Alumni talk @ CBL

Imperial College London

How *Accurate* Gaussian Processes can help Deep Learning

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Apr 30, 2021

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Today, I'll be talking about some research from the last few years.

Overview

Goal: Towards automatic model selection in deep learning.

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Talk outline:

1. The promises of Bayesian Model Selection

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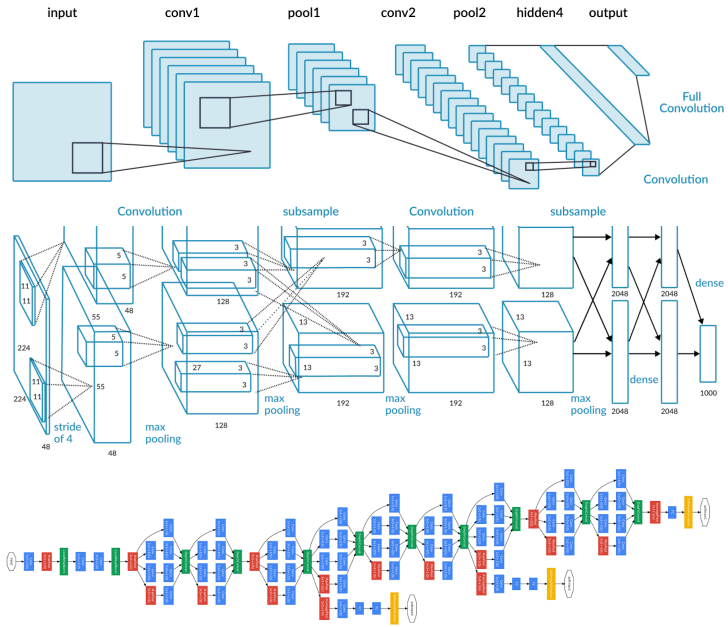
Talk outline:

1. The promises of Bayesian Model Selection
2. Accurate Gaussian process inference
3. GPs in Deep Learning
4. Other approaches: Ensembles and Architecture Search

Model Selection

Every time we train a NN we need to decide on hyperparameters:

- How many layers? How many units in a layer?
- What layer structure? Convolutional? Skip connections?
- Data augmentation parameters?



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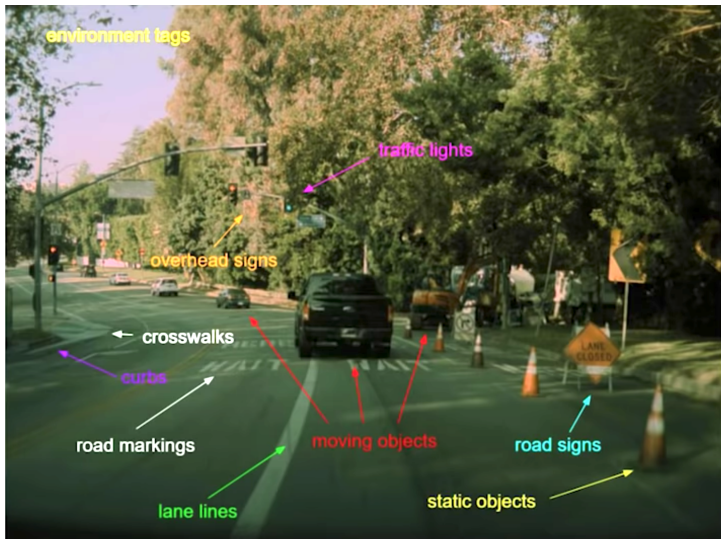
As architectures get more complex, so does design! E.g. multitask.

- Which layers to share?
- What kind of task-specific layers?
- How much capacity to assign to each task?



[Karpathy, ICML 2019]

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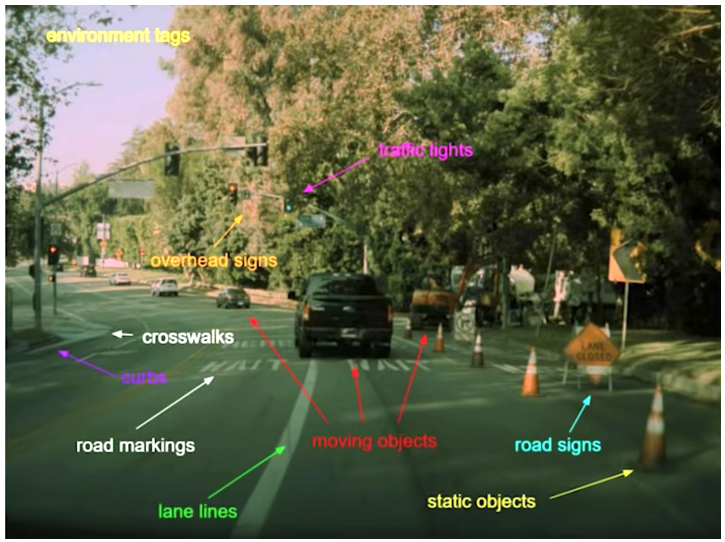

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Main tool is **crossvalidation**.

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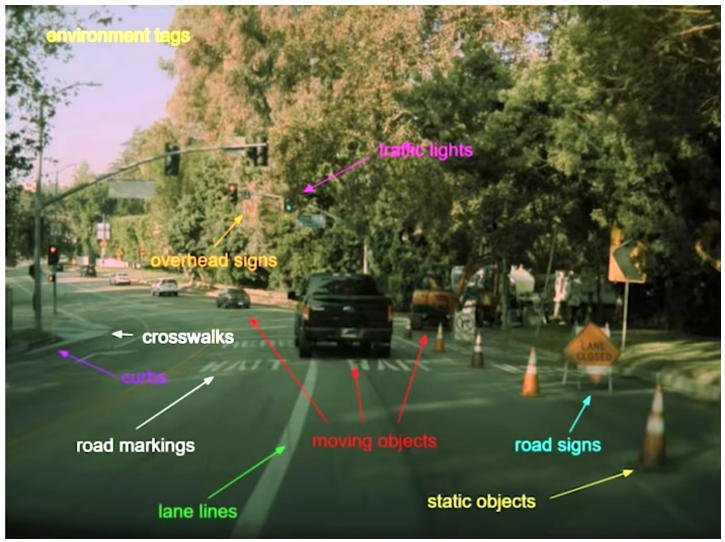

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Main tool is **crossvalidation**.

Goal: Make it as easy as learning weights.

Overview

The Promise of Bayesian Model Selection

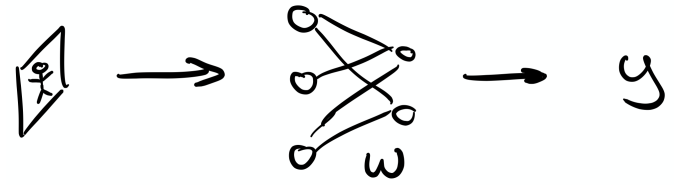
Accurate Inference in Gaussian Processes

Gaussian Processes in Deep Learning

Ensembles and Architecture Search

Conclusion

Bayesian Inference



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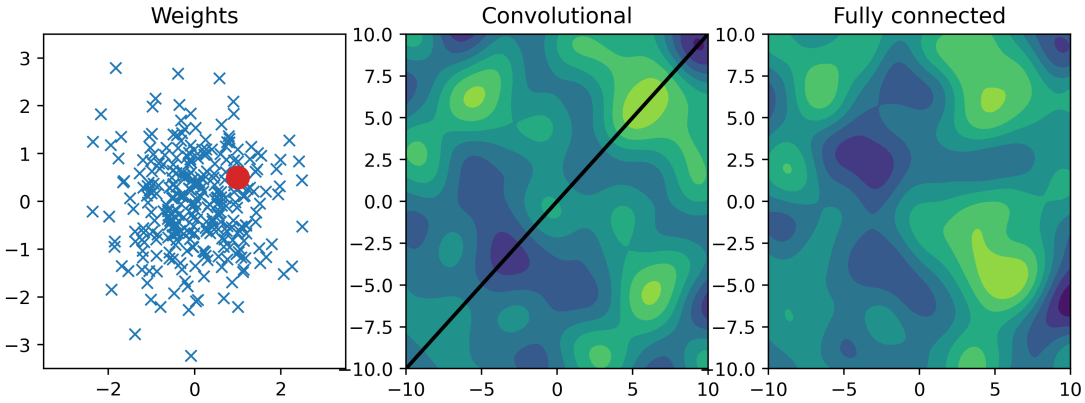
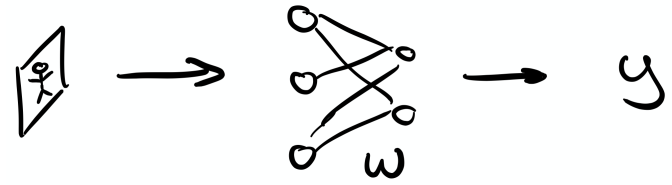
$$\mathbf{x} \mapsto f_{\mathbf{w}}(\mathbf{x}) \quad (2)$$



- A prior on parameters leads to a prior on functions
- Architectural **hyperparameters** influence prior on functions
- BDL focusses mostly on uncertainty in the function:

$$p(f|\mathbf{y},\theta) = \frac{p(\mathbf{y}|f)p(f|\theta)}{p(\mathbf{y}|\theta)} \quad (3)$$

