PAC-Bayes with Backprop

Omar Rivasplata
DeepMind
rivasplata@google.com

Vikram M Tankasali
DeepMind
tvikram@google.com

Csaba Szepesvari
DeepMind
szepi@google.com

Abstract
We explore a method to train probabilistic neural networks by minimizing risk upper bounds, specifically, PAC-Bayes bounds. Thus randomization is not just part of a proof strategy, but part of the learning algorithm itself. We derive two training objectives, one from a previously known PAC-Bayes bound, and a second one from a novel PAC-Bayes bound. We evaluate both training objectives on various data sets and demonstrate the tightness of the risk upper bounds achieved by our method. Our training objectives have sound theoretical justification, and lead to self-bounding learning where all the available data may be used to learn a predictor and certify its risk, with no need to follow a data-splitting protocol.

1 Introduction

An interesting take on neural network learning considers the weights as random outcomes of a probability distribution, rather than having fixed deterministic values. For instance this approach may be realized by injecting noise into the components of a fixed architecture. The intuition is that a probabilistic neural network may lead to better predictions, overcoming the limited generalization ability of a single weight vector (Neal [1993]). Another argument in favour of the probabilistic framework for neural networks might be enforcing robustness properties (Blundell et al. [2015]).

Training methods for probabilistic neural networks may be developed from a Bayesian perspective, where a data-dependent posterior distribution over possible network weight vectors is found by updating a prior distribution over weights with the data-dependent likelihood factor. The ideas go back to MacKay [1992a,b] who argued that Bayesian techniques are suitable for developing and comparing different network architectures, as well as addressing their generalization ability.

Blundell et al. [2015] proposed a training method derived from a variational Bayes perspective that showed competitive test set accuracy. They called their method ‘Bayes by Backprop’ (BBB) since their training objective reuses the gradients of backpropagation (Hecht-Nielsen [1992], Rumelhart et al. [1985]) and so stochastic gradient descent (SGD) optimization could be done at little extra computational cost. BBB also takes advantage of the computationally tractable approximations to the posterior of the variational Bayes (Attias [2000], Jaakkola and Jordan [1997]) approach. The BBB objective regularizes the weights using the Kullback-Leibler divergence, which is inspired by the variational objective, but the regularization factor introduced in BBB has no explicit justification. In fact, BBB uses the regularization factor as a hyperparameter that requires tuning.

In this paper we take on probabilistic neural networks from a different point of view. Our approach to learning a randomized neural network is based on minimization of an upper bound on the risk, specifically a PAC-Bayes bound, hence we call the method ‘PAC-Bayes with Backprop’ (PBB). Based on Seeger [2002]’s PAC-Bayes bound on the binary Kullback-Leibler divergence (actually, the enhanced form of Maurer [2004]) we derive two training objectives. The first training objective follows the PAC-Bayes-λ bound of Thiemann et al. [2017], which regularizes the Kullback-Leibler divergence, but unlike Blundell et al. [2015] the regularization parameter is part of the risk upper bound, hence the optimization itself sets the value of this parameter, without requiring any extra.

Preprint. Under review.
effort. The second training objective follows what we call the PAC-Bayes-quadratic bound, whose derivation involves solving a quadratic inequality, hence the name. Thus, via PBB a data-dependent distribution over weight vectors is found by minimizing a training objective that balances loss to data with loss to a ‘prior’ distribution over weights. However, PBB does not restrict these distributions to be related by a likelihood factor. In fact, the comparatively rather general PAC-Bayes framework (Shawe-Taylor and Williamson [1997], McAllester [1998]) gives a lot of flexibility in the choice of these distributions. We used Laplace distributions and Gaussian distributions in our experiments.

We report on two sets of experiments exploring the potential of PBB. To compare apples to apples, we also replicated the experiments of Blundell et al. [2015], i.e. the BBB method, in both sets of experiments. A set of experiments was run on MNIST with two training objectives (see Section 5), namely, PAC-Bayes-λ and PAC-Bayes-quadratic. We experimented with Gaussian and with Laplace distributions in both cases. In all cases the optimization of training objectives was carried out by stochastic gradient descent (SGD); and ‘prior’ distributions were centered at the randomly initialized weights. This choice of priors was crucial for computing non-vacuous bounds with tight values. Our conclusions from these experiments are (1) that PBB is comparable to Blundell et al. [2015]’s BBB method in terms of test set error (∼0.014), while (2) the minimal value of the upper bound that we achieve (∼0.023) is a significant improvement over Dziugaite and Roy [2017, 2018], i.e. we further close the gap between the risk bound certificate and the test set risk estimate. Another set of experiments was run on some UCI datasets with the same two training objectives as our experiments on MNIST, again showing tightness of the gap between risk certificate and risk estimate.

