On the Importance of Priors in Bayesian Deep Learning

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RIKEN AIP (remotely)

April 2022

Agenda

- Pathologies of common BNN priors
  - BNN priors and the cold posterior effect
  - The role of data augmentation
- How to find better priors
  - Empirical Bayes using the marginal likelihood
  - (PAC-)Bayesian meta-learning
- How to use function-space priors
  - Repulsive deep ensembles
  - GP priors in the latent space

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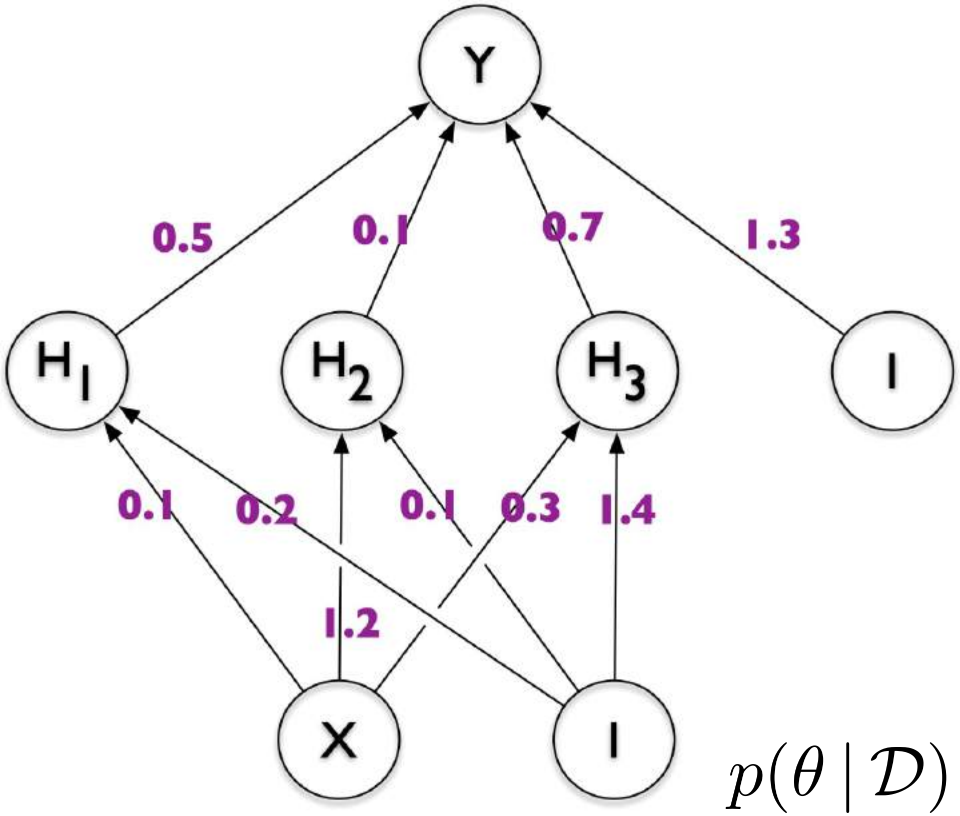
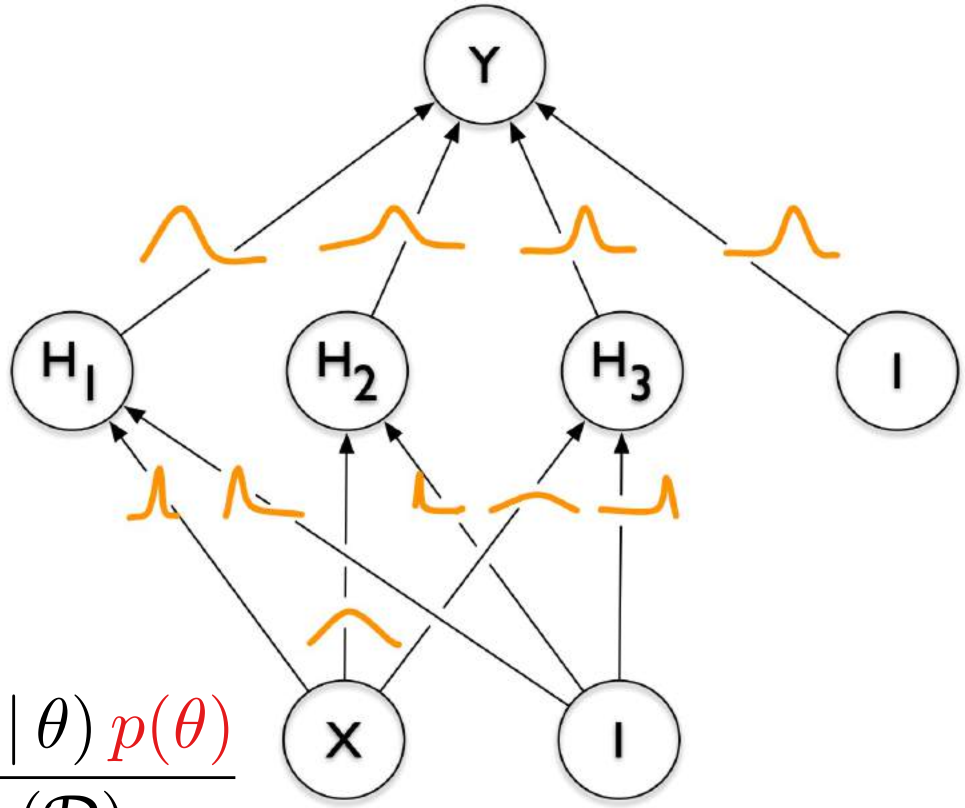
Background: Bayesian Neural Networks

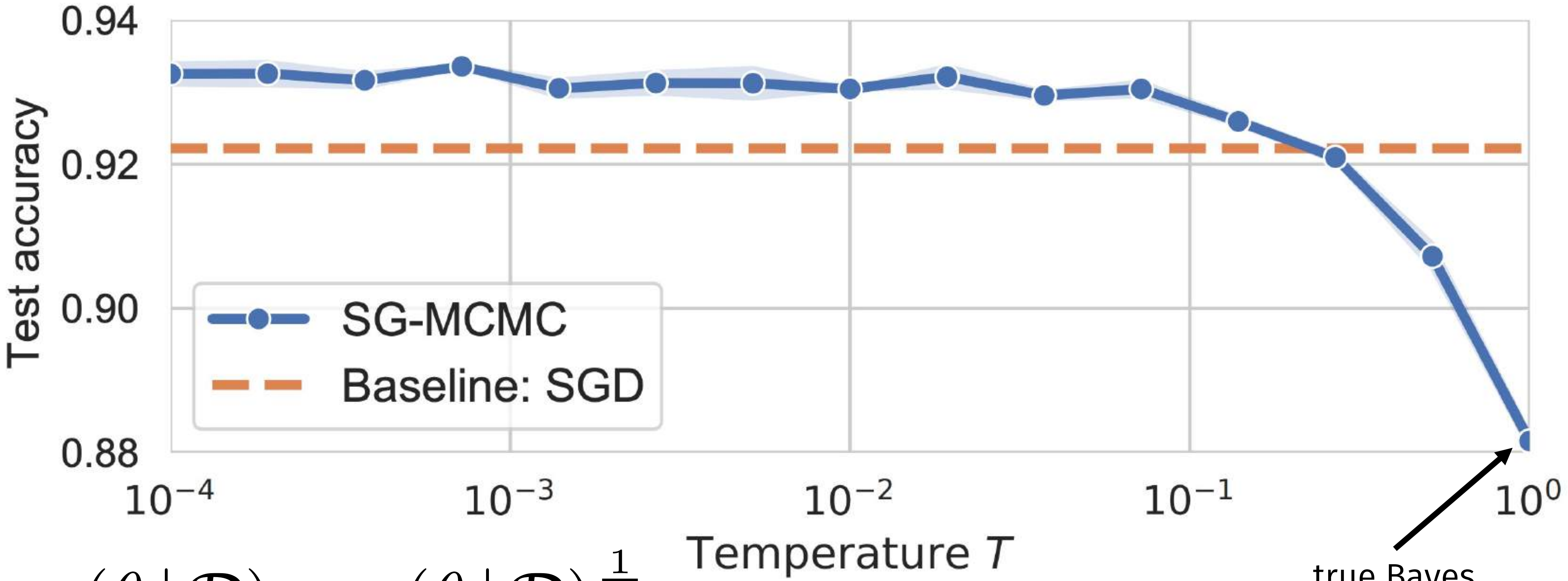




$$p(\theta \,|\, \mathcal{D}) = \frac{p(\mathcal{D} \,|\, \theta)\, {\color{red} p(\theta)}}{p(\mathcal{D})}$$

[Blundell, Cornebise, Kavukcuoglu, Wierstra 2015]

Motivation: Cold-posterior effect



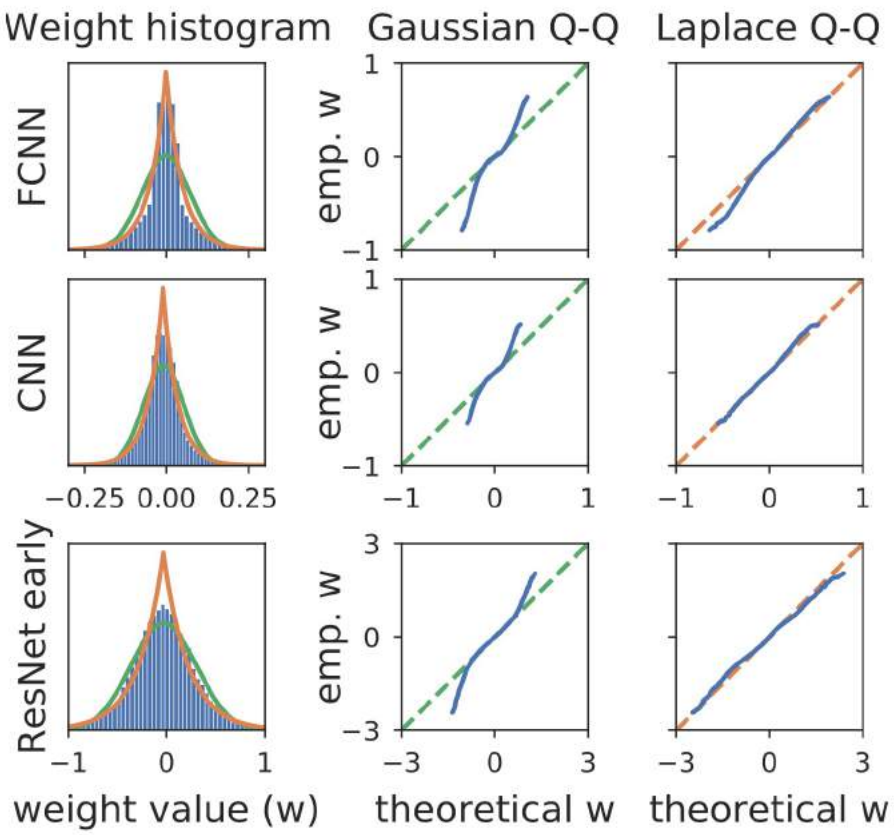
$$p_T(\theta \,|\, \mathcal{D}) \propto p(\theta \,|\, \mathcal{D})^{\frac{1}{T}}$$