Bayesian Inference



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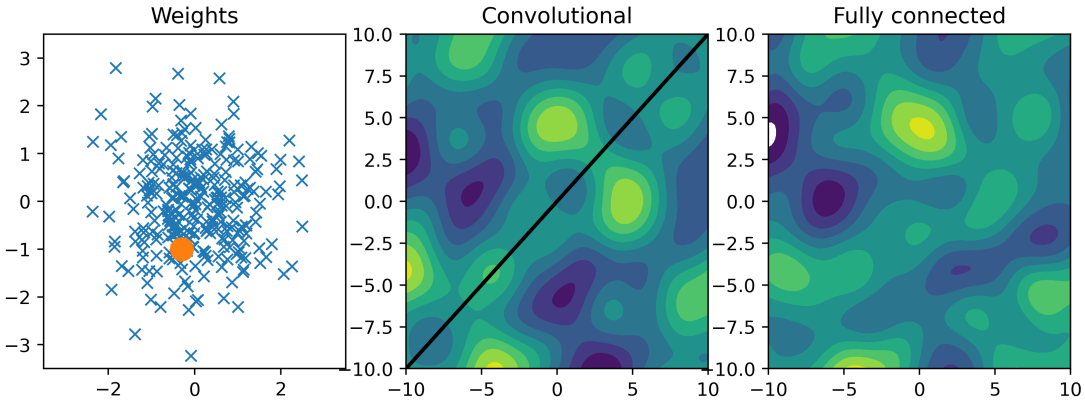

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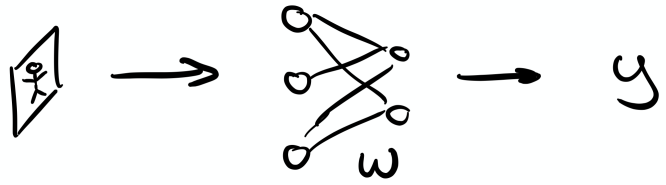

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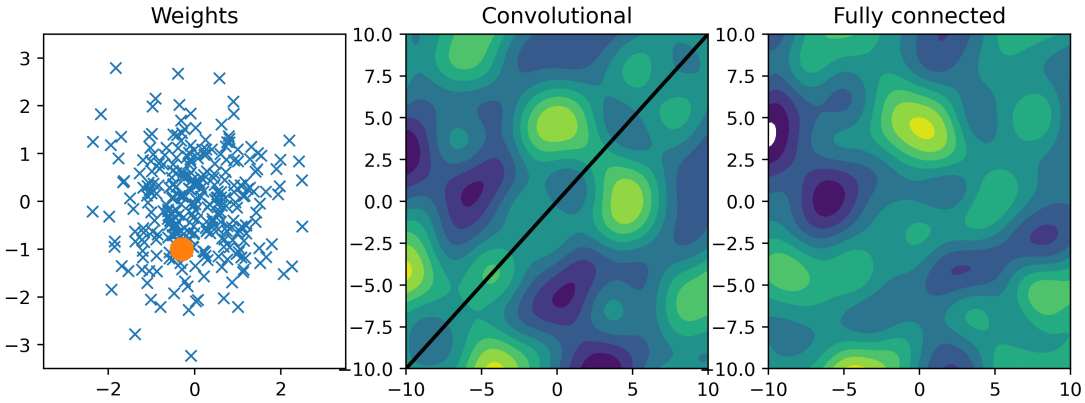

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But we want to determine the hyperparameters θ too!

Bayesian Model Selection

Bayes tells us: Just find the posterior over all your unknowns!

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... if we can compute $p(\mathbf{y} \mid \theta)$

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- Quality of posterior is linked to the accuracy of lower bound!

Learning Invariances

Learning Invariances using the Marginal Likelihood

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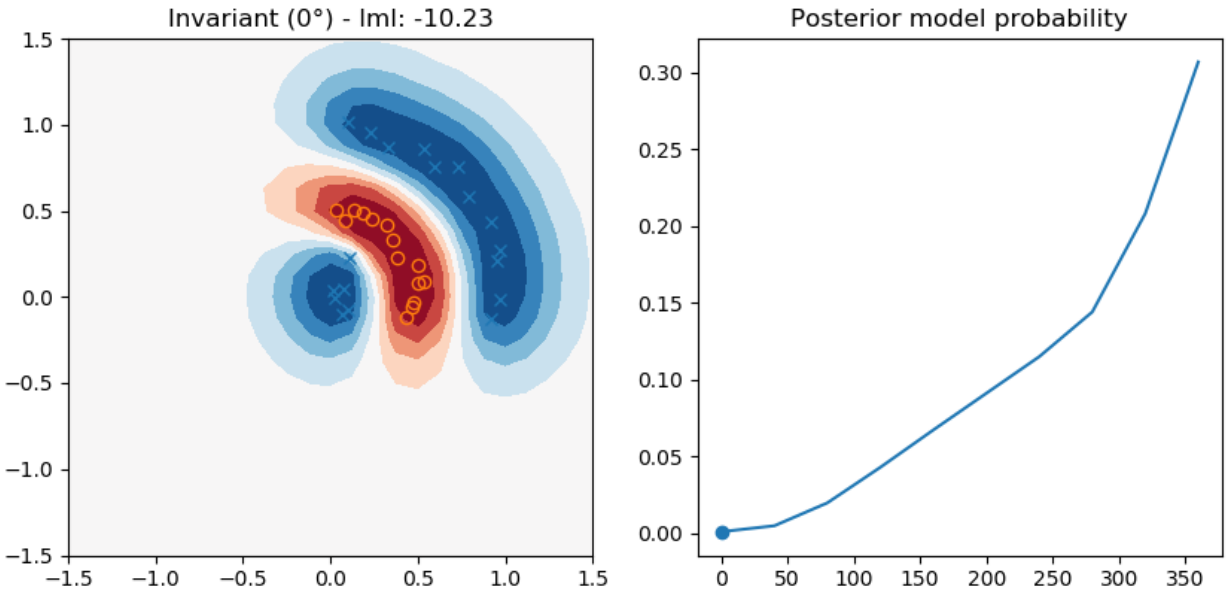

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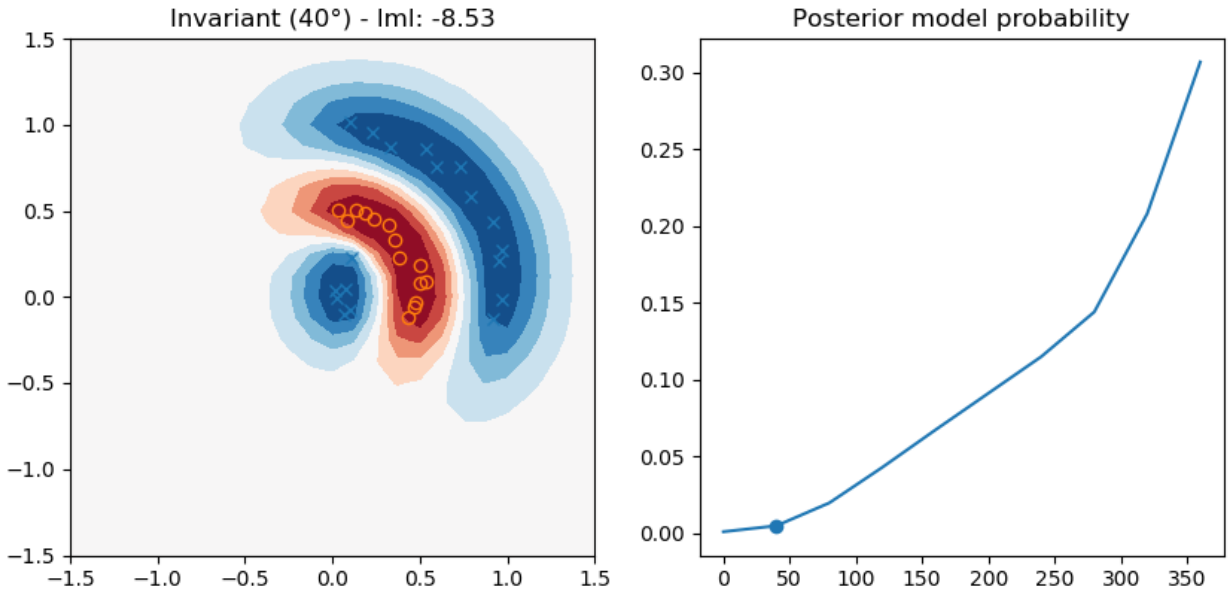

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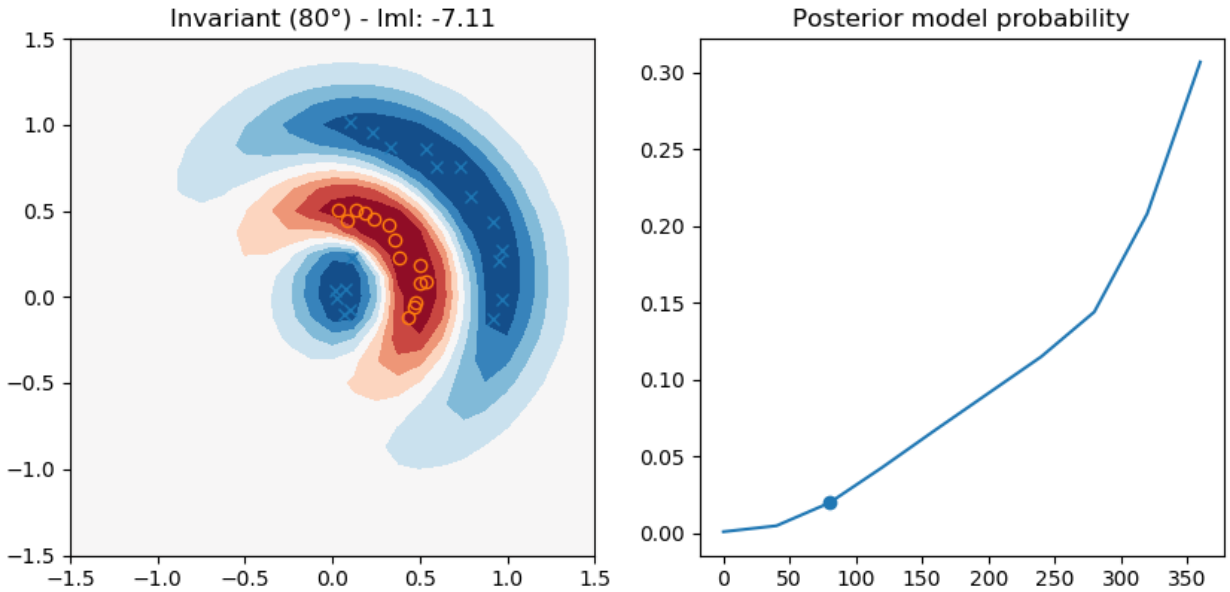