As the error on unseen examples of the data-dependent predictors found by minimizing a risk upper bound is guaranteed to be no more than the minimal value of the upper bound, PBB is an instance of certified learning, where a learned predictor is reported together with a performance certificate that is valid on unseen examples. Moreover, in view of the tightness of our computed bounds, PBB leads to self-bounding algorithms (Freund [1998], Langford and Blum [2003]) that use all the available data to produce a predictor together with a risk certificate. This is an advantage over methods that evaluate a risk estimate on a test set, which require data-splitting (thus potentially losing expensive samples available for training) and extra computation.

The rest of this paper is organized as follows. In Section 2 we briefly discuss some notions of the supervised learning framework. Then in Section 3 we discuss the PAC-Bayes framework and two PAC-Bayes bounds to be used by our method. Section 4 discusses the BBB method and Section 5 discusses our proposed method, PBB. Section 6 presents our experimental results for both methods. We conclude and discuss future directions in Section 7. The Appendix A displays two KL divergence formulas for convenience.

2 Generalization through risk upper bounds

In the context of supervised learning, an algorithm that trains a neural network receives a finite list of training examples and produces a weight vector \( w \in \mathcal{W} \subset \mathbb{R}^p \) which will be used to predict the label of unseen examples. The ultimate goal is for the algorithm to find a weight that generalizes well, meaning that the decisions arrived at by using the learned \( w \) should give rise to a small loss on unseen examples.\(^1\) Turning this into precise statements requires some formalizations, briefly discussed next. The experienced readers should feel free to skip the next couple of paragraphs which aim to recall these formalizations as well as setting the notation for the rest of the paper.

Let \( Z_{1:n} = (Z_1, \ldots, Z_n) \) denote the size-\( n \) list of training examples, each belonging to a space \( \mathcal{Z} \). The approach of statistical learning theory is to regard the training examples as independent copies of a \( \mathcal{Z} \)-valued random variable, with an unknown underlying probability distribution\(^2\) \( P \in \mathcal{M}_1(\mathcal{Z}) \). The form of the example space in supervised learning is \( \mathcal{Z} = \mathcal{X} \times \mathcal{Y} \) with \( \mathcal{X} \subset \mathbb{R}^d \) and \( \mathcal{Y} \subset \mathbb{R} \), each example being a pair \( Z_i = (X_i, Y_i) \) consisting of an input \( X_i \) and its corresponding label \( Y_i \).

It is understood that each possible weight vector \( w \in \mathcal{W} \) maps to a function \( h_w : \mathcal{X} \to \mathcal{Y} \) that will assign a label \( h_w(X) \in \mathcal{Y} \) to each new input \( X \in \mathcal{X} \). While statistical inference is largely concerned with learning properties of the unknown data-generating distribution, the main focus of

\(^1\) In statistical learning theory there is a precise meaning of when does a method generalize [Shalev-Shwartz and Ben-David, 2014]. We use the word generalization in a slightly broader sense here.

\(^2\) \( \mathcal{M}_1(\mathcal{Z}) \) denotes the set of all probability measures over \( \mathcal{Z} \).
machine learning is on the quality of predictors, measured by a loss function \( \ell \). With these components, regression is defined as the problem when \( Y = \mathbb{R} \) and the loss function is the squared loss \( \ell(w, z) = (y - h_w(x))^2 \), while binary classification is defined with \( Y = \{0,1\} \) (or \( Y = \{-1,+1\} \)) and setting the loss to the zero-one loss: \( \ell(w, z) = I[y \neq h_w(x)] \).

