UNIVERSITY OF CAMBRIDGE

Bayesian Methods in Deep Learning

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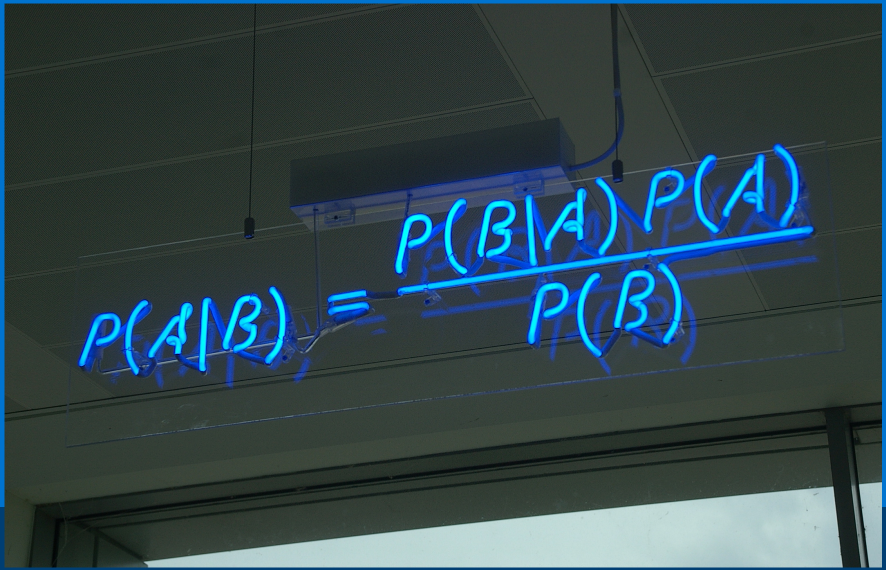
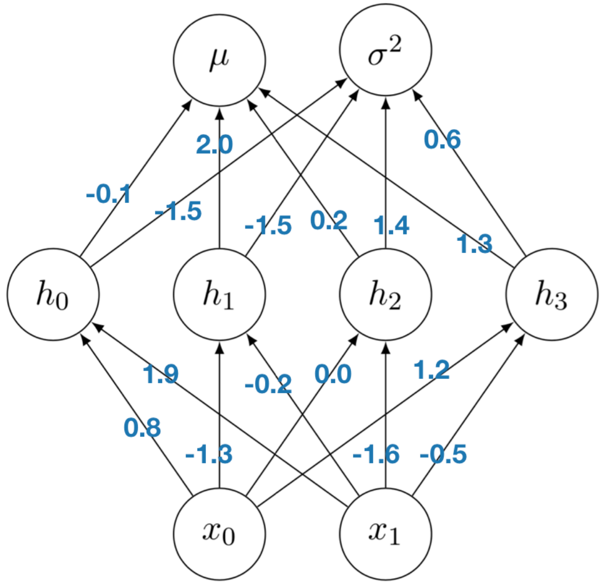
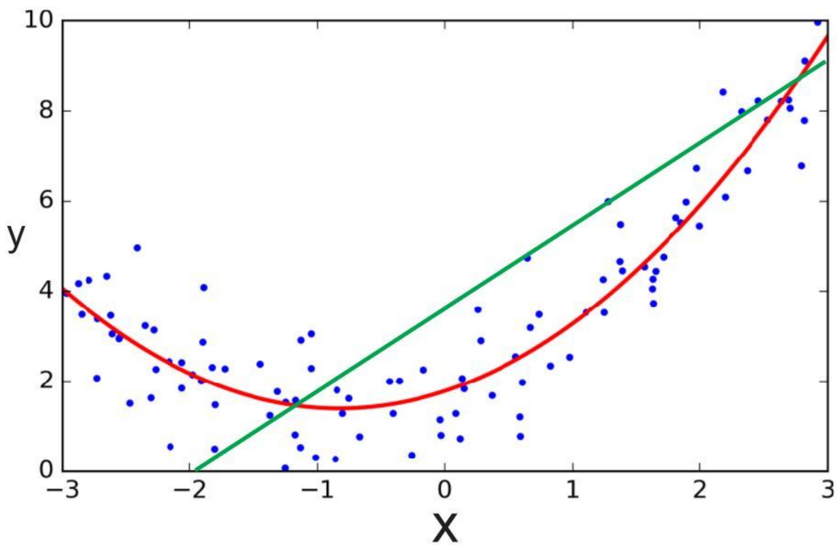


Feel free to interrupt at any time :)

Deep learning

- Overparametrised non-linear models
- ML / MAP inference + Stochastic optimisation
- Needs lots of data



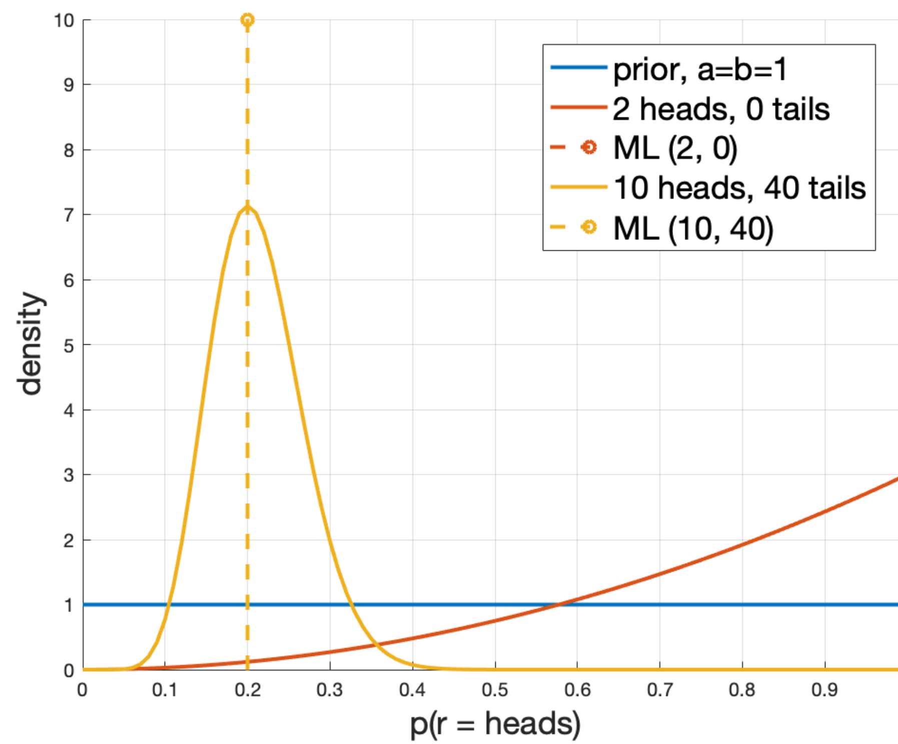


Probabilistic Inference: A biased coin

Likelihood

Prior

$$p(\mathbf{w}|\mathscr{D}) = \frac{p(\mathscr{D}|\mathbf{w})p(\mathbf{w})}{p(\mathscr{D})}$$

