

HWA: AVERAGING HYPERPARAMETERS IN BAYESIAN NEURAL NETWORKS LEADS TO BETTER GENERALIZATION.

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ABSTRACT

Bayesian Deep Learning presents itself as the most useful tool for adding uncertainty estimation to traditional Deep Learning models that only produce point estimates predictions as outputs. Confidence of the model and the predictions at inference time are left alone. Applying randomness and Bayes Rule to the weights of a deep neural network is a step towards achieving this goal. Current state of the art optimization method for training a Bayesian Neural Network are relatively slow and inefficient, compared to their deterministic counterparts. In this paper, we propose HWA (Hyperparameters Weight Averaging) algorithm that leverages averaging procedure in order to train faster and achieve a better accuracy. We develop our main algorithm using the simple averaging heuristic and demonstrate its effectiveness on the space of the hyperparameters of the neural networks random weights. Numerical applications confirm the empirical benefits of our method.

1 INTRODUCTION

While Deep Learning methods have shown increasing efficiency in various domains such as natural language processing, computer vision or robotics, sensible areas including autonomous driving or medical imaging not only require accurate predictions but also uncertainty quantification. In (Neal, 2012), authors develop a bayesian variant of plain feedforward multilayer neural networks in which weights and biases are considered as random variables. For supervised learning tasks, deterministic models are prone to overfitting and are not capable of estimating uncertainty in the training data resulting in making overly confident decisions about the correct class, *i.e.* miscalibration (Guo et al., 2017; Kendall & Gal, 2017). Nevertheless, representing that aforementioned uncertainty is crucial for decision making.

Bayesian methods display a hierarchical probabilistic model that assume a (prior) random distribution over the parameters of the parameters and are useful for assessing the uncertainty of the model via posterior predictive distribution quantification (Blundell et al., 2015; Kingma et al., 2015). Current training methods for Bayesian Neural Networks (BNN) (Neal, 2012) include Variational Inference (Graves, 2011; Hoffman et al., 2013) or BayesByBackprop (Blundell et al., 2015) based on Evidence Lower Bound (ELBO) maximization task. Naturally, Bayesian methods, and in particular BNNs, are thus highly sensitive to the parameters choice of the prior distribution and current state-of-the-art models are not as efficient and robust as traditional deep learning models.

In this paper, we introduce a new *optimization* algorithm to alleviate those challenges. Our main contributions read as follows:

- We introduce Hyperparameter Weight Averaging (HWA), a training algorithm that leverages stochastic averaging techniques (Polyak & Juditsky, 1992) and posterior sampling methods.
- Given the high nonconvexity of the loss landscape, our method finds heuristic explanation from theoretical works on averaging and generalization such as (Keskar et al., 2016; He et al., 2019) and more practical work on Deep Neural Networks (DNN) optimization such as (Izmailov et al., 2018).
- Plots to show how HWA adapts to the curvature and reaches a better testing accuracy (but worst training loss). Plots with hyperparameters landscape and HWA trajectory on PCA subspace.
- We provide numerical examples showcasing the effectiveness of our method on simple and complex supervised classification tasks.

The remaining of the paper is organized as follows. Section 2 presents the related works in the fields of optimization, Variational Inference and posterior sampling. Section 3 introduces the HWA algorithm which is the main contribution of our paper. Section 4 highlights the benefits of our averaging procedure on simple and complex numerical classification tasks. Section 5 concludes our work.

2 RELATED WORK

Posterior Prediction. Due to the nonconvexity of the loss landscapes involved in modern and complex deep learning tasks, direct sampling from the posterior distribution of the weights is not an option. Depending on the nature and in particular the dimensionality of the problem, Markov Chain Monte Carlo (MCMC) methods have been employed to overcome this intractability issue. By constructing a Markov chain, the samples drawn at convergence are guaranteed to be drawn from the target distribution. Hamiltonian Monte Carlo (HMC) (Neal et al., 2011) or Metropolis Hastings (MH) (Hastings, 1970) are two standard solutions used. Their stochastic gradients counterpart are extensively studied in (Ma et al., 2015).

Variational Inference (VI). When tackling an optimization problem, exact posterior sampling may be computationally involved and not even required. variational inference was proposed in (Graves, 2011), in the particular case of BNNs, in order to fit a Gaussian variational posterior approximation over the weights of neural networks. Through a simple reparameterization trick (Blundell et al., 2015), several methods have emerged to train BNNs leveraging the ease of use and implementation of VI (Kingma et al., 2015; Blundell et al., 2015; Molchanov et al., 2017). Though, those methods appear to be inefficient for large-scale datasets and newer methods were proposed to alleviate this issue such as the use of normalizing flows (Louizos & Welling, 2017), deterministic VI (Wu et al., 2018) or dropout VI (Gal & Ghahramani, 2016).

Stochastic Averaging. Averaging methods include the seminal papers of (Polyak, 1990) and (Ruppert, 1988), both based on the combination of past iterates along a stochastic approximation trajectory. For nonconvex loss objectives, this averaging procedure has been adapted to Stochastic Gradient Descent (SGD) trajectory (Zhou & Cong, 2017). In particular, in modern deep learning examples, Izmailov et al. (2018) develops a novel method that averages snapshots of a deep neural networks (DNN) through the iterations and shows empirical benefits leading to a better generalization. Those experimental discoveries are then backed by theoretical understanding of the DNN loss landscape and the impact of averaging successive iterates in (Keskar et al., 2016; He et al., 2019).