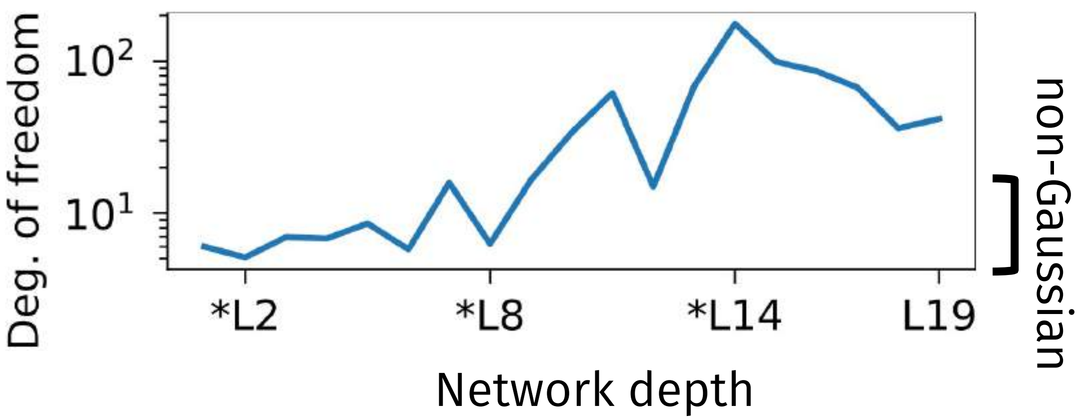
true Bayes posterior

[Wenzel, Roth, Veeling, Swiatkowski, Tran, Mandt, Snoek, Salimans, Jenatton, Nowozin 2020]

Empirical FCNN weights are heavy-tailed

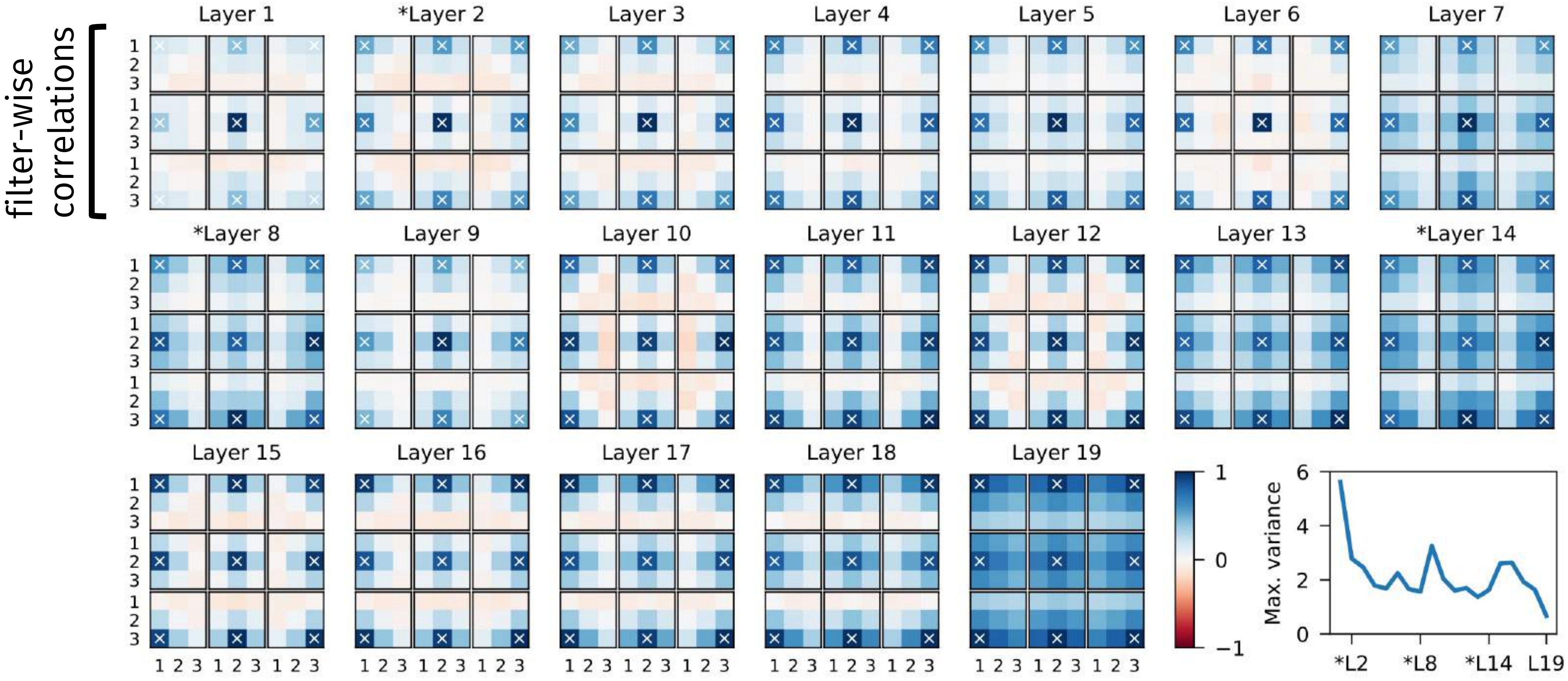
[F, Garriga-Alonso, Ober, Wenzel, Rätsch, Turner, van der Wilk, Aitchison. ICLR 2022]





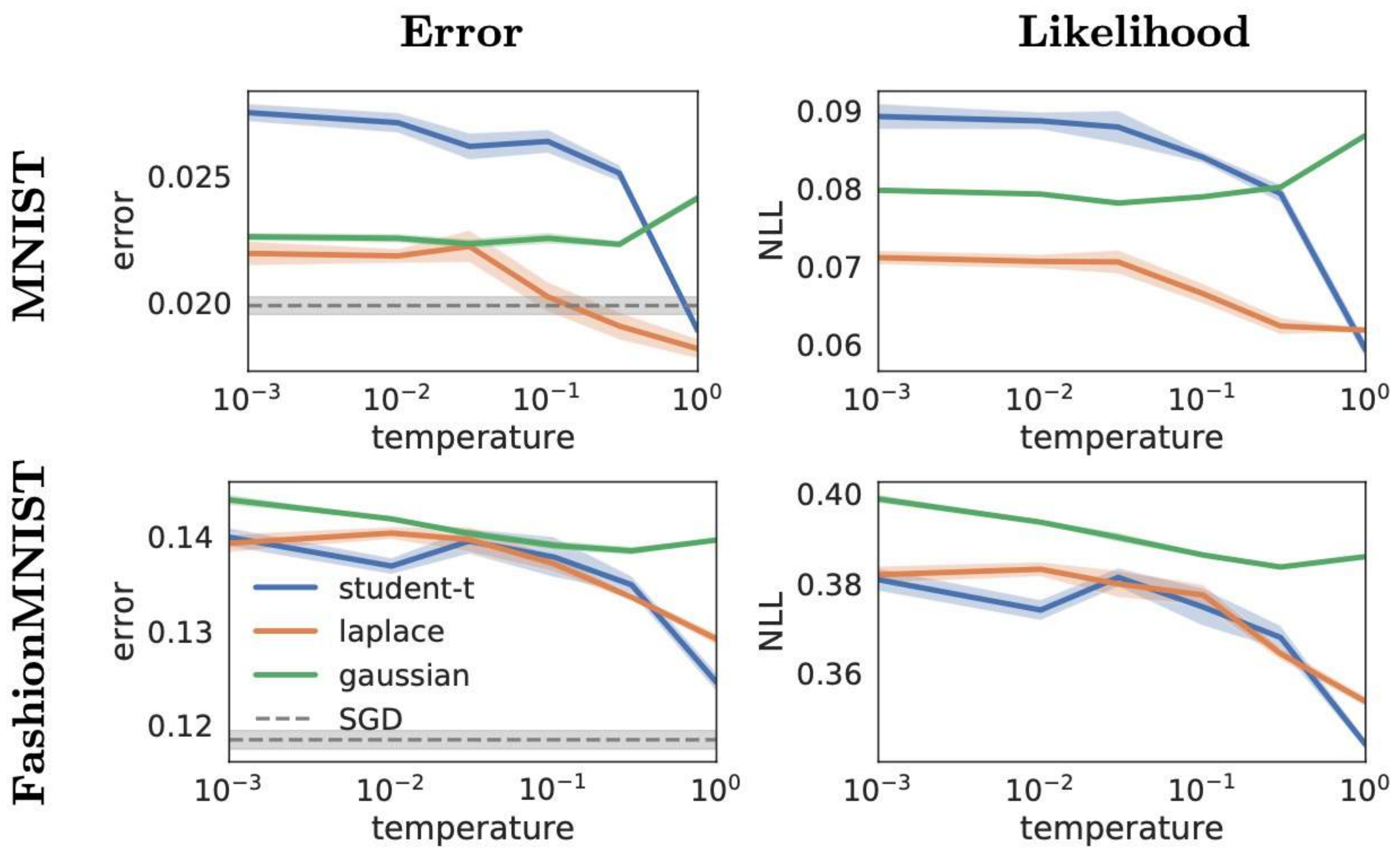
Empirical CNN weights are correlated

[F, Garriga-Alonso, Ober, Wenzel, Rätsch, Turner, van der Wilk, Aitchison. ICLR 2022]



