Sampling-Free Variational Inference of Bayesian Neural Nets

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Abstract

We propose a new Bayesian Neural Net (BNN) formulation that affords variational inference for which the evidence lower bound (ELBO) is analytically tractable subject to a tight approximation. We achieve this tractability by decomposing ReLU nonlinearities into an identity function and a Kronecker delta function. We demonstrate formally that assigning the outputs of these functions to separate latent variables allows representing the neural network likelihood as the composition of a chain of linear operations. Performing variational inference on this construction enables closed-form computation of the evidence lower bound. It can thus be maximized without requiring Monte Carlo sampling to approximate the problematic expected log-likelihood term. The resultant formulation boils down to stochastic gradient descent, where the gradients are not distorted by any factor besides minibatch selection. This amends a long-standing disadvantage of BNNs relative to deterministic nets. Experiments on four benchmark data sets show that the cleaner gradients provided by our construction yield a steeper learning curve, achieving higher prediction accuracies for a fixed epoch budget.

1 Introduction

The advent of data-flow libraries has made fast prototyping of novel neural net architectures possible by writing short and simple high-level code. Availability of these tools triggered an explosion of research output on application-specific neural net design, which in turn allowed a period of fast improvement of prediction performance in almost all fields of application where machine learning is used. At present, we can at least speculate about whether the era of large accuracy leaps is over. The next grand challenge is to solve mainstream machine learning problems with more time-efficient, energy-efficient, and interpretable models that make predictions with an attached uncertainty estimate. For industry-scale applications, we require models less vulnerable to adversarial attacks [7, 43].

The Bayesian modeling approach provides principled solutions to all of the aforementioned next-stage challenges of machine learning. Bayesian Neural Networks (BNNs) [27] lie at the intersection of deep learning and the Bayesian approach that learns the parameters of a machine learning model via posterior inference [28, 51]. A neural net having an arbitrary architecture and loss function can be turned into a BNN simply by corrupting its synaptic connection weights with noise, thereby upgrading from deterministic parameters to latent random variables that follow a prior distribution.

Unfortunately, the non-linear activation functions at the neuron outputs render direct methods to estimate the posterior distribution of BNN weights analytically intractable. A recently established technique for approximating this posterior is Stochastic Gradient Variational Bayes (SGVB) [17], which suggests reparameterizing the variational distribution and then Monte Carlo (MC) integrating the intractable expected data fit part of the ELBO. Sample white noise for a cascade of random

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Preprint. Work in progress.
variables distorts the gradient signal, leading to unstable training. Improving the sampling procedure to reduce the variance of the gradient estimate is an active research topic. Recent advances in this vein include the local reparameterization trick [16] and variance reparameterization [30, 33].

We here present a novel BNN construction that makes variational inference possible with a closed-form ELBO, obviating the need for Monte Carlo sampling and the associated precautions required for variance reduction. Without a substantial loss of generality, we restrict the activation functions of all neurons of a net to the Rectified Linear Unit (ReLU), which is shown to be sufficient to improve the state of the art in numerous cases [9, 40]. We build our formulation on the fact that the ReLU function can be expressed as the product of the identity function and Kronecker delta: \( \max(0, u) = u \times \delta_{u>0} \). Exploiting the fact that we are up to devising a probabilistic learner, we assign a separate latent variable \( z \) to the Kronecker delta. We relax the Kronecker delta factor by \( z \sim \delta_{f>0} \approx \text{Bern}(\sigma(Cf)) \) for some large \( C \), where \( \text{Bern}(\cdot) \) is a Bernoulli mass function and \( \sigma(u) = 1/(1 + \exp(-u)) \) is the standard sigmoid. The idea is illustrated in Figure 1. We show how the asymptotic account of this relaxation converts the likelihood calculation into a chain of linear matrix operations, giving way to closed-form computation of the data fit term of the Evidence Lower Bound (ELBO) in mean-field variational BNN inference. In our construction, the data fit term lends itself as the sum of a standard neural net loss (e.g. Mean-Squared Error (MSE) or cross entropy) on the expected prediction output and the prediction variance. We discover the plausible property of our construction that the predictor variance term has a recursive form, describing how the predictor variance back-propagates through the layers of a BNN. We refer to our model as Variance Back-Propagation (VBP).

Unlike the present gold standard in BNNs, the closed-form ELBO of our model does not require any Monte Carlo integration step. Keeping the ELBO gradients free from multiplicative [16] or additive [30] white noise distortion, VBP boosts learning. Experiments on four benchmark data sets and two different network architectures show that VBP accelerates learning within widely-adopted training budgets. Last but not least, VBP presents a generic formulation that is directly applicable to all weight prior selections as long as their Kullback-Leibler (KL) divergence with respect to the variational distribution is available in closed form, including the common log-uniform [16, 30], normal [5, 41], and horseshoe [24] densities.

2 Bayesian Neural Nets with Decomposed Feature Maps

We assume to have a continuous-output feed-forward neural net that uses the ReLU activation function. Decomposing the ReLU function as \( \max(0, u) = u \times \delta_{u>0} \), here \( \delta \) being the Kronecker delta function, the feature map vector \( h_{l+1} \) of data point at layer \( l + 1 \) expressed as

\[
f_l = W_l^T h_l, \quad z_l = \delta_{W_l^T h_l>0}, \quad h_{l+1} = f_l \circ z_l,
\]

where \( h_l \) is the feature map vector of the same data point at layer \( l \), the matrix \( W_l \) contains the synaptic connection weights between the neurons of layers \( l \) and \( l + 1 \) and \( \circ \) denotes the element-wise

Figure 1: **Left:** We decompose the ReLU function into an identity function and a Kronecker delta function. Then, we approximate the step function output with a Bernoulli distribution, the parameter of which is first amplified by a factor \( C \) and passed through a sigmoid \( \sigma(\cdot) \). **Right:** We build a Bayesian Neural Net, exemplified here with two hidden layers, the feature maps of which are decomposed into random variables following an amplified Bernoulli (\( z_1 \) and \( z_2 \)) and the linear activation. This decomposition makes the likelihood on \( y \) depend on the weights \( W_1 \) and \( W_2 \) and the binary outputs \( z_1 \) and \( z_2 \) through only a chain of linear operations, allowing an analytically tractable approximation for the evidence lower bound, unlike all previous studies.
We assign an individual factor to each feature map output. We follow prior art \cite{16, 30} and adopt the mean-field assumption that the variational distribution factors across individual weights. We also assume each factor to follow $q(w^l_{ij}) = \mathcal{N}(w^l_{ij} \mid \mu^l_{ij}, (\sigma^l_{ij})^2)$. We assign an individual factor to each feature map output $z^l_j$ of each data point. Rather than handcrafting the functional form of this factor, we calculate its ideal form having other factors fixed, as detailed in Section 2.3.4. The final variational distribution is
\[
q(\theta | \phi) = \prod_{l=1}^{L} \prod_{i=1}^{J_l} \prod_{j=1}^{J_l} q(z^l_j) q(w^l_{ij}),
\]
where \( L \) is the number of hidden layers and \( J_l \) denotes the number of neurons at layer \( l \).

