An Ensemble of Neural Nets

Rahul Ramesh

STAT-991

Problem Setting

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and is well-calibrated.

$$\gamma = \mathbb{P}(Y|p_h(Y|X) = q)$$
$$c(h) = \mathop{\mathbb{E}}_{q}\left[d(\gamma, q)\right]$$

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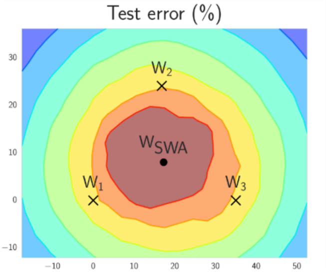

Figure: See Izmailov et al. (2018)

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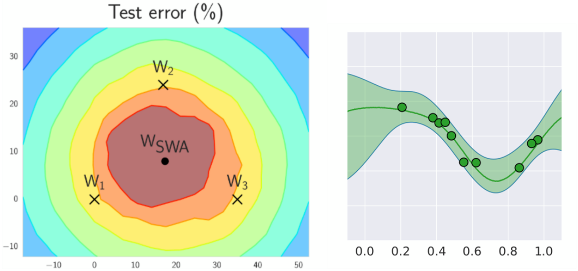

Figure: See Izmailov et al. (2018) and Ovadia et al. (2019)

Outline

We discuss some popular Bayesian methods for deep learning.

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We explore some recent results that make use of ensembles.

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The Bayes posterior

Consider a dataset $D = \{x_i, y_i\}_{i=1}^n$ and the negative log-likelihood

$$U(\theta) = -\log p(\theta) - \sum_{i=1}^{n} \log p(y_i | x_i, \theta).$$

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Instead, we hedge our bets and consider a distribution over parameters

$$p(\theta|D) \propto p(D|\theta)p(\theta) = \exp(-U(\theta))$$

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$$\theta_1, \theta_2, \cdots \theta_k \sim p(\theta|D),$$

and use them to make predictions.

$$p(y|x, D) \approx \frac{1}{k} \sum_{i=1}^{k} p(y|x, \theta_i)$$

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2. Markov-chain Monte-carlo (MCMC)

Variational Approximation

The ELBO forms the basis of VI methods (Blundell et al., 2015; Wen et al., 2018; Louizos and Welling, 2016)

$$\log p(y|x) \geq \mathbb{E}_{q_w(\theta)}[\log p(y|x,\theta)] - \mathbb{E}_{q_w(\theta)}\left[\log \frac{q_w(\theta)}{p(\theta)}\right]$$

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$w = (\mu, \Sigma)$ are now the learnable parameters. We assume $p(\theta) = \mathcal{N}(0, \mathbb{I})$.

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Consider dropout (Gal and Ghahramani, 2016), which randomly sets some parameters to 0 during training.

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is the gradient with dropout.
The second term is usually absent in an implementation of dropout

$$\mathbb{E}_{q_\mu(\theta)}[\log \frac{q_\mu(\theta)}{p(\theta)}]$$

but approximately corresponds to the L2-penalty.

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Parameters with low losses are sampled more frequently.

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Consider the stochastic differential equation (SDE)

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Hence, if we simulate the SDE, we will converge to the stationary distribution

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Introduce a ”velocity” variable and attempt to conserve the Hamiltonian of the system.

A closer look at Bayesian posteriors

How Good is the Bayes Posterior in Deep Neural Networks Really?

Florian Wenzel[* 1] **Kevin Roth**[* + 2] **Bastiaan S. Veeling**[* + 3 1] **Jakub Świątkowski**[4 +] **Linh Tran**[5 +]
Stephan Mandt[6 +] **Jasper Snoek**[1] **Tim Salimans**[1] **Rodolphe Jenatton**[1] **Sebastian Nowozin**[7 +]

What Are Bayesian Neural Network Posteriors Really Like?

Pavel Izmailov[1] **Sharad Vikram**[2] **Matthew D. Hoffman**[2] **Andrew Gordon Wilson**[1]

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MCMC is compute intensive but accurate.

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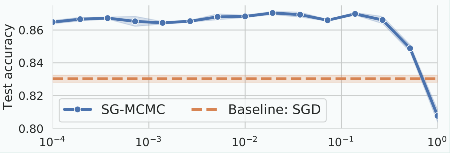

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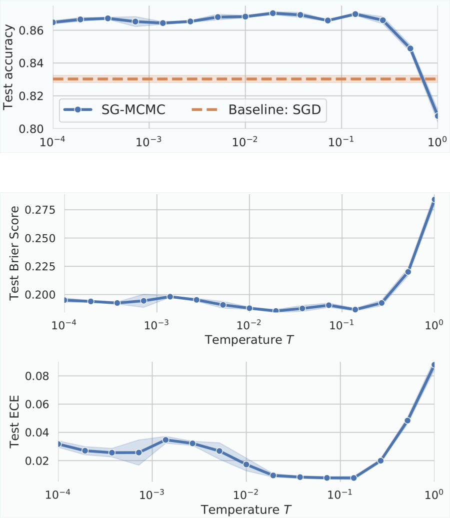

Cold posteriors

Most MCMC methods in literature use a cold-posterior.