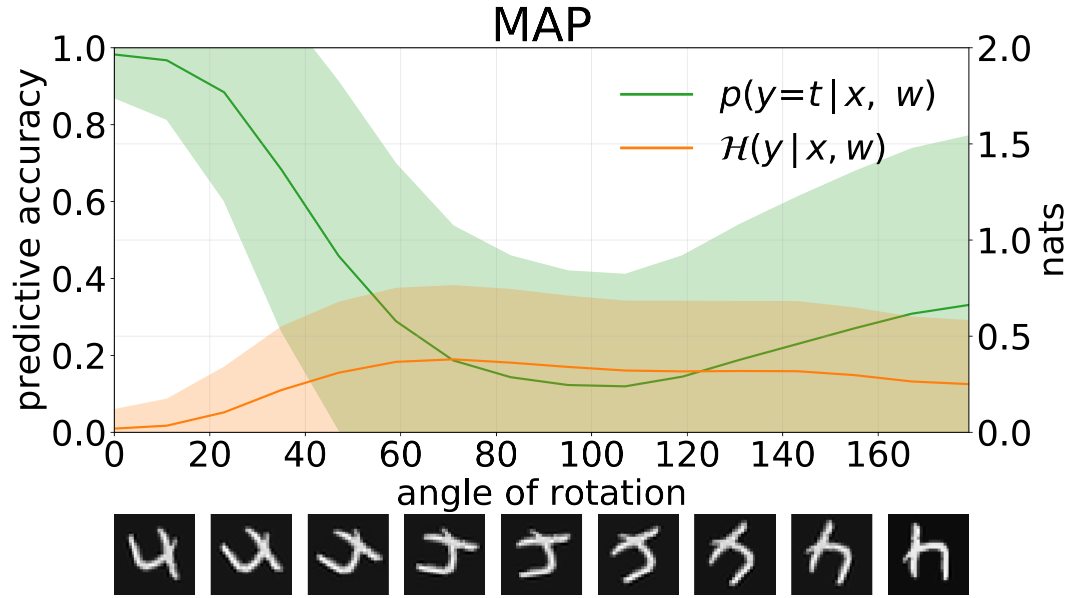


The Problem With MAP / ML

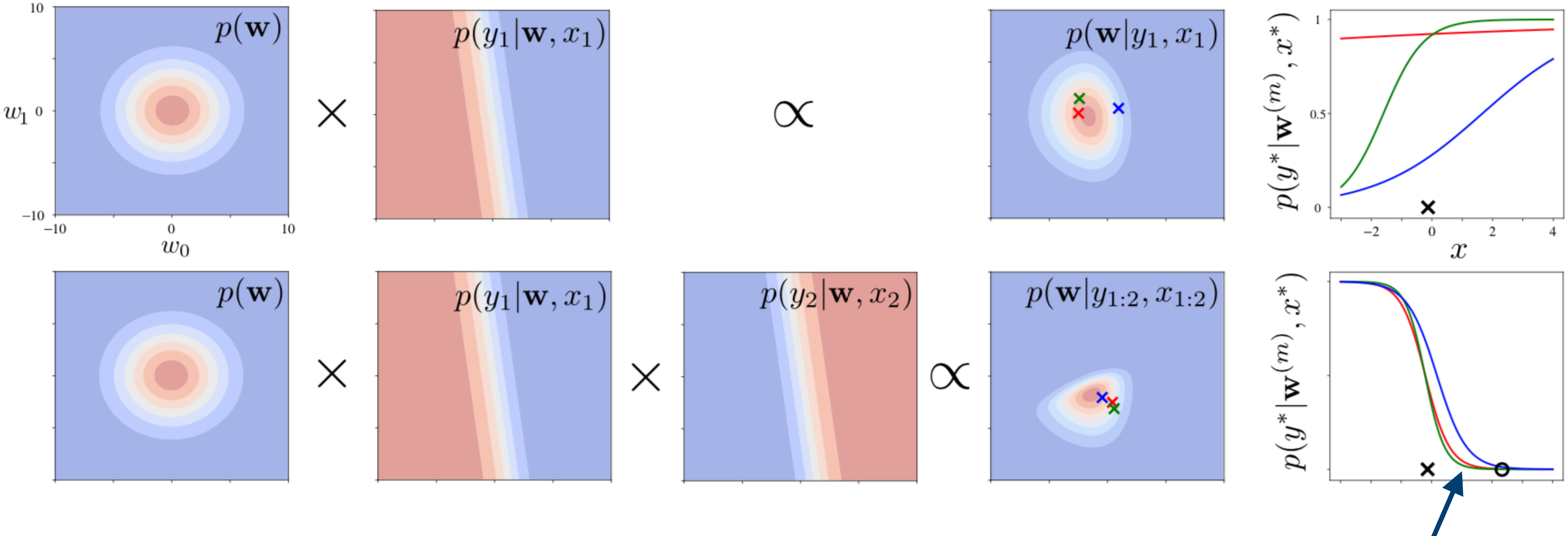
Given a dataset $\mathscr{D} = \{\mathbf{X}, \mathbf{Y}\}$ composed of inputs $\mathbf{X} = \{\mathbf{x}_1 \dots \mathbf{x}_n\}$ and targets $\mathbf{Y} = \{\mathbf{y}_1 \dots \mathbf{y}_n\}$, and a neural network parametrised by $\mathbf{w}$, the maximum likelihood criterion:

$$\mathbf{w}_{ml} = \arg\max_{\mathbf{w}} p(\mathscr{D}|\mathbf{w}) = \arg\max_{\mathbf{w}} \log p(\mathscr{D}|\mathbf{w}) \tag{2.1}$$

- MAP / ML returns the parameter setting that best explains the data.
- It may not be the only good explanation.
- No guarantees about unseen data. These must be introduced through priors.



1-d Probabilistic Logistic Regression



$p(\mathbf{w})$ $\times$ $P(\mathcal{Y}|\mathbf{w}, \mathcal{X})$ $\propto$ $p(\mathbf{w}|\mathcal{Y}, \mathcal{X})$

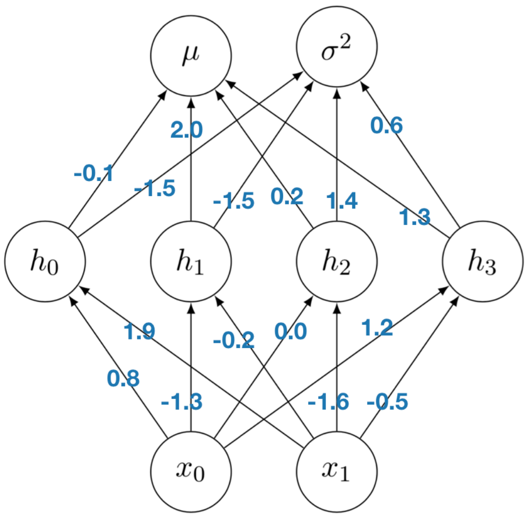
prior
what we knew
before seeing data

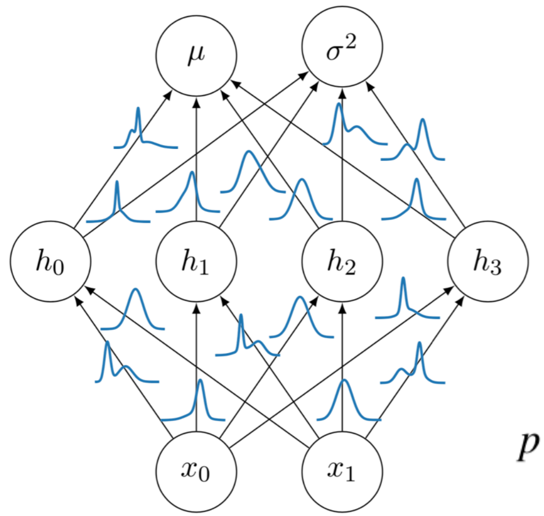
likelihood of $\mathbf{w}$
what the
data told us

posterior
what we know
after seeing data

Variability among samples of **w** is model uncertainty

Bayesian Neural Networks (BNNs)

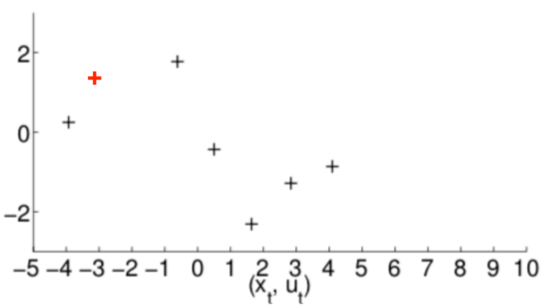


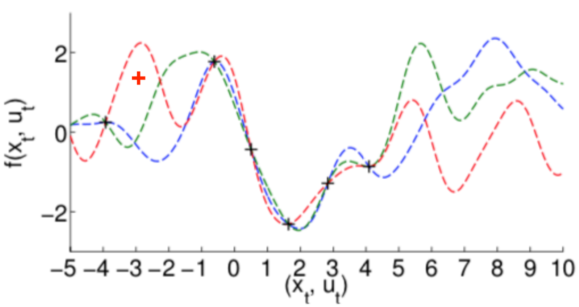


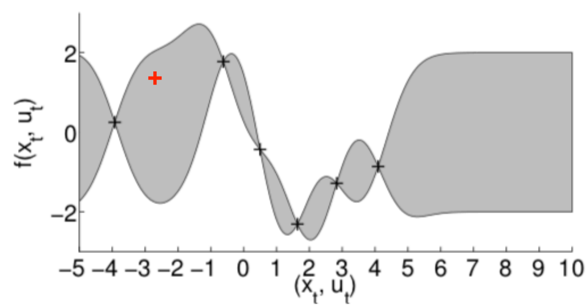
- Predictions incorporate model uncertainty!

$$p(\mathbf{Y}^*|\mathbf{X}^*, \mathscr{D}) = \int p(\mathbf{Y}^*|\mathbf{X}^*, \mathbf{w}) p(\mathbf{w}|\mathscr{D})\, d\mathbf{w}$$

