{\mathbf{w}})=0, \mathbf{w}\in\Omega\right)\right) p_\Omega \\ &\qquad+ \mathbb{E}_{\mathbf{w}\sim\pi}\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\right)\middle| l_\Delta(\Omega)=0, \mathbf{w}\in\Omega\right)\right)(1-p_\Omega).\end{aligned}$$

Using Lemma 8.1 we have that

$$\begin{aligned}&\mathbb{E}_{\mathbf{w}\sim\pi}\Big(\mathbb{E}_{S\sim\mathcal{D}^m}\Big(\exp\Big(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\Big)\Big| l_\Delta(\tilde{\mathbf{w}})=0, \mathbf{w}\in\Omega\Big)\Big) \\ &\qquad\leq \sum_{k=0}^{m}\binom{m}{k}\exp\left(\frac{kt^2C^2}{8}\right)p_\Delta^{m-k}(1-p_\Delta)^k \\ &\qquad= \left(p_\Delta + (1-p_\Delta)\exp\left(\frac{t^2C^2}{8}\right)\right)^m\end{aligned}$$

and

$$\mathbb{E}_{\mathbf{w}\sim\pi}\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\right)\middle| l_\Delta(\Omega)=0, \mathbf{w}\in\Omega\right)\right) \leq \exp\left(\frac{mt^2C^2}{8}\right).$$

We get the top inequality as we can think of the sum as only involving k terms rather than m as only k are potentially non-zero. Letting $\lambda = mt$ we get that

$$\begin{aligned}&\mathbb{E}_{\mathbf{w}\sim\pi}\Big(\mathbb{E}_{S\sim\mathcal{D}^m}\Big(\exp\Big(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\Big)\Big| l_\Delta(\tilde{\mathbf{w}})=0, \mathbf{w}\in\Omega\Big)\Big) \\ &\qquad\leq \left(p_\Delta + (1-p_\Delta)\exp\left(\frac{\lambda^2C^2}{m^2}\right)\right)^m\end{aligned}$$

and

$$\mathbb{E}_{\mathbf{w}\sim\pi}\left(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(tm\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\right)\Big|l_\Delta(\Omega)=0,\mathbf{w}\in\Omega\right)\right)\leq\exp\left(\frac{\lambda^2C^2}{8m}\right).$$

Therefore,

$$\begin{aligned}\mathbb{E}_{\mathbf{w}\sim\pi}\Big(\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(\lambda\left(R(\mathbf{w})-\hat{R}(\mathbf{w})\right)\right)\right)\Big|l_\Delta(\Omega)=0\Big)&\\ \leq p_\Omega\left(p_\Delta+(1-p_\Delta)\exp\left(\frac{\lambda^2C^2}{m^2}\right)\right)^m&\\ +(1-p_\Omega)\exp\left(\frac{\lambda^2C^2}{8m}\right).&\end{aligned}$$

Applying Fubini's theorem we can exchange the order of taking expectations to deduce that

$$\begin{aligned}\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(\lambda\left(R(\pi)-\hat{R}(\pi)\right)\right)\Big|l_\Delta(\Omega)=0\right)\leq&p_\Omega\left(p_\Delta+(1-p_\Delta)\exp\left(\frac{\lambda^2C^2}{m^2}\right)\right)^m\\ &+(1-p_\Omega)\exp\left(\frac{\lambda^2C^2}{8m}\right)=:B(\lambda,m,p_\Delta,p_\Omega).\end{aligned}$$

We can now apply Lemma 8.3 to deduce that

$$\mathbb{E}_{S\sim\mathcal{D}^m}\left(\exp\left(\sup_{\rho\in\mathcal{M}(\mathcal{W})}\left(\lambda\left(R(\rho)-\hat{R}(\rho)\right)\right)-\mathrm{KL}(\rho,\pi)-\log\left(B(\lambda,m,p_\Delta,p_\Omega)\right)\right)\Big|l_\Delta(\Omega)=0\right)\leq 1$$

to which we can apply Markov's inequality to get that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(\sup_{\rho\in\mathcal{M}(\mathcal{W})}\left(\lambda\left(R(\rho)-\hat{R}(\rho)\right)\right)-\mathrm{KL}(\rho,\pi)-\log\left(B(\lambda,m,p_\Delta,p_\Omega)\right)>s\Big|l_\Delta(\Omega)=0\right)\leq e^{-s}$$

for fixed $s>0$. Letting $s=\log\left(\frac{1}{\delta}\right)$ and taking the complement we get that

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R(\rho)\leq\hat{R}(\rho)+\frac{\log\left(B(\lambda,m,p_\Delta,p_\Omega)\right)+\mathrm{KL}(\rho,\pi)+\log\left(\frac{1}{\delta}\right)}{\lambda}\Big|l_\Delta(\Omega)=0\right)\geq 1-\delta,$$

which completes the proof of the theorem. □

8.2 Uniform Bounds

The power of our assumptions is that they tell us the shape of the underlying distribution on the region $\Delta\subset\mathcal{Z}$. Now suppose that we have a reasonably accurate approximate of p_Δ, so that in the following we can say 'calculate' instead of 'approximate'. With this we can calculate

$$p_\Delta=\int_\Delta\mathcal{D}(z)dz$$

and if we let $\Delta'=\mathcal{Z}\setminus\Delta$ we can define the distributions

$$\mathcal{D}_\Delta(z)=\begin{cases}\frac{\mathcal{D}(z)}{p_\Delta} & z\in\Delta\\ 0 & \text{otherwise,}\end{cases}\quad\mathcal{D}_{\Delta'}(z)=\begin{cases}\frac{\mathcal{D}(z)}{1-p_\Delta} & z\in\Delta'\\ 0 & \text{otherwise.}\end{cases}$$

