A Symmetry-Aware Exploration of Bayesian DNN Posteriors

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Motivations

Most successful deep learning uncertainty quantification methods — Deep Ensembles, SWA(G), MC Dropout, etc — seek to approximate the Bayesian posterior via marginalization over the weights:

$$p(y \mid \boldsymbol{x}, \mathcal{D}) = \int_{\omega \in \Omega} p(y \mid \boldsymbol{x}, \omega) p(\omega \mid \mathcal{D}) d\omega$$

However, in modern deep neural networks, there exists a large or infinite number of corresponding weight configurations.

- Scaling the weights by sequences of coefficients and their inverses leaves the function unchanged.
- Reordering the weights using sequences of permutation matrices and their inverses does not change the function.

→ Symmetries impact optimization, generalization via the loss landscape.

? What is the impact of symmetries on Bayesian posteriors and their estimation by uncertainty quantification methods?

Contributions & Presentation layout

A - Express the theoretical impact of perm./scaling symmetries on the posterior.

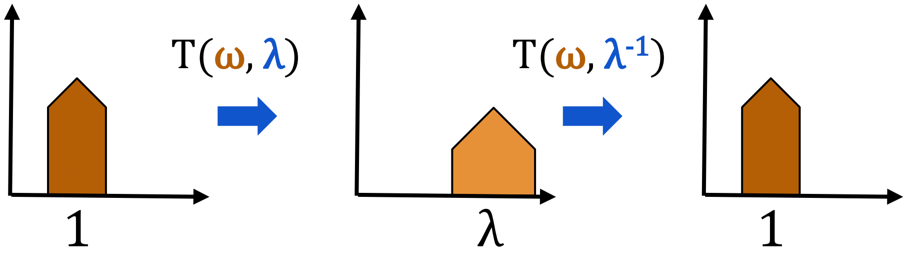
B - Evaluate & discuss the impact of symmetries on UQ methods through quantitative performance & diversity analysis.

C - The min. of the weight decay on scaling symmetries has a unique solution.

D - "Checkpoints": dataset of medium-sized independently trained models.

Notations & Theory

- Permutation symmetries
- Scaling symmetries
- other symmetries (partially accounted for)



Scaling symmetries & activations

Proposition:

With the *r.v.* of the scaled and sorted weights, the final posterior is a continuous mixture of discrete mixtures of the "original" posterior $p(\tilde{\Omega} \mid \mathcal{D})$:

$$p(\Omega \mid \mathcal{D}) = |\mathbb{\Pi}|^{-1} \int_{\Lambda \in \mathbb{\Lambda}} \sum_{\Pi \in \mathbb{\Pi}} \mathcal{T}_p(\mathcal{T}_s(p(\tilde{\Omega} \mid \mathcal{D}), \Lambda), \Pi) p(\Lambda) d\Lambda$$

Corollary:

With independent and layer-wise constant initializations, $p(\omega_{i,j}^{[l]} | \mathcal{D}) = p(\omega_{0,j}^{[l]} | \mathcal{D})$, for all i, j at layer l.

Uncertainty Performance & Posterior quality estimation

A — Perf. & Aleatoric Uncertainty

➡ Multi-mode methods obtain better scores in accuracy, calibration and Brier score *i.e.* better aleatoric uncertainty estimation.

B — Epistemic Uncertainty

➡ Multi-mode methods consistently perform better.

➡ No clear correlation with posterior quality estimation.

C — ID & OOD Diversity

➡ Multi-mode methods exhibit more diversity either in- and out- of-distribution.