$\mu(x_t)$
$\sigma = 0$

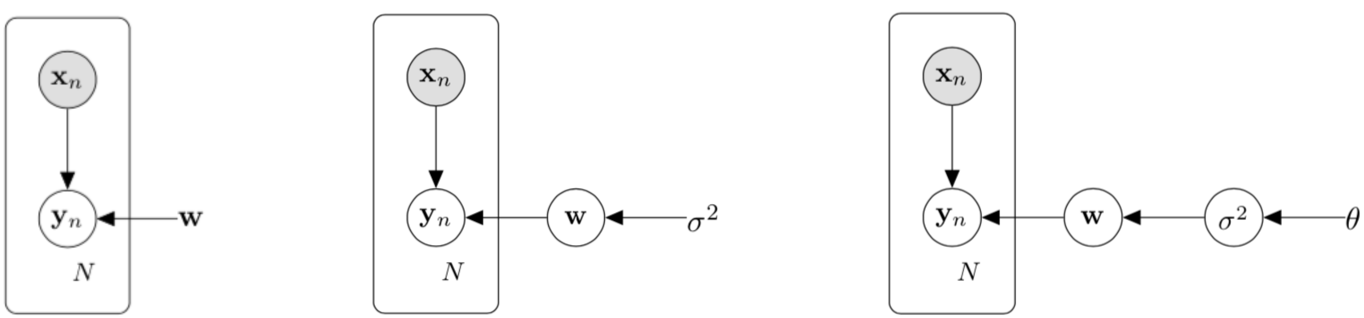






Practical Forms of Prior

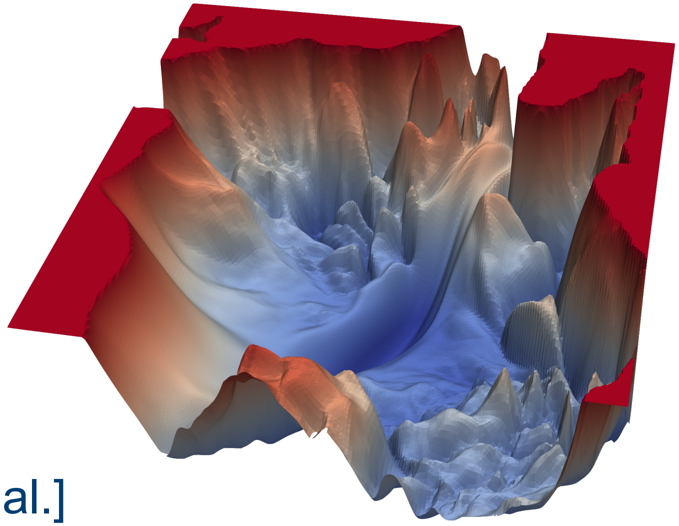
- ML / MAP **a)**
- Symmetric tractable prior **b)**
  - Gaussian, Laplace, Student-T, etc
  - Type-2 Maximum Likelihood
  - Previous posterior (Bayesian update)
- Conjugate hyper-prior + Gibbs sampling (hierarchical model) **c)**



a) **b)** **c)**

Inference with BNNs

- The data's likelihood under a BNN model is a very complex, high dimensional and multimodal function.



[Li et al.]

- **Intractable evidence:**

$$p(\mathscr{D}) = \int p(\mathscr{D}|\mathbf{w})p(\mathbf{w})\,d\mathbf{w}$$

- **Intractable predictive:**

$$p(\mathbf{Y}^*|\mathbf{X}^*,\mathscr{D}) = \int p(\mathbf{Y}^*|\mathbf{X}^*,\mathbf{w})p(\mathbf{w}|\mathscr{D})\,d\mathbf{w}$$

- Must resort to **Approximate Inference**

Variational Inference

Calculus of variations is like finding optima of a function but instead of finding a value of (x, y) which yields the optima, you find a function which yields the optima.

Kullback–Leibler (KL) divergence $\mathrm{KL}(q(\mathbf{w})||p(\mathbf{w})) = \int q(\mathbf{w}) \log \frac{q(\mathbf{w})}{p(\mathbf{w})} \mathrm{d}\mathbf{w}$

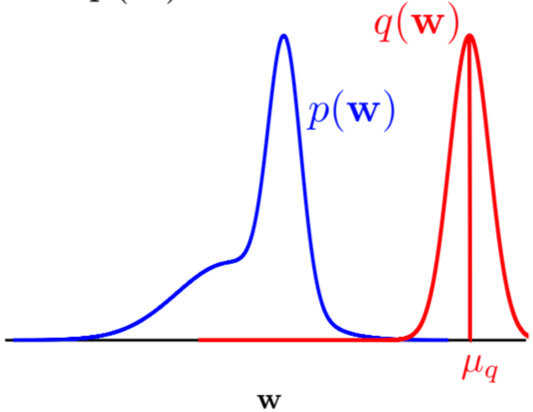
1. non-negative

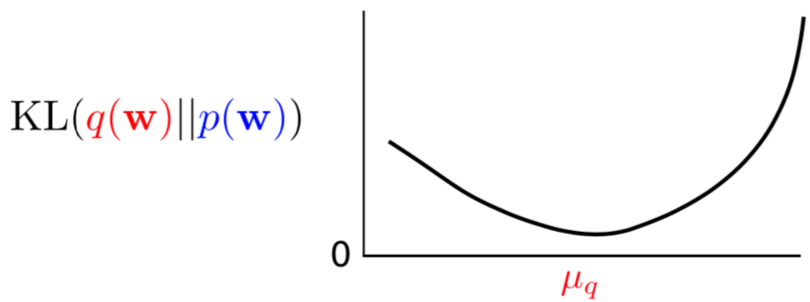
$$\frac{\delta^2}{\delta q^2}\mathrm{KL}(q(\mathbf{w})||p(\mathbf{w})) = \frac{1}{q(\mathbf{w})} \geq 0$$

2. zero (minimised) when $q(\mathbf{w}) = p(\mathbf{w})$

$$\mathrm{KL}(p(\mathbf{w})||p(\mathbf{w})) = \int p(\mathbf{w}) \log \frac{p(\mathbf{w})}{p(\mathbf{w})} \mathrm{d}\mathbf{w} = 0$$

First grad = 0 only if q=p.
Second grad -> strictly convex

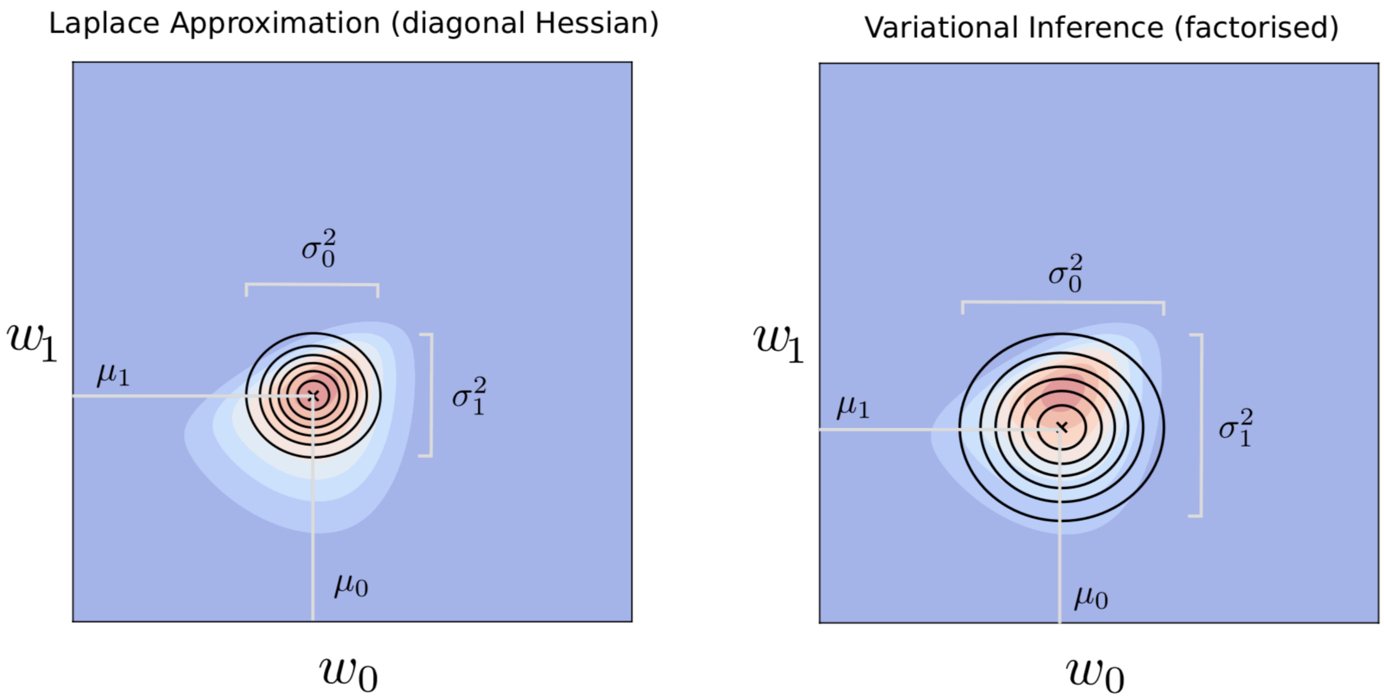




3. can be computed up to an additive constant w/o needing normalisation for $p(\mathbf{w})$

