ETH zürich

UNIVERSITY OF CAMBRIDGE

On the Importance of Priors in Bayesian Deep Learning

Dr. Vincent Fortuin

Bayesian World Meeting

Montreal, June 2022

Agenda

- Pathologies of common BNN priors
- How to find better priors using the marginal likelihood
- PAC-Bayesian meta-learning for priors

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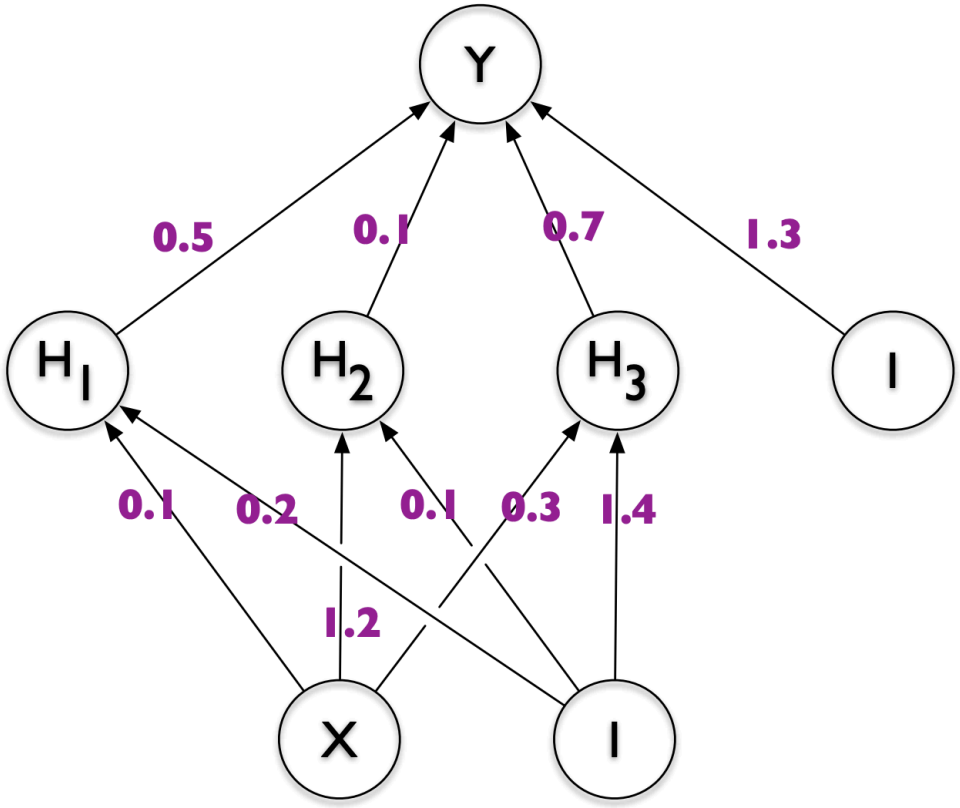
Background: Bayesian Neural Networks



[Blundell, Cornebise, Kavukcuoglu, Wierstra 2015]

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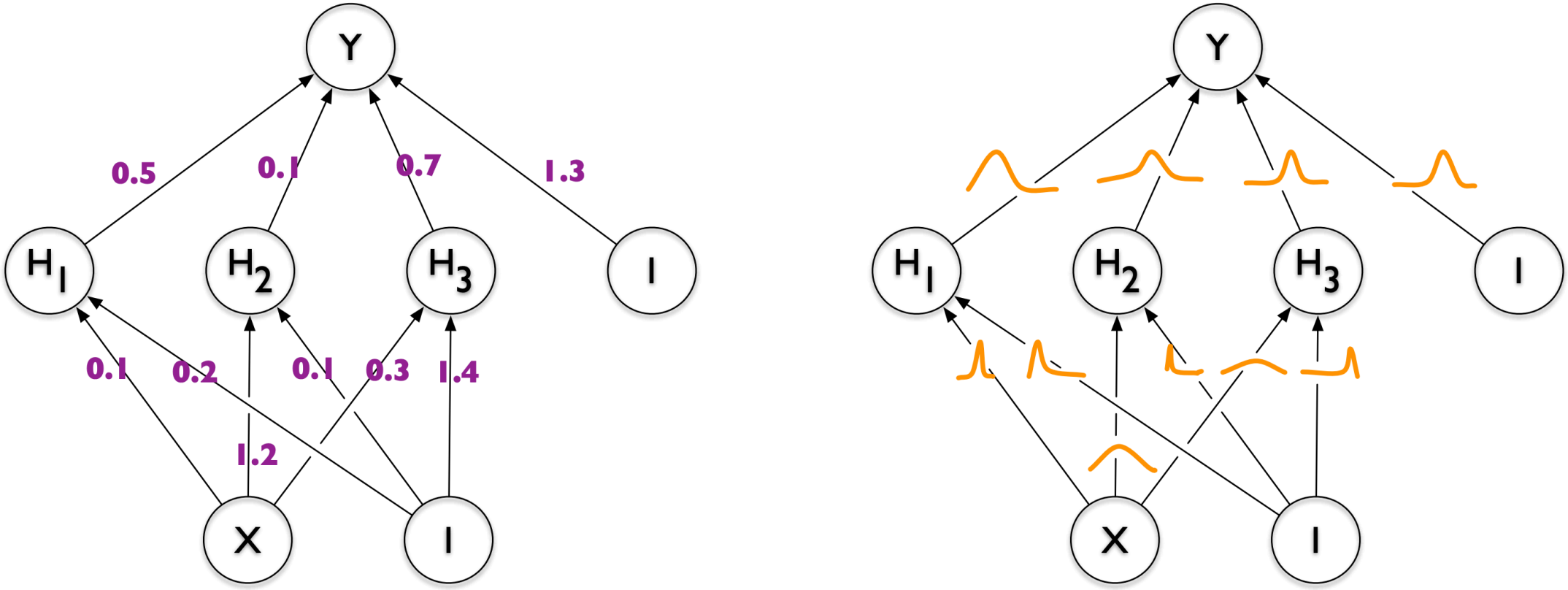

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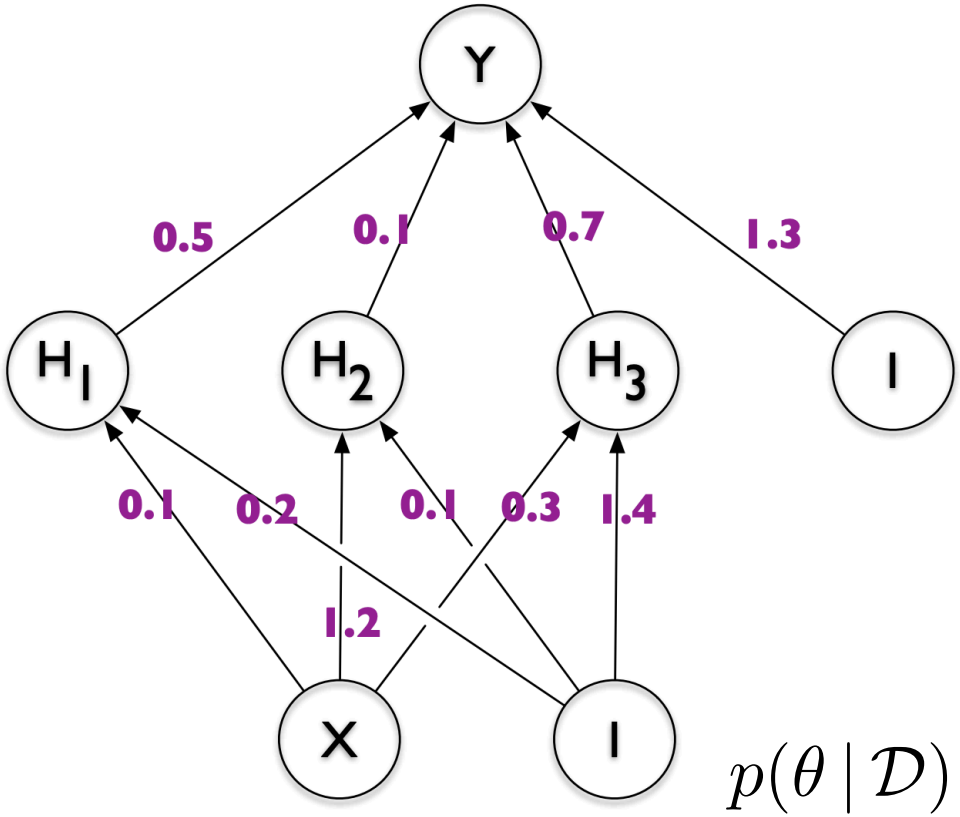
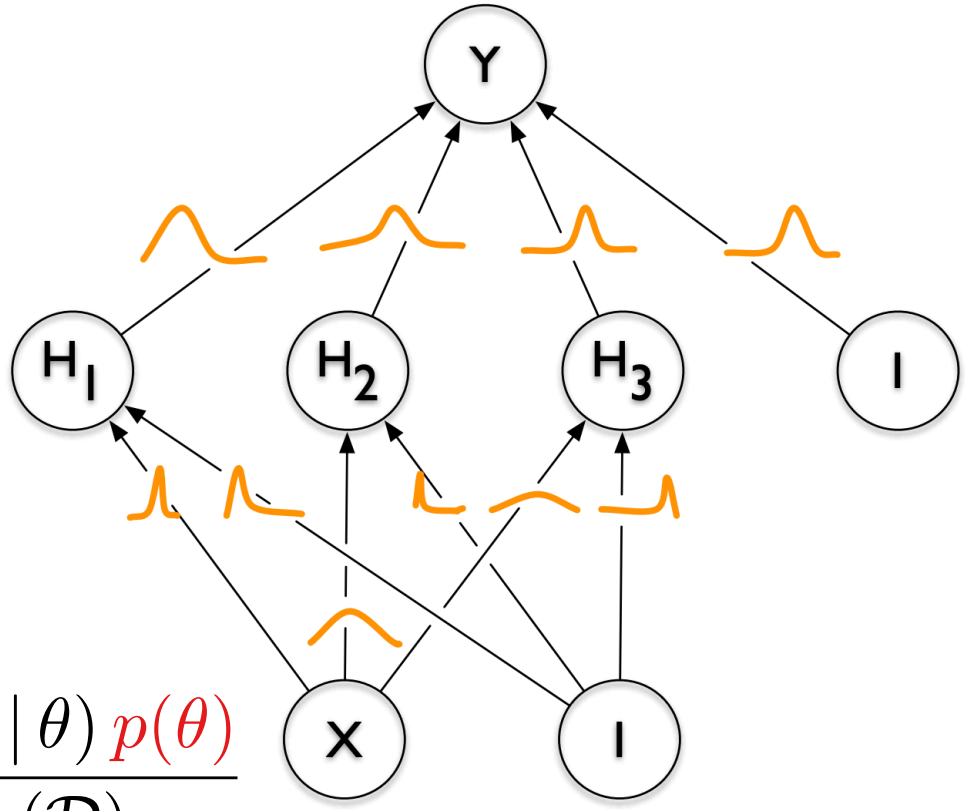
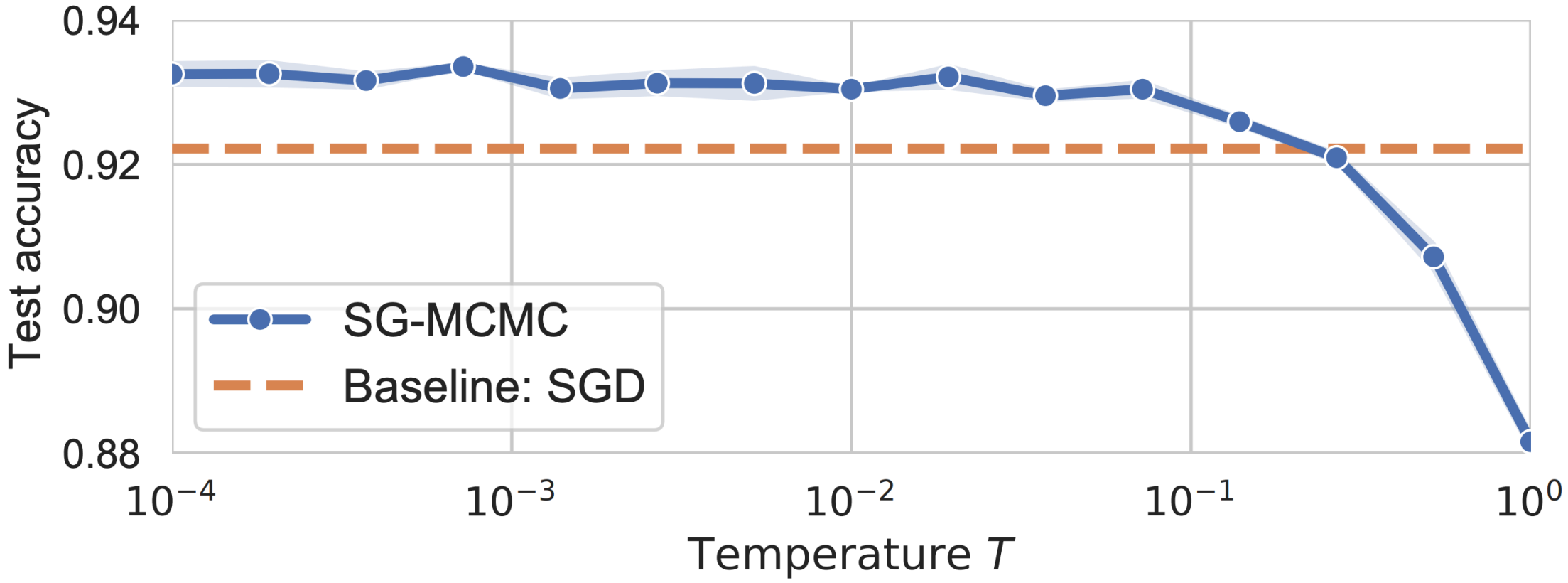