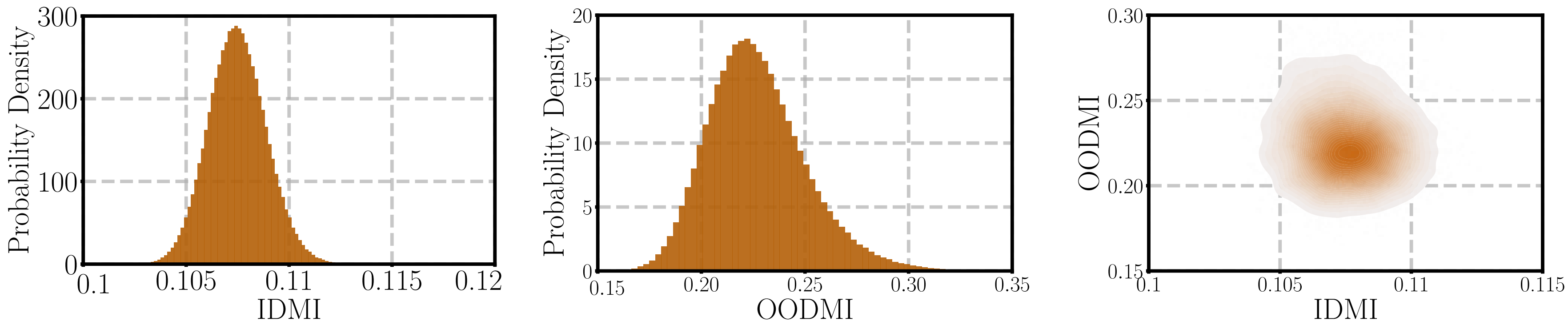
			Posterior quality			Calibration			OOD detection		Diversity	
		Method	MMD ↓	NS ↓	Acc ↑	ECE ↓	ACE ↓	Brier ↓	AUPR ↑	FPR95 ↓	**IDMI** ↓	**OODMI** ↑
CIFAR100	**One Mode**	Dropout	4.5	7.5	74.2	14.7	3.2	38.8	76.4	47.7	5.7	9.1
		vBNN	2.0	10.2	57.9	24.6	3.0	63.7	60.9	79.1	2.7	4.2
		SWAG	6.7	7.2	70.9	2.3	1.2	38.9	86.2	48.0	2.4	6.3
		Laplace	5.7	7.0	75.1	**0.9**	0.9	34.6	81.3	42.4	27.6	63.3
		SGHMC	7.5	7.9	73.7	4.9	1.0	36.2	79.4	62.3	**0.2**	0.5
	Multi Mode	Dropout	0.7	4.5	**79.5**	4.3	1.0	29.2	78.2	48.1	20.5	46.3
		vBNN	6.1	5.6	66.5	2.8	2.0	45.3	71.9	71.7	45.5	81.1
		SWAG	5.0	5.4	72.8	1.5	1.1	36.9	**89.1**	50.6	6.5	19.7
		Laplace	0.6	4.3	78.9	6.9	0.8	30.3	82.9	**41.3**	44.1	**98.5**
		DE	**0.0**	**0.0**	**79.5**	1.6	**0.6**	**28.7**	81.1	45.6	22.5	58.0
TinyImageNet	**One Mode**	Dropout	9.5	4.9	63.2	16.4	2.4	53.9	48.8	81.1	8.3	8.4
		SWAG	9.1	3.9	66.4	10.5	0.7	46.2	61.9	57.7	3.0	4.5
		Laplace	5.5	6.1	33.1	6.0	3.6	77.1	48.8	77.7	200.7	228.0
		SGHMC	9.8	5.3	58.3	**2.6**	1.0	54.1	56.3	72.7	**0.24**	0.30
	M. Mode	Dropout	4.3	1.8	70.2	9.9	1.2	42.1	74.8	58.2	34.1	60.0
		SWAG	6.7	5.4	69.3	3.6	**0.6**	41.3	**96.5**	55.9	17.6	32.1
		Laplace	0.5	3.1	37.0	10.9	3.3	75.1	48.4	72.5	219.5	**254.7**
		DE	**0.0**	**0.0**	**70.3**	6.5	0.7	**40.9**	86.3	**50.2**	38.4	83.4

Comparison of popular methods approximating the Bayesian posterior - ResNet-18

Functional Collapse & Diversity

We take 1000 independent networks from "**Checkpoints**" and compute mutual information over the test set for each pair.

$$\mathrm{MI} = \mathcal{H}\left(\frac{1}{M}\sum_{m=1}^{M} P_{\omega_m}(\hat{y}|\boldsymbol{x},\mathcal{D})\right) - \frac{1}{M}\sum_{m=1}^{M}\mathcal{H}(P_{\omega_m}(\hat{y}|\boldsymbol{x},\mathcal{D}))$$



Pairwise mutual information - ResNet-18 - CIFAR-100/SVHN

→ Very **low** dispersion of the **in-distribution diversity**.

→ **Greater** dispersion of the **OOD diversity**.

→ **ID** & **OOD diversities** seem only very **weakly correlated**.

Scaling Symmetries & Representation Cost

The minimization of the L2 norm of the weights (the representation cost)

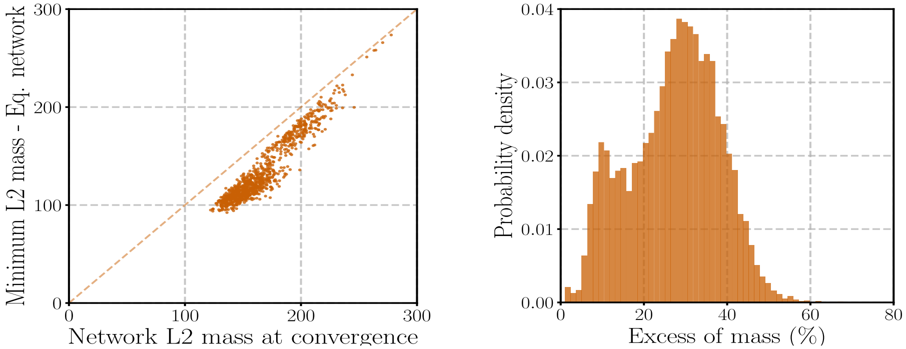
$$m^* = \min_{\Lambda \in \mathbb{\Lambda}} |\mathcal{T}_s(\bar{\omega}, \Lambda)|_2^2$$

over scaling symmetries is log-log strictly convex.

→ Unique solution found via convex optim.

Gaussian-regularized training (weight decay) empirically never converges towards the minimal scaling coefficient for the scaled representation cost.

→ Negligible gradients vs. SGD noise.



Mass profiles of simple ConvNets

⚠ Batch normalization → degenerate problem.

Dataset & PyTorch Library

"Checkpoints" @ 🤗

Easy to download models & scripts:

- 1,024 ResNet-20 FRN/SiLU – CIFAR-10
- 2,048 ResNet-18 – CIFAR-10
- 9,216 ResNet-18 – CIFAR-100
- 2,048 ResNet-18 – TinyImageNet

huggingface.co/torch-uncertainty

TorchUncertainty

Open-source uncertainty for deep learning models in PyTorch 🌱

Uncertainty-aware routines for training classification, segmentation, regression & monocular depth in PyTorch with lightning.

torch-uncertainty.github.io