Issues with VI

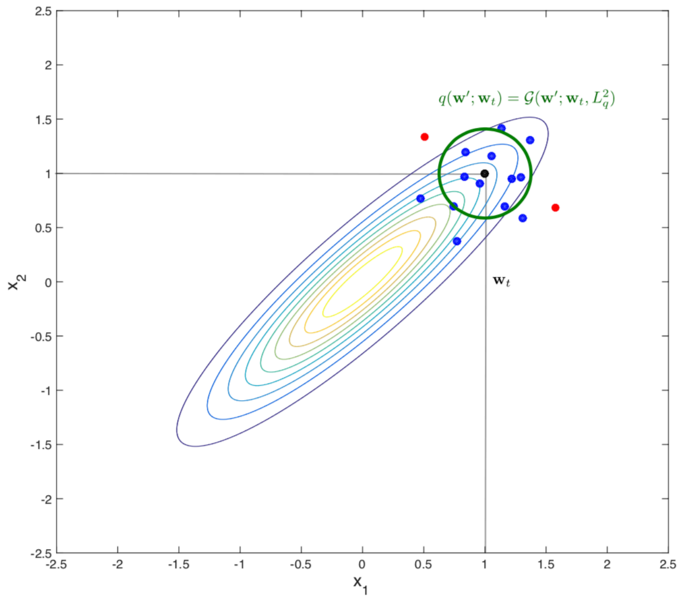
- Mode seeking behaviour
- Overly simple approximate posteriors (complexity vs tractability)



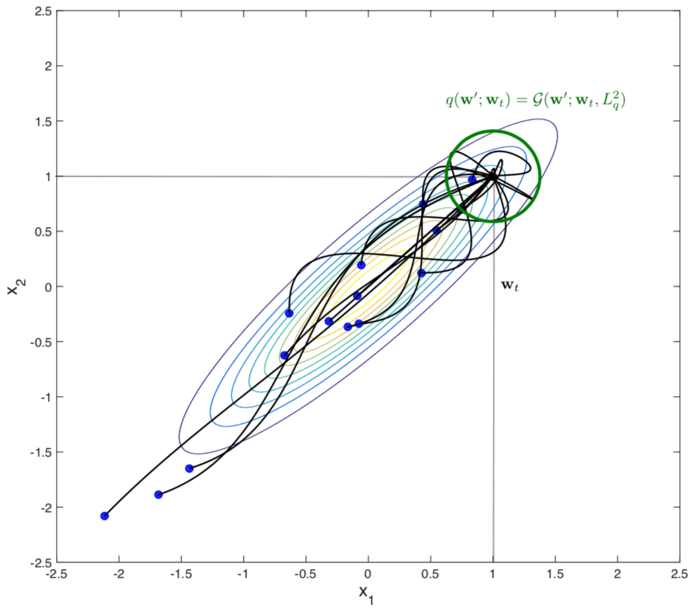
Markov Chain Monte Carlo

$$p(\mathbf{Y}^*|\mathbf{X}^*,\mathscr{D}) \approx \sum_{k=1}^{K} p(\mathbf{Y}^*|\mathbf{X}^*,\mathbf{w}_k); \quad \mathbf{w}_k \sim p(\mathbf{w}|\mathscr{D})$$