$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta)\, p(\theta)}{p(\mathcal{D})}$$



[Blundell, Cornebise, Kavukcuoglu, Wierstra 2015]

Motivation: Cold-posterior effect



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

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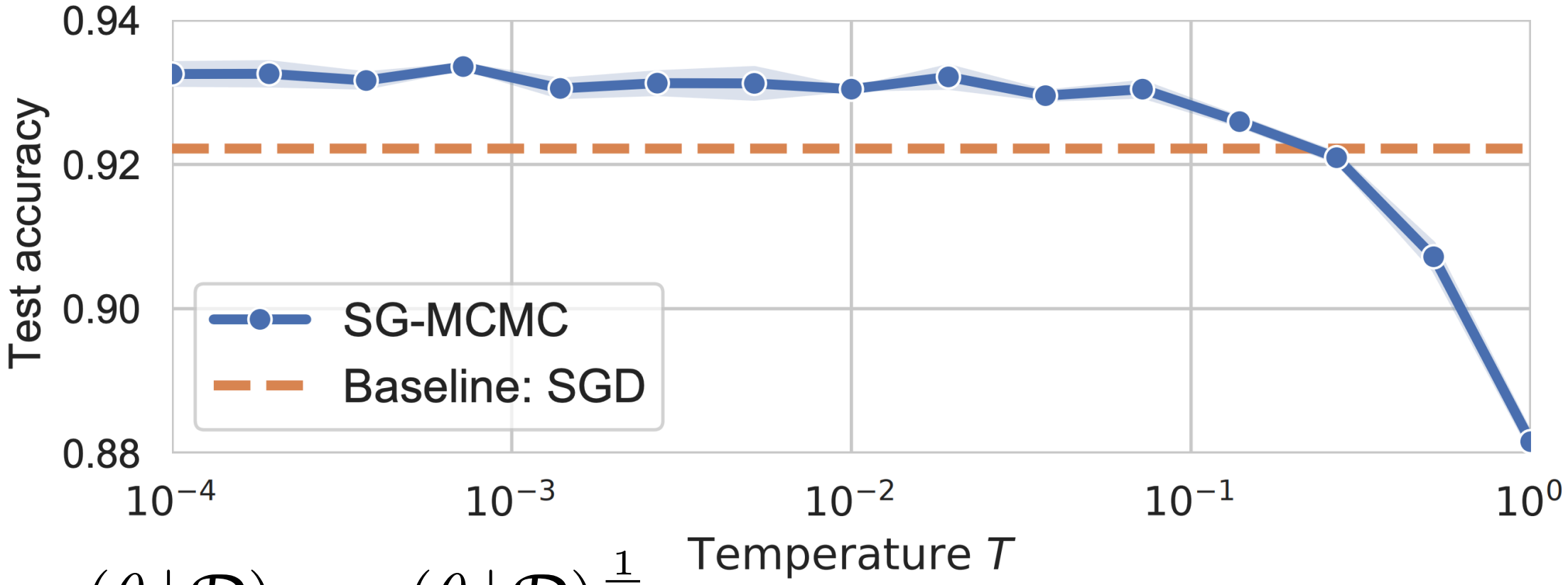

$$p_T(\theta \mid \mathcal{D}) \propto p(\theta \mid \mathcal{D})^{\frac{1}{T}}$$

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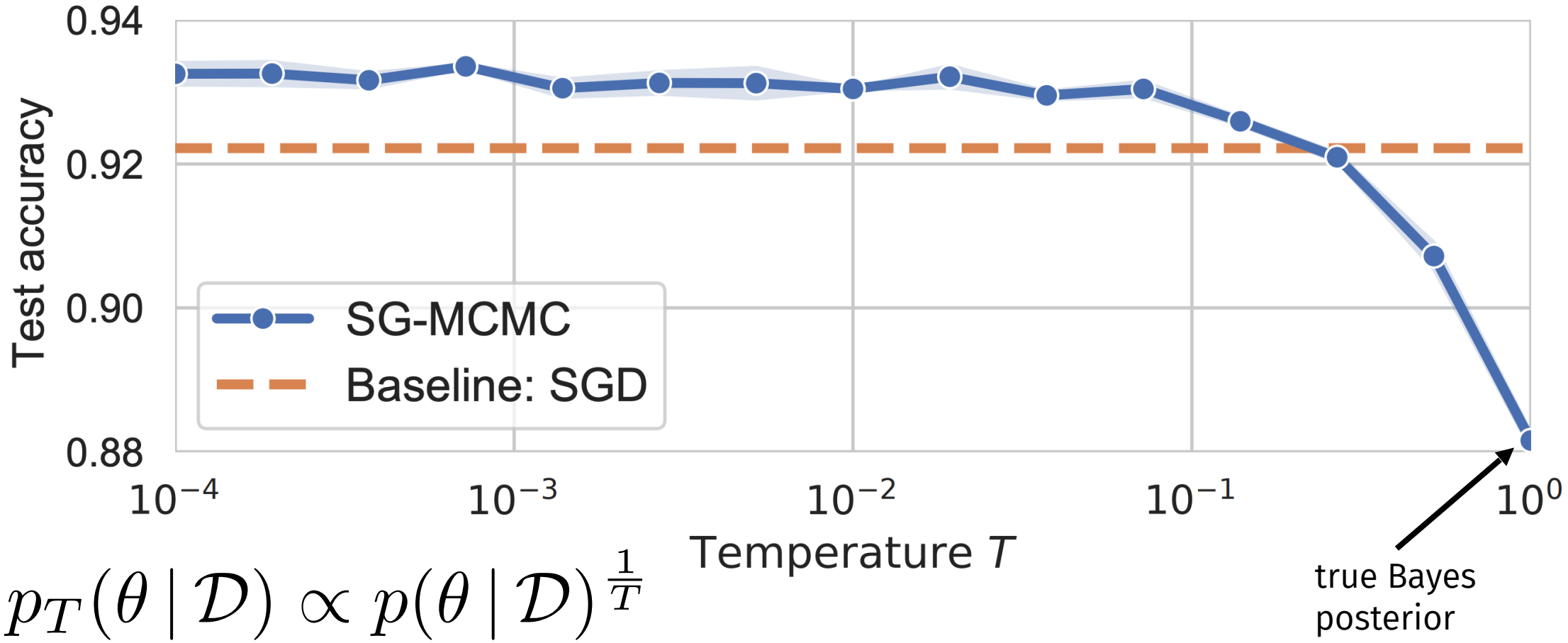

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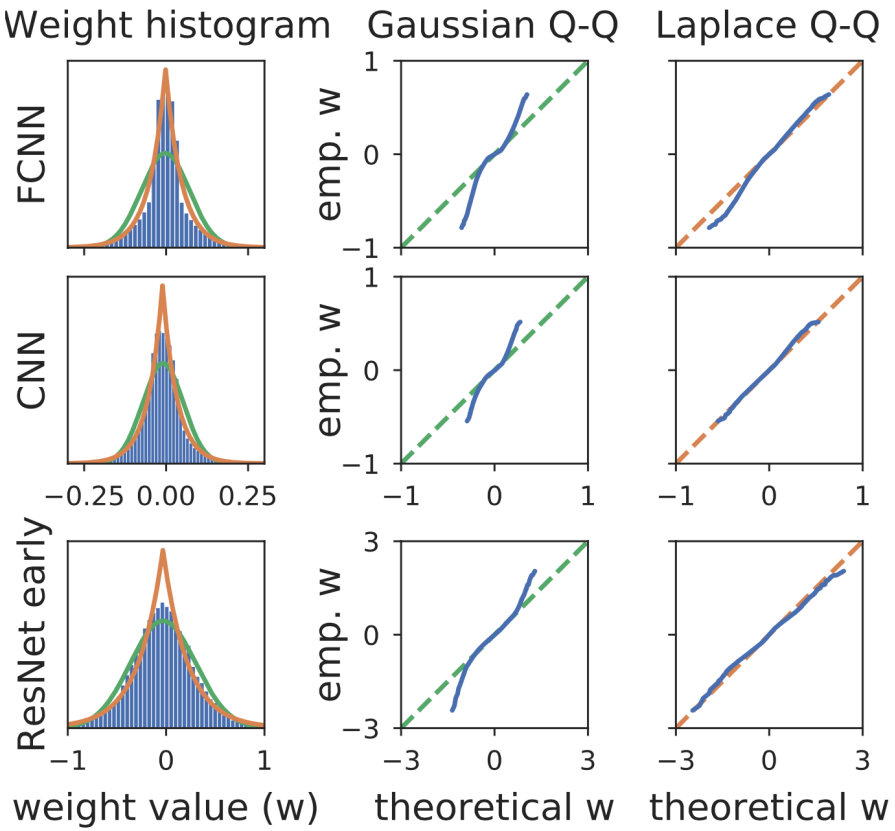
Empirical FCNN weights are heavy-tailed