Our contribution concerns calculation of \( \mathcal{L}_{data} \) in closed form, which has thus far been approximated by MC integration in the previous work. For a BNN with identity-step decomposed feature maps and linear activations denoted as \( f^{l}_{r}(x, \theta) \) for output channel \( r \) of layer \( l \), the data fit term reads

\[
\mathcal{L}_{data} = -\frac{\beta}{2} \sum_{r=1}^{R} \mathbb{E}_{q(\theta|a)} \left[ (y_r - f^{L}_{r}(x, \theta))^2 \right] - \mathbb{E}_{q(\theta|a)} \left[ \text{KL}(q(Z)||p(Z|\theta, H)) \right]
\]

\[
= -\frac{\beta}{2} \sum_{r=1}^{R} \left\{ y_r^2 - 2y_r \mathbb{E}_{q(\theta|a)}[f^{L}_{r}(x, \theta)] + \mathbb{E}_{q(\theta|a)}[f^{L}_{r}(x, \theta)^2] \right\} - \mathbb{E}_{q(\theta|a)} \left[ \text{KL}(q(Z)||p(Z|\theta, H)) \right]
\]

\[
= -\frac{\beta}{2} \sum_{r=1}^{R} (y_r - \mathbb{E}_{q(\theta|a)}[f^{L}_{r}(x, \theta)])^2 + \text{Var}[f^{L}_{r}(x, \theta)] - \mathbb{E}_{q(\theta|a)} \left[ \text{KL}(q(Z)||p(Z|\theta, H)) \right],
\]

where \( y_r \) is the observation at the \( r \)th output channel. In its eventual form, the first term is the MSE evaluated at the mean of the predictor \( f(\cdot) \) and the second term is its variance. This largely overlooked form of the data fit has some interesting implications. Firstly, \( \text{Var}[f^{L}_{r}(x, \theta)] \) infers the total amount of model variance to account for the epistemic uncertainty in the learning task [15]. Secondly, shrinking \( \text{Var}[f^{L}_{r}(x, \theta)] \) would also shrink \( \mathcal{L}_{comp} \) to a certain extent, as the posterior will converge from all possible \( q(\theta|\phi) \)'s to a deterministic net. Thirdly, shrinking \( \mathcal{L}_{comp} \) does not necessarily shrink \( \text{Var}[f^{L}_{r}(x, \theta)] \). As \( \mathcal{L}_{comp} \) approaches zero, we end up with Gaussian Dropout [42].

As our ultimate goal is to obtain the ELBO in closed form, any prior on weights that lends itself to a closed form \( \mathcal{L}_{comp} \) is acceptable. We have a list of attractive and well-settled possibilities to choose from, including: i) the normal prior [1, 5] for mere model selection, ii) the log-uniform prior [16, 30] for atomic sparsity induction and aggressive synaptic connection pruning, and iii) the horseshoe prior [24] for group sparsity induction and neuron-level pruning.

### 2.3 Closed-form calculation of the data fit term

When all feature maps of the predictor are identity-delta decomposed and \( z_j^{l} \)'s are approximated by a Bernoulli-sigmoid mass as described in Section 2.1, the expectation of \( f(x_n, \theta) \) with respect to \( q(\theta|\phi) \) can be calculated in closed form, as \( f(x_n, \theta) \) consists only of linear operations with which the expectation can commute operation orders. This order interchangeability results in a mere forward pass where each weight takes its mean value with respect to its related factor in the approximate distribution \( q(\theta|\phi) \). For instance, for a Bayesian neural net with two hidden layers, we have

\[
\mathbb{E}_{q(\theta|\phi)}[f^{L}_{r}(x, \theta)] = \mathbb{E}_{q(\theta|\phi)}[w_3^{T}(z_2 \circ W_2^{T}(z_1 \circ W_1^{T}x))] = \mathbb{E}[w_3^{T}](\mathbb{E}[z_2] \circ \mathbb{E}[W_2]^{T} \mathbb{E}[z_1] \circ \mathbb{E}[W_1]^{T}x). \tag{1}
\]

Consequently, the MSE part of \( \mathcal{L}_{data} \) can be calculated in closed form. This interchangeability property of linear operations against expectations holds as long as we keep independence between the layers, hence the MSE can be calculated in closed form also in the non-mean-field case.

#### 2.3.1 Updating the feature map activations

While we update the variational parameters of the synaptic connection weight factors towards the gradient of the ELBO, for the feature map activation distribution \( q(z_j^l) \), we choose to perform the update at the function level. Benefiting from variational calculus, we fix all other factors in \( q(\theta|\phi) \) except for a single \( q(z_j^l) \) and find the optimal functional form for this remaining factor. We first devise in Proposition 1 a generic approach for calculating variational update rules of this sort. The proofs of all propositions can be found in the Supplementary Material.

**Proposition 1.** Consider a Bayesian model including the generative process excerpt below

\[
\cdots, \quad a \sim p(a), \quad z|a \sim \delta_{a>0}, \quad b|z, a \sim p(b|g(z, a)), \quad \cdots
\]
for some arbitrary function \( q(z, a) \). If the variational inference of this model is to be performed with an approximate distribution \( \mathcal{Q} = \cdots q(a)q(z) \cdots \), the optimal closed-form update for \( z \) is

\[
q(z) \leftarrow \delta_{E[q(a)|a]>0}.
\]

Following Proposition 1, the variational update of \( z_j^l \) turns out to be \( q(z_j^l) \leftarrow \delta_{E[w_j^l|x|\theta_t]E[h_{j-1}^l]>0} \). Note that the expectation of a delta function is the binary outcome of the condition it tests. Because \( q(z_j^l) = \mathbb{E}[z_j^l] \) is an intermediate step while computing \( \mathbb{E}[q(\theta^t)|f_j^l(x, \theta^t)] \), the \( q(z_j^l) \) updates can be done concurrently with this computation. A side benefit of the resultant \( q(z_j^l) \) and the general structure of \( \mathcal{L}_{\text{data}} \) is that the complicated \( \mathbb{E}[q(\theta^t)|\mathbb{KL}(q(Z)||p(Z, H))] \) term can be calculated analytically subject to a controllable degree of relaxation.