Related work that uses $T < 1$ posteriors in SG-MCMC. The following table lists work that uses SG-MCMC on deep neural networks and tempers the posterior.[3]

Reference	Temperature T
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This is problematic since we artificially sharpen the posterior and scale the variance of the prior.

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- Inadequate prior
- SGD does not work with Bayesian methods

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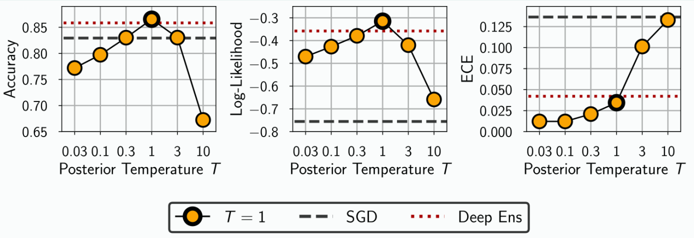

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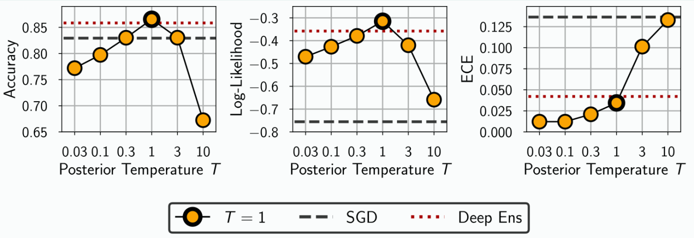

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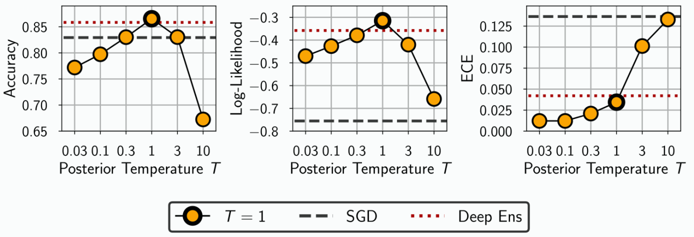

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  - Compute hungry
  - Doesn't work with augmentations yet
- We want an inexpensive and accurate model that captures the Bayes posterior

Ensembles

Emergence of Ensembles

Revisiting earlier experiments

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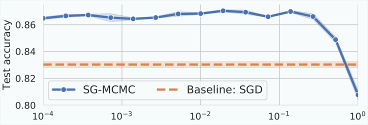

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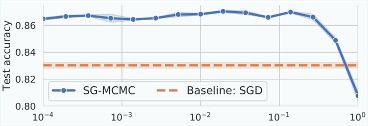

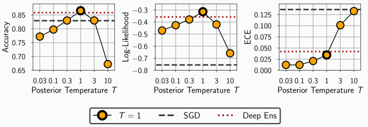

- Cold posteriors are better
- Deep ensembles match the accuracy and calibration of HMC.

Emergence of Ensembles

We focus on ensembles, which are finite particle approximations of the posterior

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Ensembles are common in machine learning (Breiman, 1996; Schapire, 1990).

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Instead of training a single neural net

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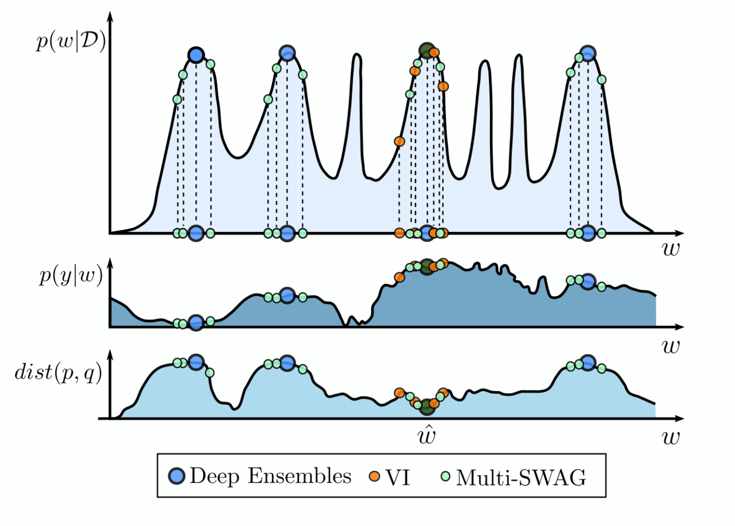
we train k copies of it, each initialized randomly:

$$\theta_1 \quad \theta_2 \quad \cdots \quad \theta_k$$

Why do they work?