Bayesian FCNNs with different priors

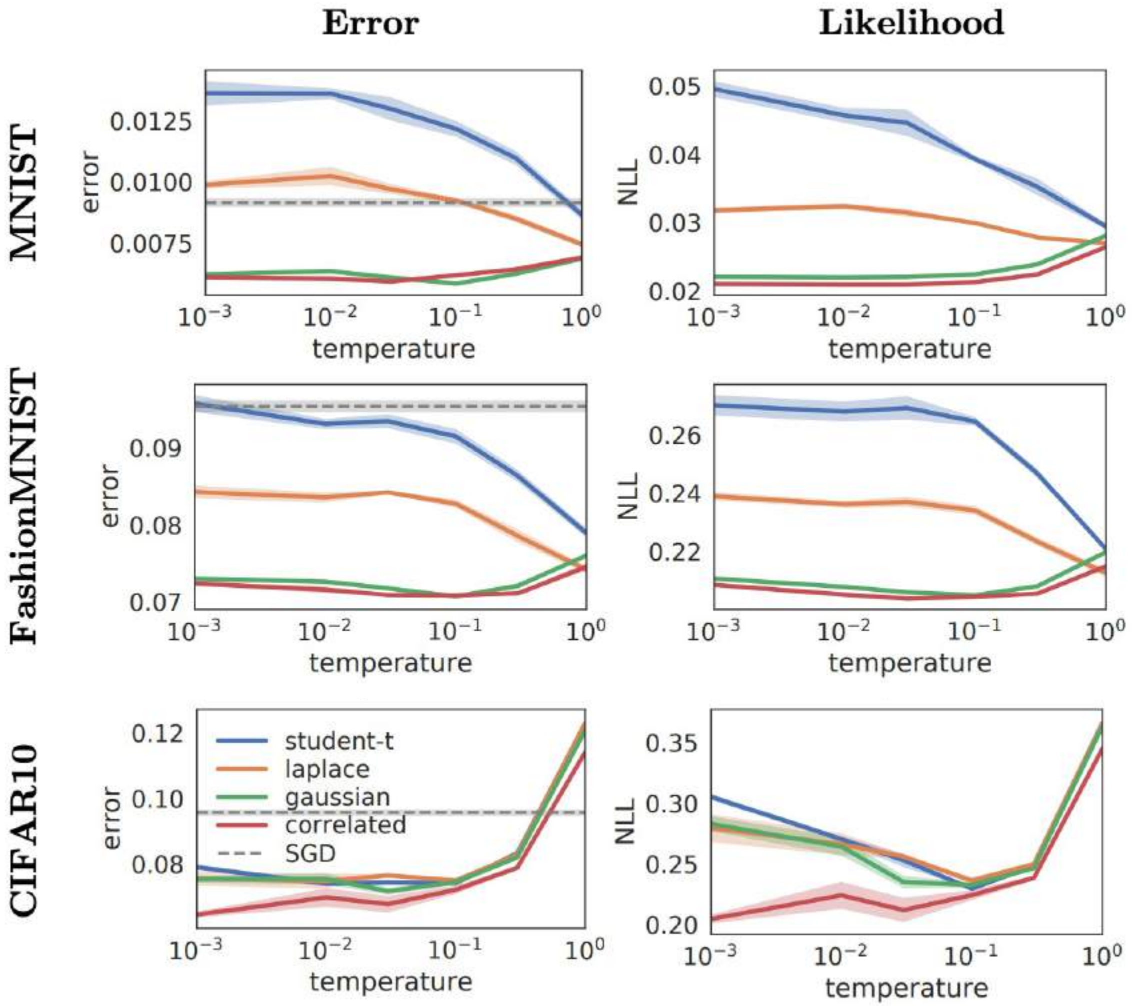
[F, Garriga-Alonso, Ober, Wenzel, Rätsch, Turner, van der Wilk, Aitchison. ICLR 2022]



heavy-tailed priors
perform better
and reduce
cold-posterior effect

Bayesian CNNs with different priors

[F, Garriga-Alonso, Ober, Wenzel, Rätsch, Turner, van der Wilk, Aitchison. ICLR 2022]



correlated prior performs better
but retains cold-posterior effect

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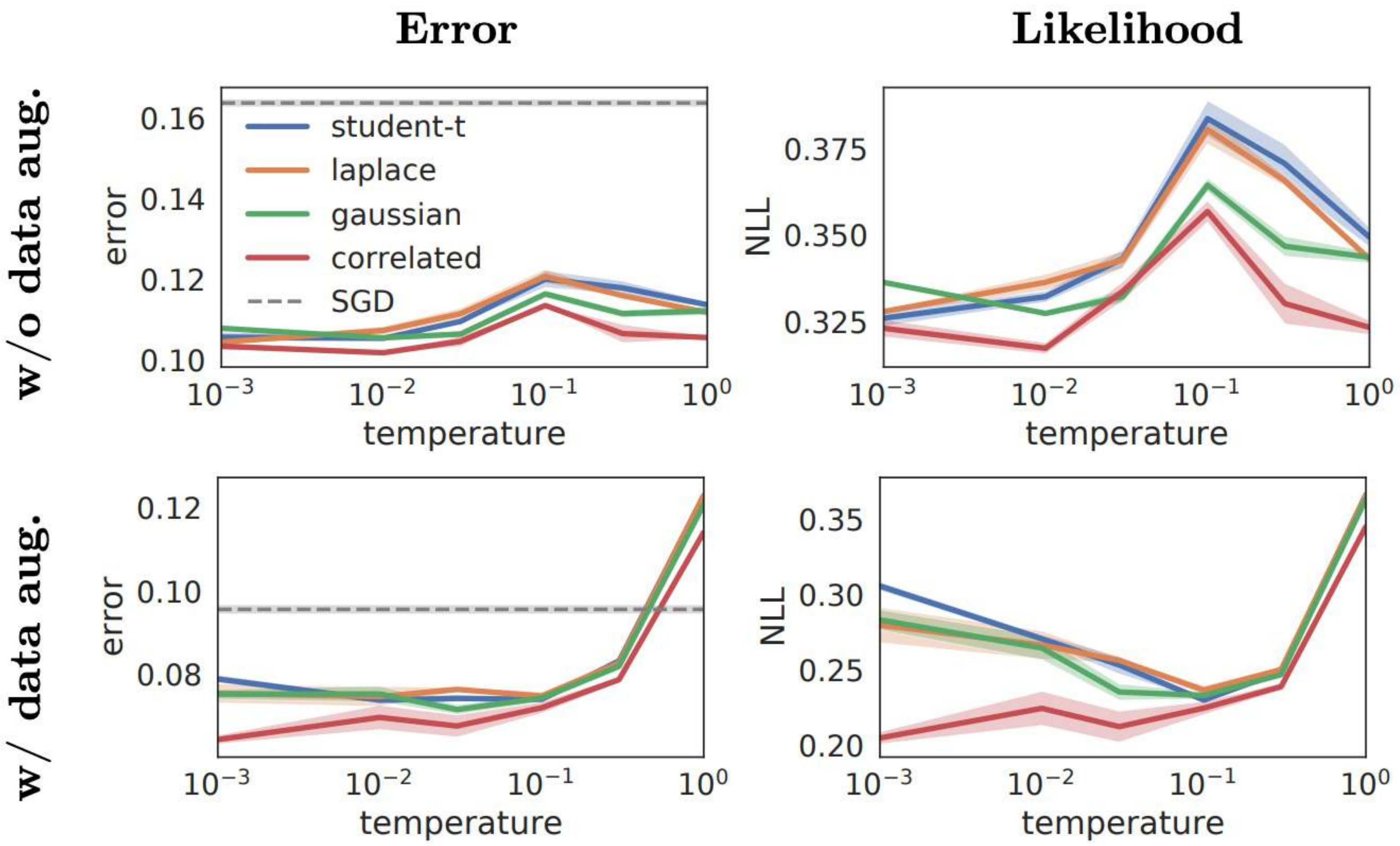
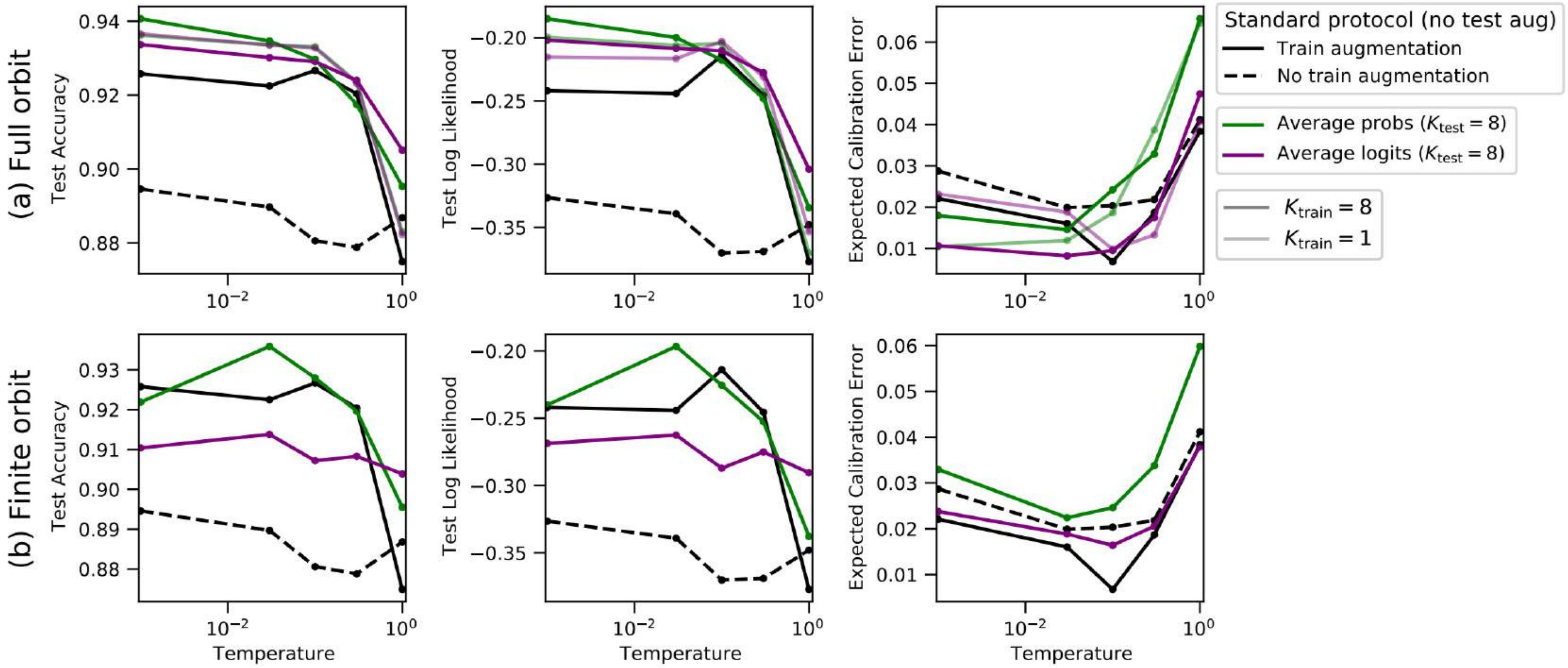
Caveat: Data augmentation plays a role!