**Proposition 2.** For the model and the inference scheme in Proposition 1 with \( q(a) = \mathcal{N}(a|\mu, \sigma^2) \), in the relaxed delta function formulation \( \delta_{a>0} \approx \text{Bern}(a|\sigma(Ca)) \) with some finite \( C > 0 \), the expression \( \mathbb{E}[q(\theta^t)|\mathbb{KL}(q(z)||p(z|a))] \) is (i) analytically tractable and (ii) its magnitude is proportional to the mass of \( q(a) \) that falls on the opposite side of the \( a = 0 \) line with respect to \( \mathbb{E}[q(a)|a] \).

Note that the approximation \( \delta_{a>0} \approx \text{Bern}(a|\sigma(Ca)) \) is extremely tight even for decently small \( C \) values. Hence, we can rescue the expected KL term from diverging to infinity by setting \( C \) to a value such as 10, without making a tangible change on the behavior of the activation function. Although this approximation would provide an analytical solution due to part (i) of Proposition 2, for practical purposes, we benefit from part (ii) and remove this term from the ELBO. The magnitude of this term depends on how tightly the mass of \( q(a) \) is concentrated around the expectation \( \mathbb{E}[q(a)|a] \). This soft constraint on the variance is already enforced by the \( \text{Var}(f(x, \theta^t)) \) term in \( \mathcal{L}_{\text{data}} \).

### 2.3.2 Handling the variance term with back-propagation

The final step in the closed-form calculation of the ELBO is the \( \text{Var}[f_L(x, \theta)] \) term. Let us recall that the likelihood function of our BNN involves a linear chain of operations that contain only sums and products of the random variables. Two identities concerning the relationship between the variances of two multiplied and added independent random variables \( a \) and \( b \) are

\[
\text{Var}(a + b) = \text{Var}(a) + \text{Var}(b),
\]

\[
\text{Var}(a \cdot b) = \text{Var}(a)\text{Var}(b) + \mathbb{E}[a]^2\text{Var}(b) + \text{Var}(a)\mathbb{E}[b]^2,
\]

\[
= \left\{\begin{array}{ll}
\text{Var}(a) + \mathbb{E}[a]^2 & \text{if } (a) = 0 \\
\text{Var}(b) + \text{Var}(a)\mathbb{E}[b]^2 & \text{otherwise}
\end{array}\right.
\]

Applying these well-known identities to the linear activation output of Layer \( l \), we attain

\[
\text{Var}_{q(\theta|\phi)}[f_j^l(x, \theta)] = \text{Var}_{q(\theta|\phi)} \left[ \sum_{i=1}^{L} w_{ij}^l z_i^l f_{i-1}^l(x, \theta) \right] = \sum_{i=1}^{L} \text{Var}_{q(\theta|\phi)}[w_{ij}^l] z_i^l E_{q(\phi)}[f_{i-1}^l(x_n, \theta)]
\]

\[
= \sum_{i=1}^{L} \mathbb{E}[z_{ni}] \mathbb{E}[w_{ij}^l] \text{Var}_{q(\theta|\phi)}[f_{i-1}^l(x_n, \theta)] + \mathbb{E}[w_{ij}^l] \text{Var}_{q(\theta|\phi)}[f_{i-1}^l(x, \theta)],
\]

\[
= \sum_{i=1}^{L} \delta_{E[w_j^l|x|\theta_t]E[h_{j-1}^l]>0} \left( \mu_{ij}^l)^2 + \sigma_{ij}^l)^2 \right) \text{Var}_{q(\theta|\phi)}[f_{i-1}^l(x_n, \theta)] + \left( \mu_{ij}^l)^2 + \sigma_{ij}^l)^2 \text{Var}_{q(\theta|\phi)}[f_{i-1}^l(x, \theta)],
\]

This formula contains two functions that are yet to be evaluated. One is \( \mathbb{E}[q(\theta|\phi)|f_{i-1}^l(x_n, \theta)] \), the calculation of which is discussed in Equation 2. The other term \( \text{Var}_{q(\theta|\phi)}[f_{i-1}^l(x, \theta)] \) is the variance of one of the linear activation outputs of the previous layer. Hence, we arrive at a recursive description of the model variance. Following this formula, we can express \( \text{Var}[f_L(x, \theta)] \) as a function of \( \text{Var}[f_{L-1}(x_n, \theta)] \), then \( \text{Var}[f_{L-1}(x_n, \theta)] \) as a function of \( \text{Var}[f_{L-2}(x_n, \theta)] \), and repeat this procedure until the observed input layer, where variance is zero. For noisy inputs, the desired homoskedastic or hetero-skedastic noise model can be injected to the input layer, which would still not break the recursion and keep the formula valid. As this formula reveals how variance back-propagates through the layers, we refer to our construction as *Variance Back-Propagation* (VBP).

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Note that \( q(b) \) might or might not exist depending on whether \( b \) is latent or observed.
2.3.3 Handling convolution and pooling

As a linear operation, convolution is directly applicable to the VBP formulation by modifying all the sums between weights and feature maps with sliding windows. Doing the same will suffice also for the calculation of $\text{Var}[f_L(x_n, \theta)]$. In VBP, one layer affects the next via only sums and products of variables, which is not the case for max-pooling. Even though convolutions are found to be sufficient for building state-of-the-art architectures [40], we show in the Supplementary Material with Proposition 3 that max-pooling is also directly applicable to VBP by extending Proposition 1.