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



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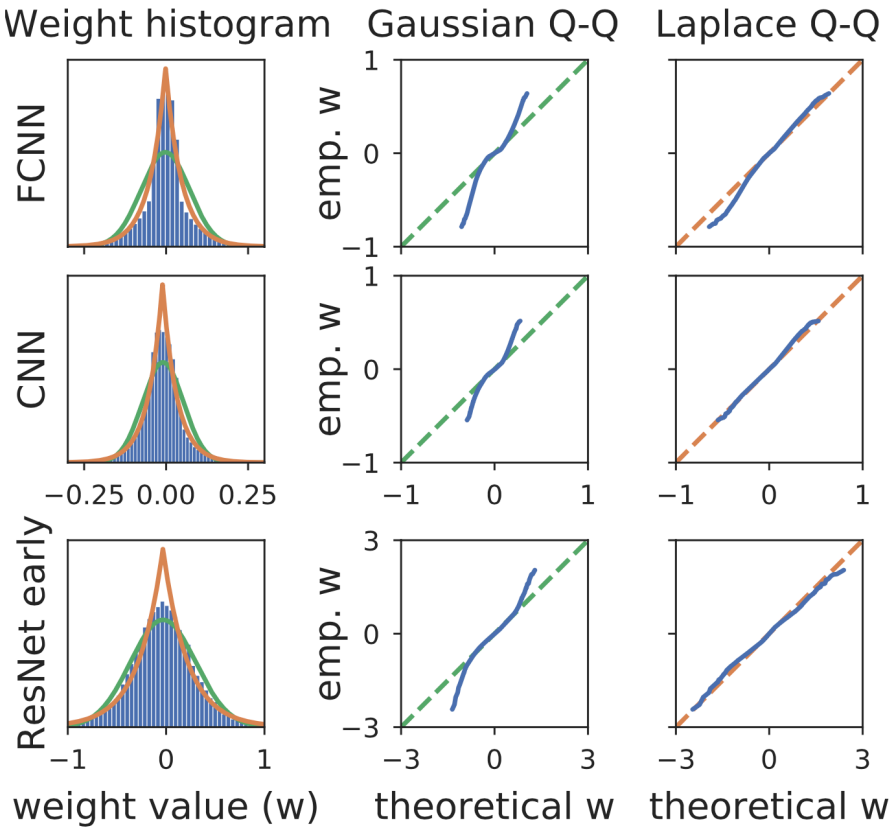

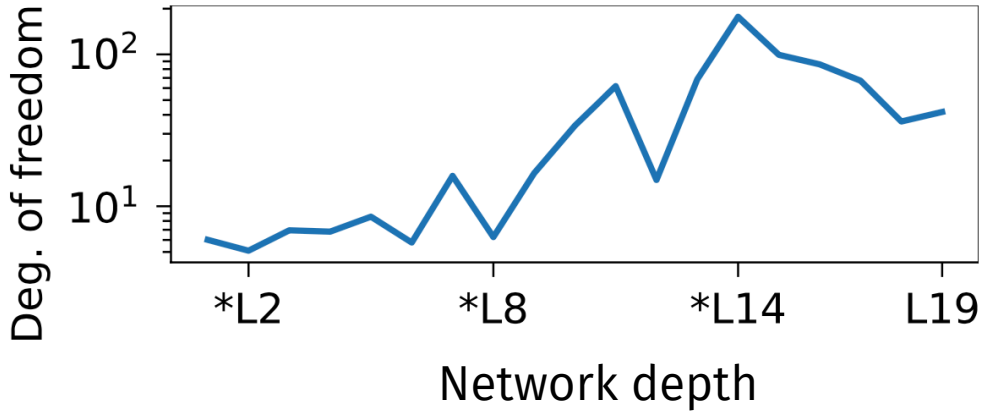

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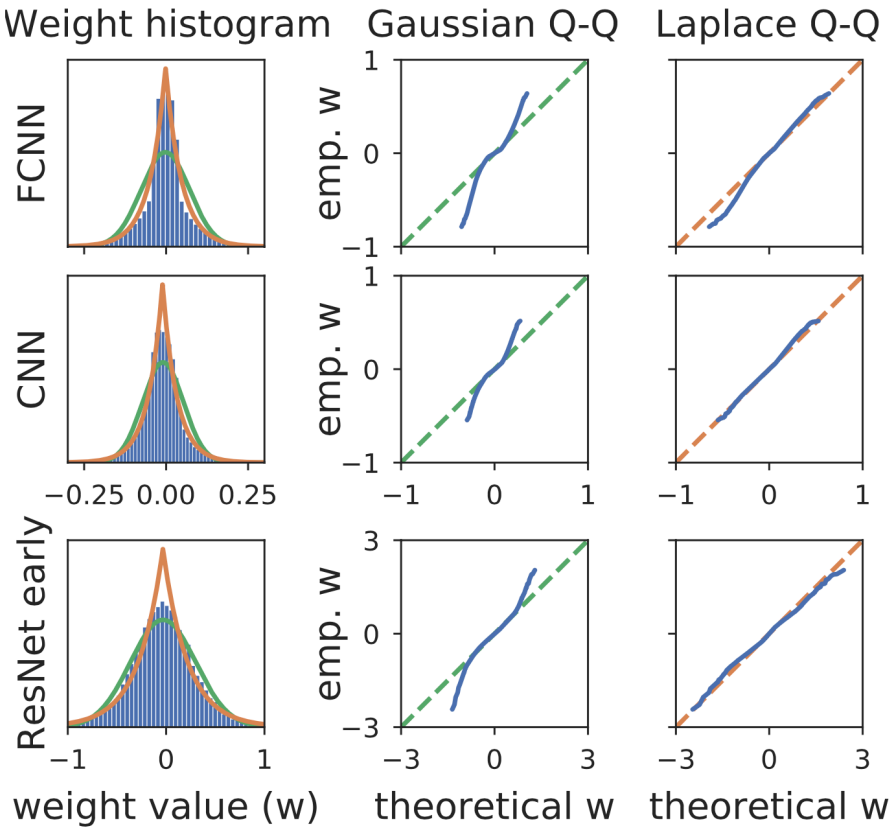
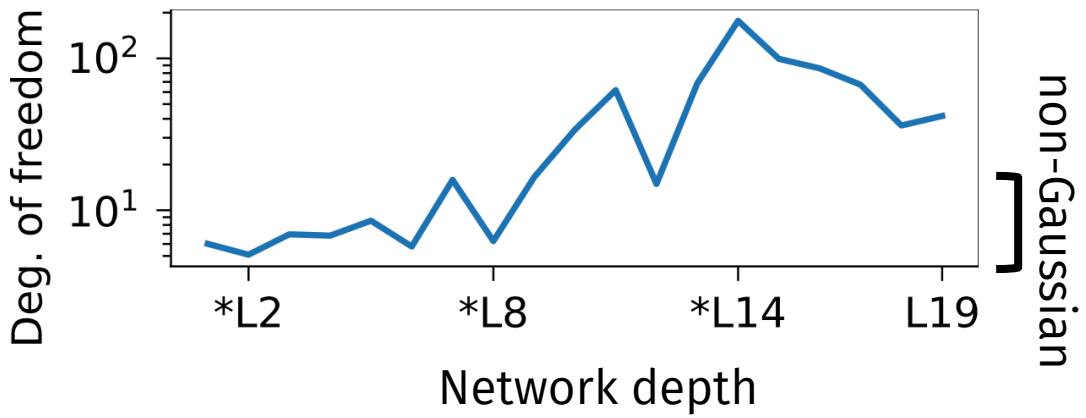
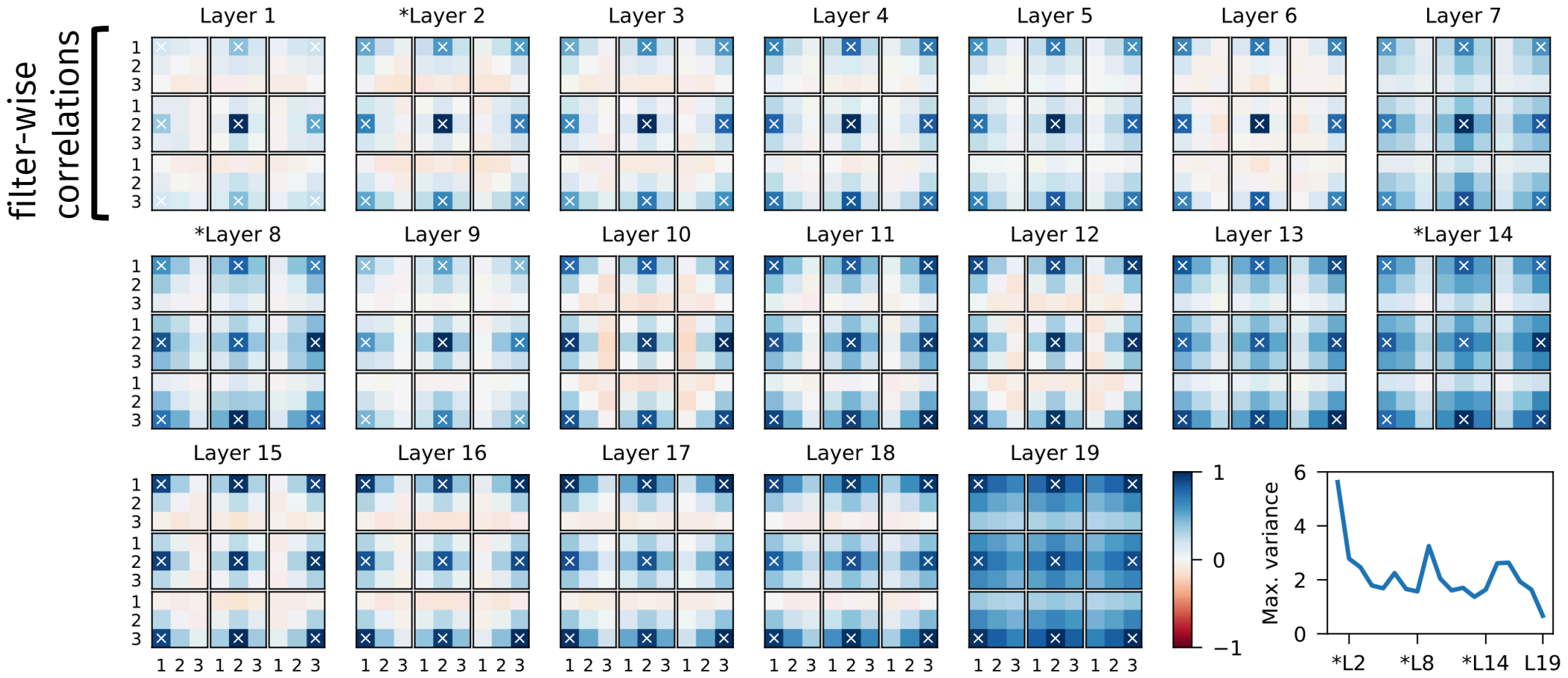