- Robust uncertainty requires sample diversity: HarleMCMC shake

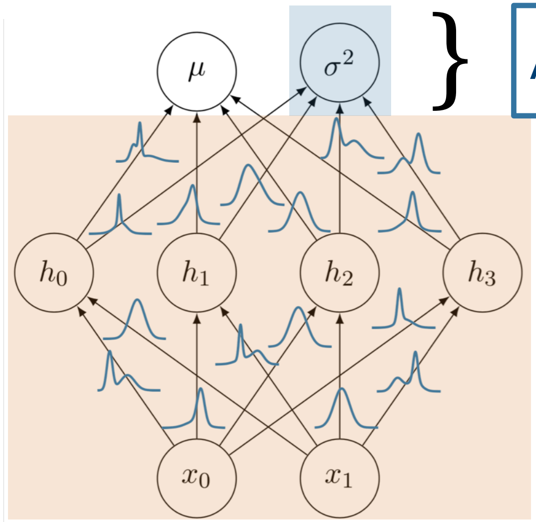


Metropolis



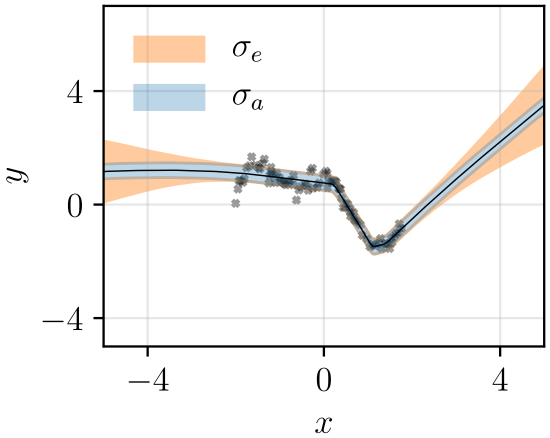
Hybrid Monte Carlo

Uncertainty Decomposition

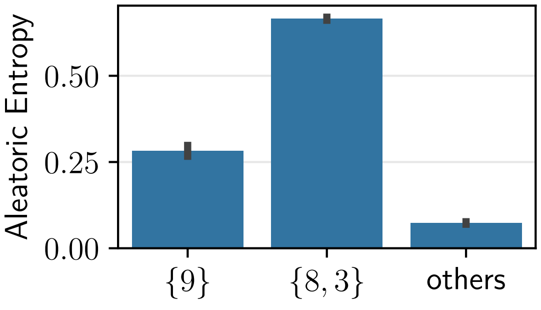


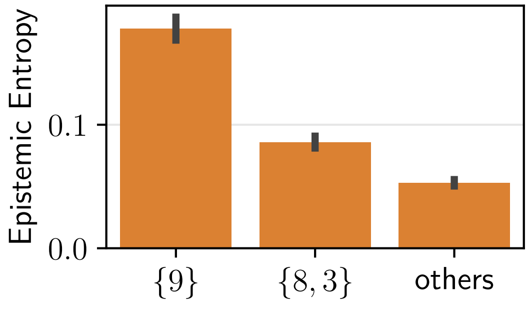
Aleatoric Uncertainty

Model Uncertainty



MNIST; Remove 80% of {9} and permute 30% {8,3}

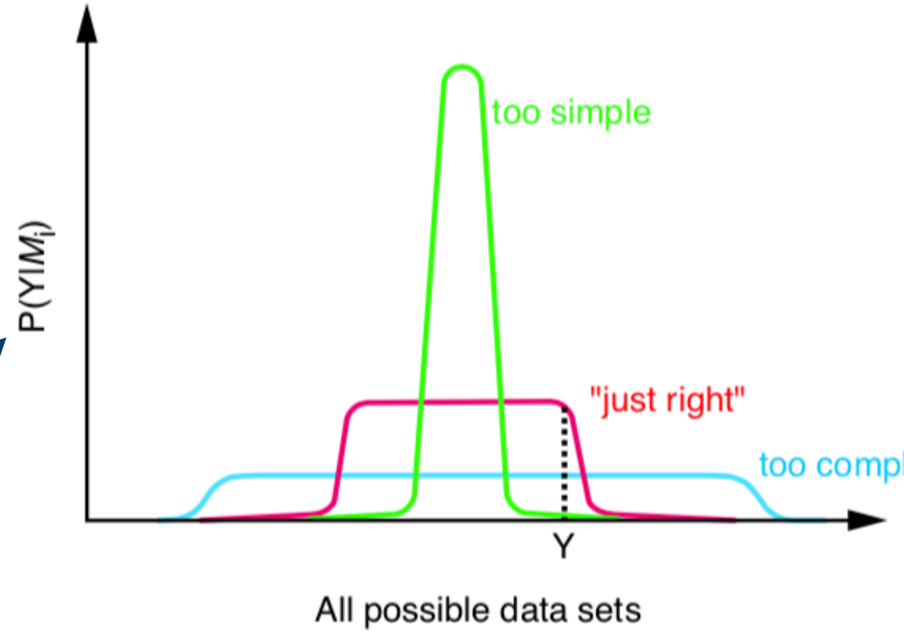




Protection Against Overfitting

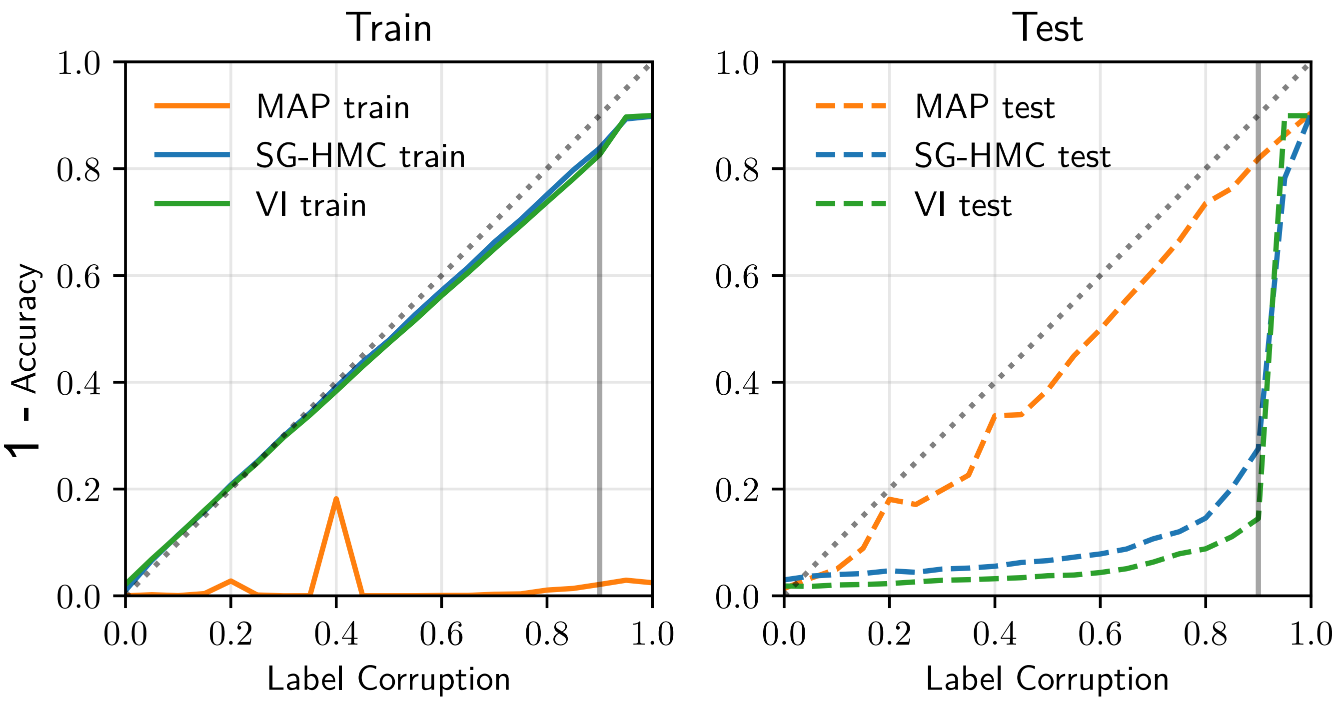
- Model uncertainty is transformed into predictive uncertainty
- With uninformative prior, automatic tradeoff between goodness of fit and model complexity: Automatic Ockham's Razor. (Related to MDL)

Marginal Likelihood



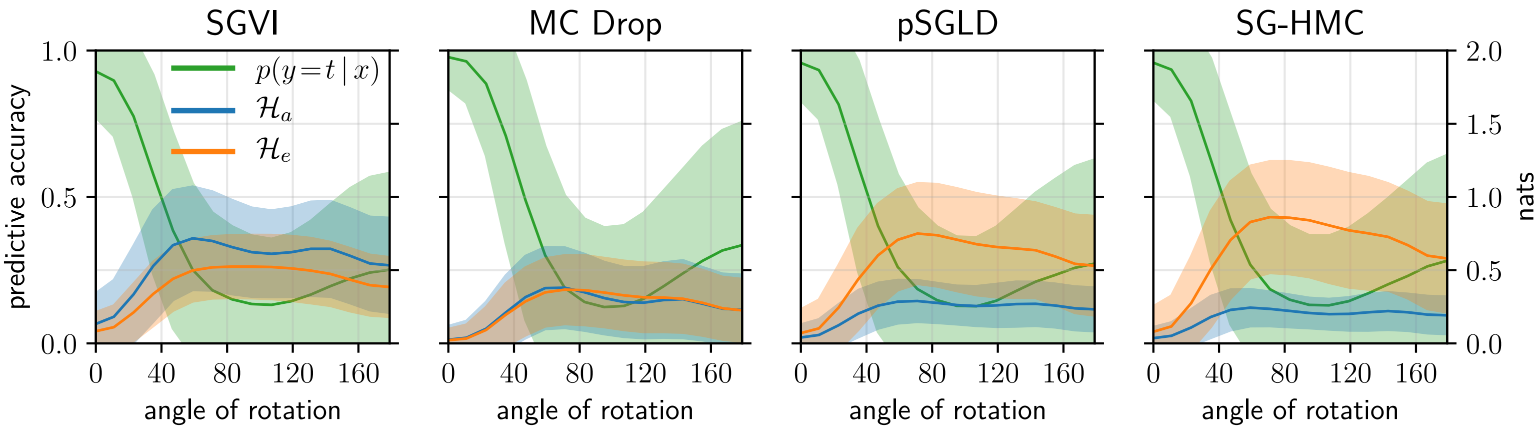
Protection Against Overfitting (cont)

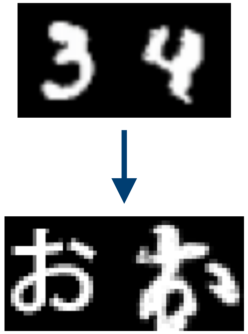
- Plot of train error and test error when training different models with increasing number of permuted samples

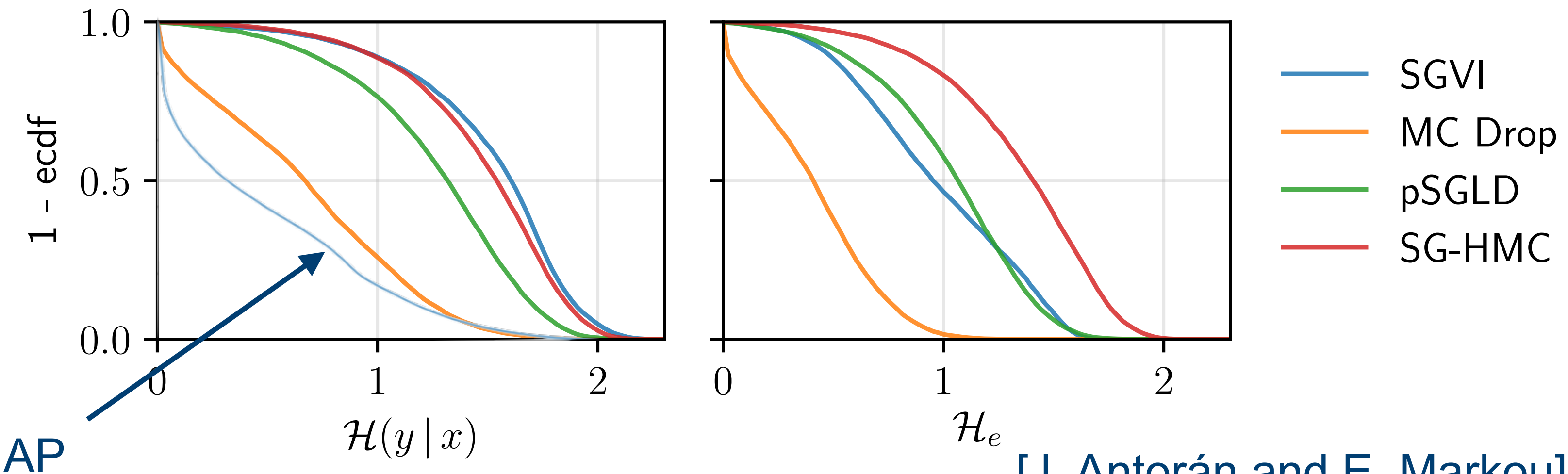


[Unpublished results]