Ensembles capture different modes (Wilson and Izmailov, 2020).



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Variational inference methods are not nearly as diverse (Fort et al., 2019).

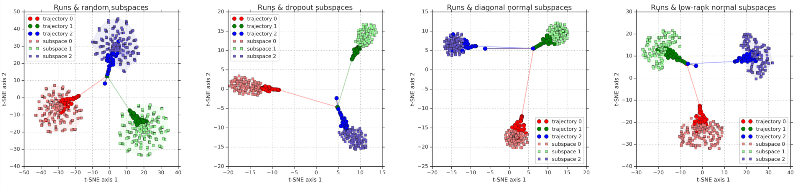

Figure: 1) Random 2) Dropout 3) Diagonal Gaussian 4) Low-rank Gaussian

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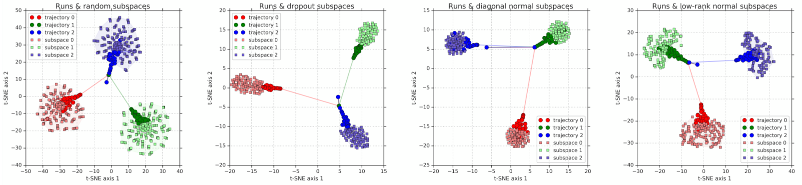

Figure: 1) Random 2) Dropout 3) Diagonal Gaussian 4) Low-rank Gaussian

Initialization influences diversity in predictions more than other factors.

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In practice, we don't use the repulsion term and find random initializations to be sufficient.

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We focus in evaluations in Imagenet, which used at most 10 models for ensembling.

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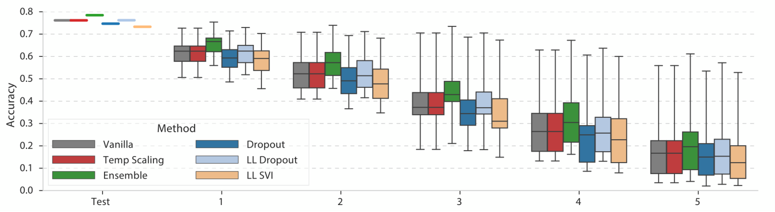

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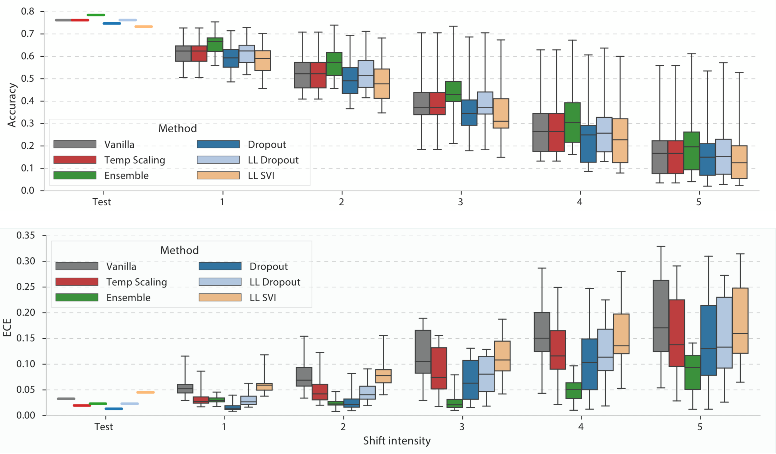

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$$U(\theta) = -\log p(\theta) + \cdots$$

includes the prior.

Usually, the prior is

$$p(\theta) \stackrel{d}{=} \mathcal{N}(0, I)$$

Wilson and Izmailov (2020); Wenzel et al. (2020) mention the importance of the prior but it is relatively unexplored beyond Gaussians.