Empirical CNN weights are correlated

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



Bayesian FCNNs with different priors

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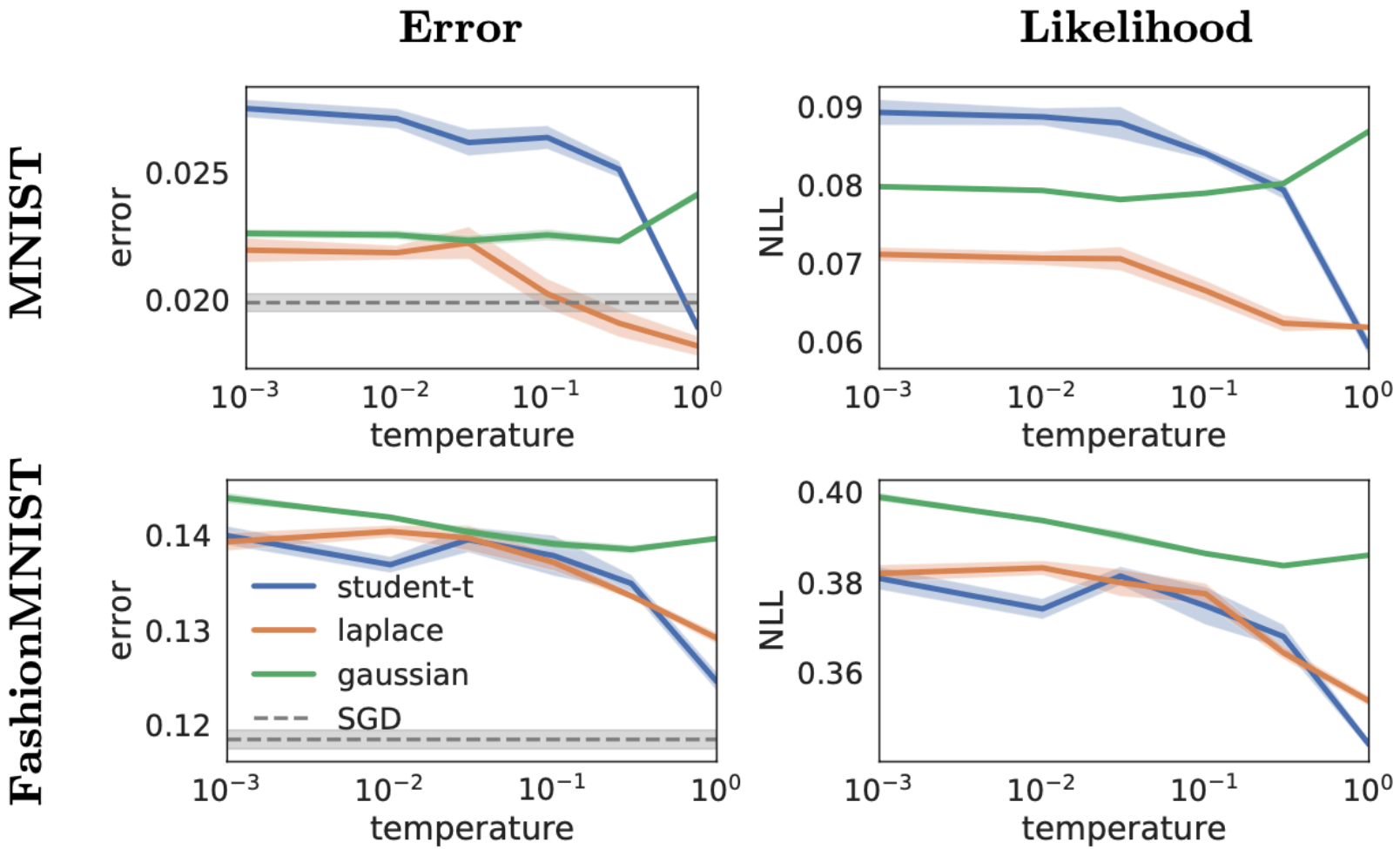

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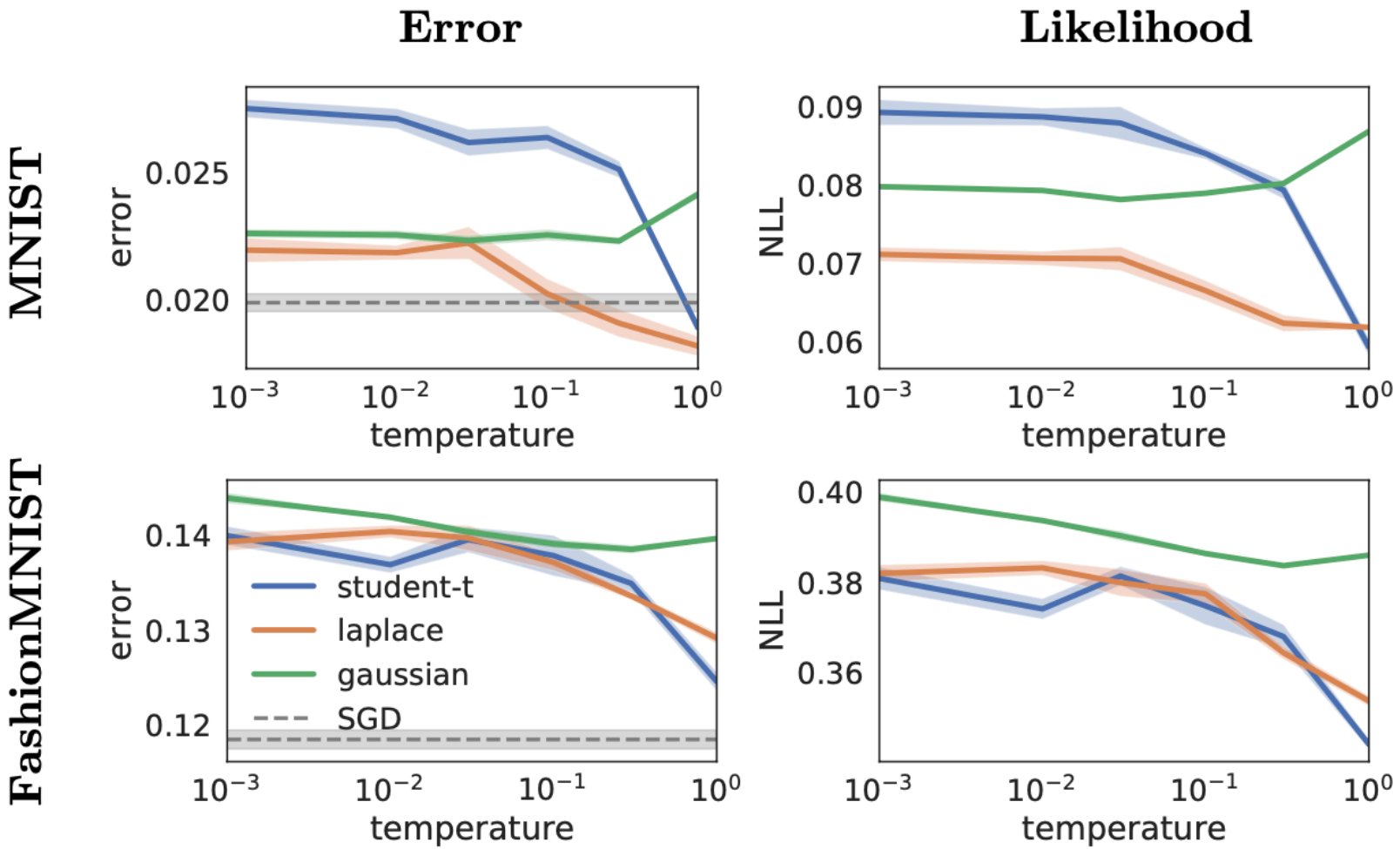

heavy-tailed priors perform better and reduce cold-posterior effect

Bayesian CNNs with different priors

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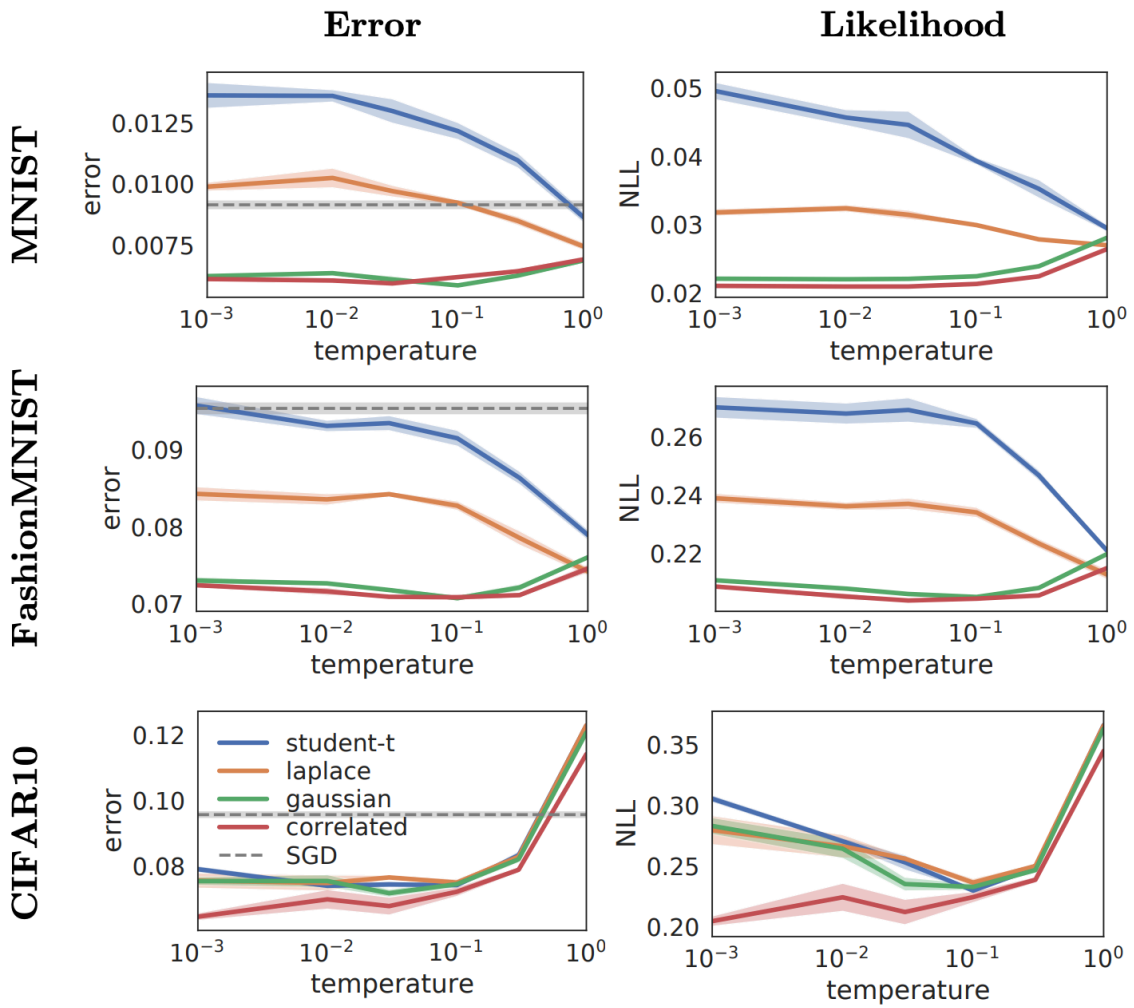

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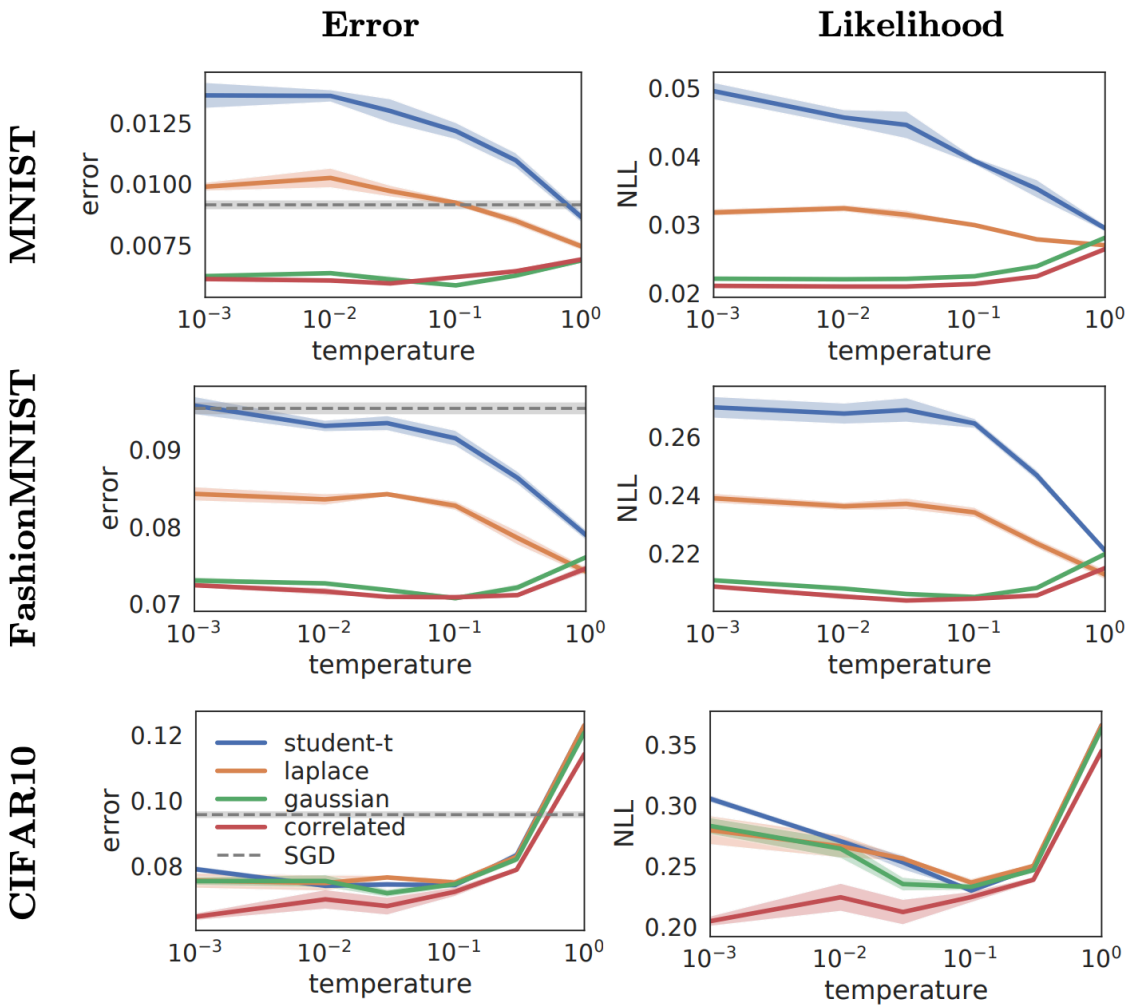

correlated prior performs better
but retains cold-posterior effect

Caveats

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- Maybe the cold posterior effect is not that bad (temperature might encode a different kind of prior knowledge)