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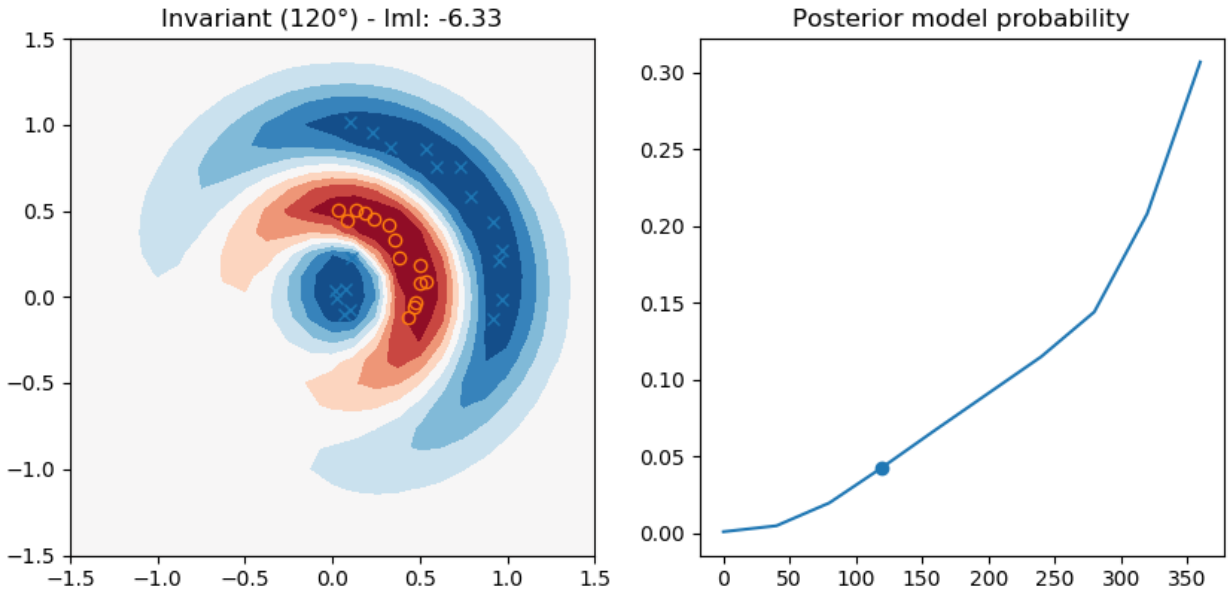

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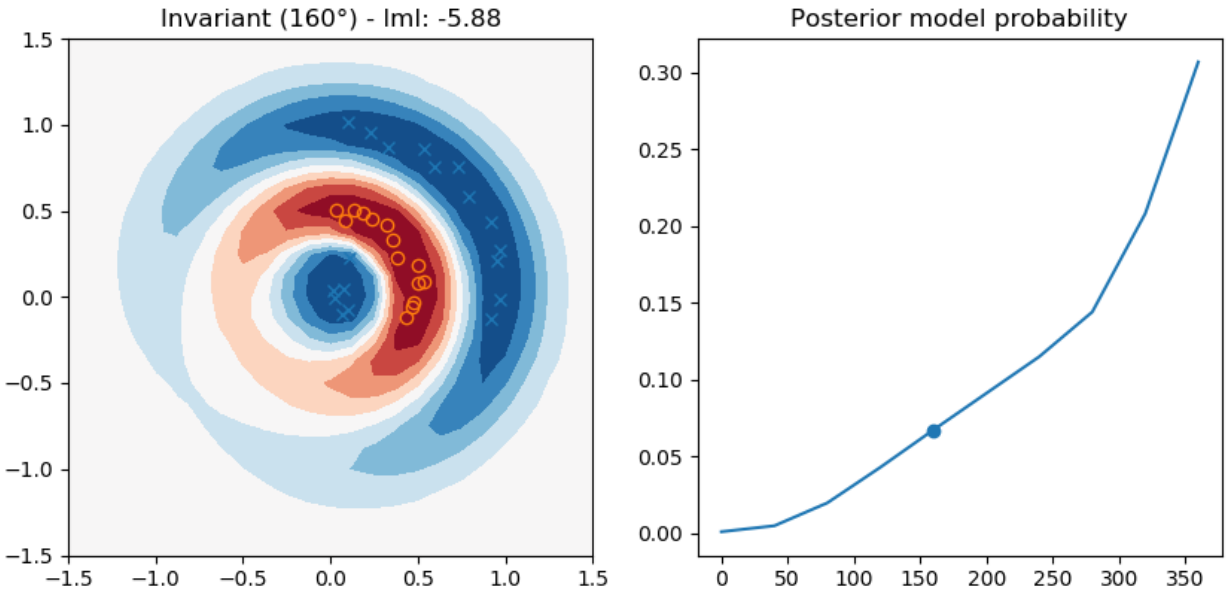

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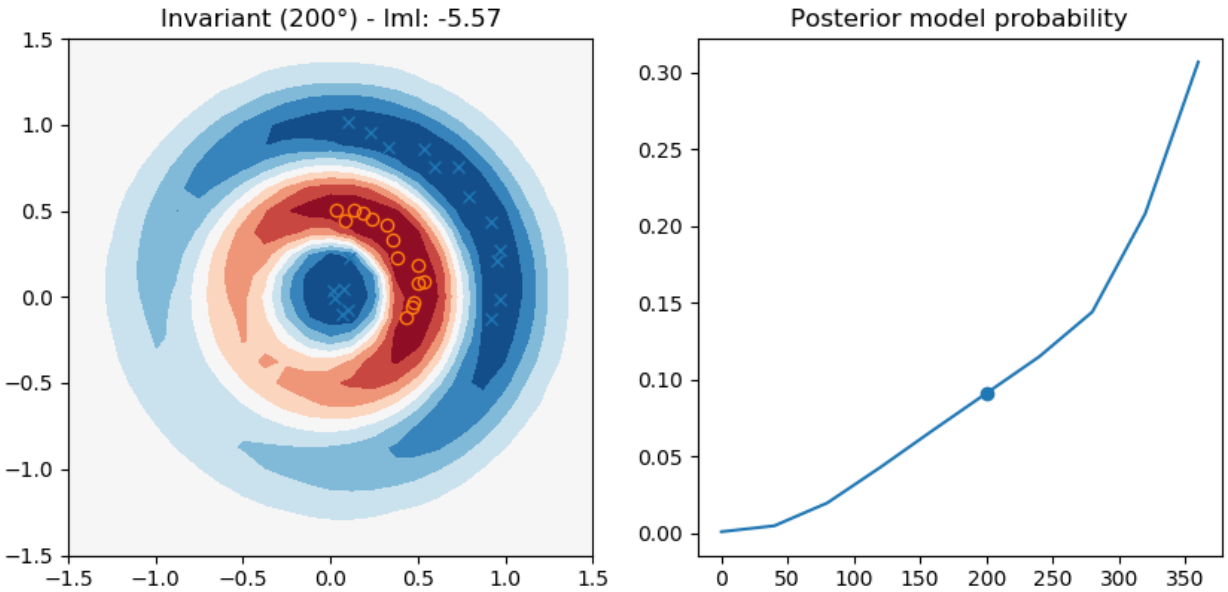

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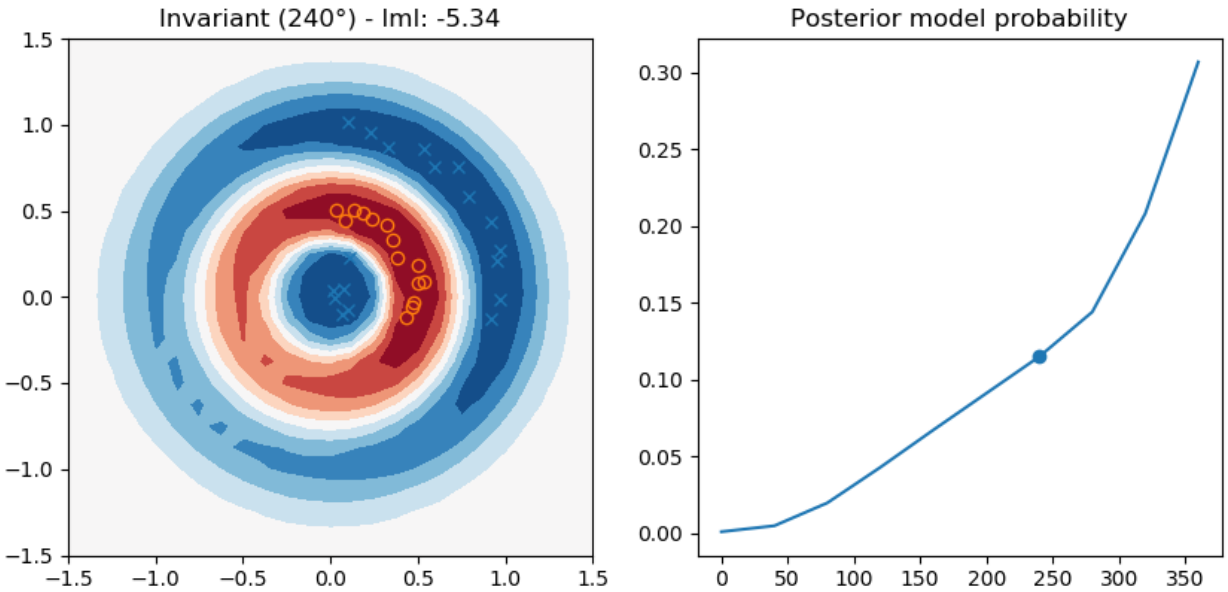