[F, Garriga-Alonso, Ober, Wenzel, Rätsch, Turner, van der Wilk, Aitchison. ICLR 2022]



Averaging logits/probs doesn't help

[Nabarro, Ganev, Garriga-Alonso, F, van der Wilk, Aitchison. arXiv 2021]



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Marginal likelihood prior selection

[Immer, Bauer, F, Rätsch, Khan. ICML 2021]

MAP solution

$$\log p(\mathcal{D}|\mathcal{M}) \approx \log q(\mathcal{D}|\mathcal{M}) := \log p(\mathcal{D}, \boldsymbol{\theta}_*|\mathcal{M}) - \frac{1}{2}\log\left|\frac{1}{2\pi}\mathbf{H}_{\boldsymbol{\theta}_*}\right|$$

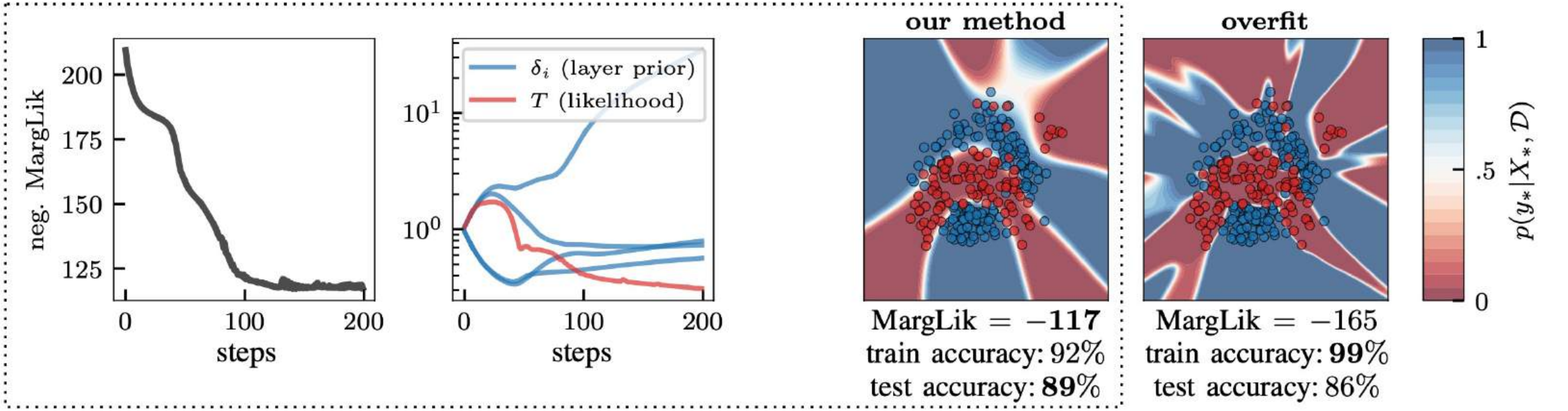
Hessian

Jacobian

$$\mathbf{H}_{\boldsymbol{\theta}} \approx \mathbf{H}_{\boldsymbol{\theta}}^{\mathrm{GGN}} = \mathbf{J}_{\boldsymbol{\theta}}^{\mathsf{T}}\mathbf{L}_{\boldsymbol{\theta}}\mathbf{J}_{\boldsymbol{\theta}} + \mathbf{P}_{\boldsymbol{\theta}}$$

$$|\mathbf{H}_{\boldsymbol{\theta}}^{\mathrm{GGN}}| \approx |\mathbf{H}_{\boldsymbol{\theta}}^{\mathrm{KFAC}}| = \prod_l \prod_{ij} \mathbf{q}_i^{(l)}\mathbf{w}_j^{(l)} + p_{\theta}^{(l)}$$

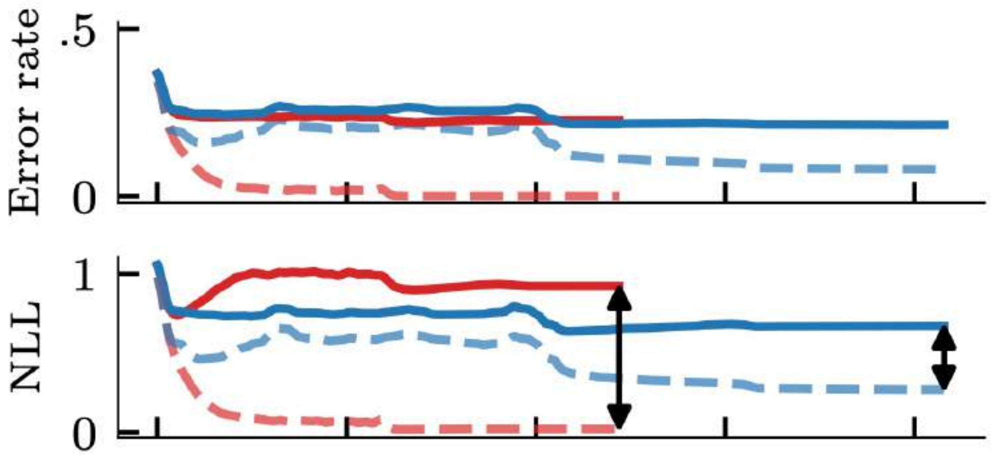
Step 1: Optimize Marginal-Likelihood wrt. hyperparameters **Step 2:** Compare marginal likelihood of models



ML-II prior improves generalization

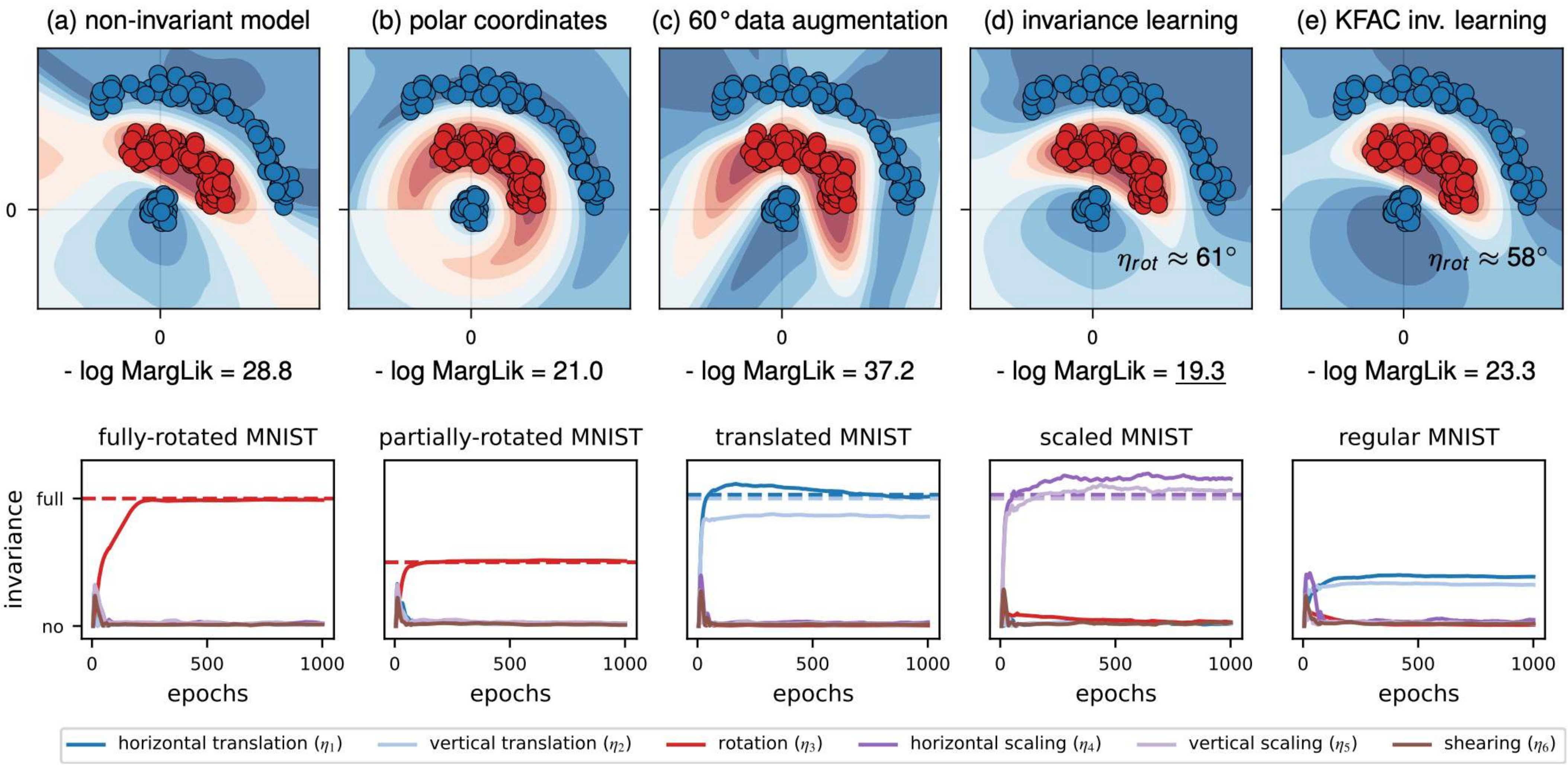
[Immer, Bauer, F, Rätsch, Khan. ICML 2021]

		cross-validation		marginal likelihood optimization					
				KFAC			diagonal EF		
Dataset	Model	accuracy	logLik	accuracy	logLik	MargLik	accuracy	logLik	MargLik
MNIST	**MLP**	98.22	−0.061	98.38	−0.053	−0.158	97.05	−0.095	−0.553
	CNN	99.40	**−0.017**	**99.46**	**−0.016**	**−0.064**	**99.45**	−0.019	−0.134
FMNIST	**MLP**	88.09	−0.347	89.83	−0.305	−0.468	85.72	−0.400	−0.756
	CNN	91.39	−0.258	**92.06**	**−0.233**	**−0.401**	91.69	**−0.233**	−0.570
CIFAR10	**CNN**	77.41	−0.680	80.46	−0.644	−0.967	80.17	−0.600	−1.359
	ResNet	83.73	−1.060	**86.11**	−0.595	**−0.717**	**85.82**	**−0.464**	−0.876