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- FCNNs induce ill-specified function-space priors, but in CNNs and Resnets on images, function-space priors can be better
  - Cold posterior effect is mostly due to data augmentation there

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Marginal likelihood prior selection

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

$$p(\mathcal{D}|\mathcal{M}) = \int \prod_{n=1}^{N} p(\mathbf{y}_n|\mathbf{f}(\mathbf{x}_n, \boldsymbol{\theta}), \mathcal{M}) p(\boldsymbol{\theta}|\mathcal{M}) \, \mathrm{d}\boldsymbol{\theta}$$

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

Marginal likelihood prior selection

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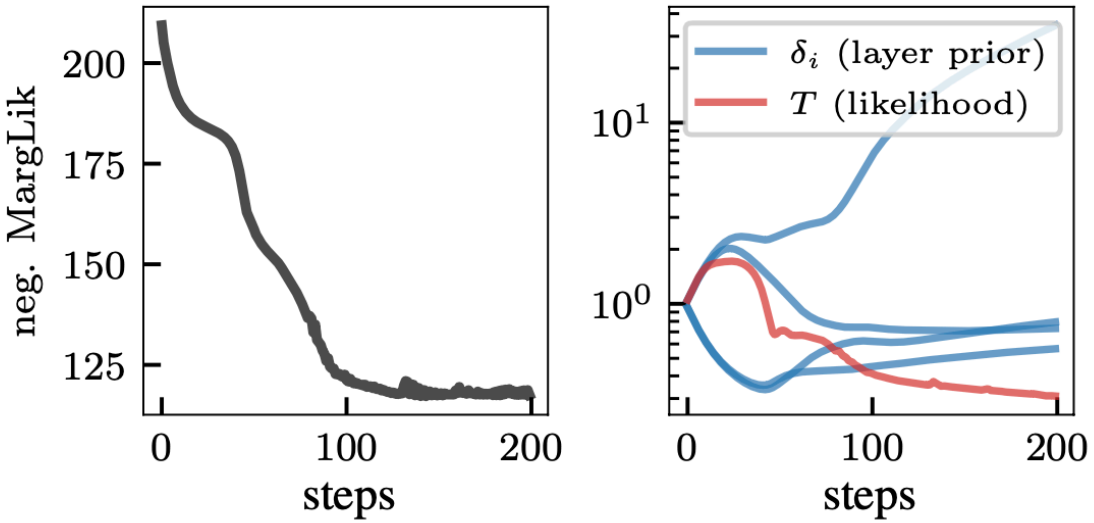
Step 1: Optimize Marginal-Likelihood wrt. hyperparameters



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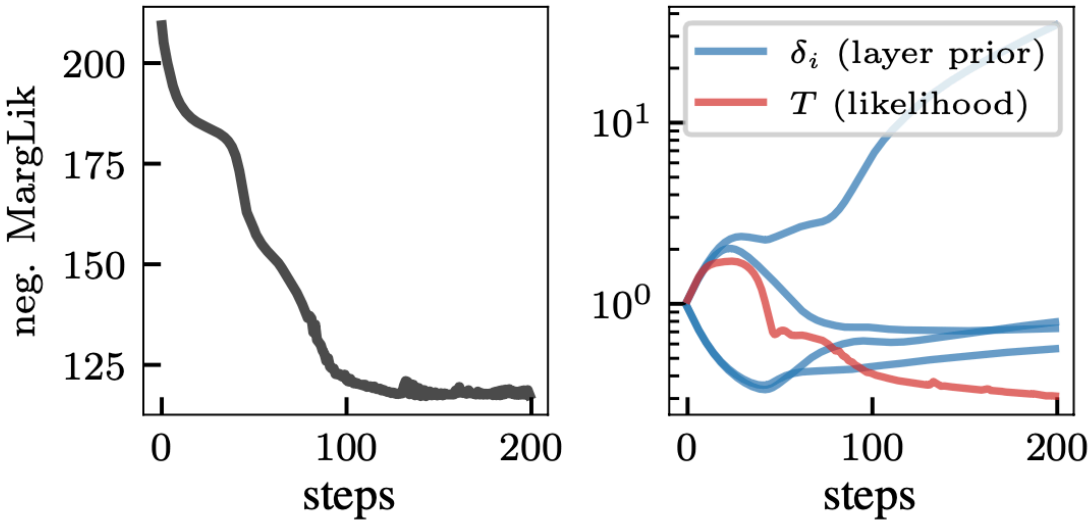
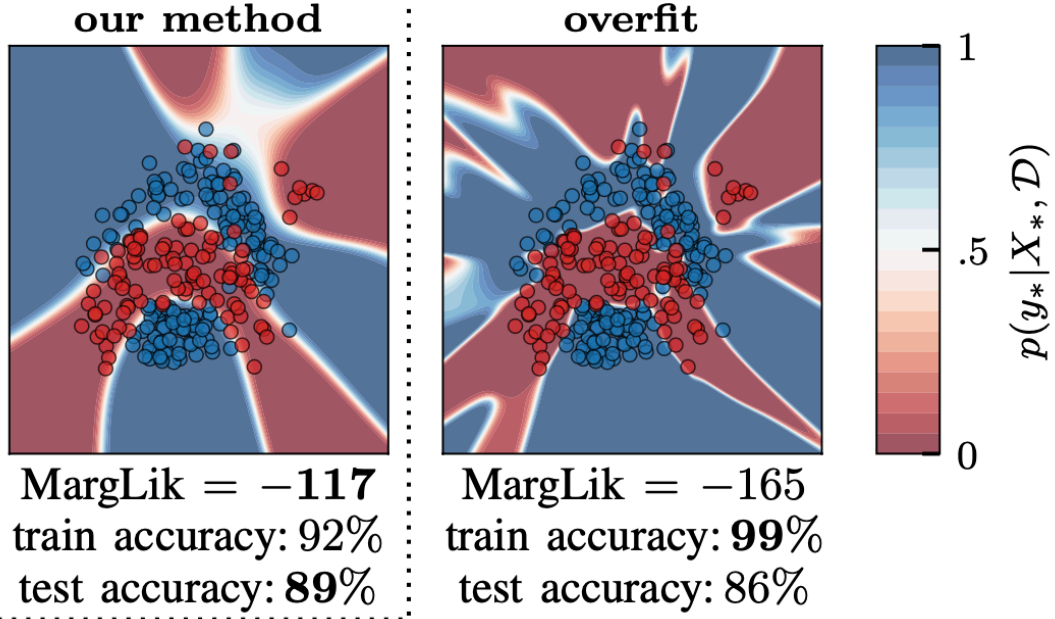


Step 2: Compare marginal likelihood of models



$\text{MargLik} = \mathbf{-117}$
train accuracy: 92%
test accuracy: **89%**

$\text{MargLik} = -165$
train accuracy: **99%**
test accuracy: 86%

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

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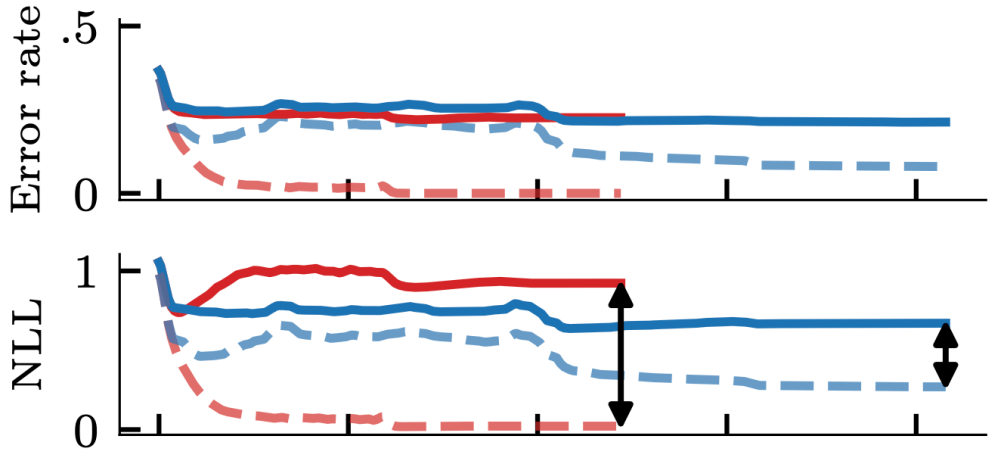
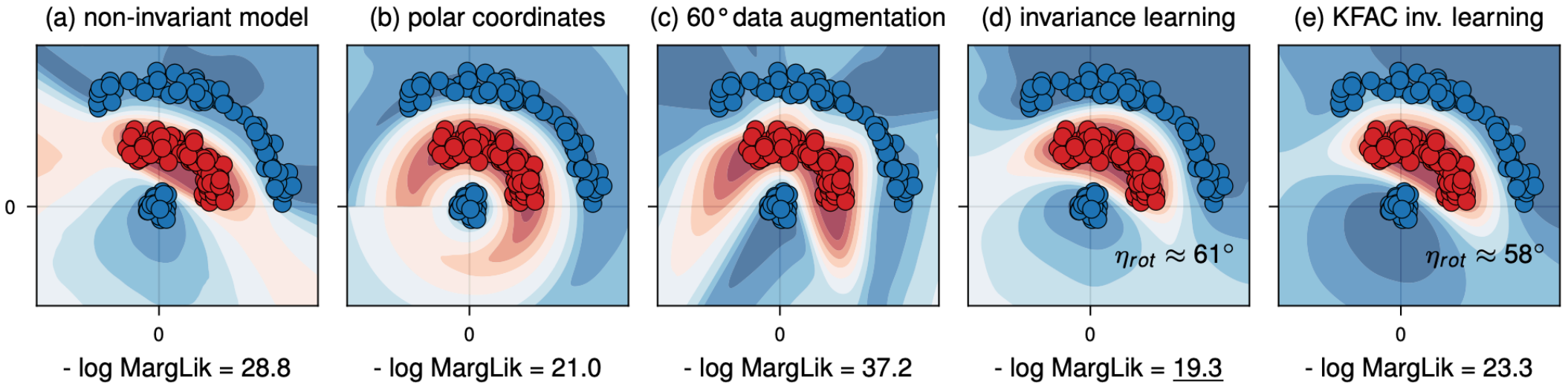