Deep Reference Priors

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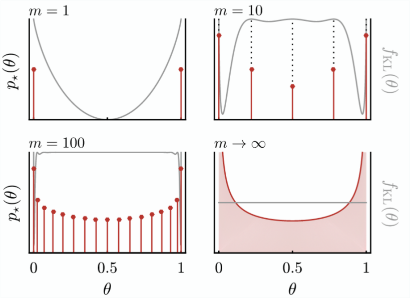

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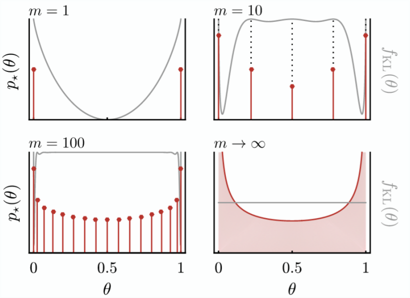
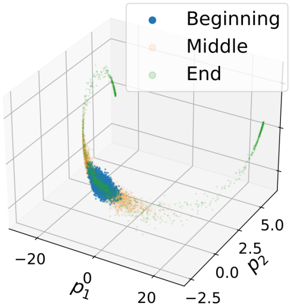
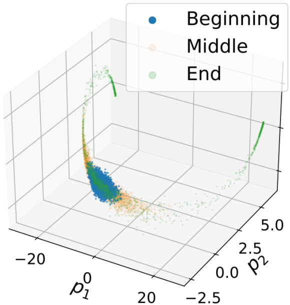


Reference priors are supported on a finite number of atoms

Deep Reference Priors



Deep Reference Priors



Method	Samples				
	50	100	250	500	1000
MixMatch	64.21	80.29	88.91	90.35	92.25
FixMatch (RA)	86.19 $\pm$ 3.37 (40)	90.12	94.93 $\pm$ 0.65	93.91	94.3
Deep Reference Prior	85.45 $\pm$ 2.12	88.53 $\pm$ 0.67	92.13 $\pm$ 0.39	92.94 $\pm$ 0.22	93.48 $\pm$ 0.24

Conclusion

We approximate the Bayes posterior using ensembles, which are effective even on large datasets.

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Can we do better?

References I

Blundell, C., Cornebise, J., Kavukcuoglu, K., and Wierstra, D. (2015). Weight uncertainty in neural network. In *International conference on machine learning*, pages 1613–1622. PMLR.

Breiman, L. (1996). Bagging predictors. *Machine learning*, 24(2):123–140.

D'Angelo, F. and Fortuin, V. (2021). Repulsive deep ensembles are bayesian. *Advances in Neural Information Processing Systems*, 34.

Fort, S., Hu, H., and Lakshminarayanan, B. (2019). Deep ensembles: A loss landscape perspective. *arXiv preprint arXiv:1912.02757*.

Gal, Y. and Ghahramani, Z. (2016). Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pages 1050–1059. PMLR.

Gao, Y., Ramesh, R., and Chaudhari, P. (2022). Deep reference priors: What is the best way to pretrain a model? *arXiv preprint arXiv:2202.00187*.

Izmailov, P., Podoprikhin, D., Garipov, T., Vetrov, D., and Wilson, A. G. (2018). Averaging weights leads to wider optima and better generalization. *arXiv preprint arXiv:1803.05407*.

Izmailov, P., Vikram, S., Hoffman, M. D., and Wilson, A. G. G. (2021). What are bayesian neural network posteriors really like? In *International Conference on Machine Learning*, pages 4629–4640. PMLR.

Louizos, C. and Welling, M. (2016). Structured and efficient variational deep learning with matrix gaussian posteriors. In *International conference on machine learning*, pages 1708–1716. PMLR.

Ovadia, Y., Fertig, E., Ren, J., Nado, Z., Sculley, D., Nowozin, S., Dillon, J., Lakshminarayanan, B., and Snoek, J. (2019). Can you trust your model's uncertainty? evaluating predictive uncertainty under dataset shift. *Advances in neural information processing systems*, 32.

Schapire, R. E. (1990). The strength of weak learnability. *Machine learning*, 5(2):197–227.

Welling, M. and Teh, Y. W. (2011). Bayesian learning via stochastic gradient langevin dynamics. In *Proceedings of the 28th international conference on machine learning (ICML-11)*, pages 681–688. Citeseer.

Wen, Y., Vicol, P., Ba, J., Tran, D., and Grosse, R. (2018). Flipout: Efficient pseudo-independent weight perturbations on mini-batches. *arXiv preprint arXiv:1803.04386*.

Wenzel, F., Roth, K., Veeling, B. S., Świątkowski, J., Tran, L., Mandt, S., Snoek, J., Salimans, T., Jenatton, R., and Nowozin, S. (2020). How good is the bayes posterior in deep neural networks really? *arXiv preprint arXiv:2002.02405*.

Wilson, A. G. and Izmailov, P. (2020). Bayesian deep learning and a probabilistic perspective of generalization. *Advances in neural information processing systems*, 33:4697–4708.