Out of Distribution Sample Detection

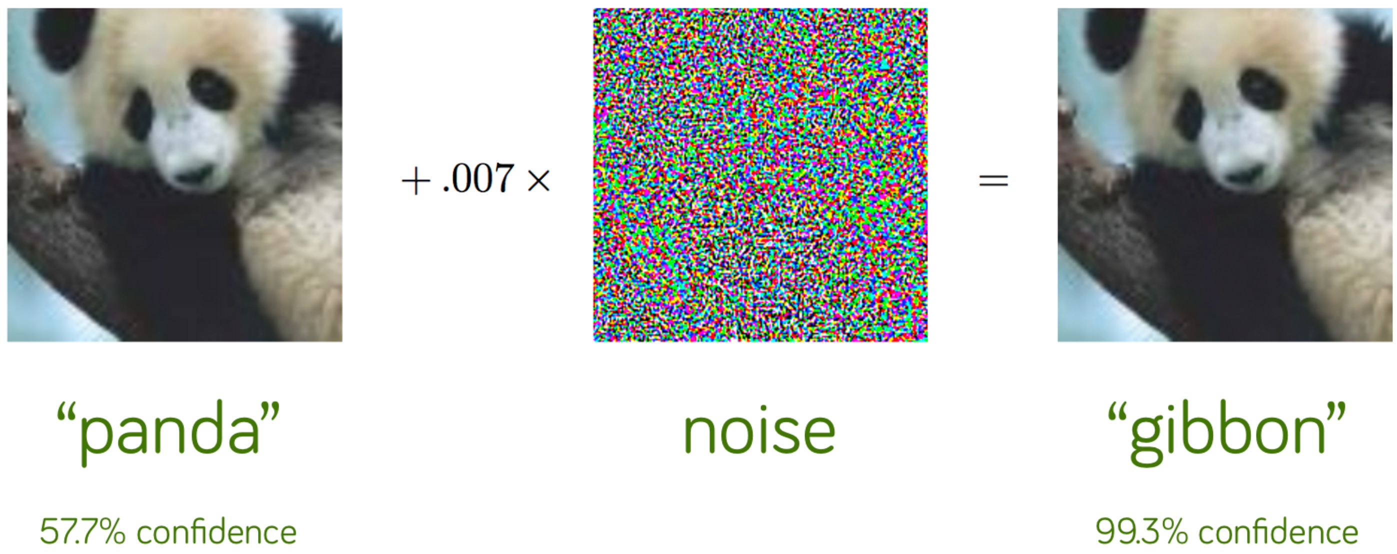




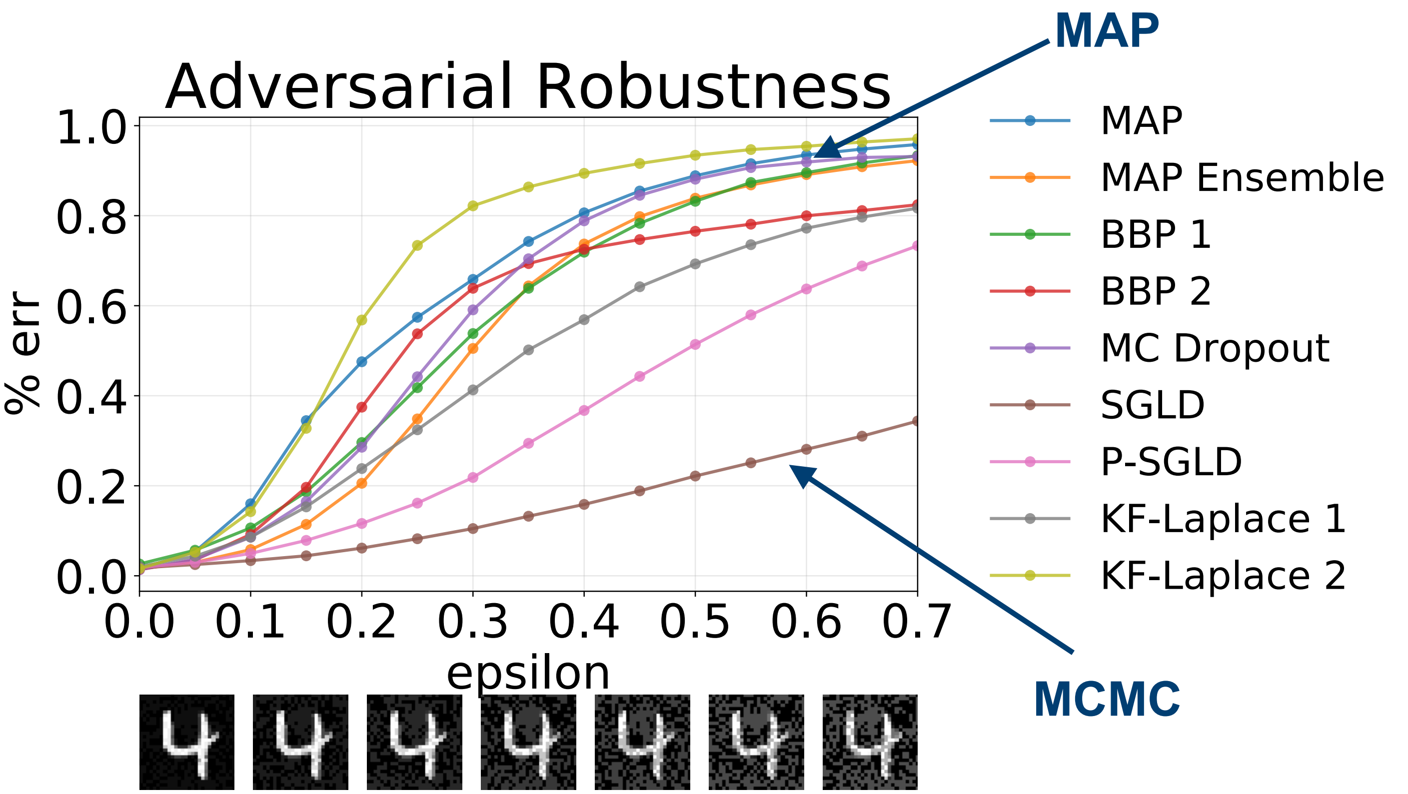


[J. Antorán and E. Markou]