Application: Learning invariances

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



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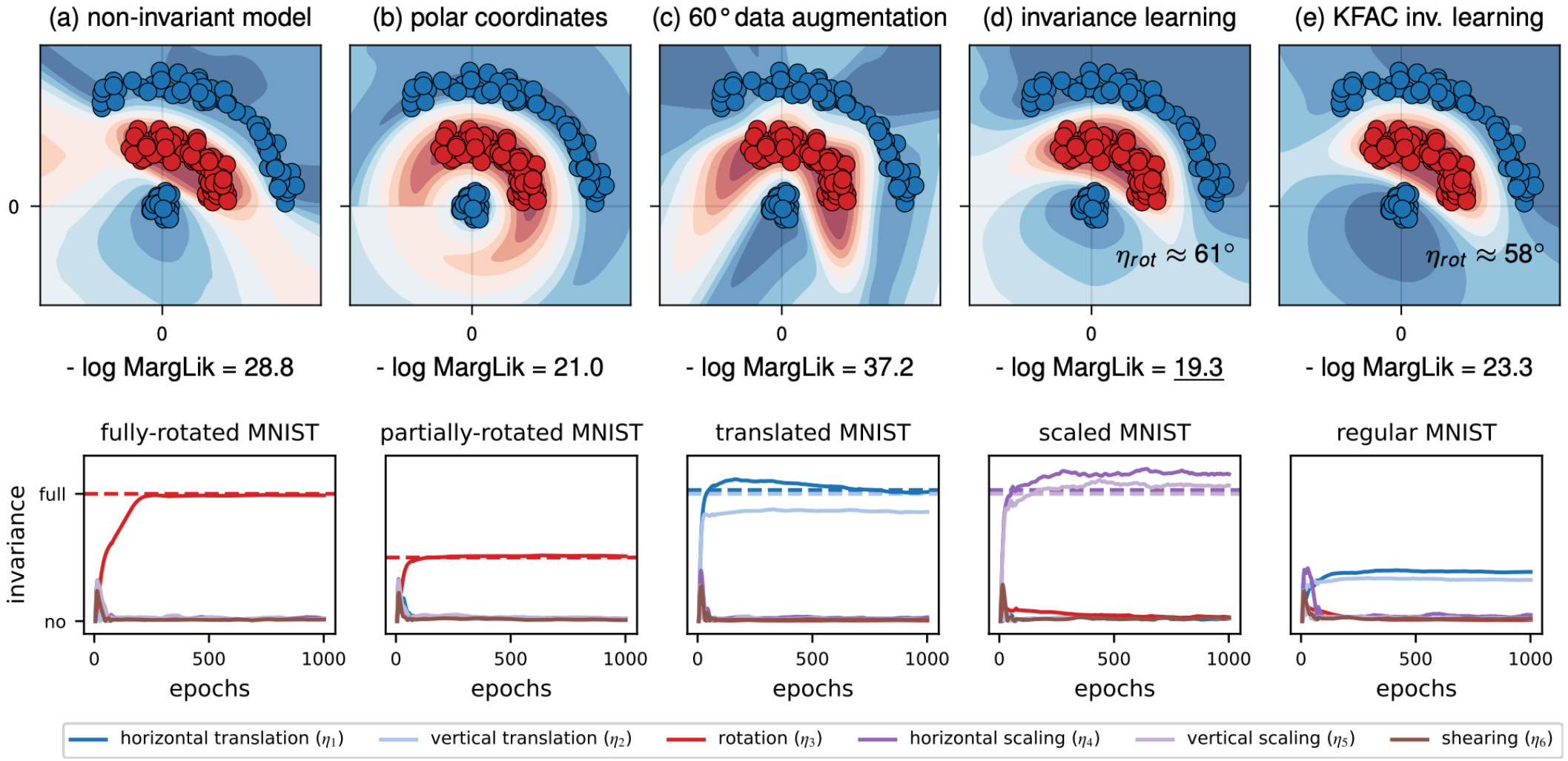
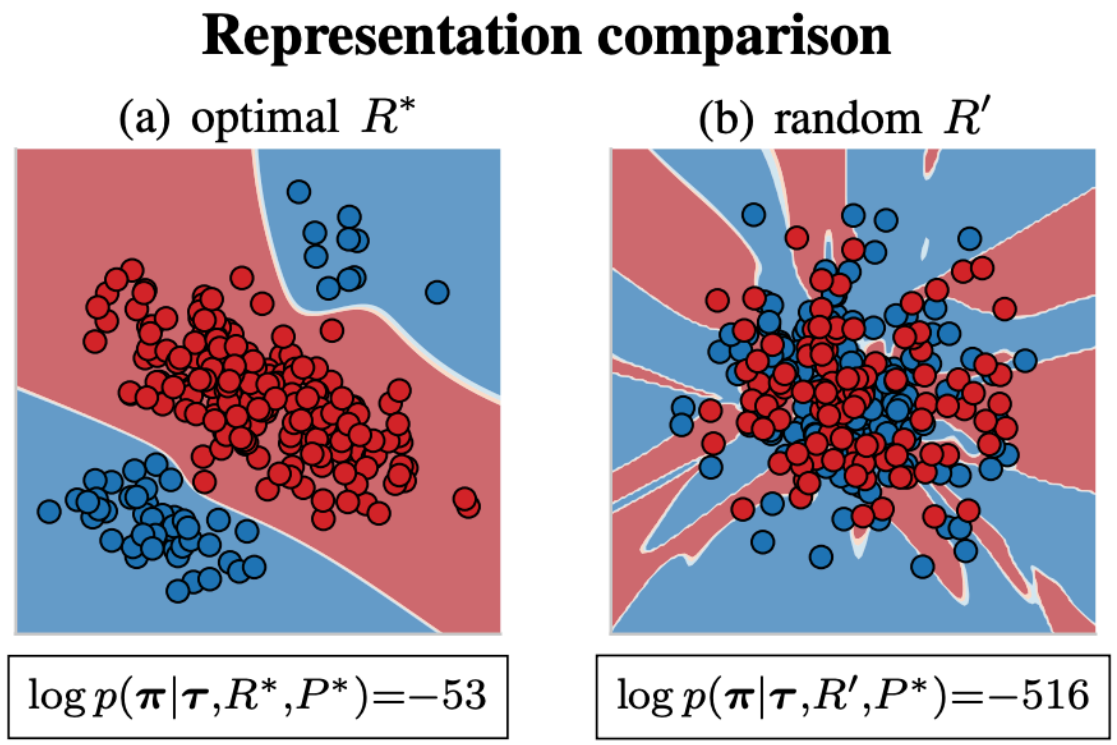


Another application: Linguistic probing

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



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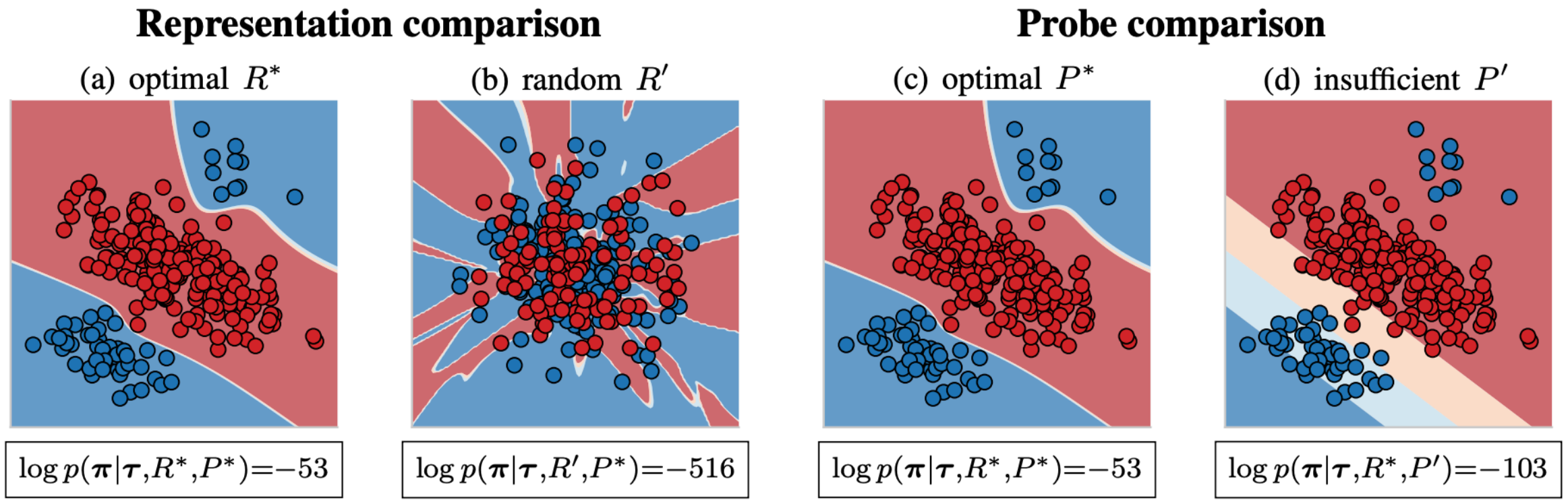

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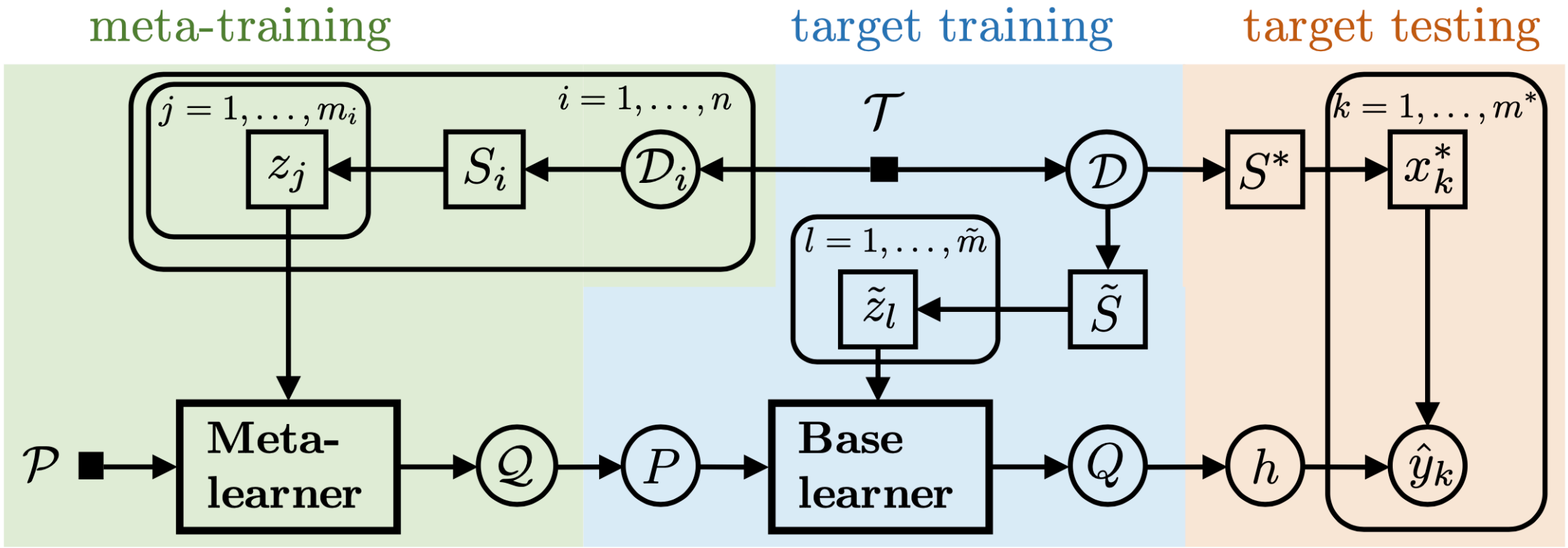
- If the prior has a lot of parameters, the marginal likelihood can still overfit
- Laplace-GGN approximation might be more akin to a ”flat minima”-style PAC-Bayes bound than true marginal likelihood

Agenda

- Pathologies of common BNN priors
- How to find better priors using the marginal likelihood
- PAC-Bayesian meta-learning for priors

PAC-Bayesian meta-learning

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



Our meta-learning PAC-bound

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

Theorem 2. *Let $Q : \mathcal{Z}^m \times \mathcal{M}(\mathcal{H}) \to \mathcal{M}(\mathcal{H})$ be a base learner, $\mathcal{P} \in \mathcal{M}(\mathcal{M}(\mathcal{H}))$ some fixed hyper-prior $\mathcal{P}$ and $\lambda, \beta > 0$. For any confidence level $\delta \in (0, 1]$ the inequality*

$$\mathcal{L}(\mathcal{Q}, \mathcal{T}) \leq \hat{\mathcal{L}}(\mathcal{Q}, S_1, ..., S_n) + \left(\frac{1}{\lambda} + \frac{1}{n\beta}\right) D_{KL}(\mathcal{Q}||\mathcal{P}) + \frac{1}{n}\sum_{i=1}^{n} \frac{1}{\beta} \mathbb{E}_{P\sim\mathcal{Q}} \left[D_{KL}(Q(S_i, P)||P)\right] + C(\delta, \lambda, \beta) \tag{4}$$

holds uniformly over all hyper-posteriors $\mathcal{Q} \in \mathcal{M}(\mathcal{M}(\mathcal{H}))$ with probability $1 - \delta$.