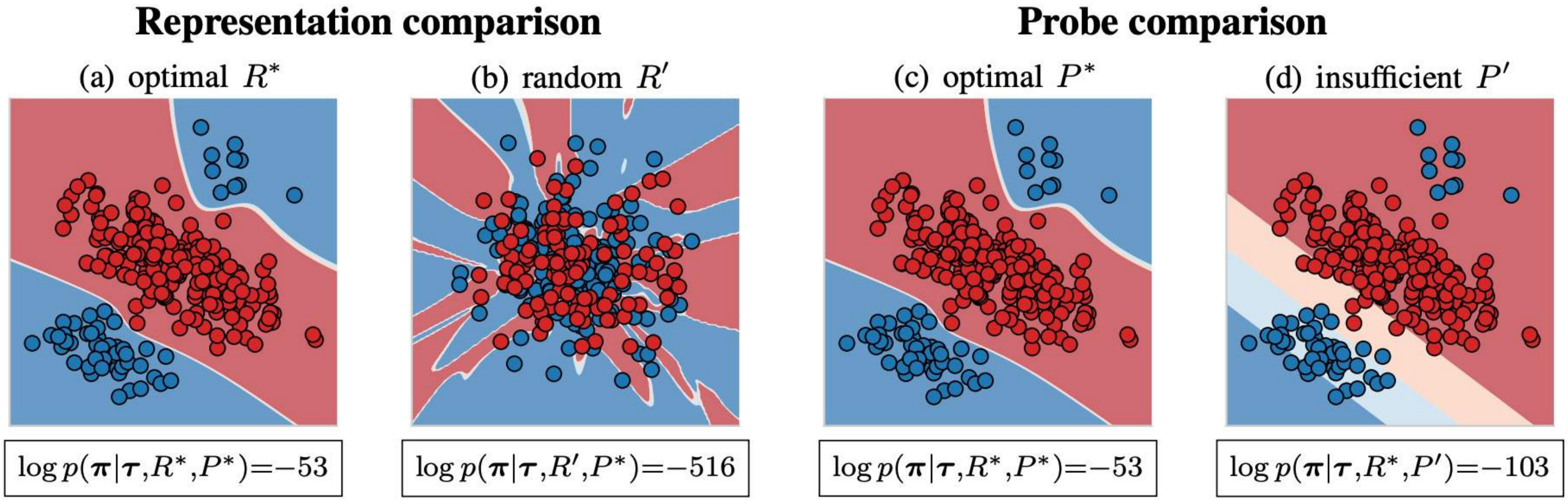
Sidenote: Learning invariances

[Immer, van der Ouderaa, F, Rätsch, van der Wilk. arXiv 2022]



Another sidenote: Linguistic probing

[Immer, Torroba-Hennigen, F, Cotterell. ACL 2022]



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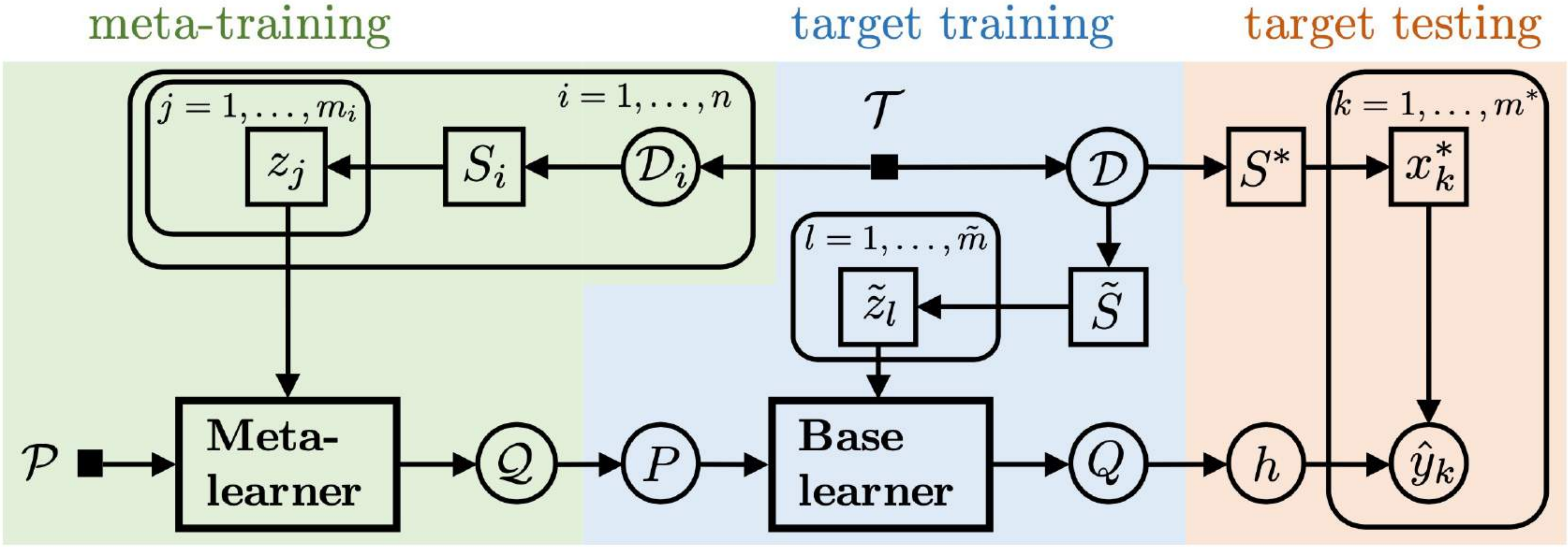
PAC-Bayesian meta-learning

[Rothfuss, F, Josifoski, Krause. ICML 2021]



PAC-Bayesian meta-learning

[Rothfuss, F, Josifoski, Krause. ICML 2021]

$$\mathcal{Q}^*(P) = \frac{\mathcal{P}(P) \exp\left(\frac{\lambda}{n\beta + \lambda} \sum_{i=1}^{n} \ln Z_\beta(S_i, P) \right)}{Z^{II}(S_1, \dots, S_n, \mathcal{P})}$$

hyperprior

marginal likelihood

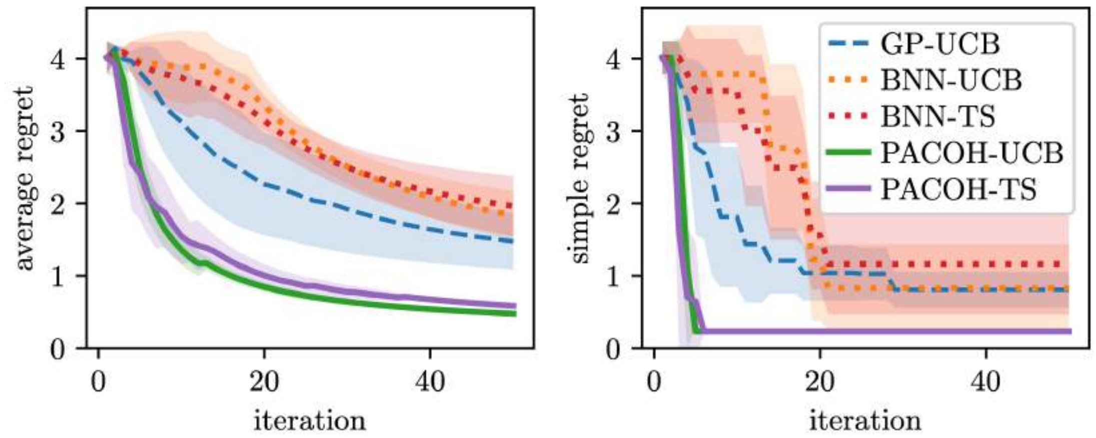
hyperposterior

PAC-Bayesian meta-learning

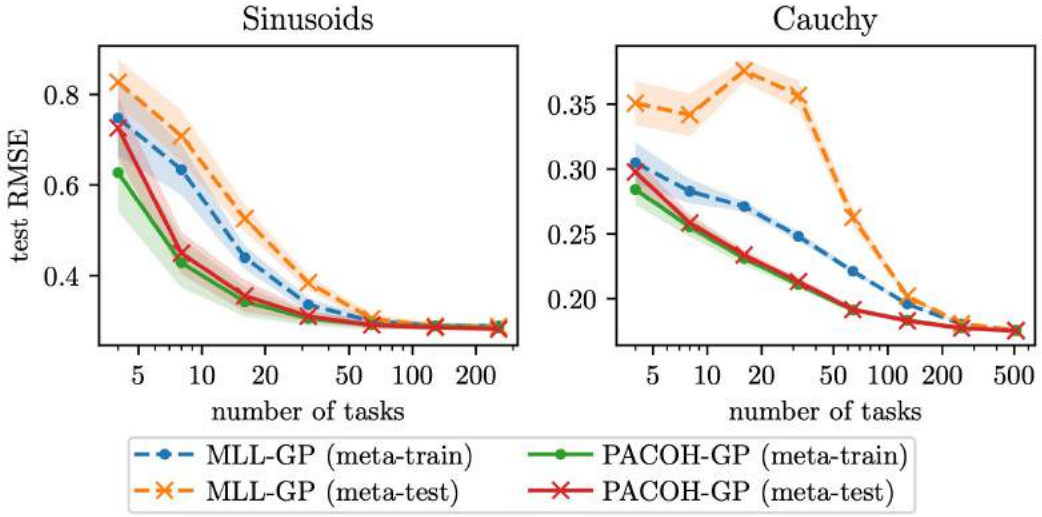
[Rothfuss, F, Josifoski, Krause. ICML 2021]