Consequently, we can also define

$$R_\Delta(\mathbf{w})=\mathbb{E}_{z\sim\mathcal{D}_\Delta}(l_z(\mathbf{w})),\text{ and }R_{\Delta'}(\mathbf{w})=\mathbb{E}_{z\sim\mathcal{D}_{\Delta'}}(l_z(\mathbf{w})).$$

Despite $l_\Delta(\mathbf{w}) = 0$ only holding for a potentially small region of the parameter space, we can explicitly calculate $R_\Delta(\mathbf{w})$ for any parameter value as we know the distribution $\mathcal{D}_\Delta$. Throughout we have had to derive results that only applied to a specific parameter value as we were utilizing the property that the empirical error on Δ is zero. Here we will instead see how we could potentially derive results that hold all parameter values. To do this we will not be able to use the fact that the training error is zero to tighten our results. Note that we can decompose the true error as

$$R(\mathbf{w}) = p_\Delta R_\Delta(\mathbf{w}) + (1 - p_\Delta) R_{\Delta'}(\mathbf{w}). \tag{1}$$

For any $\mathbf{w} \in \mathcal{W}$ we can calculate explicitly each term on the right-hand side except for $R_{\Delta'}(\mathbf{w})$. We can incorporate this decomposition into PAC bounds to deduce results of the form,

$$\mathbb{P}_{S\sim\mathcal{D}^m}\left(R_{\Delta'}(\mathbf{w}) \leq \frac{\hat{R}(\mathbf{w}) + B(\delta, m) - p_\Delta R_\Delta(\mathbf{w})}{1 - p_\Delta}\right) \geq 1 - \delta,$$

that hold for all $\mathbf{w} \in \mathcal{W}$ and $\delta \in (0, 1)$. It may seem as though verifying performance for regions increases our bound and therefore undesirable. However, as p_Δ the probability density for $z \in \Delta'$ under $\mathcal{D}_{\Delta'}(z)$ increases and so $R_{\Delta'}(\mathbf{w})$ increases accordingly.

8.2.1 Experiments

We can investigate the uniform approach in a similar way as we did in the main report.

1. Obtain a sample of size m from our data space according to a discrete underlying distribution defined by 30000 (we use this reduced sample size to reduce computation time).
2. Partition the data set according to some parameter ξ.
   (a) Use ξm data points to determine the region Δ.
      - As before $\eta\xi m$ points will be used to approximate p_Δ, and
      - $(1 - \eta)\xi m$ points will be used to train a network to determine the region Δ.
   (b) Use $(1 - \xi)m$ points to evaluate our bound.
      - Where $(1 - \zeta)(1 - \xi)m$ will be used to train the model, and
      - $\zeta(1 - \xi)m$ will be used to evaluate the empirical errors for the bound.

From our investigations in the report, we conduct this experiment with $m = 10000$, $\zeta = 0.3$, $\gamma = 0.8$, $\alpha = \delta = 0.025$,

- η taking five equally spaced values in the interval $[0.01, 0.1]$, and
- $\xi \in \{0.3, 0.5, 0.7\}$.

For each set of parameter values, we perform the experiment three times to get an average. The bound we use is that of Theorem 3.1, and from the experiments, we observe the value of

$$\hat{R}(\mathbf{w}) + B(\delta, \zeta(1 - \xi)m) - p_L R_\Delta(\mathbf{w}),$$

as from Equation 1 it is clear that this our absolute uncertainty in the value of $R(\mathbf{w})$ that holds with confidence of $1 - \delta - \alpha(1 - \delta)$.

1. $\hat{R}(\mathbf{w})$ is the empirical error of the model trained by the partition of size $(1 - \xi)(1 - \xi)m$ on the partition of size $\zeta(1 - \xi)m$.
2. p_Δ is referring to the lower bound on p_Δ calculated using the partition of size $\eta\xi m$ using the region identified by the training a model on the partition of size $(1 - \eta)\xi m$ and verifying its performance.
3. We can calculate $R_\Delta(\mathbf{w})$ as we know the shape of Δ.

4. $B(\delta, \zeta(1-\xi)m)$ is the bound of Theorem 3.1.

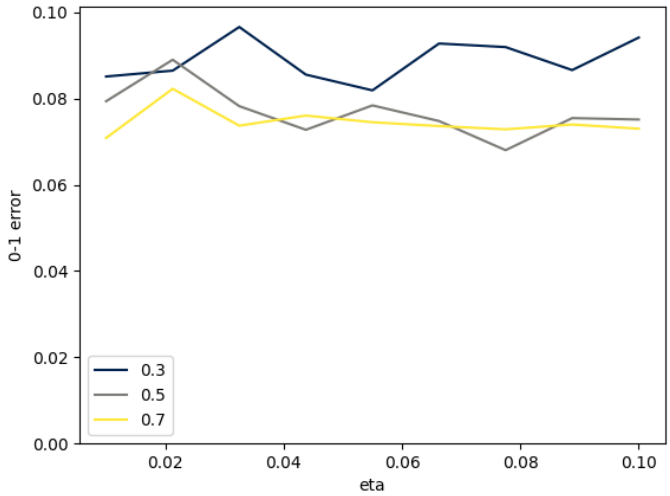


Figure 5: The bound on our absolute uncertainty of the true error. Each line corresponds to the value of ζ used in the experiment.

From Figure 5 we see that for certain values of ξ we get comparable bounds to those calculated via the method in the main report.