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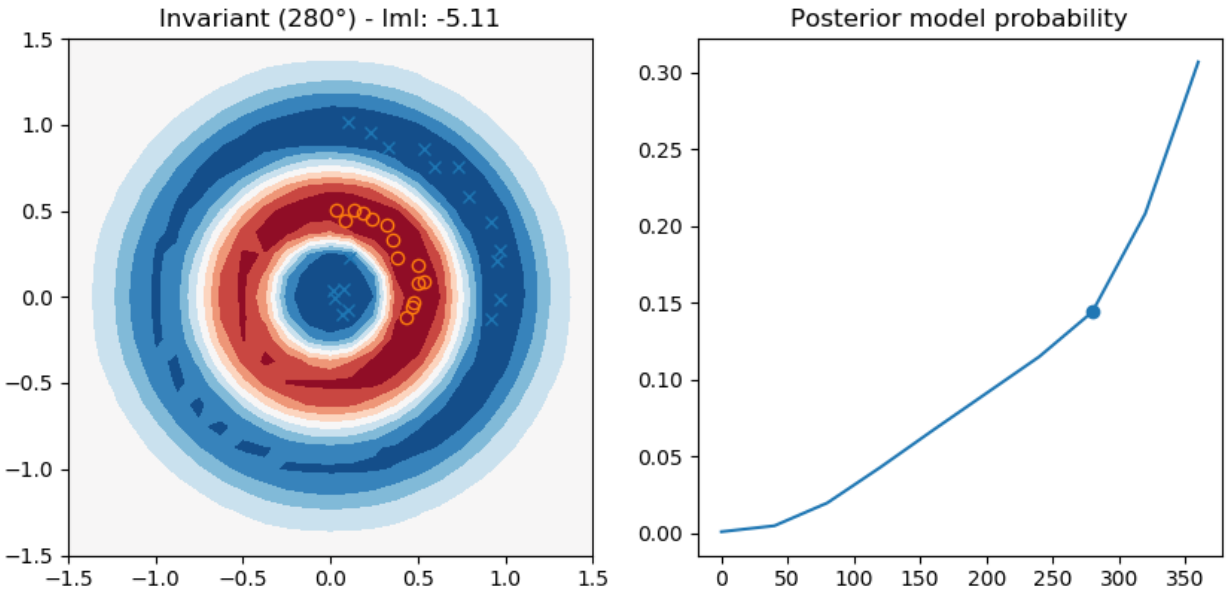

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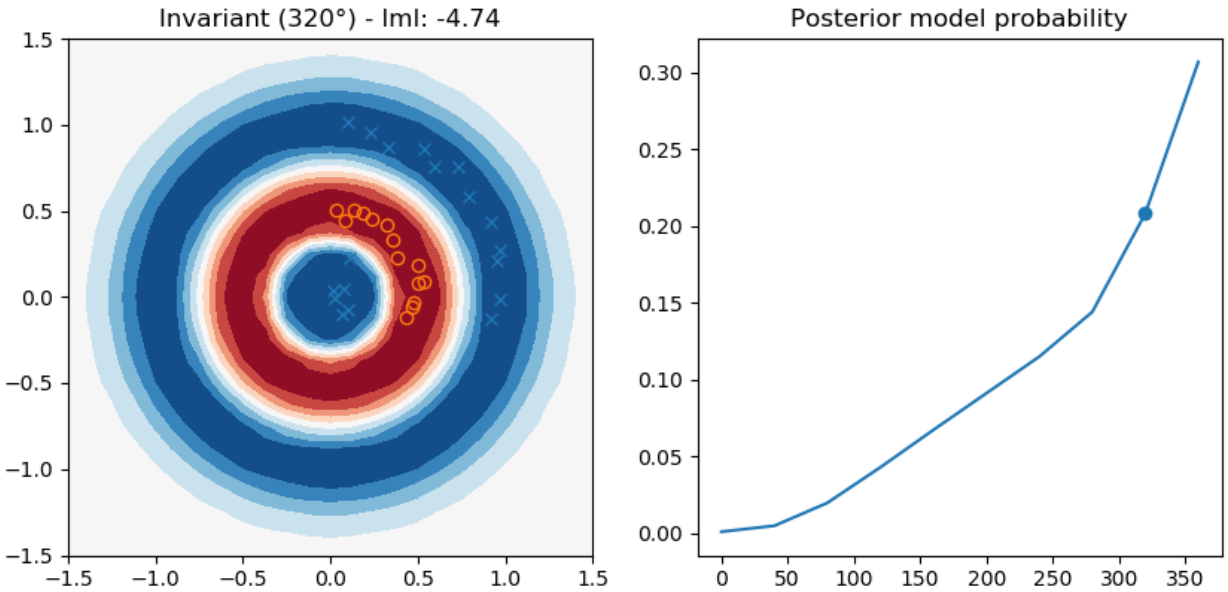

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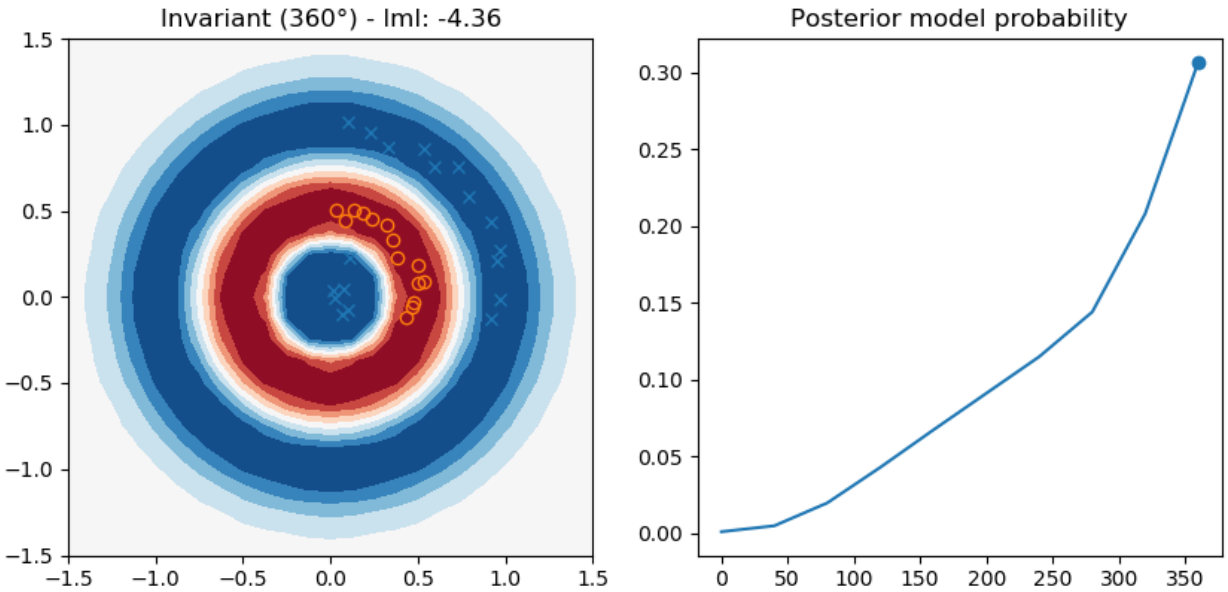

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Learning Invariances using the Marginal Likelihood

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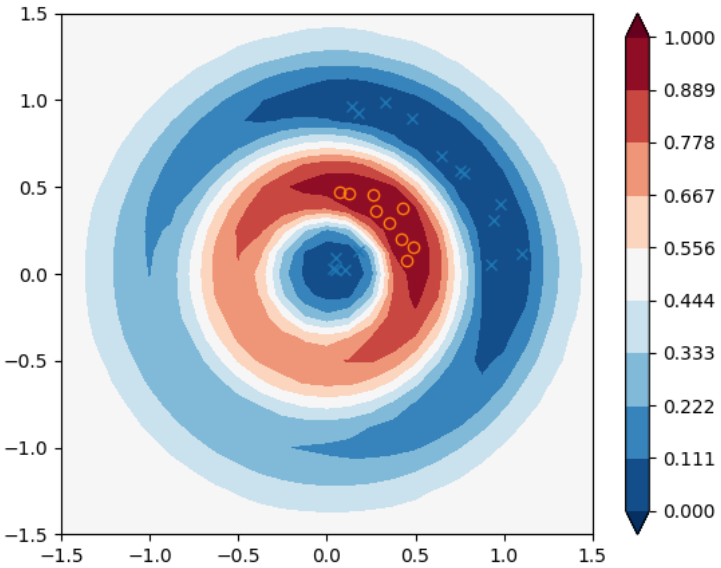

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- (First?[a]) Bayesian treatment of data augmentation
- *Learnable* invariance / data augmentation using **gradients** and only the **training set**
  - Learnable means: Same set-up learns different invariance for different dataset

[a] https://statmodeling.stat.columbia.edu/2019/12/02/a-bayesian-view-of-data-augmentation/