2.4 Handling classification

For binary classification, we treat $y$ as a vector of latent decision margins and squash it with a binary-output likelihood $p(t|y)$. From [10], the log-marginal likelihood of the resultant model is

$$\log p(t|x) = \log \int p(t|y)p(y|x)dy \geq \log \int p(t|y)\exp(L_{reg})dy = L_{clsf},$$

where $L_{clsf}$ is the new ELBO for classification. Choosing $p(t|x) = \prod_{r=1}^{R} \Phi(y_r)^{t_r}(1 - \Phi(y_r))^{1-t_r}$, where $\Phi(\cdot)$ is the Probit function, we get

$$L_{clsf} = \log \int \left[ \prod_{r=1}^{R} (\Phi(y_r)^{t_r}(1 - \Phi(y_r))^{1-t_r}) e^{-\frac{1}{2}((y_r - \mathbb{E}[f_L^c(x_n, \theta)]^2 + \text{Var}[f_L^c(x_n, \theta)] - L_{\text{comp}})dy_r} \right]$$

$$= \sum_{r=1}^{R} \left[ t_r \Phi \left( \frac{\mathbb{E}[f_L^c(x_n, \theta)]}{\sqrt{\beta^{-1}+1}} \right) + (1 - t_r) \left( 1 - \Phi \left( \frac{\mathbb{E}[f_L^c(x_n, \theta)]}{\sqrt{\beta^{-1}+1}} \right) \right) \right] + \text{Var}[f_L^c(x_n, \theta)] - L_{\text{comp}}.$$ 

Approximating $\Phi(\cdot)$ by a sigmoid function and setting $\beta^{-1} \to 0$, the new ELBO boils down to three terms: i) negative binary cross-entropy loss evaluated at the mean of the predictor, ii) the variance of the predictor, and iii) the regularization term. Note that both in regression and classification cases, the first term is a standard loss evaluated at the mean of the predictor and the remaining two terms are identical. Extension to multiple classes follows similar lines, which we skip due to space constraints.

3 Related Work

Several approaches have been introduced for approximating the intractable posterior of BNNs. One line is model-based Markov Chain Monte Carlo (MCMC), such as Hybrid (Hamiltonian) Monte Carlo [32] and Stochastic Gradient Langevin Dynamics [44]. Later work has adapted HMC to stochastic gradients [3] by quantifying the entropy overhead stemming from the stochasticity of minibatch selection. This study has made HMC applicable to large data sets and modern neural network architectures [39]. Follow-up studies on merging the strengths of HMC and SGLD [6] also exist.

While being actively used for a wide spectrum of models, successful application of variational inference to deep neural nets has taken place only recently. The earliest study to infer a Bayesian neural net with variational inference [12] was applicable for only one hidden layer. This limitation has been overcome only recently [8] by approximating intractable expectations by numerical integration. Further scalability has been achieved after SGVB [17] (a.k.a. Stochastic Back-Prop [18]) is made applicable to BNN inference using weight reparameterization [1].

Dropout has strong connections to variational inference of BNNs [42]. Gal et al. [5] developed a theoretical link between a dropout network and a deep Gaussian process [4] inferred by variational inference. It has later been shown that extending the Bayesian model selection interpretation of Gaussian Dropout [16] with a log-uniform prior on model weights leads to a BNN inferred by SGVB.

A fundamental step in reduction of ELBO gradient variance has been taken by Kingma et al. [16] with local reparameterization, which suggests taking the Monte Carlo integrals by sampling the linear activations rather than the weights. Further variance reduction has been achieved by defining the variances of the variational distribution factors as free parameters and the dropout rate as a function of them [30]. Theoretical treatments of the same problem have also been recently studied [29] [38].

SGVB has been introduced initially for fully factorized variational distributions, which provides limited support for feasible posteriors that can be inferred. Strategies for improving the approximation
Table 1: MNIST classification comparison with Bayes by Backprop (BBB) [1]. The experiment setup and the BBB results are taken from [1]. The networks consist of two hidden fully-connected layers with (400/800/1200) units each. Our results are averaged over five runs.

| MODEL                              | (Test Error in %) | 400   | 800   | 1200  |
|------------------------------------|-------------------|-------|-------|-------|
| BBB, Normal prior                  | 1.82              | 1.99  | 2.04  |
| BBB, Mixture prior                 | 1.36              | 1.34  | 1.32  |
| VBP, Normal prior                  | 1.60 ± 0.10       | 1.47 ± 0.03 | 1.40 ± 0.01 |

The quality of variational BNN inference include employment of structured versions of dropout matrix normals [25], repetitive invertible transformations of latent variables (Normalizing Flows) [37] and their application to variational dropout [26]. Lastly, there is active research on enriching variational inference using its interpolative connection to expectation propagation [11, 23, 22].

4 Experiments

We evaluate the proposed model on a variety of datasets and settings. Unless otherwise indicated we rely on our own implementation of each method to ensure comparability and fairness. The source code to replicate the experiments is available online. Details on the hyperparameters can be found in the Supplementary Material.

Classification with fully connected networks. As a first baseline we compare against Bayes by Backprop (BBB) [1], which considers classification on MNIST [21] with densely connected nets having two hidden layers of 400, 800, or 1200 units. The prior placed over the weights is either a normal prior or a scale mixture prior of two normal distributions whose combination allows for placing most of the mass around zero, while still allowing for heavy tails. We only report results for VBP with a normal prior to avoid an expensive grid search over the hyperparameters [1] mention, as it performs better than BBB+Normal coming close to its mixture prior performance (see Table 1).

Classification with convolutional layers. Our main experiment is an evaluation on four datasets, MNIST [21], SVHN [35], Cifar-10, and Cifar-100 [20]. A commonly reported problem of BNNs is their inability to cope with increasing network depth, requiring a lot of tricks such as initialization from a pretrained deterministic net or an annealing of the KL term in the ELBO. In order to focus our analysis on the steepness of the learning curves, we avoid such tricks and stick to a small LeNet-sized architecture consisting of two convolutional and two fully connected layers, where the two Cifar datasets get more filters per layer. As mentioned in Section 2.3.3 VBP can handle max-pooling layers, but they require a careful tracking of indices between the data fit and variance terms, which comes at some extra runtime cost in present deep learning libraries. Instead, we provide a reference implementation on how to do this, but stick in the experiments with strided convolutions following the recent trend of “all-convolutional-nets” [36, 40, 45].

We compare VBP with Variational Dropout (VarOut) as introduced by [16] in the improved version of [30]. Their approach places a log-uniform prior and a factorized normal distribution as the variational posterior over the weights. The KL between these two is evaluated via a tight approximation. We use the same setup and approximation to the KL for VBP. The models are trained with Adam [19] with the default hyperparameters and a learning rate which is linearly reduced to zero from $10^{-4}$ over 100 epochs. The learning curves are shown in Figure 2 the final performance on each dataset is summarized in Table 2. Avoiding the sampling step leads to a clear improvement in all four datasets. VBP achieves a lower error rate than VarOut consistently in all four data sets.