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PAC-bound for Bayesian base learners

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

Corollary 1. *When choosing a Gibbs posterior* $Q^*(S_i, P) := P(h)\exp(-\beta\hat{\mathcal{L}}(S_i, h))/Z_\beta(S_i, P)$ *as a base learner, under the same assumptions as in Theorem 2, we have*

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with probability at least $1 - \delta$.

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

	Accuracy	Calibration error
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MLAP (Amit & Meir, 2018)	0.700 ± 0.0135	0.108 ± 0.010
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BMAML (Kim et al., 2018)	0.764 ± 0.025	0.191 ± 0.018
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Few-shot learning on Omniglot

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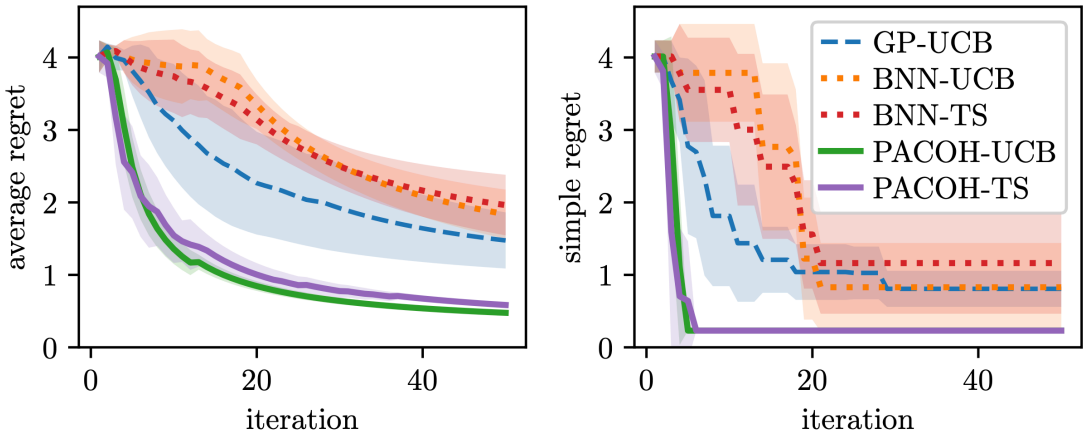

Bandit task

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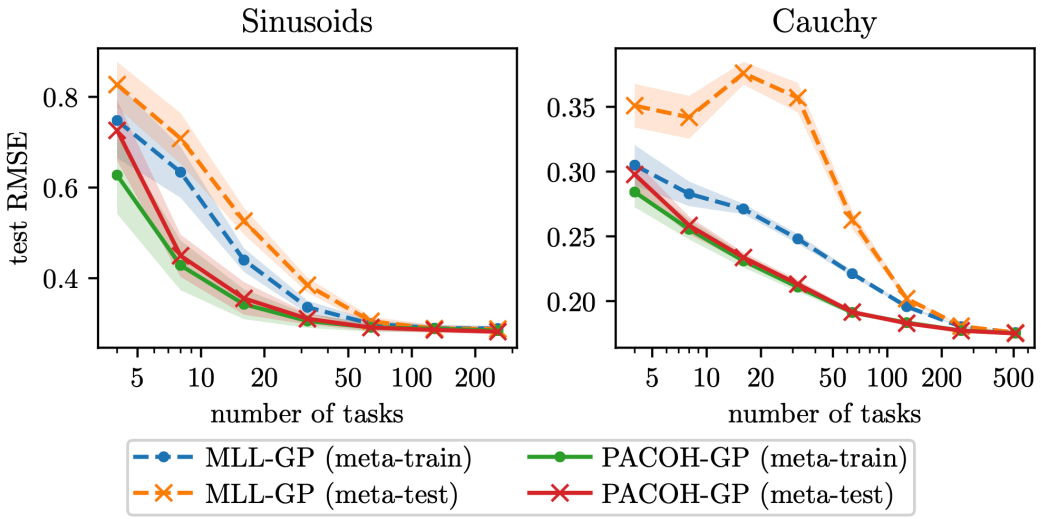
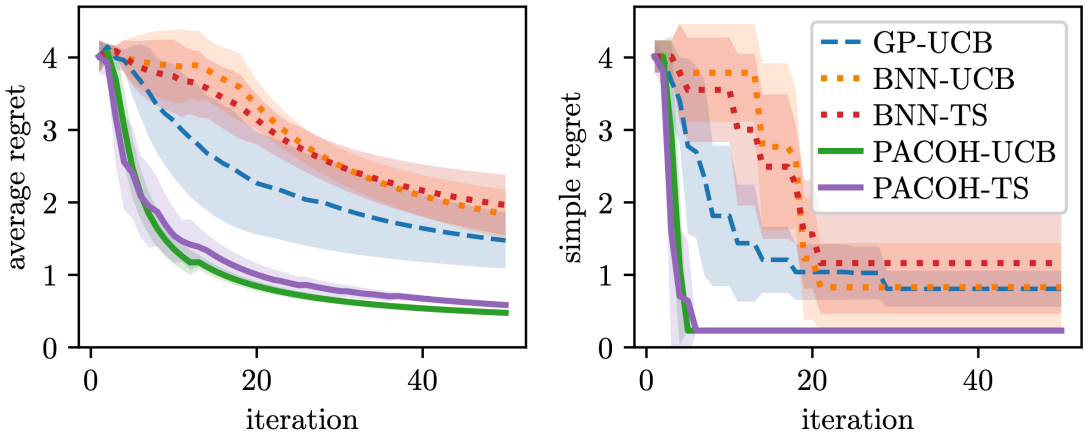


Meta-overfitting



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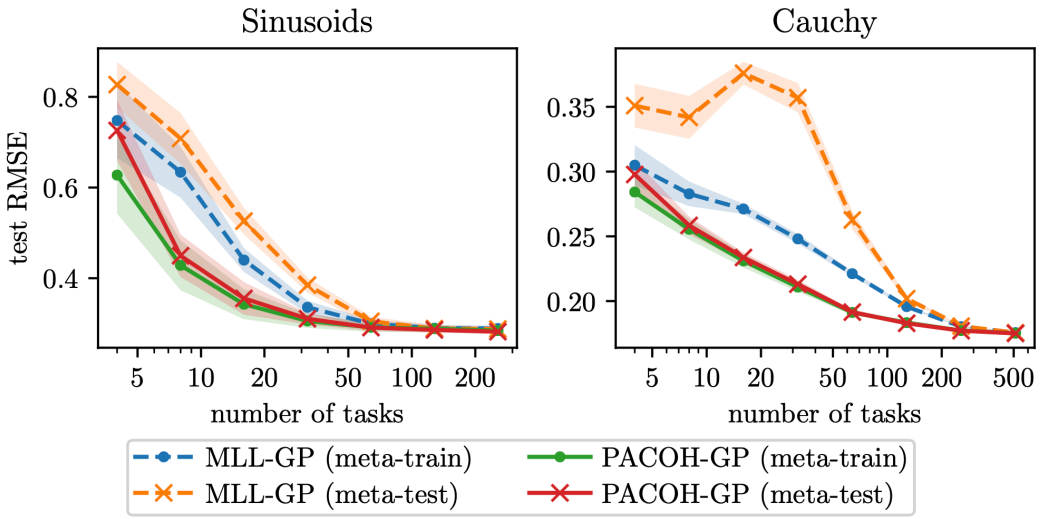

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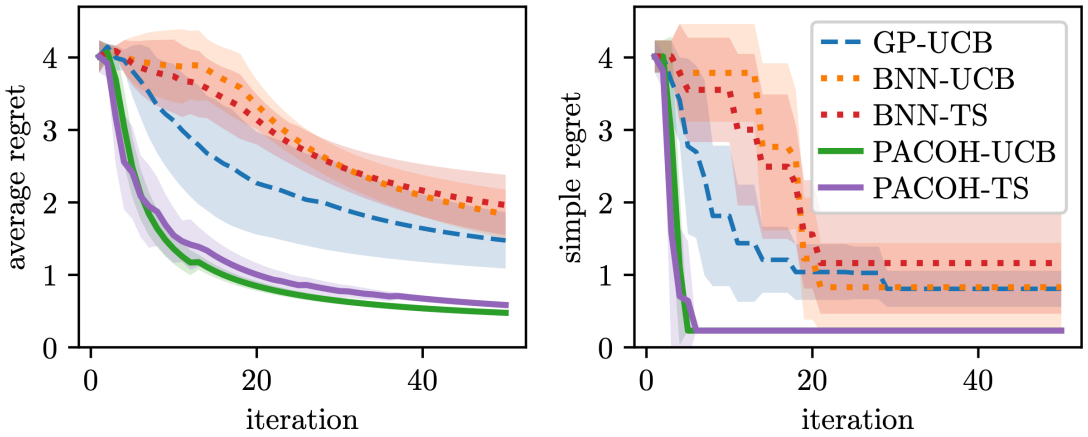

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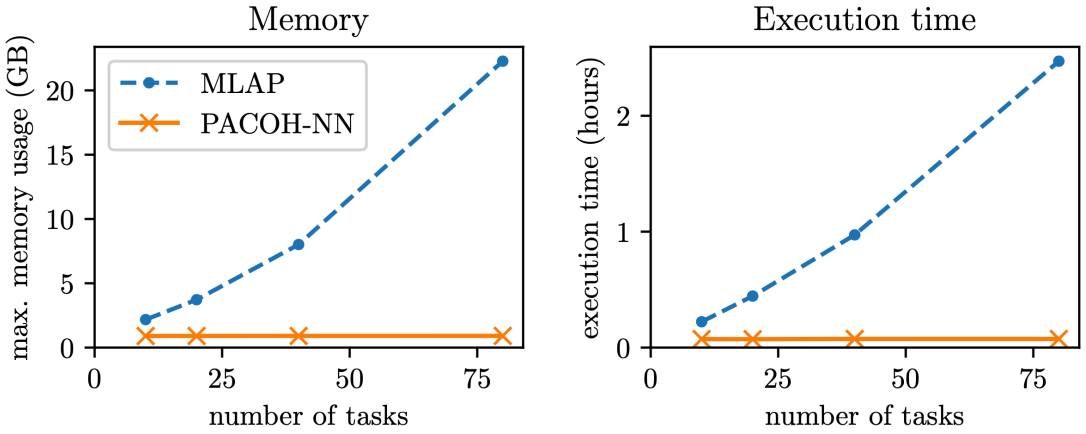