The Ingredients

We need

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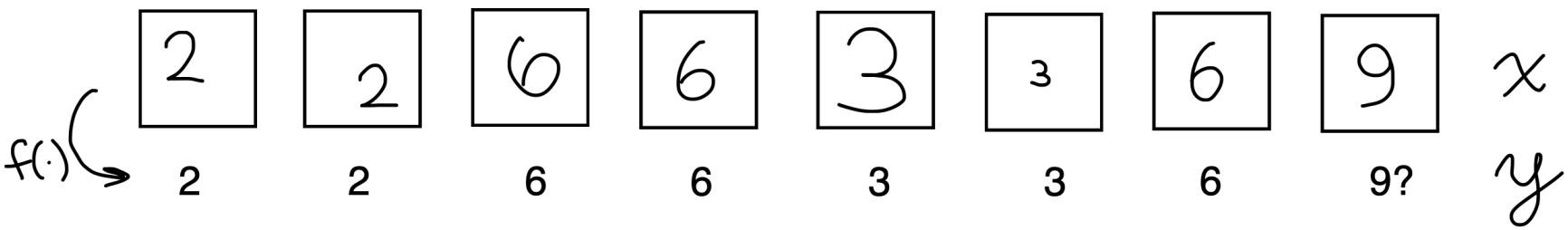
1. A way to **constrain** our learnable function to be invariant



$$f(\mathbf{x}) \approx f(t(\mathbf{x};\alpha)) \qquad \forall \alpha \in \mathcal{A}_\theta$$

$$P\Big([f(t(\mathbf{x};\alpha)) - f(\mathbf{x})]^2 > L\Big) < \delta \qquad \alpha \sim p(\alpha \mid \theta)$$

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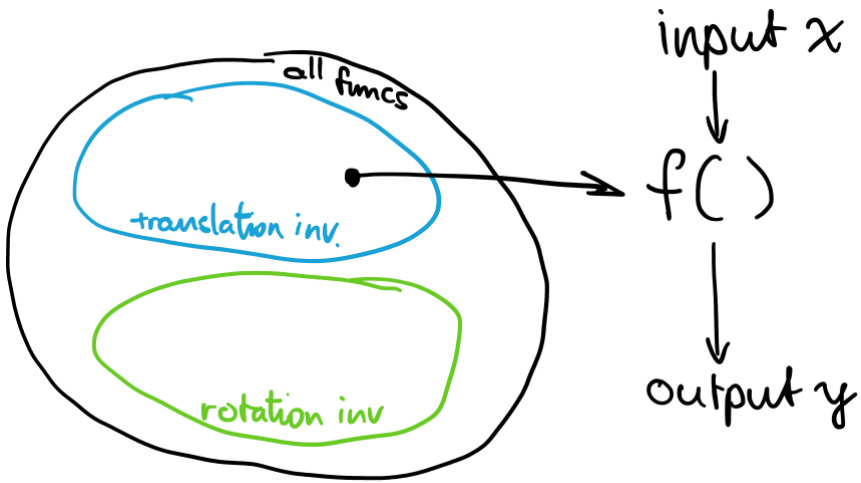

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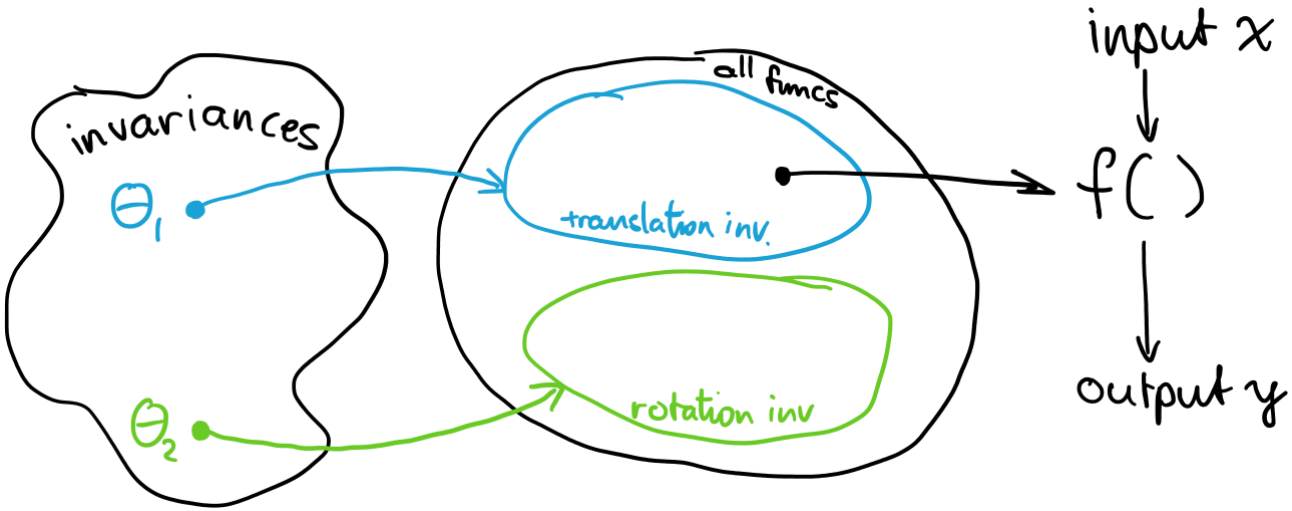
1. A way to **constrain** our learnable function to be invariant
2. A way to **parameterise** different sets of invariant functions.



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We need

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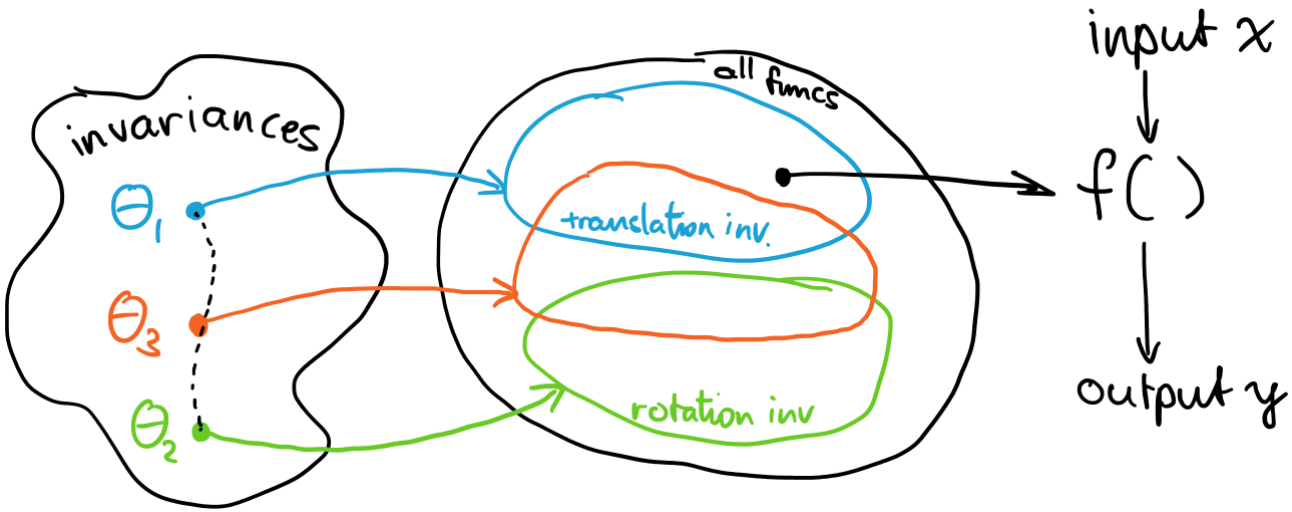
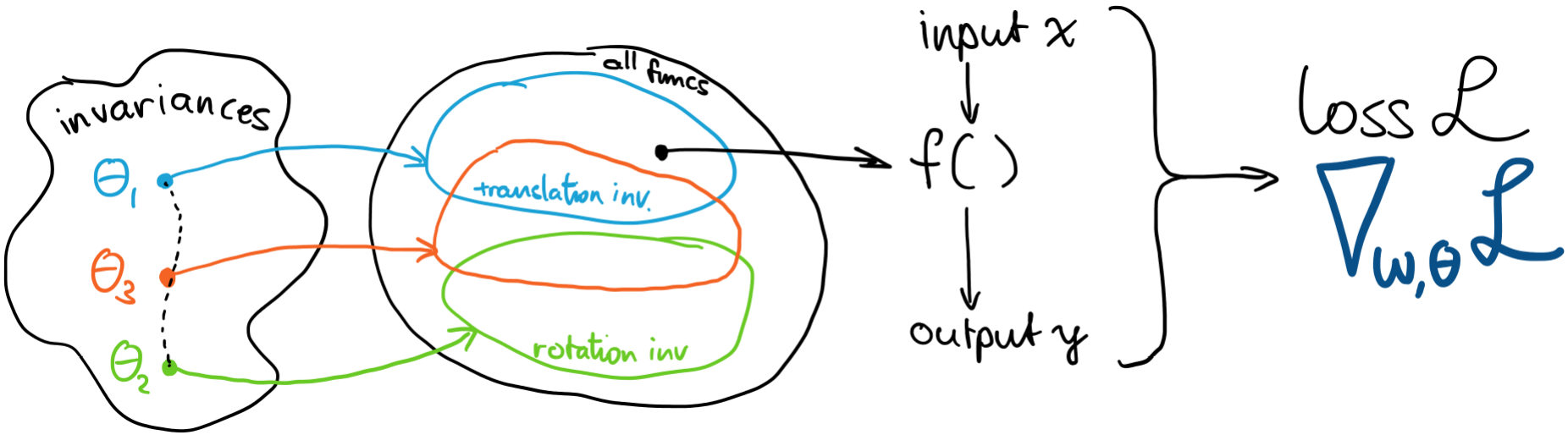
2. A way to **parameterise** different sets of invariant functions. **Differentiably**.



The Ingredients

We need

1. A way to **constrain** our learnable function to be invariant
2. A way to **parameterise** different sets of invariant functions. **Differentiably**.
3. An objective function for learning **both** the function (i.e. weights), and invariance (i.e. θ): The ELBO $\mathcal{L}(q(f), \theta)$.



Invariant functions (skip)

How do we parameterise the invariant function $f(\cdot)$?

- Sum (convolve) a non-invariant function over set of transformations we want to be invariant to!