The goal of learning is to find a weight vector that minimizes the expected loss on unseen examples, also called the risk:

\[
L(w) = \mathbb{E}[\ell(w, Z)] = \int_Z \ell(w, z)P(dz). \tag{1}
\]

If the data-generating distribution \( P \) was known, then \( L(w) \) would be the optimization objective and all efforts could focus on finding its minimizer(s). Since \( P \) is unknown, \( L(w) \) is an unobservable objective, in practice one replaces the expectation of the loss with the average loss, giving rise to the problem of finding the minimum of the empirical risk functional:

\[
\hat{L}(w, Z_{1:n}) = \frac{1}{n} \sum_{i=1}^n \ell(w, Z_i). \tag{2}
\]

When the size-\( n \) sample \( Z_{1:n} \) is clear from the context, we will abbreviate \( \hat{L}(w, Z_{1:n}) \) to \( \hat{L}_n(w) \). In practice, the minimization of \( \hat{L} \) is often done with some version of gradient descent. Since the zero-one loss gives rise to a piecewise constant loss function, in classification it is common to replace it with a smooth(er) loss, such as the cross-entropy loss, while changing the range of \( h_w \) to \( [0,1] \).

Under certain conditions, minimizing the empirical risk leads to a weight that is guaranteed to have a small risk. Examples of such conditions are when the set of functions \( \{h_w: w \in \mathbb{R}^p\} \) representable has a small capacity relative to the sample size or the map that produces the weights given the data is stable, or the same map is implicitly constructed by an algorithm such as stochastic gradient descent (see e.g. Bottou [2012] and references). However, oftentimes minimizing the empirical risk can lead to a situation where the risk of the learned weight is larger than desired – a case of overfitting. To prevent overfitting, various methods are commonly used. These include complexity regularization, early stopping, injecting noise in various places into the learning process, etc (e.g. Srivastava et al. [2014], Wan et al. [2013], Caruana et al. [2001], Hinton and van Camp [1993]).

An alternative to these is to minimize a surrogate objective which is guaranteed to give an upper bound on the risk. As long as the upper bound is tight and the optimization gives rise to a small value for the surrogate objective, the user can be sure that the risk will also be small: In this sense, overfitting is automatically prevented, while we also automatically get a self-bounded method in the sense of Freund [1998] (see also Langford and Blum [2003]). In this paper we follow this last approach, where the risk upper bound is arrived at through the so-called PAC-Bayes bounds, which we introduce in the next section.

### 3 Two PAC-Bayes bounds

Probabilistic neural networks are realized as probability distributions over the weight space. While a classical neural network learns a data-dependent weight vector \( \hat{w} \), a probabilistic neural network learns a data-dependent distribution over weights, say \( Q \in M_1(W) \), and makes randomized predictions according to this distribution. To make a prediction on a fresh example \( X \) the randomized predictor draws a weight vector \( W \) at random according to \( Q \) and applies \( h_W \) to \( X \): Each new prediction requires a fresh draw. In this case the performance measures are lifted by averaging with respect to the randomizing distribution. The average empirical loss is \( Q[\hat{L}_n] = \int_W \hat{L}_n(w)Q(dw) \) and the average theoretical loss is \( Q[L] = \int_W L(w)Q(dw) \).

Given two probability distributions \( Q, Q' \in M_1(W) \), the Kullback-Leibler (KL) divergence from \( Q \) and \( Q' \), also known as relative entropy, is defined as follows:

\[
\text{KL}(Q \| Q') = \int_W \log \left( \frac{dQ}{dQ'} \right) dQ.
\]

Here \( dQ/dQ' \) denotes the Radon-Nikodym derivative. Clearly the KL gives a finite value when \( Q \) is absolutely continuous with respect to \( Q' \), otherwise the KL is infinite. For Bernoulli distributions with parameters \( q \) and \( q' \) we will write \( \text{kl}(q \| q') = q \log \left( \frac{q}{q'} \right) + (1-q) \log \left( \frac{1-q}{1-q'} \right) \).
The PAC-Bayes theorem (Seeger [2002], Maurer [2004]) concludes that, with high probability, the binary KL from $Q[\hat{L}_n]$ and $Q[L]$ is upper bounded as follows:

$$\text{kl}(Q[\hat{L}_n]\|Q[L]) \leq \frac{\text{KL}(Q\|Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{n}.$$ 

Inversion of the binary KL divergence based on the inequality $\text{kl}(\hat{p}\|p) \leq (p - \hat{p})^2/(2p)$ valid for $\hat{p} < p$ (see e.g. [Boucheron et al., 2013, Lemma 8.4]) then gives:

$$Q[L] - Q[\hat{L}_n] \leq \sqrt{\frac{2\text{KL}(Q\|Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{n}}.$$ 

On the one hand, using (3) combined with the inequality $\sqrt{ab} \leq \frac{a}{2}(\lambda a + \frac{b}{2})$ valid for all $\lambda > 0$, plus some algebra, leads to the PAC-Bayes-$\lambda$ bound of Thiemann et al. [2017]:

**Theorem 1.** For any $n$, for any $P \in M_1(X)$, for any $Q^0 \in M_1(W)$, for any loss function with range $[0, 1]$, for any $\delta \in (0, 1)$, with probability $\geq 1 - \delta$ over size-$n$ i.i.d. samples, simultaneously for all $Q \in M_1(W)$ and $\lambda \in (0, 2)$ we have

$$Q[L] \leq Q[\hat{L}_n] + \frac{\text{KL}(Q\|Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{n\lambda(1 - \lambda/2)}.$$ 

On the other hand, solving the quadratic inequality (3) for $\sqrt{Q[L]}$ leads to the following bound:

**Theorem 2.** For any $n$, for any $P \in M_1(X)$, for any $Q^0 \in M_1(W)$, for any loss function with range $[0, 1]$, for any $\delta \in (0, 1)$, with probability $\geq 1 - \delta$ over size-$n$ i.i.d. samples, simultaneously for all $Q \in M_1(W)$ we have

$$Q[L] \leq \left(\sqrt{Q[\hat{L}_n] + \frac{\text{KL}(Q\|Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}} + \sqrt{\frac{\text{KL}(Q\|Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}}\right)^2.$$ 

Below in Section 5 we describe how these two bounds are used by our method.

Notice that the conclusion of both theorems is an upper bound on $Q[L]$ that holds simultaneously for all distributions $Q$ over weights, with high probability (over samples). The relevant case, of course, is when $Q$ is a data-dependent distribution, i.e. $Q$ learned from training data. On the other hand, $Q^0$ is supposed to be a fixed ‘non data-dependent’ distribution, external to the training process.

### 4 Bayes by Backprop (BBB)

The ‘Bayes by backprop’ of Blundell et al. [2015] is inspired by a variational Bayes argument, which, in our notation, leads to the objective

$$f(Q) = Q[\hat{L}_n] + \eta \frac{\text{KL}(Q\|Q^0)}{n},$$

where $Q^0$ plays the role of a prior distribution over the weights and $\eta > 0$, a hyperparameter, is introduced in a heuristic manner to make the method more flexible. Note in particular that the variational Bayes argument gives $\eta = 1$. When $\eta$ is treated as a tuning parameter, the method can be interpreted as searching in “KL balls” centered at $Q^0$ of various radii. Thus, the KL term then plays the role of penalizing the complexity of the model space searched. Blundell et al. [2015] propose to optimize this objective (for a fixed $\eta$) using stochastic gradient descent (SGD), which randomizes over both mini-batches (randomly selected subsamples of the training examples, Bottou [2012]) and also over the weights and uses the so-called pathwise gradient estimate (Price [1958], Jankowiak and Obermeyer [2018]). This latter assumes that $Q = Q_\theta$ for $\theta \in \mathbb{R}^k$ with some $k > 0$ is such that sampling from it can be accomplished by a smooth $\theta$-dependent transformation of a random variable sampled from a fixed distribution $P_\theta$ while the density of $Q_\theta$ (with respect to some fixed reference measure) is also available in closed form. They propose to choose $P_\theta$ to be $p$-wise independent distribution and the transformation to act affine linearly component by component and argue that the resulting procedure has a computational cost similar to backpropagation – hence the name of their method. The hyperparameter $\eta > 0$ is chosen using a validation set, which is also often used to select the best performing model among those that were produced during the course of running SGD (as opposed to using the model obtained when the optimization procedure finishes).
5 PAC-Bayes with Backprop (PBB)

The essential idea of our approach will be to train a neural network by minimizing the upper bounds (4) and (5). This will be done by alternating minimization with respect to $\lambda$ and $Q$. By choosing $Q$ appropriately, we use the pathwise gradient estimator as done by Blundell et al. [2015].

Notice that neural networks are trained to minimize the cross-entropy loss, which is unbounded, while the PAC-Bayes bounds (Theorem 1 and Theorem 2) require bounded losses. Hence in the experiments (below) we enforced an upper bound “$L_{\text{max}}$” on the cross-entropy loss by setting a lower bound on the probabilities. Using a surrogate loss, like the cross-entropy loss, is beneficial for making the error surface better behaved (continuous and piecewise differentiable), while it introduces a mismatch between the actual target (i.e. the misclassification loss) and the optimization objective.