Runtimes

Caveats

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- The bounds themselves are still very loose (and possibly vacuous), so optimizing them is not guaranteed to help

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- Choosing λ and β trades off asymptotic consistency with tightness on low data

Take-home messages

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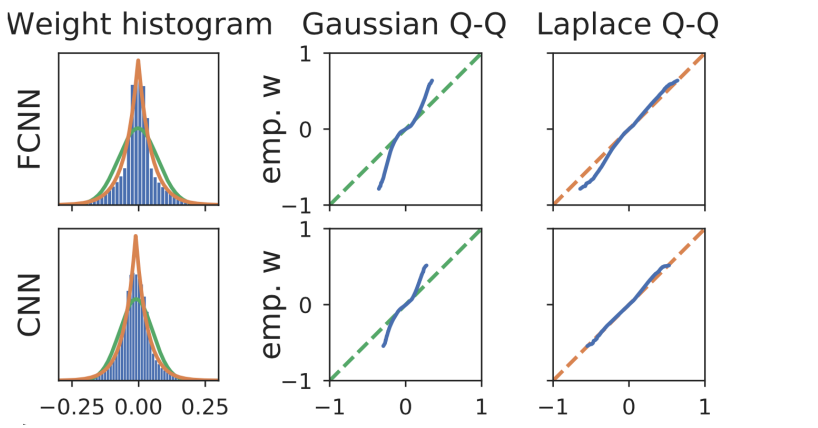
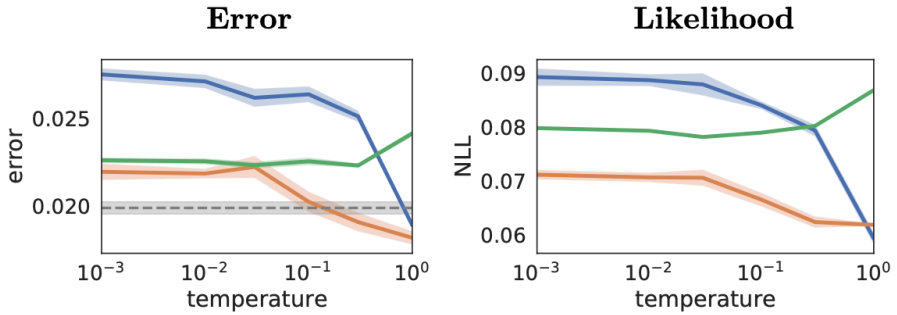
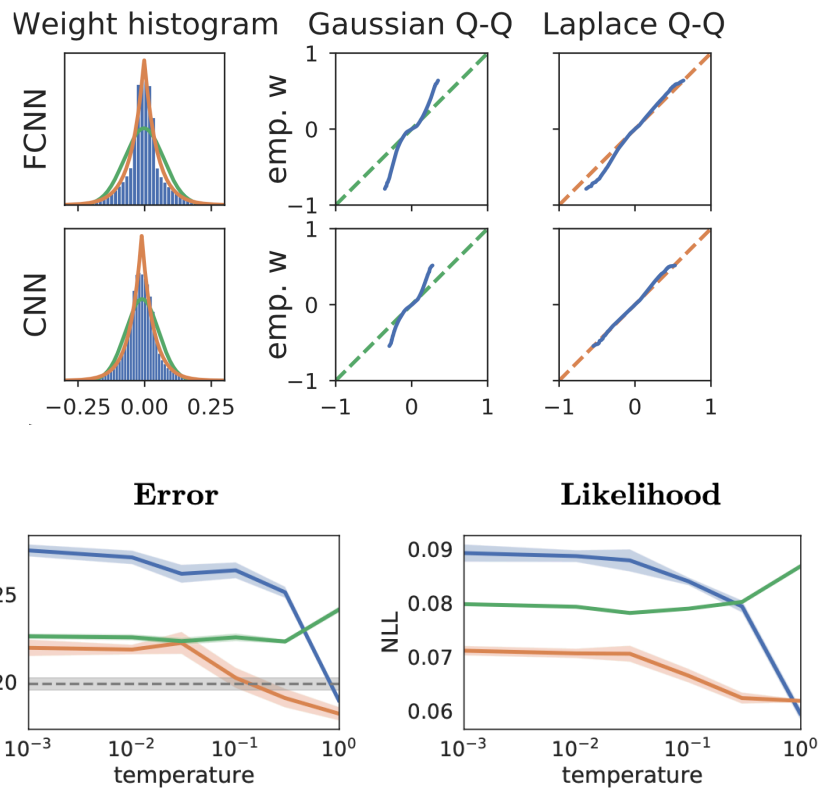




Common Bayesian neural network priors yield sub-optimal performance

Take-home messages



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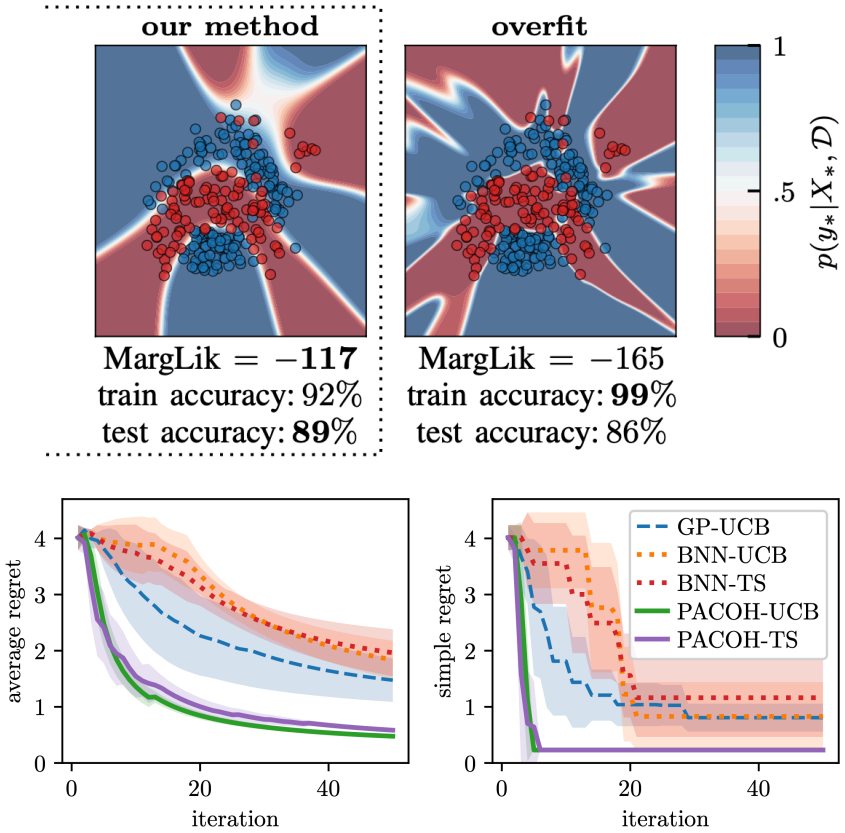

We can find better priors using ML-II or (PAC-Bayesian) meta-learning

Further reading

International Statistical Review / Early View

Original Article | Open Access

Priors in Bayesian Deep Learning: A Review

Vincent Fortuin

First published: 11 May 2022

https://doi.org/10.1111/insr.12502

Thank you!

Deepmind

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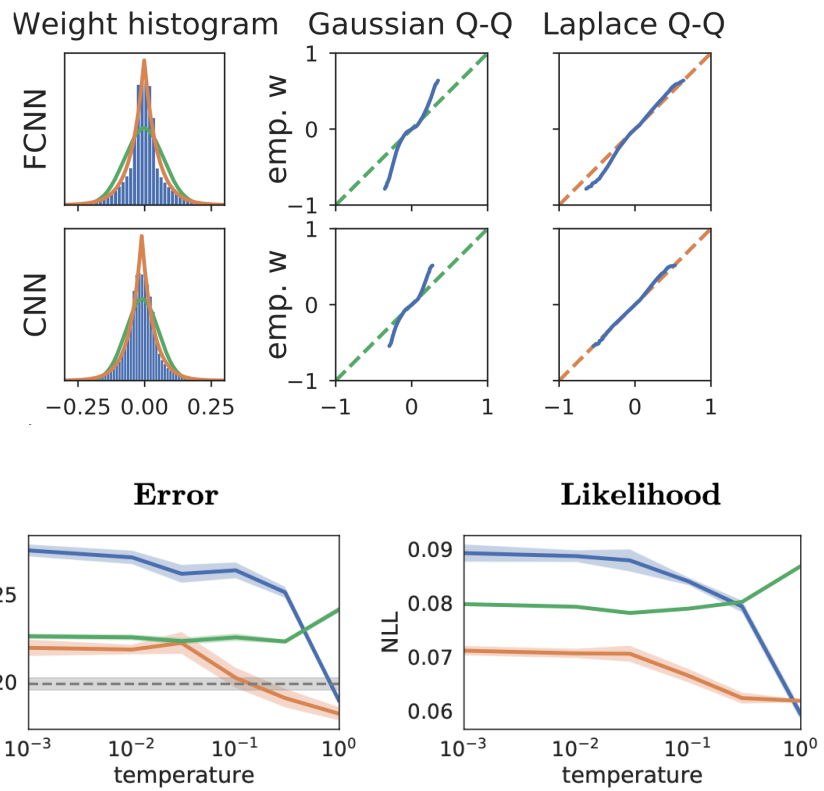
Take-home messages



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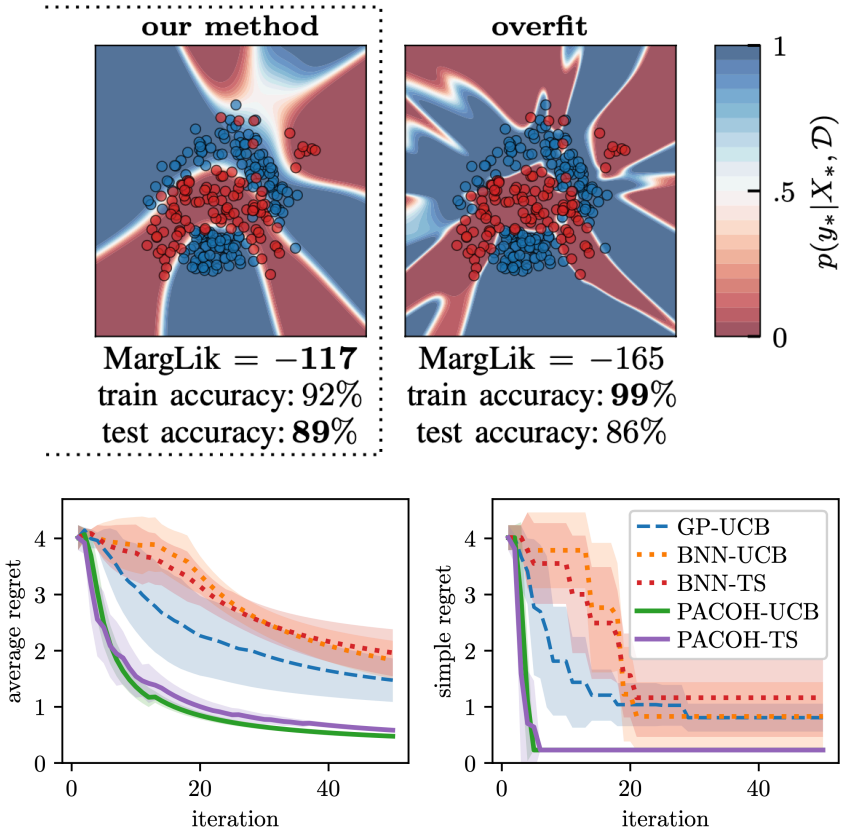

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