Sparsification. The log-uniform prior is motivated for its sparsification properties. [30] prune all weights with $\log \alpha > 3$, where $\alpha = \sigma^2 / \mu^2$, for $q(w) = \mathcal{N}(w | \mu, \sigma^2)$. This roughly translates to dropping all weights with a binary dropout rate of larger than 0.95. For VBP, this strict pruning rule tends to be suboptimal. Instead we follow [24] and place the threshold based on a visual evaluation

[https://github.com/manuelhaussmann/vbp](https://github.com/manuelhaussmann/vbp)

[13] recently showed that the improper log-uniform prior will usually lead to an improper posterior. This can be avoided [34] by using a Student-t distribution with a tiny d.o.f. parameter (approximating log-uniform).
Table 2: Classification error (in %) averaged over five runs. (orig) refers to unpruned performance, (fixed) to pruning with a fixed threshold of 3 as in [30], (var) prunes with a the flexible threshold based on visual inspection as suggested by [24]. The numbers in the parentheses denote |W|.

|                  | MNIST             | SVHN              | Cifar-10          | Cifar-100         |
|------------------|-------------------|-------------------|-------------------|-------------------|
| VarOut (orig)    | 1.46 ± 0.06 (1)   | 13.21 ± 0.21 (1)  | 41.30 ± 0.70 (1)  | 72.37 ± 0.19 (1)  |
| VBP (orig)       | 1.02 ± 0.04 (1)   | 11.23 ± 0.27 (1)  | 31.90 ± 0.56 (1)  | 66.36 ± 0.71 (1)  |
| VarOut (fixed)   | 1.69 ± 0.08 (50.5)| 13.74 ± 0.22 (23.7) | 41.93 ± 0.53 (230.2) | 72.68 ± 0.25 (160.1) |
| VarOut (var)     | 1.58 ± 0.09 (16.3)| 13.66 ± 0.26 (6.9) | 41.45 ± 0.61 (68.6) | 72.43 ± 0.27 (40.0) |
| VBP (fixed)      | 1.90 ± 0.15 (49.7)| 14.85 ± 1.02 (15.3) | 38.74 ± 1.38 (85.7) | 72.88 ± 0.65 (58.5) |
| VBP (var)        | 1.33 ± 0.1 (13.67)| 11.94 ± 0.10 (2.77) | 32.27 ± 0.67 (24.3) | 67.24 ± 0.45 (24.0) |

Figure 2: Learning curves (test set error over time). Each plot shows five runs per method in thin lines, and their average in bold ones. The datasets are MNIST, SVHN, C10, C100 (from left to right).

of the histogram of the log α which allows us to rank the weights and trade sparsity for accuracy. See Table 2 for the results, where a fixed pruning (fixed) strategy tends to a larger sparsity over the variable (var) one, but also a greater cost in accuracy. See the Supplementary Material for details.

Influence of Sampling. As a final experiment, we allowed the VarOut variation to estimate $L_{data}$ with multiple samples instead of one. However, similar to the results reported in the context of VAEs [2] it could only marginally improve its performance with an increase in the number of samples (up to 30), while drastically increasing the computational requirements. We conjecture that one would require a similar importance weighing scheme as [2] introduce to solve this. See Table 3 for results.

Table 3: Influence of taking multiple samples with VarOut to estimate the gradient. The results are on SVHN and averaged over 3 runs. VBP reaches 11.23 ± 0.27, outperforming even VarOut that takes as many as 30 MC samples.

| Nr. of samples | 1       | 5       | 10      | 20      | 30      |
|----------------|--------|--------|--------|--------|--------|
| Test error (in %) | 13.21 ± 0.24 | 12.86 ± 0.16 | 12.87 ± 0.18 | 12.69 ± 0.38 | 12.64 ± 0.19 |

5 Discussion

Our experiments demonstrate that VBP follows a steeper learning curve than its sampling-based counterpart. The consistency in performance improvement illustrates the price SGVB has to pay for keeping the model probabilistic. As Table 2 shows, cleaning the gradients from sampling noise improves not only the prediction performance but also the model selection effectiveness. VBP is able to discover a less sparse but more effective architecture than VarOut, although it still prunes the far majority of the synaptic connections in three data sets, more than half on the fourth.

Following the No-Free-Lunch theorem, our closed-form available ELBO comes at the expense of a number of restrictions, such as a fully factorized approximate posterior, sticking to ReLU activations, and inapplicability of Batch Normalization [14]. An immediate implication of this work is to explore ways to relax the mean-field assumption and incorporate normalizing flows without sacrificing from the closed-form solution. Because Equations 3 and 4 extend easily to dependent variables after adding the covariance of each variable pair, our formulation is applicable to structured variational inference schemes without major theoretical obstacles. We speculate that the same should be true for normalizing flows after designing transformation functions carefully.
References