We empirically evaluated the training objectives on the two training objectives above lead to (1) test set performance comparable to that of Blundell et al. [2015], while (2) computing non-vacuous bounds with tighter values than those obtained by Dziugaite and Roy [2017, 2018]. We do claim that our contributions are significant.

We will use both the optimization objective from Theorem 1:

$$f_{\text{lamb}}(Q) = \frac{Q[\hat{L}_n]}{1 - \lambda/2} + \frac{\text{KL}(Q||Q^0) + \log\left(2\sqrt{n}/\delta\right)}{n\lambda(1 - \lambda/2)},$$

(7)

and also the optimization objective from Theorem 2:

$$f_{\text{quad}}(Q) = \left(\sqrt{Q[\hat{L}_n]} + \frac{\text{KL}(Q||Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}\right)^2 + \sqrt{\frac{\text{KL}(Q||Q^0) + \log\left(\frac{2\sqrt{n}}{\delta}\right)}{2n}}.$$  

(8)

For the sake of clarification, we are not claiming to be the first to train a probabilistic neural network by minimizing a PAC-Bayes bound. However, as will be demonstrated below, our experiments based on the prior distribution in [0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 4e−2, 3e−2, 2e−2, 1e−2, 5e−3, 1e−3]. The initial value of the variance of the posterior distribution over model parameters was initialized to \(\frac{\lambda}{2}\). The posterior distribution is the same kind as the prior in each case. The results can be seen in Fig. 1. We note 'pbquad' with Laplace prior achieves minimum value of the risk upper bound. However we observed that test error achieved by 'pb_quad' with either prior was similar. The prior distribution to use is problem-dependent but we found both Gaussian and Laplace priors achieve good risk upper bounds across different datasets. In the Fig. 1 we also plot the normalized KL divergence ($\text{KL}(Q||Q^0)/\mu_{\text{lamb}}$). The KL divergence starts at 0.0 increases quickly and then starts decreasing later in the training.

6 Experiments

We empirically evaluated the training objectives $f_{\text{lamb}}$ and $f_{\text{quad}}$ of Eq. (7) and Eq. (8), respectively, on MNIST and on various UCI data sets (Dua and Graff [2017]). We compared our methods $\text{pb}_{\text{lamb}}$ ($f_{\text{lamb}}$) and $\text{pb}_{\text{quad}}$ ($f_{\text{quad}}$) with BBB (Blundell et al. [2015]) and vanilla SGD with momentum optimizer. In all the experiments on various data sets we performed a grid sweep over all the relevant hyper parameters and then selected the run with the best risk upper bound. We experimented with Laplace and Gaussian prior distributions on model weights for both BBB and our methods. Our prior distributions $Q^0$ were centered at the randomly initialized weights. Also the model is initialized with the same random weight. We did a grid sweep over variance parameter of the prior distribution in $[0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 4e^{-2}, 3e^{-2}, 2e^{-2}, 1e^{-2}, 5e^{-3}, 1e^{-3}]$. The initial value of the variance of the posterior distribution over model parameters was initialized to prior distribution variance. We observed that higher variance leads to instability during training and lower variance does not explore the weight space. The lambda value in $f_{\text{lamb}}$ was optimized using alternate minimization using SGD with fixed learning rate of $1e^{-4}$. For BBB and our methods the predictions were obtained using the randomly sampled model weights. For BBB we performed additional sweep over the KL trade-off coefficient in $[1e^{-6}, 1e^{-5}, \ldots, 1e^{-1}]$.

6.1 The choice of the prior distribution

We studied the performance on MNIST with different prior distributions over the model. We used the same experimental setup as described below in Section 6.2. We experimented with Gaussian and Laplace priors. The posterior distribution is the same kind as the prior in each case. The results can be seen in Fig. 1. We note ‘pbquad’ with Laplace prior achieves minimum value of the risk upper bound. However we observed that test error achieved by ‘pb_quad’ with either prior was similar. The prior distribution to use is problem-dependent but we found both Gaussian and Laplace priors achieve good risk upper bounds across different datasets. In the Fig. 1 we also plot the normalized KL divergence ($\text{KL}(Q||Q^0)/\mu_{\text{lamb}}$). The KL divergence starts at 0.0 increases quickly and then starts decreasing later in the training.
As pointed out above, our prior distributions were centered at the random initialization of the weights. The attentive reader may object that, according to the PAC-Bayes theorems, priors are supposed to be non-random. To clarify, the conditions of these theorems require a prior distribution to be non data-dependent. The randomness in the initialization of the weights is non data-dependent, hence it is external to the training process. This justifies that using priors centered at the randomly initialized weights is perfectly valid.

