On Symmetries in Variational Bayesian Neural Nets

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Abstract

Probabilistic inference of Neural Network parameters is challenging due to the highly multi-modal likelihood functions. Most importantly, the permutation invariance of the neurons of the hidden layers renders the likelihood function unidentifiable with a factorial number of equivalent (symmetric) modes, independent of the data. We show that variational Bayesian methods that approximate the (multi-modal) posterior by a (uni-modal) Gaussian distribution are biased towards approximations with identical (e.g. zero-centred) weights, resulting in severe underfitting. This explains the common empirical observation that, in contrast to MCMC methods, variational approximations typically collapse most weights to the (zero-centred) prior. We propose a simple modification to the likelihood function that breaks the symmetry using fixed semi-orthogonal matrices as skip connections in each layer. Initial empirical results show an improved predictive performance.

1 Introduction

The probabilistic approach to learning deep neural networks promises several appealing advantages compared to point estimates, s.a. reducing overfitting, estimating epistemic uncertainty [3], and enabling online/continual learning methods [5, 6]. Despite a growing scientific interest, Bayesian neural networks (BNN) are still rarely used in practical applications. Variational methods s.a. Bayes by Backprop [1] result in severe underfitting in case of small dataset sizes or large models [2].

We hypothesize that underfitting is primarily caused by the bias of the evidence lower bound (ELBO) objective, providing a tighter bound for posterior approximations with identical (e.g. zero-centred) weights. Neural networks are known to be invariant (wrt. a factorial number of permutations of the neurons) in every hidden layer, resulting in the same likelihood function for different parametrisations. For commonly used priors such as the standard normal distribution (or mixtures of zero-centred diagonal Gaussians), the resulting posterior is therefore also a symmetric mixture with a factorial number of equivalent modes. It can be shown easily that the ELBO (with a uni-modal posterior approximation) is tighter/looser if the symmetric modes of the "true" posterior are overlapping/well separated. A notable special case in which all modes overlap is in case where the distribution over the weights is centred at zero, i.e. collapsing to the prior.

Reducing this additional bias of the ELBO is essential to avoid the severe underfitting of variational BNNs; this could potentially be achieved through one of the following (non-exclusive) routes:

- likelihood: 'hard' symmetry-breaking by modifying likelihood function.
- prior: 'soft' symmetry-breaking by assigning low probability to symmetric modes.
- variational: approximate the symmetric-mixture posterior.
- objective: modify the ELBO to reduce the bias, e.g. approximate the additional gap between single-mode and symmetric-mixture posterior.

In this work, we focus on breaking the permutation and sign-flip symmetries through skip connections with fixed semi-orthogonal matrices. We formulate the permutation invariance problem in Sec. 2, describe approach to break the symmetries in Sec. 3, and show initial results in Sec. 4.

Workshop on Bayesian Deep Learning (NeurIPS 2021), Sydney, Australia.

2 Permutation symmetries and variational posterior approximation

Neural networks are known to be invariant wrt. permutations of the neurons in every hidden layer. This implies that the likelihood function of neural networks is non-identifiable and has no global optimum. For maximum likelihood/a posteriori point estimation through stochastic gradient descent, this does not pose a significant problem since any of the equivalent optima suffices. However, the non-identifiability complicates probabilistic inference, especially the variational Bayesian approach.

2.1 Symmetric-mixture posterior

Consider a Multi-Layer-Perceptron (MLP) with L hidden layers. Written in pre-activations form, each layer indexed by l, computes the representation

$$h_l = W_l f_l(h_{l-1}) + b_l \tag{1}$$

using weights $W_l \in \mathbb{R}^{N_l \times N_{l-1}}$, biases $b_l \in \mathbb{R}^{N_l}$ and element-wise activation functions f_l. The first activation is the input data, that is, $h_0 := x$ and f_1 is the identity function. This parameterisation is invariant to permutations of the neurons (dimensions of the representation) in each hidden layer

$$\begin{aligned} h_{l+1} &= W_{l+1} f_{l+1}(P_l^T P_l h_l) + b_{l+1} \\ &= \underbrace{W_{l+1} P_l^T}_{W'_{l+1}} f_{l+1}(\underbrace{P_l W_l}_{W'_l} f_l(h_{l-1}) + \underbrace{P_l b_l}_{b'_l}) + b_{l+1}, \end{aligned} \tag{2}$$

where $P_l \in \mathbb{R}^{N_l \times N_l}$ is a permutation matrix (each row consists of all 'zeros' except a single 'one'). The permutation invariance is follows from the activation functions being applied element-wise s.t. the permutation matrix P_l^T in Eq. (2) can be "pulled out" of f_{l+1}.[1] W'_{l+1}, W'_l and b'_l then denote the weights and biases corresponding to one of the equivalent modes. For every hidden layer l, there are $N_l!$ possible permutations, totalling $\prod_{l=1}^{L} N_l$ equivalent modes.[2]