[1] C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wiestra. Weight uncertainty in neural networks. In ICML, 2015.
[2] Y. Burda, R. Grosse, and R. Salakhutdinov. Importance weighted autoencoders. In ICLR, 2016.
[3] T. Chen, E.B. Fox, and C. Guestrin. Stochastic gradient Hamiltonian monte carlo. In ICML, 2017.
[4] A. Damianou and N.D. Lawrence. Deep Gaussian processes. In AISTATS, 2013.
[5] Y. Gal and Z. Ghahramani. Dropout as a Bayesian approximation: Representing model uncertainty in deep learning. In ICML, 2016.
[6] M. Girolami and B. Calderhead. Riemann manifold Langevin and Hamiltonian monte carlo methods. Handbook of Markov Chain Monte Carlo, 73(2):123–214, 2011.
[7] I.J. Goodfellow, J. Shlens, and C. Szegedy. Explaining and harnessing adversarial examples. In ICLR, 2015.
[8] A. Graves. Practical variational inference for neural networks. In NIPS, 2011.
[9] K. He, G. Gkioxari, P. Dollár, and R. Girshick. Mask r-cnn. In ICCV, 2017.
[10] J. Hensman, N. Fusi, and N.D. Lawrence. Gaussian processes for big data. In UAI, 2013.
[11] J.M. Hernandez-Lobato, Y. Li, M. Rowland, D. Hernandez-Lobato, T. Bui, and R. Turner. Black-box α-divergence minimization. In ICML, 2016.
[12] G.E. Hinton and D. van Camp. Keeping neural networks simple by minimizing the description length of the weights. In COLT, 1993.
[13] J. Hron, A.G. Matthews, and Z. Ghahramani. Variational Gaussian dropout is not Bayesian. arXiv preprint arXiv:1711.02989, 2017.
[14] S. Ioffe and C. Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In ICML, 2015.
[15] A. Kendall and Y. Gal. What uncertainties do we need in Bayesian deep learning for computer vision? In NIPS, 2017.
[16] D. Kingma, T. Salimans, and M. Welling. Variational dropout and the local reparameterization trick. In NIPS, 2015.
[17] D. Kingma and M. Welling. Auto-encoding variational Bayes. In ICLR, 2014.
[18] D. Kingma and M. Welling. Stochastic backpropagation and approximate inference in deep generative models. In ICML, 2014.
[19] D.P. Kingma and J. Ba. Adam: A method for stochastic optimization. In ICLR, 2015.
[20] A. Krizhevsky and G. Hinton. Learning multiple layers of features from tiny images. 2009.
[21] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86(11):2278–2324, 1998.
[22] Y. Li and Y. Gal. Dropout inference in Bayesian neural networks with alpha-divergences. In ICML, 2017.
[23] Y. Li and R.T. Turner. Rényi divergence variational inference. In NIPS, 2016.
[24] C. Louizos, K. Ullrich, and M. Welling. Bayesian compression for deep learning. In NIPS, 2017.
[25] C. Louizos and M. Welling. Structured and efficient variational deep learning with matrix Gaussian posteriors. In ICML, 2016.
[26] C. Louizos and M. Welling. Multiplicative normalizing flows for variational Bayesian neural networks. In ICML, 2017.
[27] D.J. MacKay. A practical Bayesian framework for backpropagation networks. Neural Computation, 4:448–472, 1992.
[28] D.J. MacKay. Probable networks and plausible predictions – a review of practical Bayesian methods for supervised neural networks. Network: Computation in Neural Systems, 6(3):469–505, 1995.
[29] A. Miller, N. Foti, A. D’Amour, and R.P. Adams. Reducing reparameterization gradient variance. In NIPS, 2017.

[30] D. Molchanov, A. Ashukha, and D. Vetrov. Variational dropout sparsifies deep neural networks. In ICML, 2017.

[31] R. Neal. Bayesian learning for neural networks. PhD Thesis, 1995.

[32] R. Neal. MCMC using Hamiltonian dynamics. Handbook of Markov Chain Monte Carlo, 54:113–162, 2010.

[33] K. Neklyudov, D. Molchanov, A. Ashuka, and D. Vetrov. Structured Bayesian pruning via log-normal multiplicative noise. In NIPS, 2017.

[34] K. Neklyudov, D. Molchanov, A. Ashuka, and D. Vetrov. Variance networks: When expectation does not meet your expectations. arXiv preprint [arXiv:1803.03764] 2018.

[35] Y. Netzer, T. Wang, A. Coates, A. Bissacco, B. Wu, and A.Y. Ng. Reading digits in natural images with unsupervised feature learning. In NIPS Workshop on Deep Learning and Unsupervised Feature Learning, 2011.

[36] J. Redmon and A. Farhadi. Yolov3: An incremental improvement. arXiv preprint [arXiv:1804.02767] 2018.

[37] D.J. Rezende and S. Mohamed. Variational inference with normalizing flows. In ICML, 2015.

[38] G. Roeder, Y. Wu, and D. Duvenaud. Sticking the landing: Simple, lower-variance gradient estimators for variational inference. In NIPS, 2017.

[39] Y. Saatchi and A.G. Wilson. Bayesian GAN. In NIPS, 2017.

[40] J.T. Springenberg, A. Dosovitskiy, T. Brox, and M. Riedmiller. Striving for simplicity: The all convolutional net. In ICLR, 2015.

[41] N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, and R. Salakhutdinov. Probabilistic backpropagation for scalable learning of Bayesian neural networks. In ICML, 2015.

[42] N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, and R. Salakhutdinov. Dropout: A simple way to prevent neural networks from overfitting. Journal of Machine Learning Research, 15:1929–1958, 2016.

[43] C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus. Intriguing properties of neural networks. In ICLR, 2014.

[44] M. Welling and Y.W. Teh. Bayesian learning via stochastic gradient Langevin dynamics. In ICML, 2011.

[45] F. Yu, V. Koltun, and T. Funkhouser. Dilated residual networks. In CVPR, 2017.
Supplementary Material for: "Sampling-Free Variational Inference of Bayesian Neural Nets"

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Proposition 1. Consider a Bayesian model including the generative process excerpt below
\[ \cdots, \ a \sim p(a), \ z | a \sim \delta_{a>0}, \ b | z, a \sim p(b | g(z, a)), \ \cdots \]
for some arbitrary function \( g(z, a) \). If the variational inference of this model is to be performed with an approximate distribution \( Q = \cdots q(a)q(z) \cdots \), the optimal closed-form update for \( z \) is
\[ q(z) \leftarrow \delta_{E_q(a)>0}. \]

Proof. Consider the below property of the Bernoulli mass function
\[ \text{Bern}(z|\sigma(a)) = \sigma(a)^z(1 - \sigma(a))^{1-z} = e^{a \cdot z} - \sigma(-a). \]
Applying this property to closed-form calculation of the optimal update rule for \( z \) reads
\[ \log q(z) \leftarrow zC \mathbb{E}_{q(a)}[a] + \mathbb{E}_{q(a)}[\log \sigma(-Ca)] + \mathbb{E}_{q(a)}[\log p(b | g(z, a))] + \text{const}. \]
The second term does not depend on \( z \), hence can be dumped into \text{const}. From the remaining two terms, the first one will dominate for \( C >> 0 \), leading to
\[ q(z) \leftarrow \sigma(C \mathbb{E}_{q(a)}[a]). \]
Setting \( C \) to infinity, we get
\[ \lim_{C \rightarrow \infty} \sigma(C \mathbb{E}_{q(a)}[a]) = \delta_{E_q(a)>0}. \]

Proposition 2. For the model and the inference scheme in Proposition 1 with \( q(a) = \mathcal{N}(a|\mu, \sigma^2) \), in the relaxed delta function formulation \( \delta_{a>0} \approx \text{Bern}(a | \sigma(Ca)) \) with some finite \( C > 0 \), the expression \( \mathbb{E}_{q(a)}[\mathbb{KL}[q(z)||p(z|a)]] \) is i) analytically tractable and ii) its magnitude is proportional to the mass of \( q(a) \) that falls on the opposite side of the \( a = 0 \) line with respect to \( \mathbb{E}_{q(a)}[a] \).