6.2 MNIST

For experiments on MNIST we trained a feed forward neural network with 2 hidden layers, with 600 units and ReLU activations in each hidden layer, followed by an output layer. We trained our models using standard MNIST dataset split of 50000 training examples and 10000 test examples. We ran all experiments for 1 million training iterations. We observe that from the Fig. 2 the methods converge around 100000 iterations. We ran the experiments longer to check if the KL divergence can be minimized further. We used training batch size of 256 for all the experiments. In all the experiments we used SGD with momentum optimizer for training and performed a grid sweep over learning rate in $[1e^{-3}, 5e^{-3}, 1e^{-2}]$ and momentum in $[0.95, 0.99]$. We found that learning rates
higher than $1e-2$ caused divergence in training and learning rates lower than $5e-3$ converged slowly.

On Fig. 2 we report the test error and the risk upper bound as a function on the number of training iterations. Our methods ‘pb_lambda’ and ‘pb_quad’ achieve similar test accuracy at the end of training compared to BBB and SGD with momentum baseline. The $\eta$ parameter in BBB which is of $O(1e-5)$ makes the KL divergence component of the loss insignificant compared to train loss. Thus in case of BBB we see marginal decrease in the KL divergence during the course of training and the solution it returns is expected to be similar to that returned with the SGD with momentum baseline. The best test error achieved by our methods 0.014 is comparable to the risk upper bound of 0.02 at the end of training. This is a significant improvement with respect to previously computed non-vacuous bounds. Also we note that for ‘pb_lambda’ method the $\lambda$ value start at 1 and decreases to 0.5 and starts increasing again after around 150000 iterations to finally reach a value of 0.75.

### 6.3 Comparison to Dziugaite and Roy [2017, 2018]

We are not the first to propose training methods or risk certificates for neural networks based on PAC-Bayes bounds. Langford and Caruana [2001] developed a method to train a stochastic neural network by randomizing the weights with Gaussian noise (adjusted via a sensitivity analysis) and computed an upper bound on the error using a PAC-Bayes bound. They run experiments on a UCI data set and a synthetic data set, and also pointed that the PAC-Bayes approach might be more fruitful for computing non-vacuous bounds. Dziugaite and Roy [2017] derived a training objective from a similar PAC-Bayes bound to train a stochastic neural network with Gaussian randomization, and computed non-vacuous bounds on a ‘Binary MNIST’ dataset. London [2017] approached the generalization of stochastic neural networks by a stability-based PAC-Bayes analysis, and run experiments on CIFAR-10. Other efforts showing further evidence in favour of the PAC-Bayes approach for neural networks are e.g. Neyshabur et al. [2017a,b], and Pitas et al. [2017].

Usually, as we also noticed, the problem is that the KL term tends to dominate and most of the work in training is targeted at reducing it. To address this issue distribution-dependent (Lever et al. [2013]) or data-dependent (Dziugaite and Roy [2018]) priors can be used. The latter derived a novel PAC-Bayes bound under differentially private (or, distributionally stable) priors and proposed a procedure to minimize the terms in the bound in connection to training neural networks. While there is no fully rigorous argument for backing up their finite-time procedure, an asymptotic argument is available. What makes their work especially relevant to us is that they also provide results of experiments on standard multiclass MNIST. The values in the following table were reported by them. We compare our result (PBB) with the best value they achieved on the test error and risk upper bound.

| Method                               | Test Error | Risk upper bound |
|--------------------------------------|------------|-----------------|
| Dziugaite and Roy [2018] ($\tau = 3e + 3$) | 0.12       | 0.21            |
| Dziugaite and Roy [2018] ($\tau = 1e + 5$) | 0.06       | 0.65            |
| Lever et al. [2013] ($\tau = 3e + 3$)   | 0.12       | 0.26            |
| Lever et al. [2013] ($\tau = 1e + 5$)   | 0.06       | 1               |
| PBB                                  | 0.014      | 0.023           |

Table 1: Test set error / Risk upper bound for standard MNIST dataset.