Adversarial Robustness

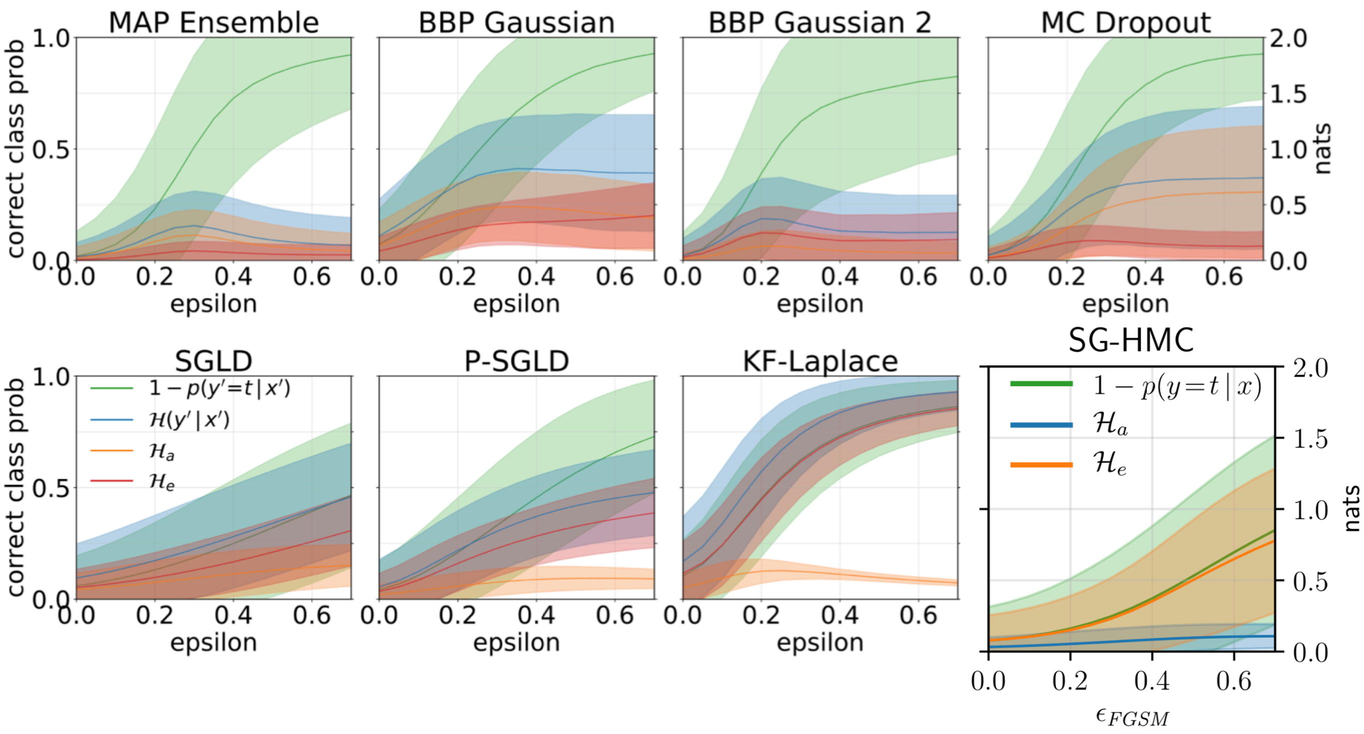


Adversarial Robustness



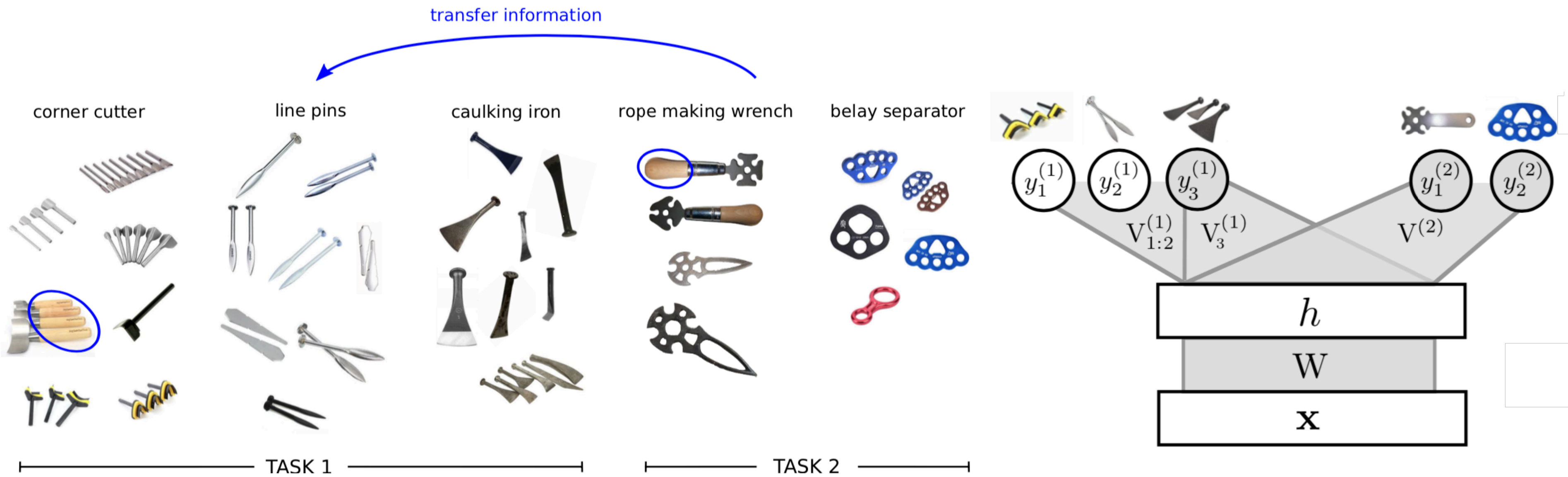
[J. Antorán and E. Markou]

Adversarial Robustness

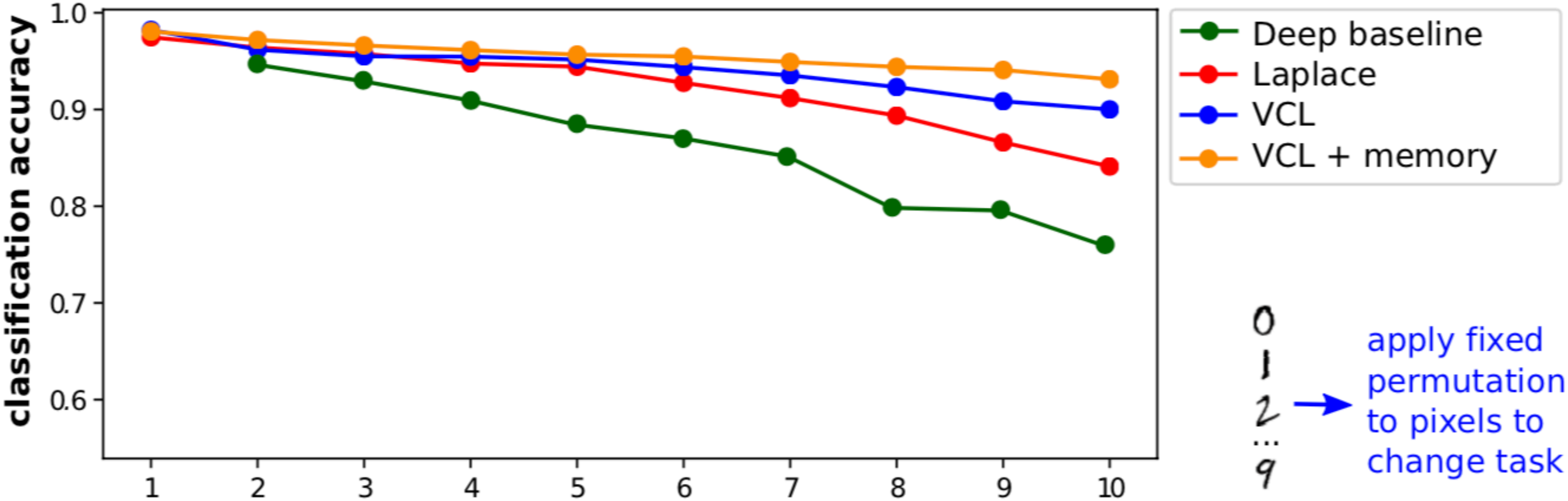


[J. Antorán and E. Markou]

Continual Learning



Continual Learning

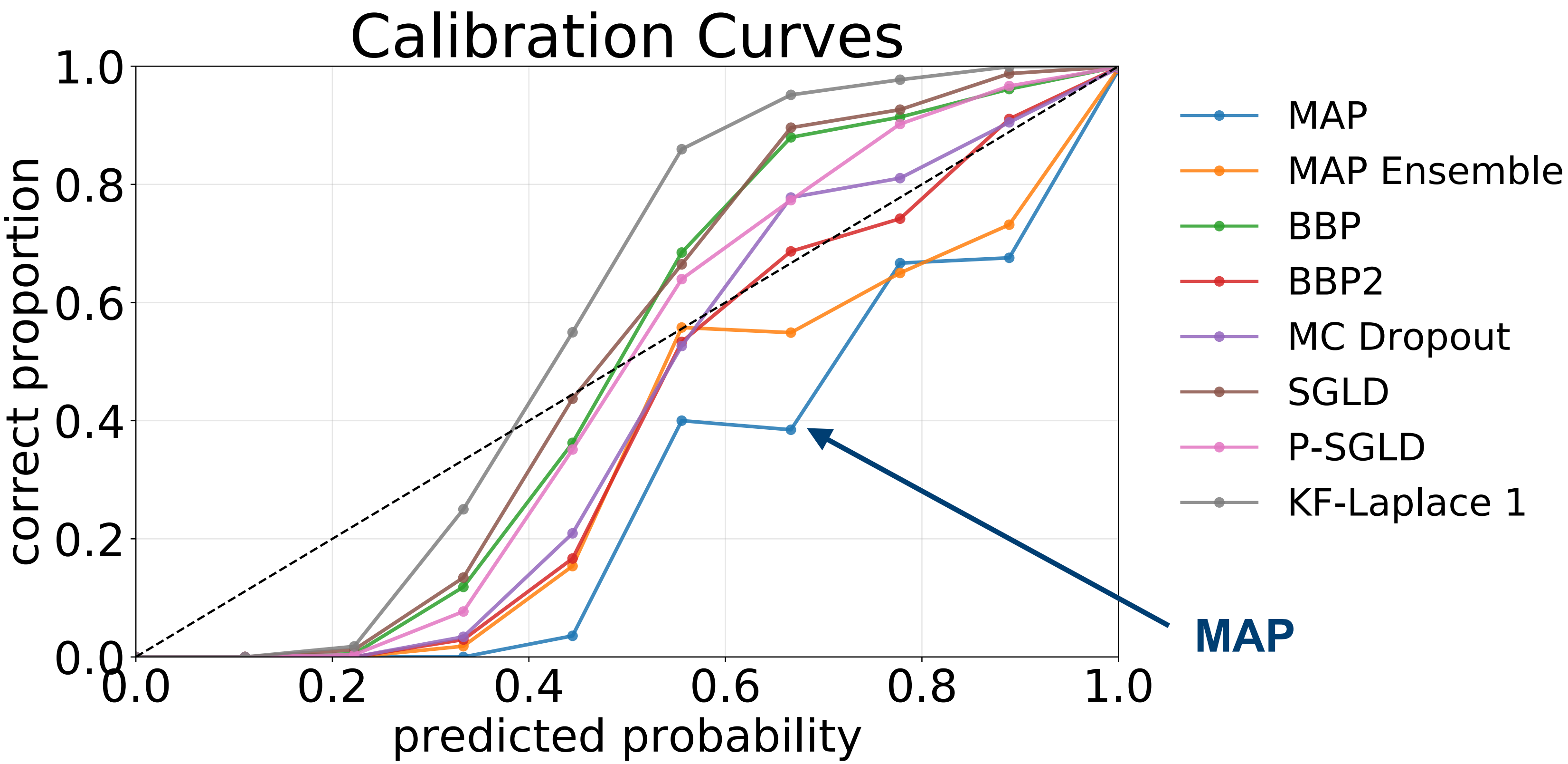


apply fixed permutation to pixels to change task

$$p(\mathbf{w}|\mathcal{D}_1,\mathcal{D}_2) = \frac{p(\mathcal{D}_2|\mathbf{w})q(\mathbf{w}|\mathcal{D}_1)}{p(\mathcal{D}_2)}$$

[C. Nguyen et al.]