Strict invariance (i.e. $f(\mathbf{x}) = f(t(\mathbf{x}; \alpha))$ with exact equality):

$$f(\mathbf{x}; \mathbf{u}, \theta) = \sum_{\alpha \in \mathcal{A}_\theta} g(t(\mathbf{x}; \alpha); \mathbf{u})$$

Weak invariance / data augmentation:

$$f(\mathbf{x}; \mathbf{u}, \theta) = \int g(t(\mathbf{x}; \alpha); \mathbf{u}) p(\alpha \mid \theta) \mathrm{d}\alpha$$

The function $g(\cdot; \mathbf{u})$ is parameterised by $\mathbf{u}$ and can be seen as a Gaussian process or a single-layer NN.

Training procedure (skip)

1. Generate a sample of transformed images (reparam trick $p(\alpha \mid \theta)$):

$$\{\mathbf{x}^{(s)} = t(\mathbf{x}, \alpha^{(s)})\}_{s=1}^{S} \qquad \alpha^{(s)} = h(\epsilon^{(s)}, \theta) \qquad \epsilon^{(s)} \overset{iid}{\sim} p(\epsilon)$$

2. Monte Carlo estimate of invariant function $f(\mathbf{x})$:

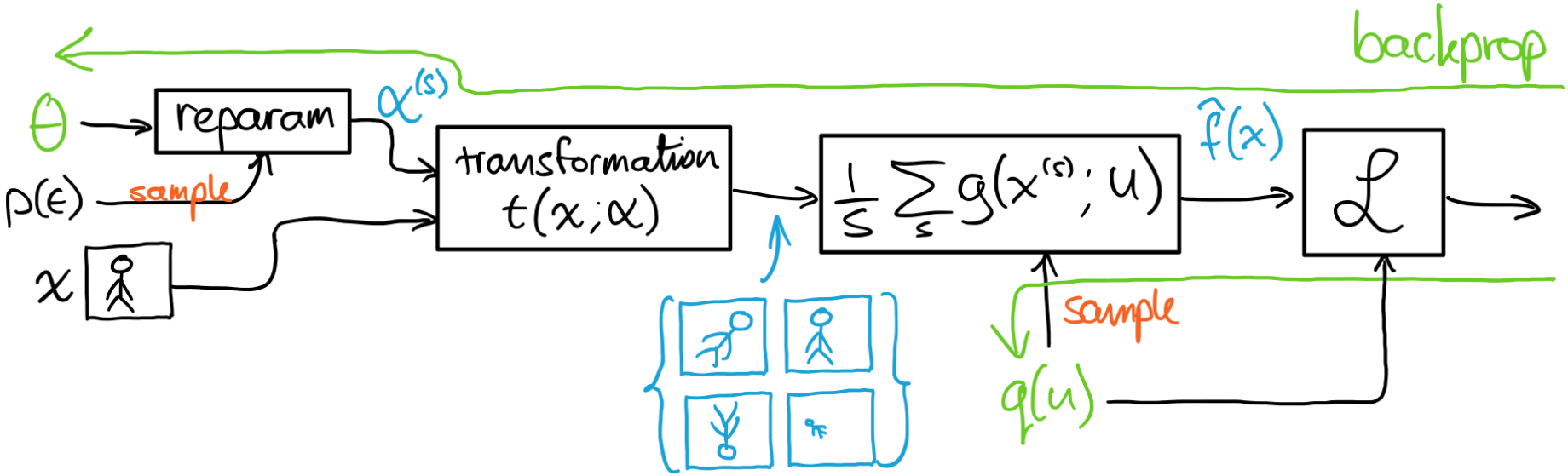
$$\hat{f}(\mathbf{x}) = \frac{1}{S} \sum_{s=1}^{S} g(\mathbf{x}^{(s)}; \mathbf{u})$$

3. Compute unbiased estimate ELBO using MC estimate of $f(\mathbf{x})$:

$$\mathcal{L} = N \cdot \mathbb{E}_{q(\mathbf{u})} \Big[\log p(y_n | \hat{f}(\mathbf{x}_n) \Big] - \mathrm{KL}[q(\mathbf{u}) || p(\mathbf{u}|\theta)]$$

4. Backpropagate to get gradients!

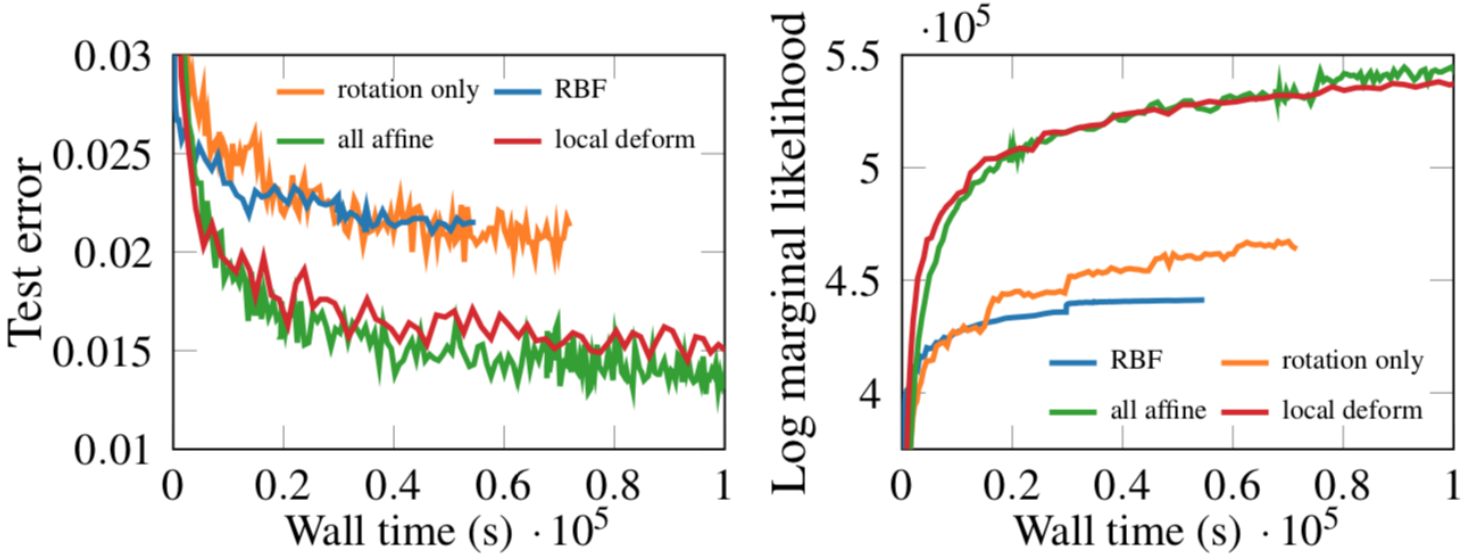
Training procedure



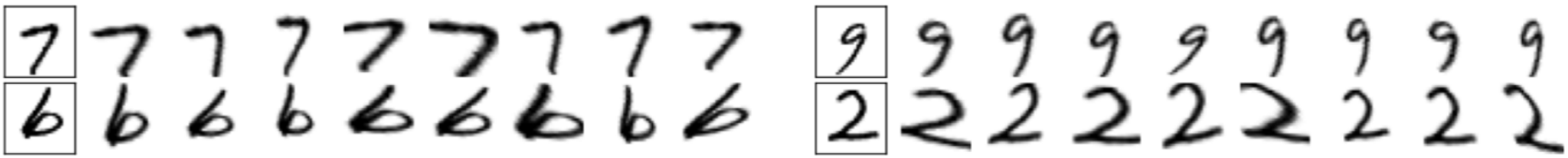
- Be Bayesian about the function $g(\cdot; \mathbf{u})$
- Averaging the output of $g(\cdot; \mathbf{u})$ (data aug)
- Compute ELBO (approximate marginal likelihood)
- Backpropagate

Results: MNIST

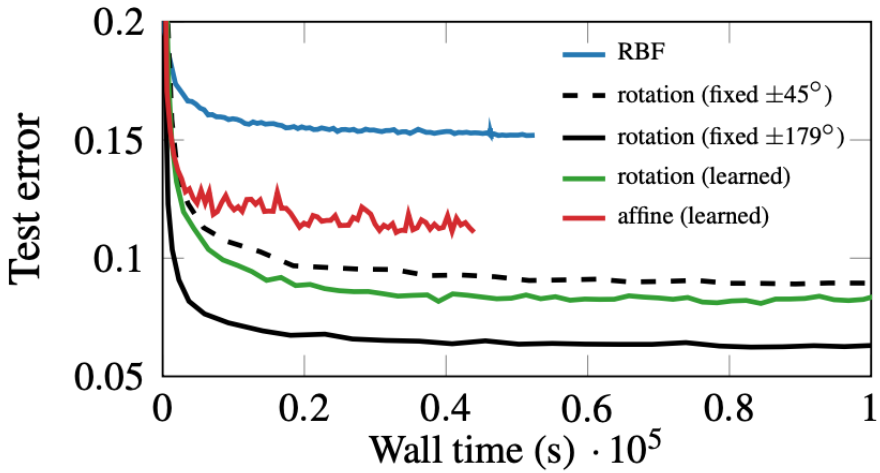
- Learns the invariance parameters through backprop
- Makes a weak Gaussian process classifier much stronger

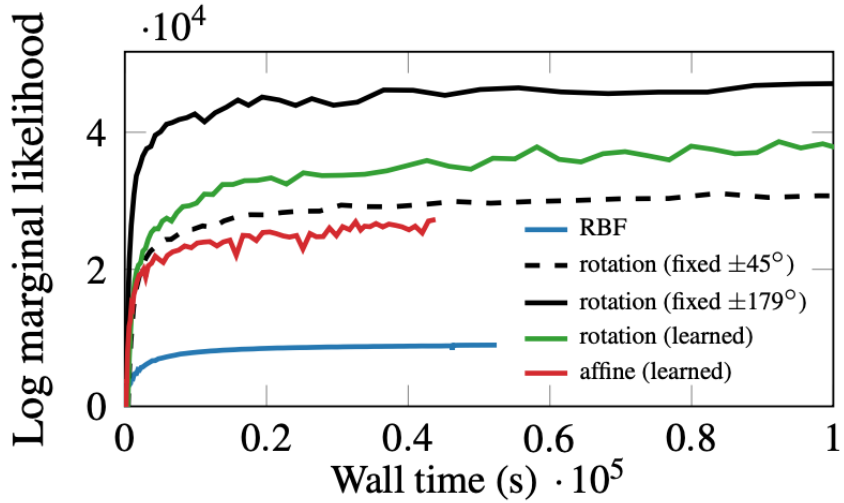


Examples of $t(\mathbf{x};\alpha)$ with $\alpha \sim p(\alpha|\theta)$, describing the **learned invariances**:



Results: MNIST-rot





- **Same** model on rotated MNIST dataset recovers **different** invariance (much more rotational invariance)
- No changes needed to the method or architecture.