	Accuracy	Calibration error
Vanilla BNN (Liu & Wang, 2016)	0.795 ± 0.006	0.135 ± 0.009
MLAP (Amit & Meir, 2018)	0.700 ± 0.0135	0.108 ± 0.010
MAML (Finn et al., 2017)	0.693 ± 0.013	0.109 ± 0.011
BMAML (Kim et al., 2018)	0.764 ± 0.025	0.191 ± 0.018
PACOH-NN (ours)	$\mathbf{0.885 \pm 0.090}$	$\mathbf{0.091 \pm 0.010}$

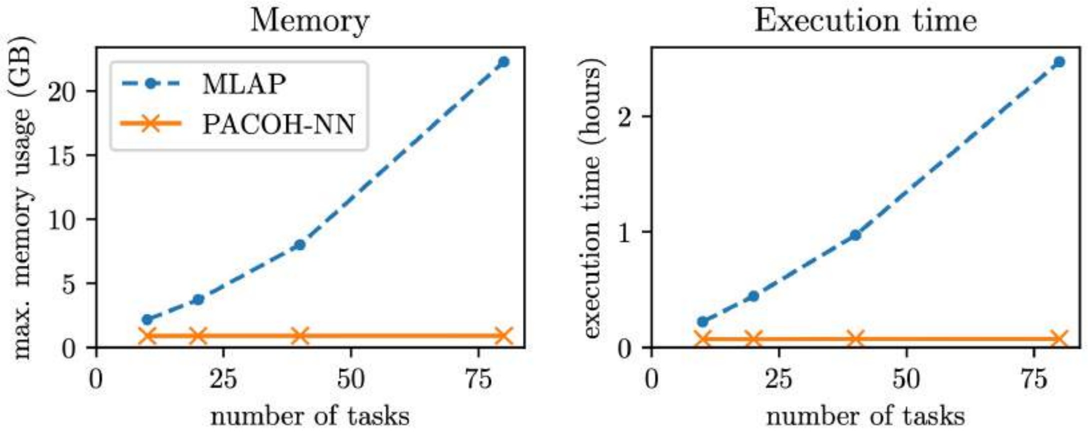
Few-shot learning on Omniglot



Bandit task



Meta-overfitting



Runtimes

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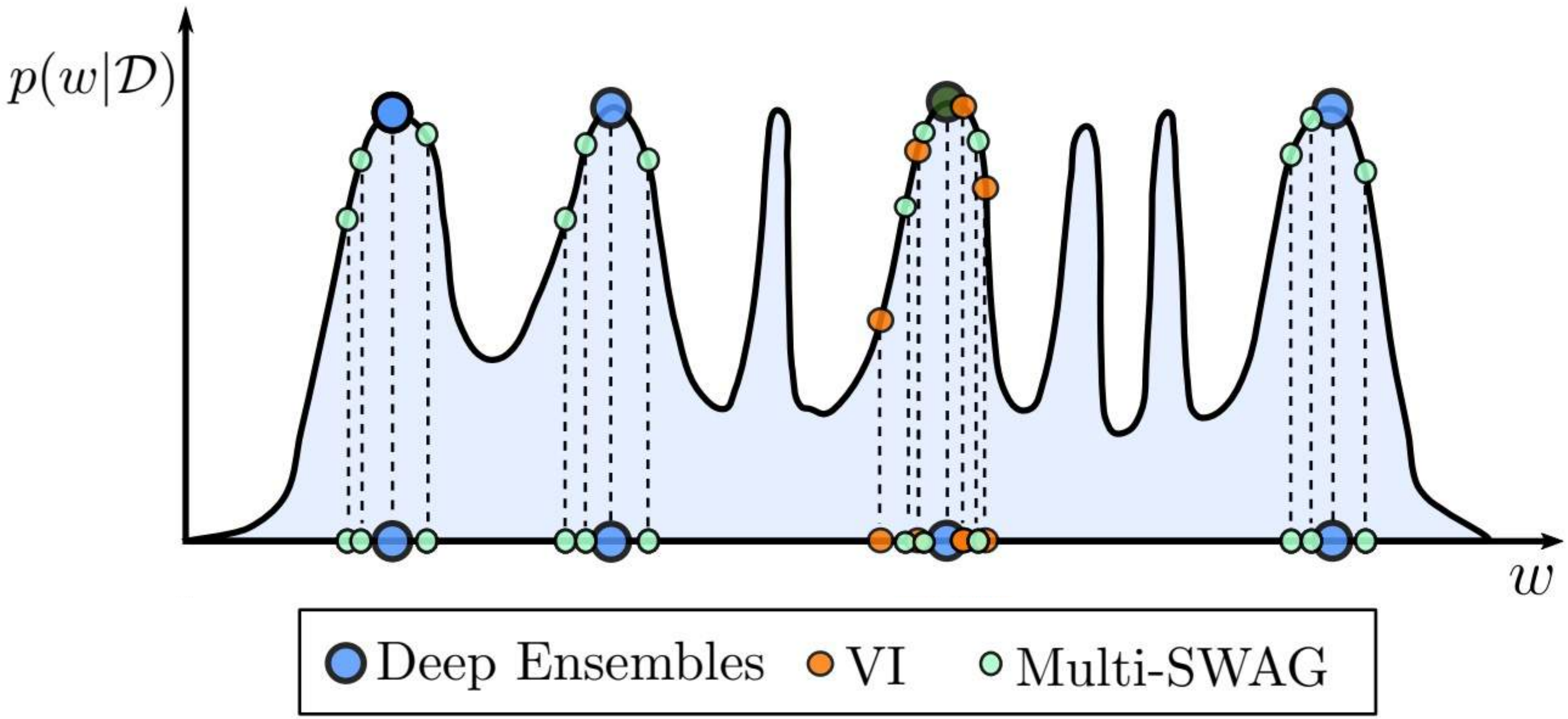
Background: Posterior coverage



[Wilson, Izmailov 2020]

Repulsive deep ensembles

[D'Angelo, F. NeurIPS 2021]

Standard deep ensembles:

$$\mathbf{w}_i^{t+1} \leftarrow \mathbf{w}_i^t + \epsilon_t \phi(\mathbf{w}_i^t)$$

$$\phi(\mathbf{w}_i^t) = \nabla_{\mathbf{w}_i^t} \log p(\mathbf{w}_i^t | \mathcal{D})$$

Repulsive deep ensembles:

kernel

$$\phi(\mathbf{w}_i^t) = \nabla_{\mathbf{w}_i^t} \log p(\mathbf{w}_i^t | \mathcal{D}) - \mathcal{R}\left(\left\{\nabla_{\mathbf{w}_i^t} k(\mathbf{w}_i^t, \mathbf{w}_j^t)\right\}_{j=1}^{n}\right)$$

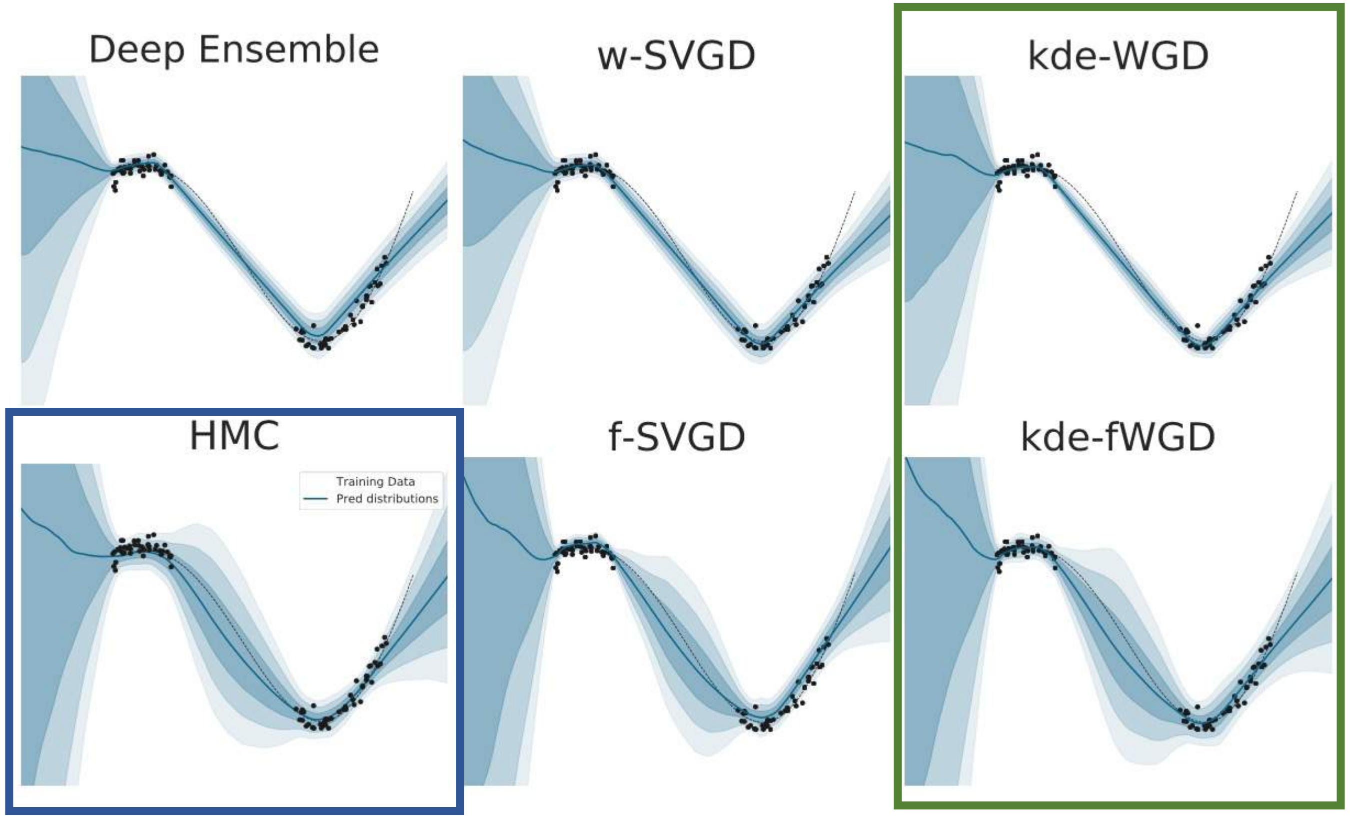
Function-space repulsive deep ensembles:

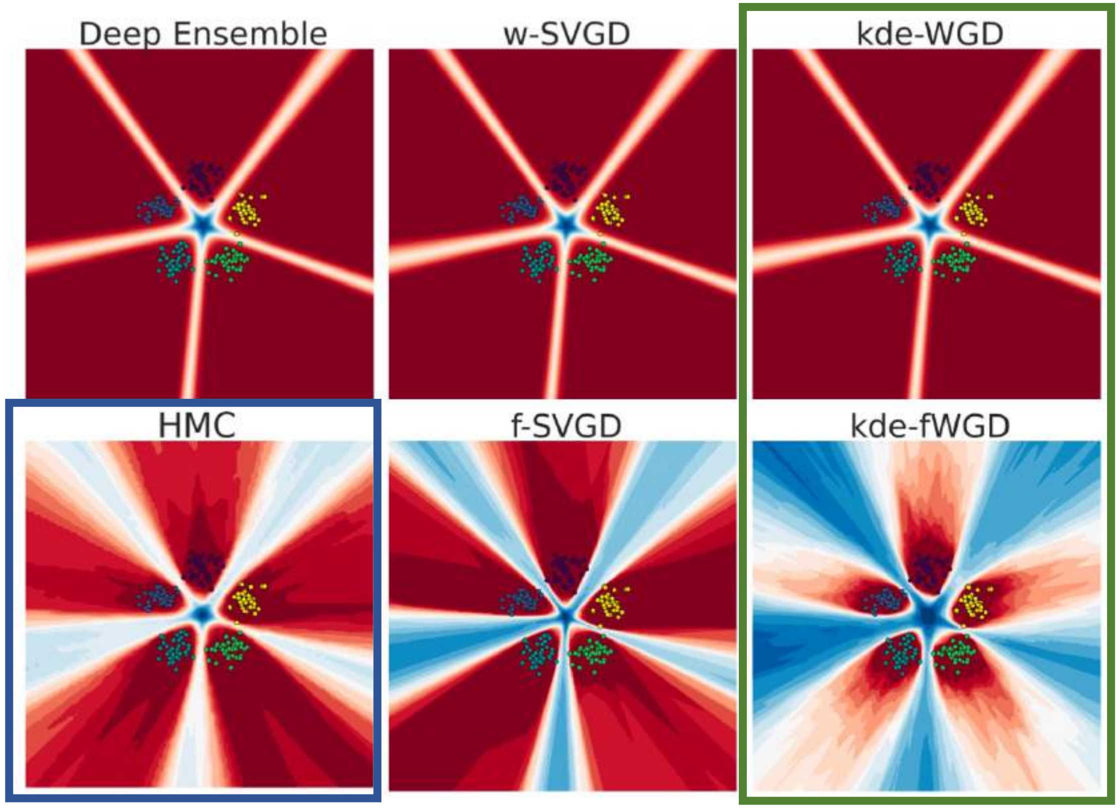
canonical projection

$$\phi(\mathbf{w}_i^t) = \left(\frac{\partial \boldsymbol{f}_i^t}{\partial \mathbf{w}_i^t}\right)^\top \left[\nabla_{\boldsymbol{f}_i^t} \log p(\boldsymbol{f}_i^t | \mathcal{D}) - \mathcal{R}\left(\left\{\nabla_{\boldsymbol{f}_i^t} k(\pi_B(\boldsymbol{f}_i^t), \pi_B(\boldsymbol{f}_j^t))\right\}_{j=1}^{n}\right)\right]$$

Repulsion approximates the posterior

[D‘Angelo, F. NeurIPS 2021]





„gold standard“

our model

„gold standard“

our model

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GP priors in the latent space

[F, Collier, Wenzel, Liu, Allingham, Tran, Lakshminarayanan, Berent, Jenatton, Kokiopoulou. AABI 2022]

SNGP-distributed latent means
(correlated across data points)

SNGP kernel
(RFF approximation)

$$\boldsymbol{f}_c \sim \mathcal{N}(\mathbf{0}, \boldsymbol{K}_\theta(\boldsymbol{x}, \boldsymbol{x}))$$

$$\boldsymbol{u}_i \sim \mathcal{N}(\boldsymbol{f}_i, \boldsymbol{\Sigma}(\boldsymbol{x}_i; \varphi))$$

heteroscedastic logits
(correlated across classes)

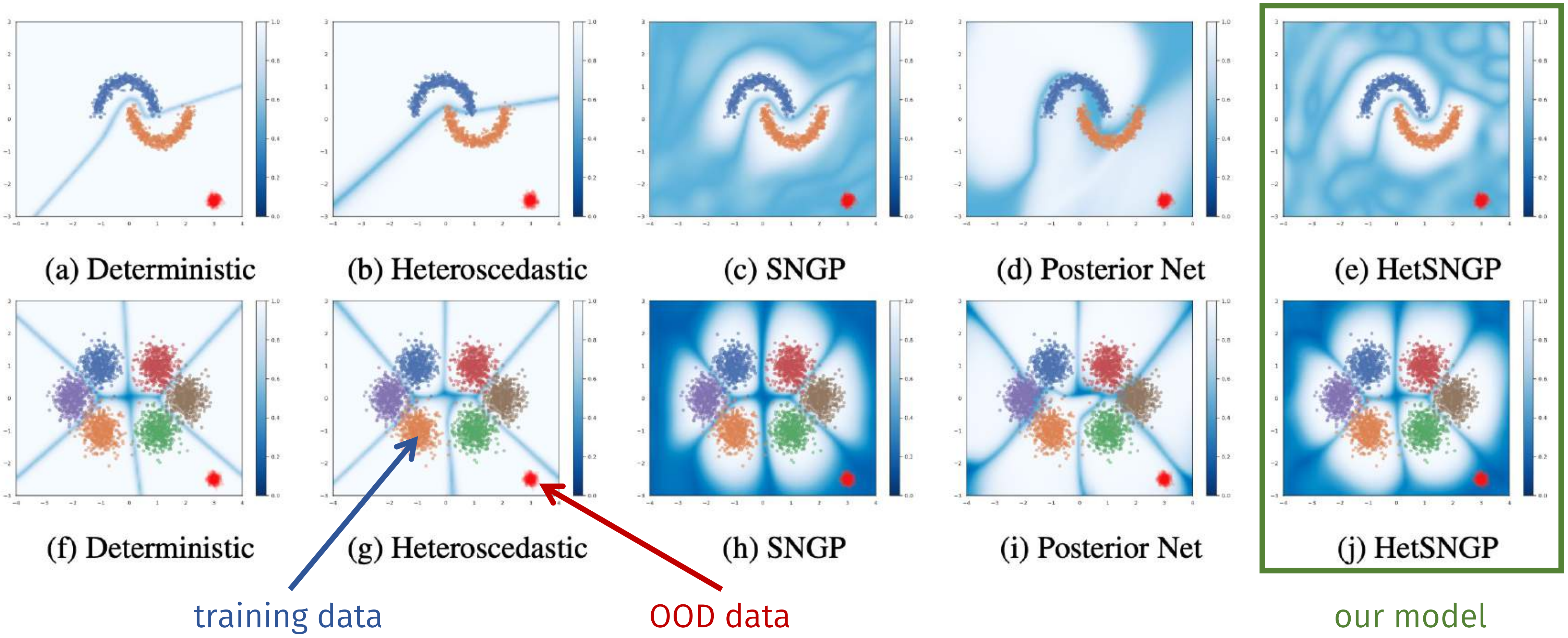
label noise covariance
(possibly low-rank)

$$p(y_i = c \,|\, \boldsymbol{u}_i) = \mathbb{1}\left[c = \arg\max_k \, u_{ik}\right]$$

output probabilities (approximated by softmax)

Distance-aware OOD uncertainties

[F, Collier, Wenzel, Liu, Allingham, Tran, Lakshminarayanan, Berent, Jenatton, Kokiopoulou. AABI 2022]