The parameter $\tau$ in their setting controls the temperature of a Gibbs distribution. In the table we display only the two values of their $\tau$ parameter which achieve best test error and risk upper bound. Notice that our method did not use data-dependent priors, while Dziugaite and Roy [2018] used data-dependent priors. The rows ‘Lever et al. [2013]’ display values achieved by minimizing a PAC-Bayes bound that uses a different approach to relate the priors to the data, namely, the priors used by Lever et al. [2013] were distribution-dependent$^3$ (see also Lever et al. [2010]). The method based on the PAC-Bayes bound of Lever et al. [2013] was implemented for neural networks by Dziugaite and Roy [2018] and used as a baseline to contrast the experimental results.

$^3$The relevant part is their treatment of stochastic exponential weights prediction schemes, although they also treated stochastic RKHS methods with Gaussian randomization.
It is interesting to compare our results with the values obtained by other methods in Table 1 above. We note that Dziugaite and Roy [2018]'s best values correspond to test accuracy of 94% or 93% while in those cases their bound values, although non-vacuous, were far from tight. On the other hand the tightest value of their bound only gives an 88% accuracy. By contrast, our method PBB achieves close to 98.6% test accuracy (or 0.014 test error) even without using a data-dependent prior. At the same time, as noted above, our optimal upper bound value (0.023) is much tighter than theirs (0.21).

To compare our results with Dziugaite and Roy [2017]'s results we also run experiments on their 'Binary MNIST' dataset where digits 0 – 4 were mapped to class 0 and digits 5 – 9 were mapped to class 1. We implemented the network architecture which achieved the best test error in their setting.

| Method                        | Test error | Risk upper bound |
|-------------------------------|------------|------------------|
| Dziugaite and Roy [2017]      | 0.013      | 0.201            |
| PBB                           | 0.015      | 0.022            |

Table 2: Test set error / Risk upper bound for 'Binary MNIST' dataset.

From the results in Table 2 we note that we achieve similar test set accuracy, while the minimal value of our risk upper bound is significantly tighter, i.e. our method PBB further tightens the gap between the risk certificate (upper bound) and the risk estimate evaluated on a test set.

6.4 UCI

For experiments on UCI datasets we trained a feed forward neural network with ReLU activations in each hidden layer, with 64 units in the first hidden layer and 32 units in the second hidden layer, followed by an output layer. We performed experiments on 7 different UCI datasets. We ran all experiments for 30000 training iterations. We used training batch size of 256 for all the experiments.

| UCI dataset  | pb_lambda | pb_quad | bbb  | sgd_momentum |
|--------------|-----------|---------|------|--------------|
| MUSHROOM     | 0.0 / 0.0 | 0.0 / 0.0 | 0.0  | 0.0          |
| BREAST       | 0.047 / 0.051 | 0.029 / 0.134 | 0.047 | 0.065        |
| AvsB         | 0.0 / 0.013 | 0.0 / 0.052 | 0.0  | 0.0          |
| IONOSPHERE   | 0.110 / 0.224 | 0.117 / 0.420 | 0.145 | 0.110        |
| SKIN         | 0.001 / 0.001 | 0.001 / 0.001 | 0.002 | 0.002        |

Table 3: Test set error / Risk upper bound for UCI datasets.

In Table 3 we list the test error / risk upper bound for various methods. We note that both ‘pb_lambda’ and ‘pb_quad’ obtain similar test accuracy to that of BBB and SGD with momentum baselines. Also the risk upper bounds are comparable to the test errors. We would like to emphasize that BBB uses cross-validation over $\eta$ in equation (6) to obtain good performance, while ‘pb_lambda’ automatically tunes the coefficient $\lambda$ which controls the weight of the various components in the objective function.

7 Conclusion and Future Work

We explored the ‘PAC-Bayes with Backprop’ (PBB) method to train probabilistic neural networks. The take-home message is that our training method is derived from a sound theoretical foundation, and outputs a model that comes with a performance guarantee at no extra cost, since PBB minimizes a risk upper bound, namely, a PAC-Bayes bound. This is an improvement over methods which are derived heuristically rather than from theoretically justified arguments, and over methods which do not include a risk upper bound. Moreover, experiments showed that PBB gives predictors with competitive test set performance and with significantly improved computed non-vacuous bounds.

We found that the biggest issue when using PBB is the KL term. In particular this is noticeable for larger networks. Besides the obvious choice of smaller networks, some ideas to deal with this issue in future work are e.g. coupling of weights to reduce the number of terms in the KL, using hierarchical priors (mixture over networks of different sizes), or using data-dependent priors. We believe that these combinations may have the chance of achieving state of the art results, while giving tight bounds which may be used as certificates of performance on unseen examples.
References

Hagai Attias. A variational Bayesian framework for graphical models. In Advances in Neural Information Processing Systems, pages 209–215, 2000.

Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight uncertainty in neural networks. In 32nd International Conference on Machine Learning, pages 1613–1622, 2015.

Léon Bottou. Stochastic gradient descent tricks. In Neural networks: Tricks of the trade, pages 421–436. Springer, 2012.

Stéphane Boucheron, Gábor Lugosi, and Pascal Massart. Concentration inequalities: A nonasymptotic theory of independence. Oxford university press, 2013.

Rich Caruana, Steve Lawrence, and C Lee Giles. Overfitting in neural nets: Backpropagation, conjugate gradient, and early stopping. In Advances in Neural Information Processing Systems, pages 402–408, 2001.

Dheeru Dua and Casey Graff. UCI Machine Learning Repository, 2017. URL http://archive.ics.uci.edu/ml.

Gintare Karolina Dziugaite and Daniel M. Roy. Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data. In UAI, 2017.

Gintare Karolina Dziugaite and Daniel M Roy. Data-dependent PAC-Bayes priors via differential privacy. In Advances in Neural Information Processing Systems, pages 8430–8441, 2018.

Yoav Freund. Self bounding learning algorithms. In Proceedings of the eleventh annual conference on Computational Learning Theory, pages 247–258. ACM, 1998.

Robert Hecht-Nielsen. Theory of the backpropagation neural network. In Neural networks for perception, pages 65–93. Elsevier, 1992.

Geoffrey E Hinton and Drew van Camp. Keeping neural networks simple. In International Conference on Artificial Neural Networks, pages 11–18. Springer, 1993.

TS Jaakkola and MI Jordan. Bayesian logistic regression: a variational approach. In Artificial Intelligence and Statistics, 1997.

Martin Jankowiak and Fritz Obermeyer. Pathwise Derivatives Beyond the Reparameterization Trick. arXiv:1806.01851, 2018.

John Langford and Avrim Blum. Microchoice bounds and self bounding learning algorithms. Machine Learning, 51(2):165–179, 2003.

John Langford and Rich Caruana. (Not) bounding the true error. In Advances in Neural Information Processing Systems, pages 809–816, 2001.

Guy Lever, François Laviolette, and John Shawe-Taylor. Distribution-dependent PAC-Bayes priors. In International Conference on Algorithmic Learning Theory, pages 119–133. Springer, 2010.

Guy Lever, François Laviolette, and John Shawe-Taylor. Tighter PAC-Bayes bounds through distribution-dependent priors. Theoretical Computer Science, 473:4–28, 2013.

Ben London. A PAC-Bayesian analysis of randomized learning with application to stochastic gradient descent. In Advances in Neural Information Processing Systems, pages 2931–2940, 2017.

David JC MacKay. A practical Bayesian framework for backpropagation networks. Neural Computation, 4(3):448–472, 1992a.

David JC MacKay. Bayesian interpolation. Neural Computation, 4(3):415–447, 1992b.

Andreas Maurer. A note on the PAC Bayesian theorem. arXiv:cs/0411099, 2004.
A  KL formulas: Laplace versus Gauss

The Laplace density with mean parameter $\mu \in \mathbb{R}$ and variance $b > 0$ is the following:

$$p(x) = (2b)^{-1} \exp\left(-\frac{|x - \mu|}{b}\right).$$

The KL divergence for two Laplace distributions is as follows:

$$KL(Lap(\mu_1, b_1) || Lap(\mu_0, b_0)) = \log\left(\frac{b_0}{b_1}\right) + \frac{\left|\mu_1 - \mu_0\right|}{b_0} + \frac{b_1}{b_0}e^{-\frac{|\mu_1 - \mu_0|}{b_1}} - 1. \quad (9)$$

For comparison, recall that the Gaussian density with mean parameter $\mu \in \mathbb{R}$ and variance $b > 0$ has the following form:

$$p(x) = (2\pi b)^{-1/2} \exp\left(-\frac{(x - \mu)^2}{2b}\right).$$

The KL divergence for two Gaussian distributions is as follows:

$$KL(Gauss(\mu_1, \sigma_1^2) || Gauss(\mu_0, \sigma_0^2)) = \frac{1}{2} \left( \log\left(\frac{b_0}{b_1}\right) + \frac{(\mu_1 - \mu_0)^2}{b_0} + \frac{b_1 - 1}{b_0} \right). \quad (10)$$