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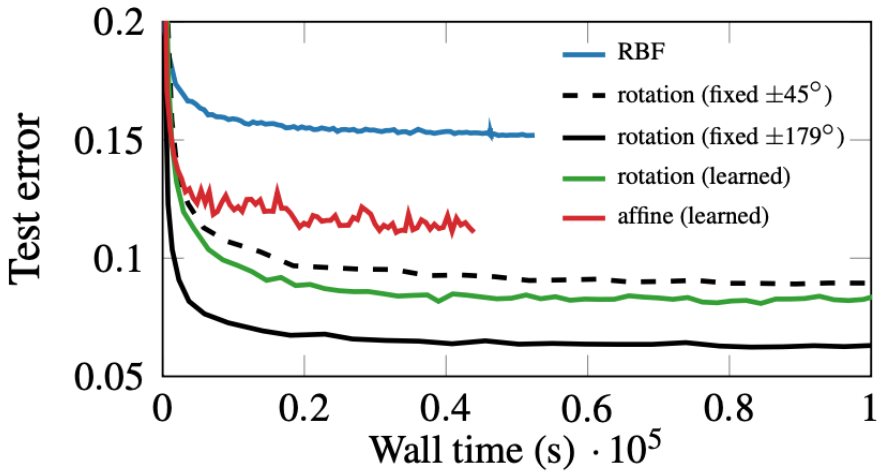

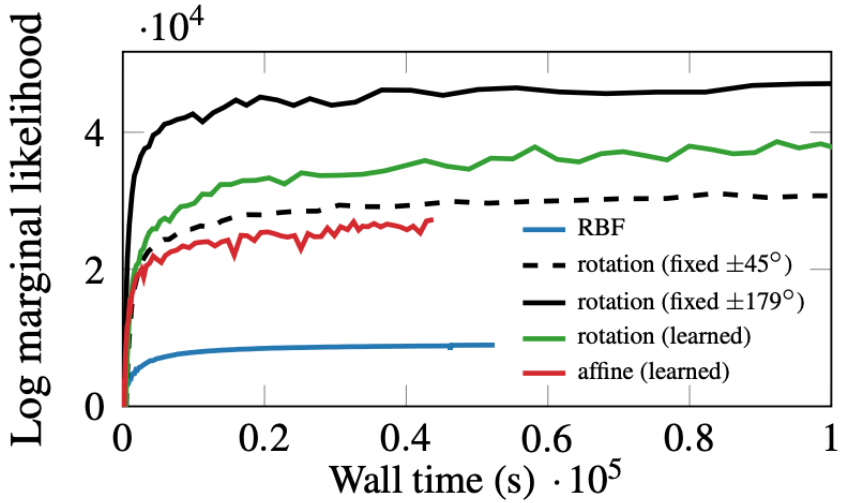

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Overview

The Promise of Bayesian Model Selection

Accurate Inference in Gaussian Processes

Gaussian Processes in Deep Learning

Ensembles and Architecture Search

Conclusion

The easiest paper I ever wrote

There were quite a few untested moving parts in the "Learning Invariances" paper. We needed:

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The method worked on the first run of the first implementation!

The easiest paper I ever wrote

"Learning invariance" was such an easy paper to write because

we had strong, working theory!

VI in GPs is very mature. In 2018 I could rely on[1]:

- Every (hyper)parameter having a clear guideline on how to set it
- Accurate, reliable approximation of the marginal likelihood
- Optimisation that converges

[1] This is not to say that training these models is easy! But their behaviour is predicted by well-understood theory.

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- How much can we blame people for not running a difficult method?

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Theory Gives Solutions

In "*Convergence of Sparse Variational Inference in Gaussian Processes Regression*" (Burt et al., 2020) we

- discussed an automatic inducing point initialisation scheme
- proved that it would give *arbitrarily accurate* results as $N \to \infty$
- proved that the asymptotic complexity was reasonable $O(N(\log N)^{2D}(\log\log N)^2))$ for SqExp, barely above linear[3]

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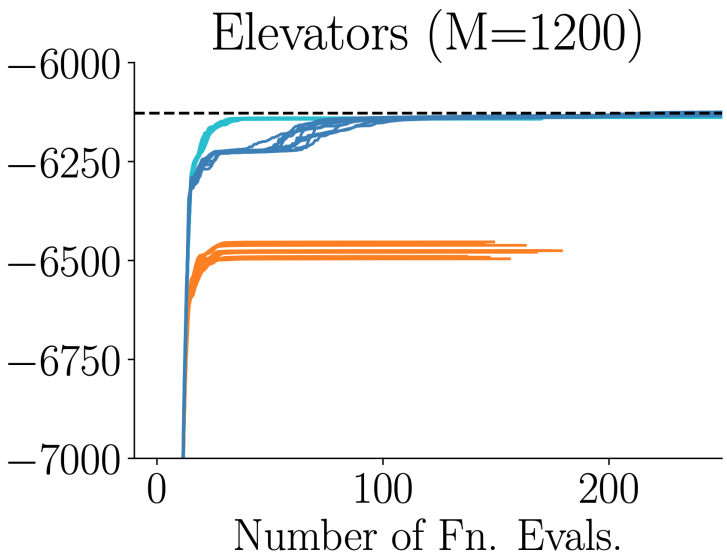
Practical implications for the Titsias (2009) method:



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Currently, little impact without good software!

- The credit you get for good software is non-linear
- Very little initially, until it becomes generally useful

The hardest paper I ever wrote

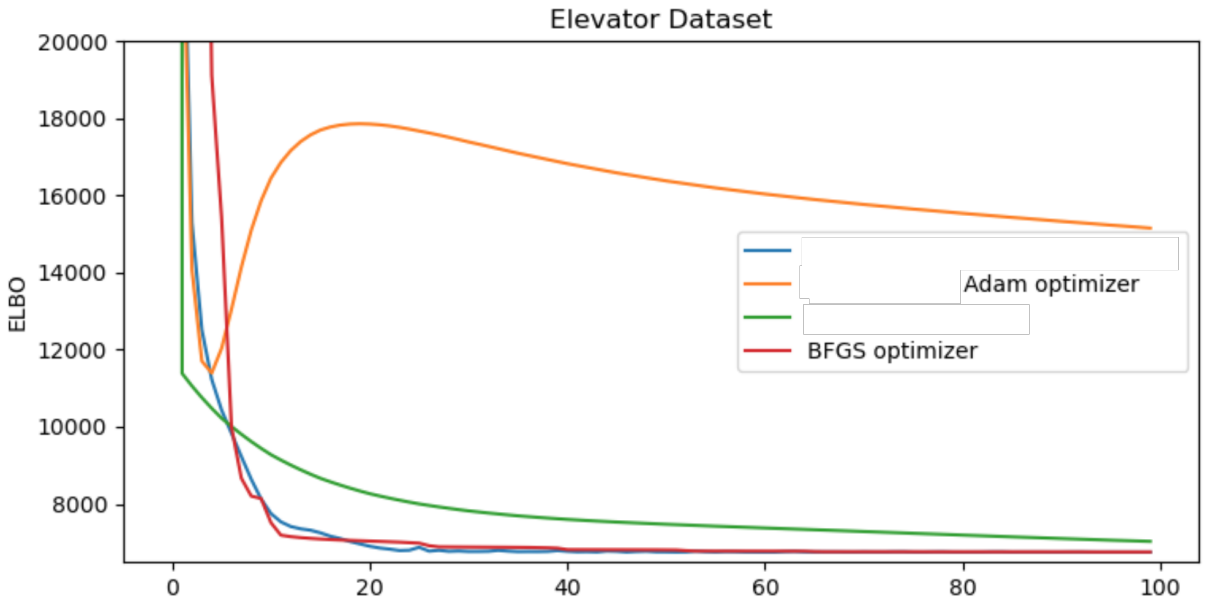
Variational Gaussian Process Models without Matrix Inverses

Mark van der Wilk MARK@PROWLER.IO
ST John ST@PROWLER.IO
Artem Artemev ARTEM@PROWLER.IO
James Hensman JAMES@PROWLER.IO
PROWLER.io

- Had idea in 2018, presented at AABI 2020, still not published.
- Very exciting: Remove bottleneck of matrix inverse.
- Can compute bound in $O(M^2)$ instead of $O(M^3)$.
- Takes far too many iterations to optimise!

Stochastic Optimisation in GPs is really bad!

Open problem: Fast stochastic optimisation in GPs



Courtesy of Maëlhann Rozé, MEng student

- Adam is a terrible stochastic optimiser for GPs!
- Stochastic optimisation is supposed to be faster than full batch!
- We really need to solve this problem if we want to make GPs usable with deep learning.