Proof. The KL divergence inside the expectation has the following form
\[ \mathbb{KL}[q(z)||p(z|a)] = \sigma(C \mathbb{E}_{q(a)}[a]) \log \frac{\text{Bern}(z = 1|\sigma(C \mathbb{E}_{q(a)}[a]))}{\text{Bern}(z = 0|\sigma(Ca))}, \]
\[ + (1 - \sigma(C \mathbb{E}_{q(a)}[a])) \log \frac{\text{Bern}(z = 0|\sigma(C \mathbb{E}_{q(a)}[a]))}{\text{Bern}(z = 0|\sigma(Ca))}, \]
\[ = \sigma(C \mathbb{E}_{q(a)}[a]) \left[ \log \sigma(C \mathbb{E}_{q(a)}[a]) - \log \sigma(Ca) \right] \]
\[ + (1 - \sigma(C \mathbb{E}_{q(a)}[a])) \left[ \log \sigma(-C \mathbb{E}_{q(a)}[a]) - \log \sigma(-Ca) \right] \]
\[ = \sigma(C \mathbb{E}_{q(a)}[a]) \left[ - \log \left(1 + e^{-C \mathbb{E}_{q(a)}[a]} \right) + \log \left(1 + e^{Ca} \right) \right] \]
\[ + (1 - \sigma(C \mathbb{E}_{q(a)}[a])) \left[ - \log \left(1 + e^{-C \mathbb{E}_{q(a)}[a]} \right) + \log \left(1 + e^{Ca} \right) \right]. \]

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Note that \( q(b) \) might or might not exist depending on whether \( b \) is latent or observed.

Preprint. Work in progress.
The expectation of this expression is then given by

$$E \left[ \sigma(CE_q(a))[a] \left( \log \frac{1 + \exp(-Ca)}{1 + \exp(-CE_q(a))[a]} \right) + (1 - \sigma(CE_q(a))[a]) \left( \log \frac{1 + \exp(Ca)}{1 + \exp(CE_q(a))[a]} \right) \right]$$

$$= E \left[ \sigma(CE_q(a))[a] \left( C(CE_q(a))[a] - a \right) + \log \frac{1 + \exp(Ca)}{1 + \exp(CE_q(a))[a]} \right]$$

$$+ (1 - \sigma(CE_q(a))[a]) \left( \log \frac{1 + \exp(Ca)}{1 + \exp(CE_q(a))[a]} \right)$$

$$= E \left[ \left( \log \frac{1 + \exp(Ca)}{1 + \exp(CE_q(a))[a]} \right) \right] = E \left[ \log(1 + \exp(Ca)) - \log(1 + \exp(CE_q(a))[a]) \right],$$

where the first term is a refactoring of the log term and the second equality is a rearrangement of all the terms and due to the fact that parts cancel out with the expectation.

Let $\zeta(\cdot) = \log(1 + \exp(\cdot))$, be the softplus function. With this we have

$$E[\zeta(Ca)] - \zeta(CE_q(a))[a]).$$

Since $\zeta$ is convex, we know for all finite $C$ that $(\ast)$ is bound below by zero (via the Jensen Inequality). Both terms contain a large factor $C$. Note that

$$\zeta(x) \approx \begin{cases} x, & \text{for } x \gg 0, \\ 0, & \text{for } x \ll 0. \end{cases}$$

That is we care mainly about the sign of the input. Splitting the integral in the first term we get

$$\int_{a>0} q(a)\zeta(Ca)da + \int_{a<0} q(a)\zeta(Ca)da - \zeta(CEa).$$

For a large $C$ this gives us approximately

$$C \int_{a>0} q(a)ada - \zeta(CEa).$$

The second term depends on the sign of the expectation.

**Case 1:** $E_q(a)[a] = 0$. In this case $\zeta(CEa) = \log(2)$ for all $C$ and

$$C \int_{a>0} q(a)ada - \log(2).$$

**Case 2:** $E_q(a)[a] > 0$. In this case $\zeta(CEa) \approx CE$ for large $C$, which leaves us with

$$C \int_{a>0} q(a)ada - CEa = C \left( \int_{a>0} q(a)ada - \int q(a)ada \right) = -C \int_{a<0} q(a)ada$$

**Case 3:** $E_q(a)[a] < 0$. In this case $\zeta(CEa) \approx 0$ for large $C$, which leaves us with

$$C \int_{a>0} q(a)ada = C \left( \int_{a>0} q(a)ada + \int_{a<0} q(a)ada - \int_{a<0} q(a)ada \right)$$

$$= CE_q(a)[a] - C \int_{a<0} q(a)ada$$

Hence we complete (ii). In each of the two practically relevant cases where $E_q(a)[a] > 0$ and $E_q(a)[a] < 0$, the magnitude of the expected KL divergence depends on how much of the mass of the distribution has the opposite sign of the expected value. The accuracy thus depends on how tightly the density is concentrated around the expectation, i.e. the size of $\text{Var}(a)$. In our case this term is already encouraged to be small by the corresponding term in $L_data$. For a normal distribution
$q(a)$, the required analytical solution can be computed as follows. For $a \sim \mathcal{N}(a|\mu, \sigma^2)$ we have with $x = a - \mu$ that

$$
\int_{a>0} a \mathcal{N}(a|\mu, \sigma^2) = \int_{x>\mu} (x+\mu) \mathcal{N}(x|0, \sigma^2) dx
$$

$$
= \int_{x>\mu} x \mathcal{N}(x|0, \sigma^2) dx + \mu \int_{x>\mu} \mathcal{N}(x|0, \sigma^2) dx
$$

$$
= \int_{x>\mu} x \mathcal{N}(x|0, \sigma^2) dx + \mu (1 - \Phi(\mu/\sigma)),
$$

where $\Phi(\cdot)$ is the cumulative density function of the normal distribution. The first term decomposes as

$$
\int_{-\mu}^{0} x \mathcal{N}(x|0, \sigma^2) dx + \int_{0}^{\infty} x \mathcal{N}(x|0, \sigma^2) dx
$$

$$
= \frac{\sigma}{\sqrt{2\pi}} \left( \exp\left(\frac{\mu^2}{2\sigma^2}\right) - 1 \right) + \frac{\sigma}{\sqrt{2\pi}} \exp\left(\frac{\mu^2}{2\sigma^2}\right)
$$

