One Simple Trick to Fix Your Bayesian Neural Network

Piotr Tempczyk\textsuperscript{1,2,3}, Ksawery Smoczyński\textsuperscript{2,4}, Philip Smolenski-Jensen\textsuperscript{1}, and Marek Cygan\textsuperscript{1,5}

\textsuperscript{1}Institute of Informatics, University of Warsaw
\textsuperscript{2}Polish National Institute for Machine Learning (opium.sh)
\textsuperscript{3}deeptale.ai
\textsuperscript{4}Faculty of Mathematics and Computer Science, Adam Mickiewicz University
\textsuperscript{5}Nomagic

July 28, 2022

Abstract

One of the most popular estimation methods in Bayesian neural networks (BNN)\cite{blundell2015weight} is mean-field variational inference (MFVI)\cite{blei2017variational}. In this work, we show that neural networks with ReLU\cite{fukushima1975neocognitron} activation function induce posteriors, that are hard to fit with MFVI. We provide a theoretical justification for this phenomenon, study it empirically, and report the results of a series of experiments to investigate the effect of activation function on the calibration of BNNs. We find that using Leaky ReLU activations\cite{maas2013rectifier} leads to more Gaussian-like weight posteriors and achieves a lower expected calibration error (ECE)\cite{guo2017calibration} than its ReLU-based counterpart.

1 Introduction

Uncertainty estimation and neural network calibration are important aspects of real-world deep learning applications\cite{wang2019bnn, lakshminarayanan2017simple, loquercio2020deep}. Especially, when dealing with out-of-distribution or noisy examples, which is often the case in robotics or autonomous driving. Currently ensemble methods provide best approaches to uncertainty estimation and are often superior to Bayesian methods, especially to variational inference, which is the fastest one (e.g. compared to MCMC), but also the most inaccurate one. This paper makes approach to change current state of
knowledge and make MFVI methods more scalable and accurate in terms of uncertainty estimation.

We start with observing that for neural networks with ReLU activation every parameter $w_i$ has an unbounded range of values for which the likelihood function $L_n$ (for a single data point $x_n, n = 1 \ldots N$) is constant and greater than 0.

**Proposition 1.** For every neuron with a ReLU activation function and non-negative input with weight $w_i$ there exists upper bound $w^*_ni$, such that if $w_i \leq w^*_ni$ then $\frac{\partial L_n}{\partial w_i} = 0$.

**Proof.** We can decompose this derivative using chain rule into: $\frac{\partial L_n}{\partial w_i} = \frac{\partial L_n}{\partial z} \frac{\partial z}{\partial a} \frac{\partial a}{\partial w_i}$, where $a = w_i h_i + \sum_{j \neq i} w_j h_j + b$ is a selected neuron output, $z = \max(0, a)$ is a ReLU activation function and $h_k$ is $k$-th input to the neuron. $\frac{\partial L_n}{\partial w_i}$ vanishes if any of the terms in the chain is equal to 0. Note, that if $h_i = 0$, then $\frac{\partial z}{\partial a} = 0$, for any value of $w_i$. Otherwise, if $h_i > 0$ then let $w^*_ni := -\frac{\sum_{j \neq i} w_j h_j + b}{h_i}$, which implies that $a \leq 0$, which in turns gives $\frac{\partial z}{\partial a} = 0$. $\square$

For neural networks with ReLU activations $h_i \geq 0$ holds for all the layers except the first one. For the whole dataset $\mathcal{L} = \prod_{n=1}^{N} L_n$. This fact and Proposition 1 implies that there is $w^*_i = \min_n w^*_ni$, such that if $w_i \leq w^*_i$ then $\frac{\partial \mathcal{L}}{\partial w_i} = 0$. Therefore, for all the weights and any dataset, there exists an infinite plateau on the loss function in some part of the weight space. The posterior resulting from $\mathcal{L}$ might be impossible to normalize (especially for improper uniform priors) and may cause problems when fitting it with MFVI. This can be to some extent alleviated by using proper priors, but the problem does not vanish because the resulting posterior’s shape may still be far from Gaussian’s and hence lead to poor approximation when using MFVI.

In this work we investigate this problem and propose a simple solution, where we change all activation functions from ReLU to LeakyReLU and optimize its negative slope parameter. We show this leads to posteriors much more suitable for fitting with Gaussian distribution without deteriorating the accuracy.

## 2 Experiments

The experiments were run with the following models: 3FC – Fully connected neural network with 3 hidden layers of size 1000, CONV – convolutional neural network with 2 hidden layers containing 128 and 256 channels respectively, and MNIST [LeCun and Cortes, 2010] and Fashion MNIST (FMNIST) [Xiao et al., 2017] datasets. We compared a family of Leaky ReLU functions with negative slope parameter ranging from $-1$ to 1. Note that, in particular, this family contains absolute value function, ReLU, and linear activation for slope values of $-1$, 0, and 1 respectively.