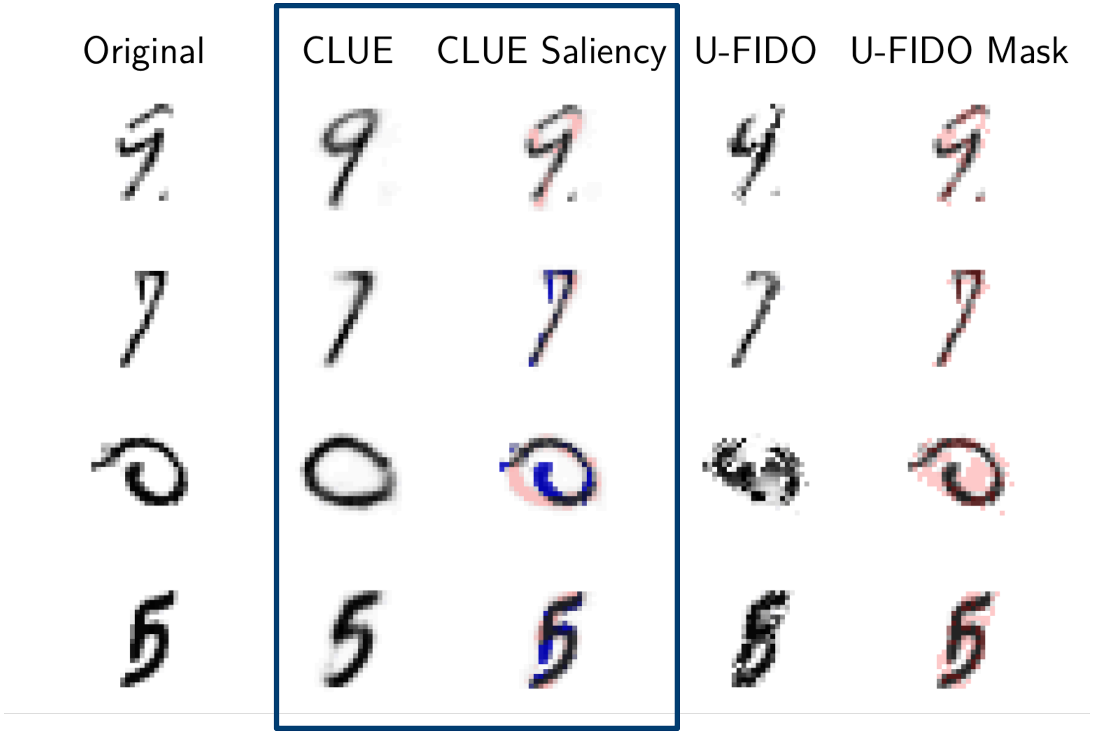
Calibration



[J. Antorán and E. Markou]

Uncertainty Interpretability

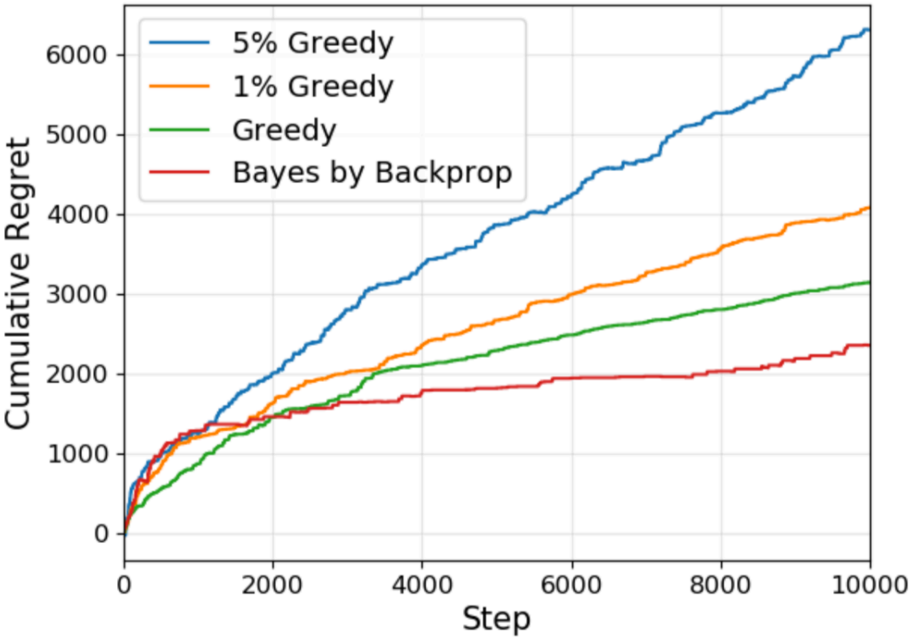
- Why is our model uncertain?



[J. Antorán]

Balancing Exploration and Exploitation: Bandits

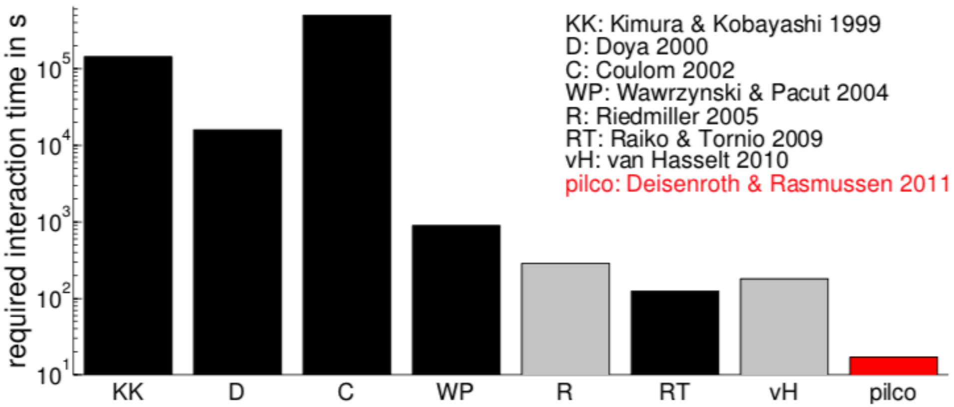
- Different mushrooms give different rewards with different probs.



- + RL / Active Learning / Bayesian Optimisation

Sample-Efficiency in Reinforcement Learning

- Probabilistic models help reduce model bias is RL
- PILCO uses a GP model and a free-form (linear, RBF, NN) controller.



PILCO learner

PILCO learner CS

[M. P. Deisenroth and C. E. Rasmussen]

Open Source BNNs

github.com/JavierAntoran/Bayesian-Neural-Networks

Bayesian-Neural-Networks

Pytorch implementations of Bayes By Backprop, MC Dropout, SGLD, the Local Reparametrization Trick, KF-Laplace and more

Jupyter Notebook ★ 140 19

Bayesian Neural Networks

License MIT | python 2.7+ | pytorch 1.0.1

Pytorch implementations for the following approximate inference methods:

- Bayes by Backprop
- Bayes by Backprop + Local Reparametrisation Trick
- MC dropout
- Stochastic Gradient Langevin Dynamics
- Preconditioned SGLD
- Kronecker-Factorised Laplace Approximation
- Stochastic Gradient Hamiltonian Monte Carlo (Coming soon)

We also provide code for:

- Bootstrap MAP Ensemble

References

- Some slides taken from Richard E. Turner

Uncertainty in Bayesian Neural Networks
J. Antorán and E. Markou.
Presented at: Workshop on The Mathematics of Deep Learning and Data Science, The Isaac Newton Institute for Mathematical Sciences, Cambridge. 2019.

Excellent textbook introductions to Bayesian machine learning:

D. J. C. MacKay Information Theory, Inference and Learning Algorithms, 2003

C. Bishop Pattern Recognition and Machine Learning, 2006

K. Murphy Machine Learning: A Probabilistic Perspective, 2012

Beautiful seminal work on Bayesian neural networks:

R. M. Neal Bayesian Learning for Neural Networks, Lecture Notes in Statistics No. 118. New York: Springer-Verlag. 1996

More References (VI and Laplace)

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G. Hinton and D. Van Camp Keeping the neural networks simple by minimizing the description length of the weights, COLT 5-13, ACM, 1993

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A. Graves Practical Variational Inference for Neural Networks, NIPS 2011

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Bayesian Learning via Stochastic Gradient Langevin Dynamics, Welling and Teh, ICML, 2011

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