Together, we complete (i) by arriving at the analytical solution as

$$
C \int_{a>0} q(a) ada = C \left[ \frac{\sigma}{\sqrt{2\pi}} \exp\left(\frac{\mu^2}{2\sigma^2}\right) + \mu (1 - \Phi(\mu/\sigma)) \right].
$$

**Proposition 3.** For a Bayesian model including the generative process excerpt as below

$$
\vdots
$$

$$
\begin{align*}
    a &\sim p(a), \\
    b &\sim p(b), \\
    c | a, b &\sim \max(a, b), \\
    d | c &\sim p(b | h(c)),
\end{align*}
$$

$$
\vdots
$$

with some arbitrary function $h(c)$, when mean-field variational Bayes is performed with an approximate distribution $Q = \cdots q(a) q(b) q(c) \cdots$, the following identities hold

(i) $\mathbb{E}[c] = \mathbb{E}[\max(a, b)] = \max(\mathbb{E}[a], \mathbb{E}[b])$.

(ii) $\text{Var}(c) = \text{Var}(\text{argmax}(\mathbb{E}[a], \mathbb{E}[b]))$.

**Proof.** Rewrite the generative process as

$$
\vdots
$$

$$
\begin{align*}
    a &\sim p(a), \\
    b &\sim p(b), \\
    z &\sim \delta_{a-b>0} \\
    c | a, b, z &\sim a z + b (1 - z) \\
    d | c &\sim p(b | h(c)),
\end{align*}
$$

$$
\vdots
$$

for a variational distribution $Q = \cdots q(a) q(b) q(z) q(c) \cdots$, then the optimal update for $z$ is

$$
q(z) \leftarrow \delta_{\mathbb{E}[a] - \mathbb{E}[b] > 0}
$$
Table 1: The Strided LeNet. For Cifar-10/Cifar-100 the convolutional layers get 192 filters instead and the number of neurons in the linear layer 1000. The activations between the layers are ReLUs.

| MODIFIED LENET-SMALL |
|-----------------------|
| Convolution (5 × 5) with 20 channels, stride 2 |
| Convolution (5 × 5) with 50 channels, stride 2 |
| Linear with 500 neurons |
| Linear with n_{class} neurons |

from Proposition 1. Then

\[ E[c] = E[\max(a, b)] = E[a]E[z] + E(1 - E[z]) = \max(E[a], E[b]), \]

which satisfies (i).

Now decompose the variance term

\[ Var(c) = Var(a, z) + Var(b(1 - z)) = zVar(a) + (1 - z)Var(b), \]

since \( z \) is a constant with zero variance. As \( z = 1 \) for \( E[a] > E[b] \), we get

\[ Var(c) = Var(\arg\max(E[a], E[b])), \]

which satisfies (ii).

This outcome can trivially be extended to \( \max(\cdots) \) functions with arbitrary number of inputs by induction referring to the identity

\[ \max(a_1, \cdots, a_n) = \max(\max(a_1, \cdots, a_{n-1}), a_n). \]

Consequently, a max-pooling layer can be plugged into our framework. The data fit term in the ELBO will use (i) while calculating the forward pass. The variance term, on the other hand, will use (ii) to during the recursion step of the max-pooling layer.

Details on the Experiments

Architectures. The fully connected neural network architecture follows the setup of Blundell et al. [1]. The structure consists of two fully connected hidden layers with \( K \in \{400, 800, 1200\} \) neurons each and ReLU activations between them.

The convolutional neural architecture we use in the convolutional classification experiments is a modified version of the classical LeNet5, without pooling layers but strided convolutions instead. The version used with MNIST and SVHN is given as presented in Table 1.

For Cifar-10/100 we increase the width of the convolutional layers to 192 channels each and the linear one to 1000, following [2]. All hidden layers are followed by ReLU activations.

Initialization. The initialization scheme is shared between all architectures and VBP/VarOut. The variational means of the weights follow the common initialization of [He]. The logarithms of their variances are sampled from \( \mathcal{N}(-9, 1e^{-3}) \).

Other Hyperparameters. We run Adam [3] with the default hyperparameters proposed by the authors, which are \( \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8} \). Each model is trained for 100 epochs during which the initial learning rate of \( 1e-4 \) is linearly reduced to zero. The batch size is 128 for all settings. Contrary to many other Bayesian neural network publications we do not anneal the KL term during the training and do constrain the variation of the parameters in any way throughout the training, except when necessitated for numerical stability, where the constraints are again equal between the models (see the code for additional details).
How to sparsify. As mentioned in the main paper, the Bayesian approach has the nice side-benefit of implicitly learning a pruning of the network. Molchanov et al. [5] suggest to prune all weights with $\log \alpha > 3$, where $\alpha = \sigma^2 / \mu^2$. Translated to a Gaussian Dropout interpretation, this is equivalent to dropping pruning weights with a dropout probability larger than 0.95. In our model we found this strict rule to be sub-optimal with respect to performance. Instead of this strict layer independent global pruning criterion we follow the approach suggested by Louizos et al. [4]. A visual inspection of the histograms over $\log \alpha$ separately for each layer shows a clear bimodal structure for most layers. Placing the pruning threshold in the valley between those, gives an criterion to prune unnecessary weights without loosing too much predictive performance. These histograms allow one to find an individual trade-off between sparsity and predictive performance. We show an example set of histograms for the C10 dataset in Figure 1.

References

[1] C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wiestra. Weight uncertainty in neural networks. In ICML, 2015.

[2] Y. Gal and Z. Ghahramani. Bayesian convolutional neural networks with Bernoulli approximate variational inference. 2015.

[3] D.P. Kingma and J. Ba. Adam: A method for stochastic optimization. In ICLR, 2015.

[4] C. Louizos, K. Ullrich, and M. Welling. Bayesian compression for deep learning. In NIPS, 2017.

[5] D. Molchanov, A. Ashukha, and D. Vetrov. Variational dropout sparsifies deep neural networks. In ICML, 2017.