We trained Bayesian models using Pyro [Bingham et al., 2019] MFVI with Adam [Kingma and Ba, 2014] optimizer, a learning rate of 0.001, and normally
2.1 Shape of the likelihood function

We trained deterministic models on all the architectures and datasets and visualized conditional likelihood functions for some random weights in the vicinity of the mode of the likelihood. We observed the phenomena we predicted theoretically for the majority of the weights in all considered architectures with ReLU, and for 10-30% of them this flat region was near the mode of the distribution
Table 1: Accuracy and ECE for different architectures, activations and datasets. Leaky stands for Leaky ReLU.

| Dataset | Model | Accuracy | ECE |
|---------|-------|----------|-----|
|         |       | Leaky    | ReLU | Leaky | ReLU |
| FMNIST  | CONV  | 0.83     | 0.83 | 0.014 | 0.079|
|         | 3FC   | 0.83     | 0.82 | 0.033 | 0.106|
| MNIST   | CONV  | 0.98     | 0.98 | 0.018 | 0.042|
|         | 3FC   | 0.97     | 0.98 | 0.007 | 0.019|

(as shown in Fig. 1), thus implying it would affect fitting the posterior using MFVI.

2.2 ECE dependence on negative slope

We ran 5 experiments for each configuration of a model, dataset, and Leaky ReLU slope. Results for one combination are shown in Fig. 2. In all configurations but one, the highest ECE corresponds to the slope of 0 (which is ReLU). In most cases, the maximum in ECE has a form of a spike, as in Fig. 2. Moreover, there is no definite domination in terms of accuracy while using ReLU which means that using Leaky ReLU leads to better calibrated models with similar accuracy.

2.3 Comparison of different architectures and datasets

In Table 1 we present average results for ECE and Accuracy for all models and datasets for Leaky ReLU negative slope equal \(-0.5\) (almost all best results for all combinations were between \(-1\) and \(-0.5\)). We can see that ReLU and Leaky ReLU models are comparable in terms of accuracy and Leaky ReLU models yield much better ECE.

2.4 Decalibration for ReLU

We observed a phenomenon that might also be related to our observation about BNNs using ReLU activations. Figure 3 shows measured metrics during the training of a model. While accuracy on the validation set increases during training with both activations, the ECE for ReLU on the validation set initially drops as expected, but then it starts to increase before the model has fully converged. This behavior has been noticed in the vast majority of experiments using ReLU (and only ReLU) activation.
Figure 3: Decalibration during ReLU training for CONV network on MNIST dataset. We plot accuracy and ECE on the validation set and Leaky ReLU model for comparison.

3 Conclusions

We have shown that Leaky ReLU leads to superior ECE scores with comparable accuracy in comparison with ReLU activations. We plan to conduct more experiments on larger architectures, bigger and non-image datasets, and verify if our observation holds in case of regression problems.

References

Eli Bingham, Jonathan P Chen, Martin Jankowiak, Fritz Obermeyer, Neeraj Pradhan, Theofanis Karaletsos, Rohit Singh, Paul Szerlip, Paul Horsfall, and Noah D Goodman. Pyro: Deep universal probabilistic programming. The Journal of Machine Learning Research, 20(1):973–978, 2019.

David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. Journal of the American statistical Association, 112(518):859–877, 2017.

Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight uncertainty in neural network. In International conference on machine learning, pages 1613–1622. PMLR, 2015.

Kunihiiko Fukushima. Cognitron: A self-organizing multilayered neural network. Biological cybernetics, 20(3):121–136, 1975.

Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. In International Conference on Machine Learning, pages 1321–1330. PMLR, 2017.
Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and scalable predictive uncertainty estimation using deep ensembles. *Advances in neural information processing systems*, 30, 2017.

Yann LeCun and Corinna Cortes. MNIST handwritten digit database. 2010. URL [http://yann.lecun.com/exdb/mnist/](http://yann.lecun.com/exdb/mnist/).

Antonio Loquercio, Mattia Segu, and Davide Scaramuzza. A general framework for uncertainty estimation in deep learning. *IEEE Robotics and Automation Letters*, 5(2):3153–3160, 2020.

Andrew L Maas, Awni Y Hannun, Andrew Y Ng, et al. Rectifier nonlinearities improve neural network acoustic models. In *Proc. icml*, volume 30, page 3. Citeseer, 2013.

Guotai Wang, Wenqi Li, Michael Aertsen, Jan Deprest, Sébastien Ourselin, and Tom Vercauteren. Aleatoric uncertainty estimation with test-time augmentation for medical image segmentation with convolutional neural networks. *Neurocomputing*, 338:34–45, 2019.

Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms, 2017.