In the Bayesian approach, we put a prior $p(w)$ over the weights and biases of the MLP and aim to infer the posterior $p(w|\mathcal{D}) \propto p(w)p(\mathcal{D}|w)$ given a dataset $\mathcal{D}$. For common priors such as a Gaussian or a Mixture of Gaussian (MoG) with the mean(s) centered at the origin and diagonal covariance(s), the posterior incurs the factorial number of modes from the likelihood function $p(\mathcal{D}|w)$. The resulting posterior is thus a symmetric mixture distribution consisting of $N = \prod_{l=1}^{L} N_l!$ mixture components

$$p(w|\mathcal{D}) = \frac{1}{N} \sum_{n=1}^{N} p_n(w|\mathcal{D}). \tag{3}$$

If we are interested in predictions only, it suffices to approximate a single mode $p_n(w|D)$, e.g. through Markov Chain Monte Carlo methods. Variational Bayesian methods however compute the entropy of the (approximate) posterior. In the subsequent section, we describes how the entropy of this degenerate model causes a bias towards underfitting.

2.2 Variational Bayesian approximation

Consider a simple diagonal Gaussian variational approximations for the posterior of the weights and biases of the neural network $q_{\theta_0}(w) = \mathcal{N}(w; \mu_0, \Sigma_0)$, $\theta_0 = \{\mu_0, \Sigma_0\}$. Inference amounts to maximizing the ELBO

$$\begin{aligned} \mathcal{L}_{\text{Gauss}}(\mathcal{D}, \theta) = \mathbb{E}_{q_{\theta_0}(w)}[\log p(\mathcal{D}|w) + \log p(w)] \\ - \mathbb{E}_{q_{\theta_0}(w)}[\log q_{\theta_0}(w)]. \end{aligned} \tag{4}$$

Notice again that both terms related to the model are invariant wrt. the permutations (for common priors). Consider now a *symmetric-MoG* posterior approximation $q_\theta(w) = \frac{1}{N} \sum_{n=1}^{N} q_{\theta_n}(w)$ for

[1] If f_l was linear, any invertible transformation would be possible, e.g. orthogonal matrices with $O^{-1} = O^T$. This could cause additional degeneracy problems if the model operates in a locally linear region, e.g. for piece-wise non-linear activations or close to the origin in case of the tanh activation.

[2] If the non-linearity is symmetric wrt. the origin, flipping the signs of incoming and outgoing weights (i.e. a "-1" in permutation matrices P_l) provides 2^{N_l} further sign-flip symmetries. Furthermore, piece-wise linear activation functions such as ReLU result in continuous scaling symmetries.

which these two terms are identical if a single Gaussian $q_{\theta_0}(w)$ is used instead of the symmetric-MoG $q_\theta(w)$. That is, $\mathbb{E}_{q_{\theta_n}(w)}[\log p(\mathcal{D}|w)] = \mathbb{E}_{q_{\theta_0}(w)}[\log p(\mathcal{D}|w)]\ \forall n$ by definition of the non-identifiability/permutation-invariance, and, similarly $\mathbb{E}_{q_{\theta_n}(w)}[\log p(w)] = \mathbb{E}_{q_{\theta_0}(w)}[\log p(w)]\ \forall n$ in case of the isotropic Gaussian prior (and MoG prior with centered means and diagonal covariance). The corresponding ELBO

$$\begin{aligned}\mathcal{L}_{\text{MoG}}(\mathcal{D}, \theta) = \mathbb{E}_{q_{\theta_0}(w)}[\log p(\mathcal{D}|w) + \log p(w)] \\ - \mathbb{E}_{q_\theta(w)}[\log q_\theta(w)]\end{aligned} \tag{5}$$

differs only in the entropy term, and the difference between the two ELBOs can thus be quantified as

$$\begin{aligned}\mathcal{L}_{\text{MoG}}(\mathcal{D}, \theta) - \mathcal{L}_{\text{Gauss}}(\mathcal{D}, \theta) &= \mathbb{E}_{q_{\theta_0}(w)}[\log q_{\theta_0}(w)] - \mathbb{E}_{q_\theta(w)}[\log q_\theta(w)] \\ &= \mathbb{E}_{q_{\theta_0}(w)}\left[\log q_{\theta_0}(w) - \log \frac{1}{N}\sum_{n=1}^{N} q_{\theta_n}(w)\right] \\ &= \text{KL}\left[\log q_{\theta_0}(w)\,||\,q_\theta(w)\right],\end{aligned} \tag{6}$$

since the expectation in the (neg.) entropy of the MoG can be taken over q_{θ_0} due to the symmetry.