3 HYPERPARAMETERS AVERAGING IN BAYESIAN NEURAL NETWORKS

In this section

3.1 BAYESIAN NEURAL NETWORKS AND ELBO MAXIMIZATION

3.2 HWA: HYPERPARAMETERS WEIGHT AVERAGING

Algorithm 1 HWA: Hyperparameters Weight Averaging

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1: Input: Trained hyperparameters  $\hat{\mu}_\ell$  and  $\hat{\sigma}$ . LR bounds  $\gamma_1$  and  $\gamma_2$ . Cycle length  $c$ .
2: Initialize the hyperparameters of the weights and  $\mu_\ell = \hat{\mu}_\ell$  and  $\mu_\ell^{HWA} = \mu_\ell$ .
3: for  $k = 0, 1, \dots$  do
4:    $\gamma \leftarrow \gamma(k)$  (Cyclical LR for the iteration)
5:    $\mu_\ell^{k+1} \leftarrow \mu_\ell^k - \gamma \nabla \mathcal{L}(\mu_\ell^k)$  (regular SVI update)
6:   if  $\text{mod}(k, c) = 0$  then
7:      $n_{\text{models}} \leftarrow k/c$  (Number of models to average)
8:      $\mu_\ell^{HWA} \leftarrow \frac{n_{\text{models}} \mu_\ell^{HWA} + \mu_\ell^{k+1}}{n_{\text{models}} + 1}$ 
9:      $\mu_\ell^{HWA} \leftarrow \frac{n_{\text{models}} \mu_\ell^{HWA} + \mu_\ell^{k+1}}{n_{\text{models}} + 1}$ 
10:   end if
11: end for

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3.3 THROUGH THE LENSES OF LOSS LANDSCAPES

4 NUMERICAL EXPERIMENTS

5 CONCLUSION

REFERENCES

- Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight uncertainty in neural networks. *arXiv preprint arXiv:1505.05424*, 2015.
- Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pp. 1050–1059, 2016.
- Alex Graves. Practical variational inference for neural networks. In *Advances in neural information processing systems*, pp. 2348–2356, 2011.
- Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. *arXiv preprint arXiv:1706.04599*, 2017.
- W Keith Hastings. Monte carlo sampling methods using markov chains and their applications. 1970.
- Haowei He, Gao Huang, and Yang Yuan. Asymmetric valleys: Beyond sharp and flat local minima. In *Advances in Neural Information Processing Systems*, pp. 2553–2564, 2019.
- Matthew D Hoffman, David M Blei, Chong Wang, and John Paisley. Stochastic variational inference. *The Journal of Machine Learning Research*, 14(1):1303–1347, 2013.
- Pavel Izmailov, Dmitrii Podoprikin, Timur Garipov, Dmitry Vetrov, and Andrew Gordon Wilson. Averaging weights leads to wider optima and better generalization. *arXiv preprint arXiv:1803.05407*, 2018.
- Alex Kendall and Yarin Gal. What uncertainties do we need in bayesian deep learning for computer vision? In *Advances in neural information processing systems*, pp. 5574–5584, 2017.
- Nitish Shirish Keskar, Dheevatsa Mudigere, Jorge Nocedal, Mikhail Smelyanskiy, and Ping Tak Peter Tang. On large-batch training for deep learning: Generalization gap and sharp minima. *arXiv preprint arXiv:1609.04836*, 2016.
- Durk P Kingma, Tim Salimans, and Max Welling. Variational dropout and the local reparameterization trick. In *Advances in neural information processing systems*, pp. 2575–2583, 2015.
- Christos Louizos and Max Welling. Multiplicative normalizing flows for variational bayesian neural networks. *arXiv preprint arXiv:1703.01961*, 2017.
- Yi-An Ma, Tianqi Chen, and Emily Fox. A complete recipe for stochastic gradient mcmc. In *Advances in Neural Information Processing Systems*, pp. 2917–2925, 2015.
- Dmitry Molchanov, Arsenii Ashukha, and Dmitry Vetrov. Variational dropout sparsifies deep neural networks. *arXiv preprint arXiv:1701.05369*, 2017.
- Radford M Neal. *Bayesian learning for neural networks*, volume 118. Springer Science & Business Media, 2012.
- Radford M Neal et al. Mcmc using hamiltonian dynamics. *Handbook of markov chain monte carlo*, 2(11):2, 2011.
- Boris T Polyak. A new method of stochastic approximation type. *Avtomat. i Telemekh.*, (7):98:107, 1990.
- Boris T Polyak and Anatoli B Juditsky. Acceleration of stochastic approximation by averaging. *SIAM journal on control and optimization*, 30(4):838–855, 1992.
- David Ruppert. Efficient estimations from a slowly convergent robbins-monro process. Technical report, Cornell University Operations Research and Industrial Engineering, 1988.
- Anqi Wu, Sebastian Nowozin, Edward Meeds, Richard E Turner, José Miguel Hernández-Lobato, and Alexander L Gaunt. Deterministic variational inference for robust bayesian neural networks. *arXiv preprint arXiv:1810.03958*, 2018.
- Fan Zhou and Guojing Cong. On the convergence properties of a k -step averaging stochastic gradient descent algorithm for nonconvex optimization. *arXiv preprint arXiv:1708.01012*, 2017.

A APPENDIX

You may include other additional sections here.