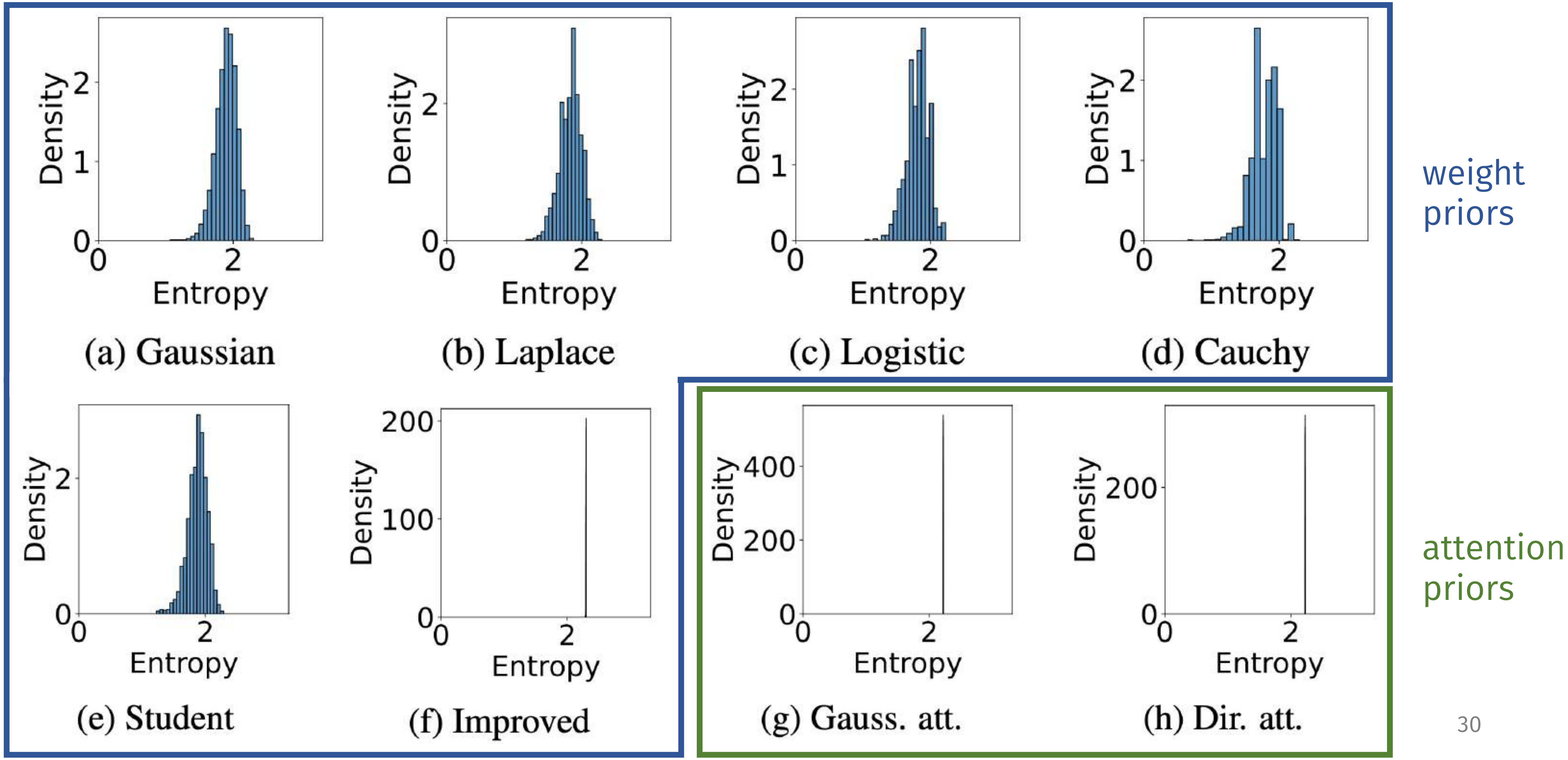
Label noise modeling in real datasets

[F, Collier, Wenzel, Liu, Allingham, Tran, Lakshminarayanan, Berent, Jenatton, Kokiopoulou. AABI 2022]

Method	↑ID prec@1	↑Im Acc	↑ImC Acc	↑ImA Acc	↑ImR Acc	↑ImV2 Acc
Det.	0.471 $\pm$ 0.000	0.800 $\pm$ 0.000	0.603 $\pm$ 0.000	0.149 $\pm$ 0.000	0.311 $\pm$ 0.000	0.694 $\pm$ 0.000
Het.	**0.480** $\pm$ 0.001	0.796 $\pm$ 0.002	0.590 $\pm$ 0.001	0.132 $\pm$ 0.004	0.300 $\pm$ 0.006	0.687 $\pm$ 0.000
SNGP	0.468 $\pm$ 0.001	0.799 $\pm$ 0.001	0.602 $\pm$ 0.000	0.165 $\pm$ 0.003	0.328 $\pm$ 0.005	0.696 $\pm$ 0.003
HetSNGP	0.477 $\pm$ 0.001	**0.806** $\pm$ 0.001	**0.613** $\pm$ 0.003	**0.172** $\pm$ 0.007	**0.336** $\pm$ 0.002	**0.705** $\pm$ 0.001

Sidenote: Attention prior in transformers

[Cinquin, Immer, Horn, F. AABI 2022]



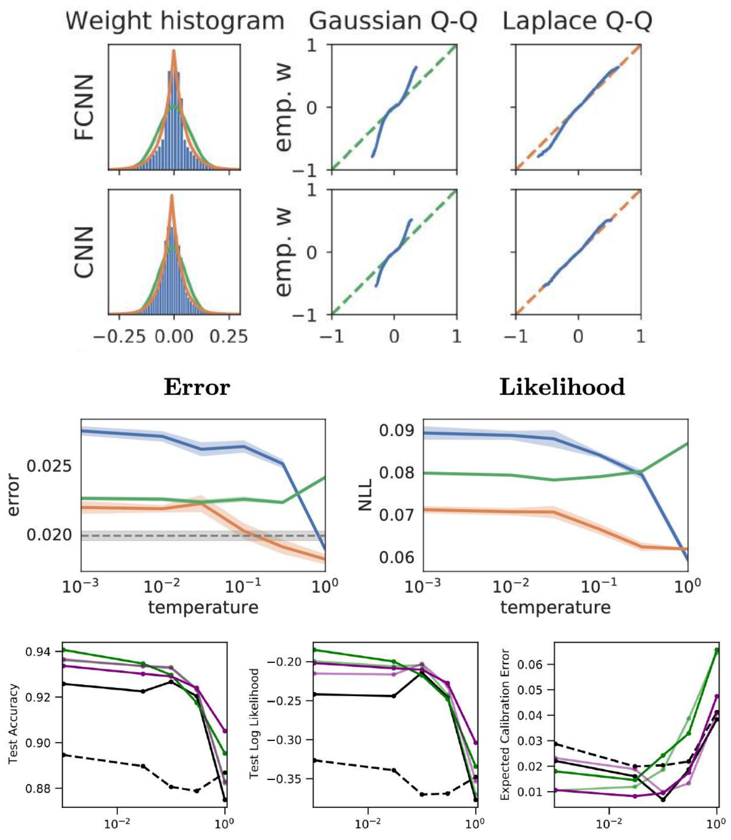
Improving the prior helps in all tasks

[Cinquin, Immer, Horn, F. AABI 2022]

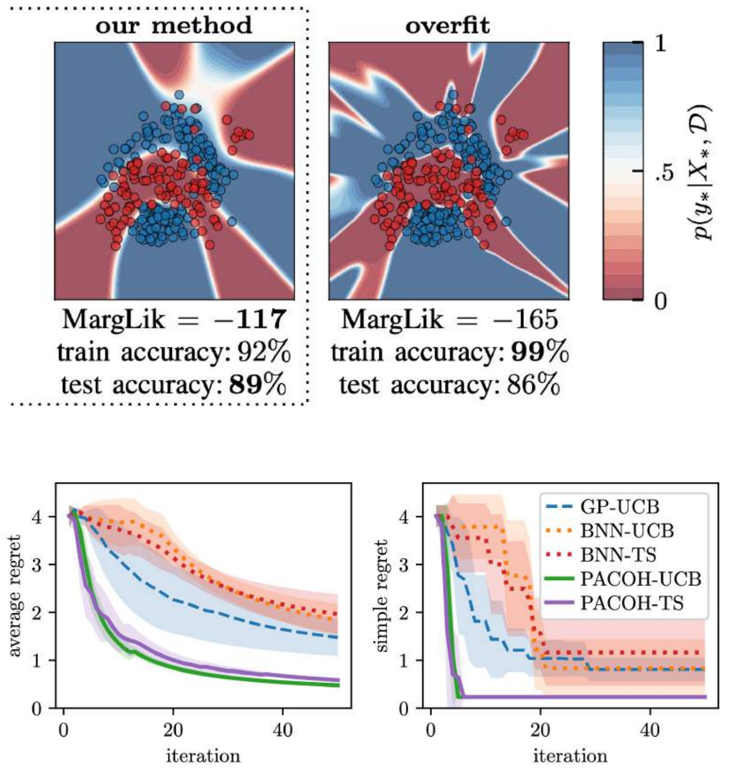
Dataset	Gauss. VI	Laplace VI	Logistic VI	Cauchy VI	Student VI
M1	1.40%	3.80%	4.12%	1.85%	2.79%
M2	2.85%	3.06%	2.76%	4.36%	2.70%
POS	0.12%	2.05%	2.16%	0.87%	-0.32%
MNIST	26.95%	33.31%	31.36%	5.66%	26.94%

Percentage of improvement changing from standard to improved prior

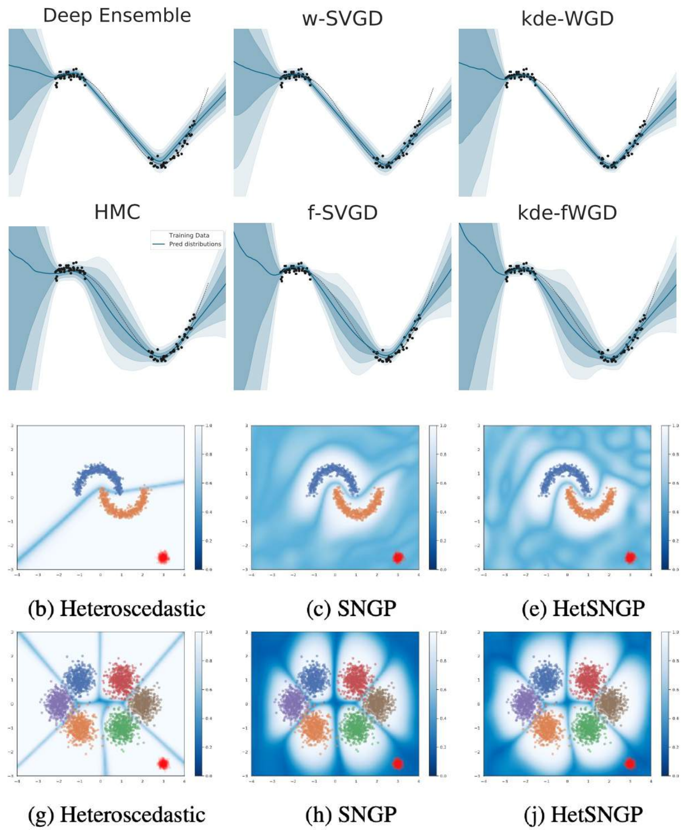
Take-home messages



Common weight-space BNN priors have several pathologies



We can find better priors using ML-II or meta-learning



Function-space priors can work better than weight-space ones

Thank you!

Deepmind

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