The resulting KL divergence is bounded between 0 and $\log \prod_{l=2}^{L} N_l!$, i.e. the log of the number of modes. The ELBO corresponding to a Gaussian posterior can thus have a significant gap wrt. the log likelihood even if the posterior is locally Gaussian. Importantly, the gap between these two ELBOs, measured by the KL in Eq. (6), is not a constant: i) the KL is minimised if the MoG has only identical modes, resulting in a single Gaussian; ii) the KL is maximised if the components of the MoG are well separated. That is, the Gaussian posterior approximation is tighter if most of the neural network weights are identical, e.g. zero. We therefore hypothesise that the variational Bayesian approach to inference in BNNs is biased towards collapsing most weights in the approximate posterior to zero.

3 Symmetry-breaking through skip connections

In this work, we address the degeneracy/symmetry problem by modifying the likelihood function s.t. the modes more no longer equivalent. Previous work enforces a bias-ordering constraint $b_l^{(1)} \leq b_l^{(2)} \leq \ldots \leq b_l^{(N_l)}$ by parameterising the log-differences the scalar biases [8]. However, if the biases take (near) zero values, the degeneracy remains (mostly) intact. Here, we modify each layer to include skip connections with *fixed* matrices O_l:

$$h_l = O_l h_{l-1} + W_l f_l\left(h_{l-1}\right) + b_l. \tag{7}$$

With this simple modification of the likelihood function, it is not possible to permute the neurons/activations since only the corresponding weight parameters are inferred (and thus permutable), but the matrices O_l remain fixed. Omitting the biases for simplicity,

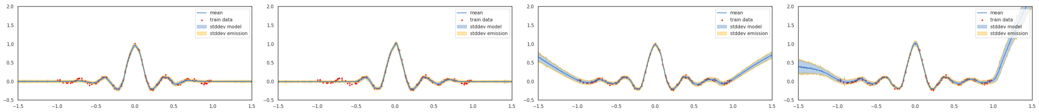
$$\begin{aligned}h_l = O_l h_{l-1} + f_l\left(P_l^T P_l W_l h_{l-1}\right) &= O_l h_{l-1} + P_l^T f_l\left(P_l W_l h_{l-1}\right) \\ &\neq P_l^T\left(O_l h_{l-1} + f_l\left(P_l W_l h_{l-1}\right)\right)\end{aligned} \tag{8}$$

The last line would be needed if we want to 'group' P^T with the subsequent layer's weights W_{l+1}.

It has been shown previously that models with residual connections [7] break the symmetry and argued that this improves the learning dynamics in ResNets. Since residual connections can be used only for layers with the same number of neurons, we use *fixed random semi-orthogonal* matrices.

4 Experiments

We trained an MLP with 5 hidden layers of 32 units each on 128 data points from a (scaled) sinc-function with additive noise. We used an isotropic Gaussian prior and a diagonal Gaussian posterior approximation. Inference is performed using the local reparameterisation trick [4] with 64 samples for training and 256 for testing. The model is trained for 200.000 full-batch iterations, with a linear annealing schedule for the KL divergence in the first half of the iterations. The predictive distributions for a standard BNN, a model with a bias ordering constraint, our proposed orthogonal skip connections, as well as the combination of both, are shown in Fig. 1. It can be seen that the baseline results in severe underfitting, while orthogonal skip connections fit the data well and provide better (albeit still not good) out of distribution uncertainty.



(a) No skip & no bias constr.

(b) Bias constr.

(c) Orthogonal skip

(d) Ortho. skip & bias constr.

Figure 1: Predictive distribution (1 std. dev) for sinc-function regression. The model is an MLP with 5 layers of 32 units and SELU activation functions. The dataset consists of 128 samples (marked red), drawn uniformly in $[-1, 1]$, mapped through the (scaled) sinc-function with additive noise with std. dev 0.2.

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