Conjugate Gradients

Alternative approach to inducing points. Tries to find $\mathbf{K}^{-1}\mathbf{v}$ by solving

$$\underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2}\mathbf{x}^\top \mathbf{K}\mathbf{x} - \mathbf{x}^\top \mathbf{b} \tag{8}$$

- **Conjugate Gradients** gives iterative solution that is exact in the limit.
- May give better speed-accuracy trade-off than inducing points.
- Has given genuinely impressive results[4]:

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Exact Gaussian Processes on a Million Data Points

Ke Alexander Wang[1*] **Geoff Pleiss**[1*] **Jacob R. Gardner**[2]
Stephen Tyree[3] **Kilian Q. Weinberger**[1] **Andrew Gordon Wilson**[1,4]
[1]Cornell University, [2]Uber AI Labs, [3]NVIDIA, [4]New York University

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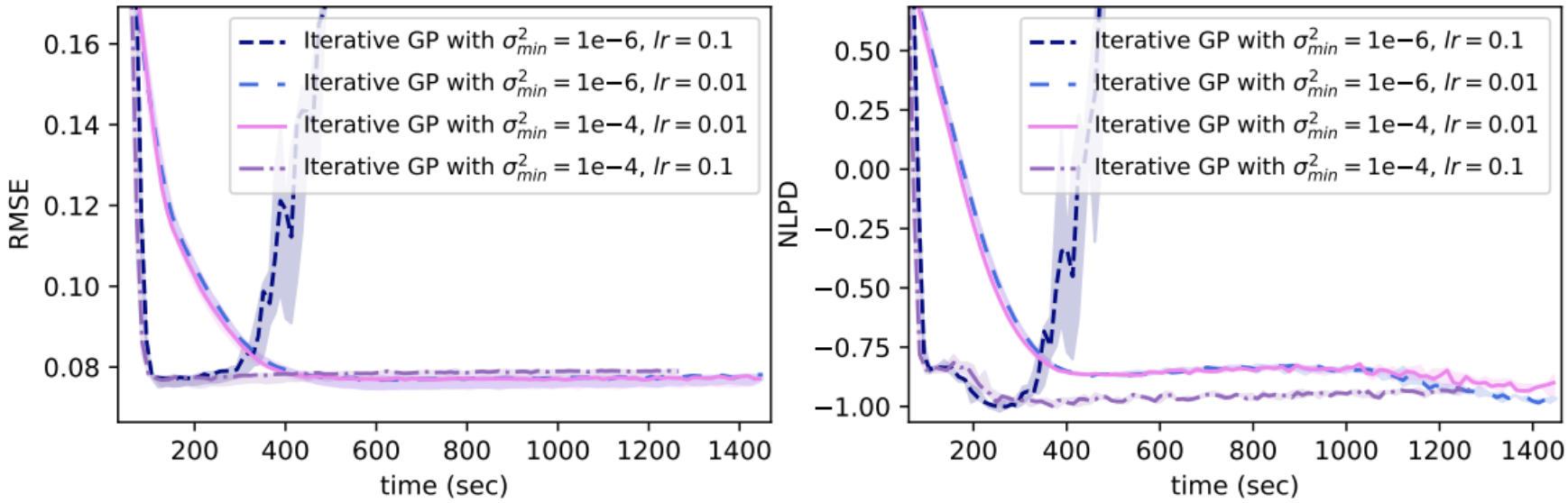
  - Wang et al. (2019) directly approximate the gradients with CG. With error introduced, it is not clear whether following them will lead to convergence.
- What convergence tolerances should be used to obtain good accuracy-speed tradeoff?
  - An "arbitrarily exact" method would require a well-defined rule, a proof, and an asymptotic computational cost analysis, as inducing points currently has (Burt et al., 2019, 2020)

Conjugate Gradients

This has practical consequences, with behaviour that you would not expect from an exact method:



This said, CG is a good idea, and inspired by the results of Wang et al. (2019), we (+ Artem Artemev, David Burt) propose some improvements.

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- VI measures quality of approximation and hyperparameters in a single objective: The ELBO.

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We develop the **Conjugate Gradient Lower Bound** (CGLB).

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- Makes it easy to design convergent algorithms: Just optimise the ELBO!
- Q: How to set parameters? A: Just optimise the ELBO!

Can we do something similar for Conjugate Gradient methods? **Yes!**

We develop the **Conjugate Gradient Lower Bound** (CGLB).

- The partial solution $\mathbf{v}$ to the CG optimisation problem to find $\mathbf{K}^{-1}\mathbf{y}$ is unified with the hyperparameter objective
  $\implies$ easier to guarantee convergence

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- Additional upper bound to automatically determine number of CG iterations.

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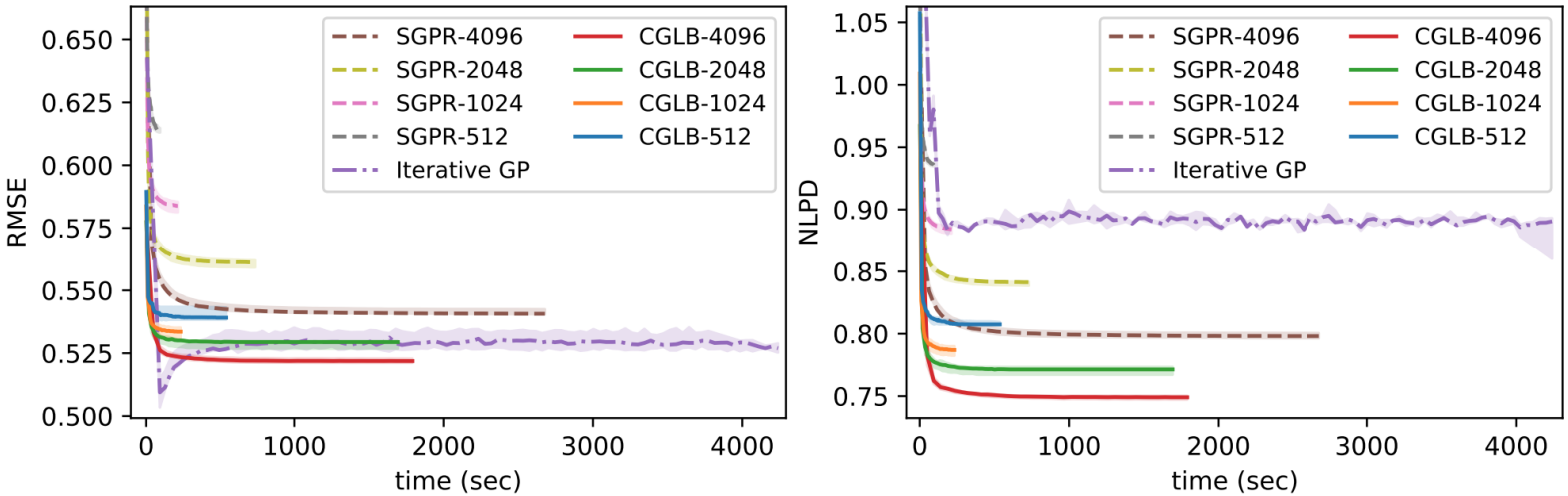
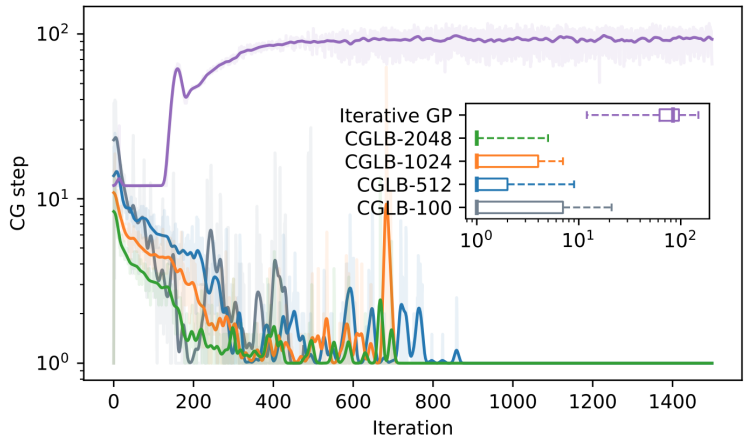
Conjugate Gradient Lower Bound





- Fewer iterations of CG $\implies$ faster.
- More guarantees for optimisation $\implies$ better performance.

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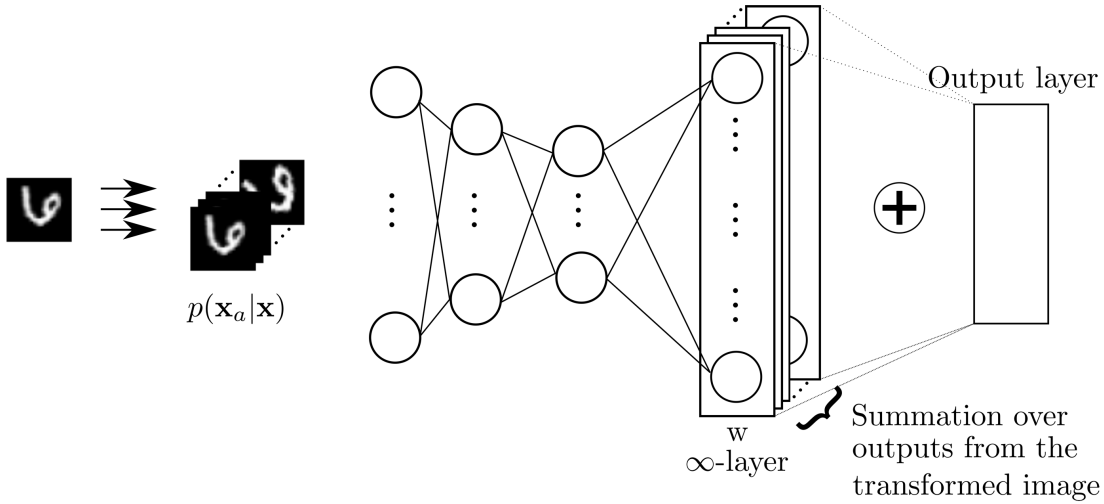
Learning Invariances in DNNs

Find invariances through backprop for a Deep Neural Network, by only computing the marginal likelihood for the last layer.



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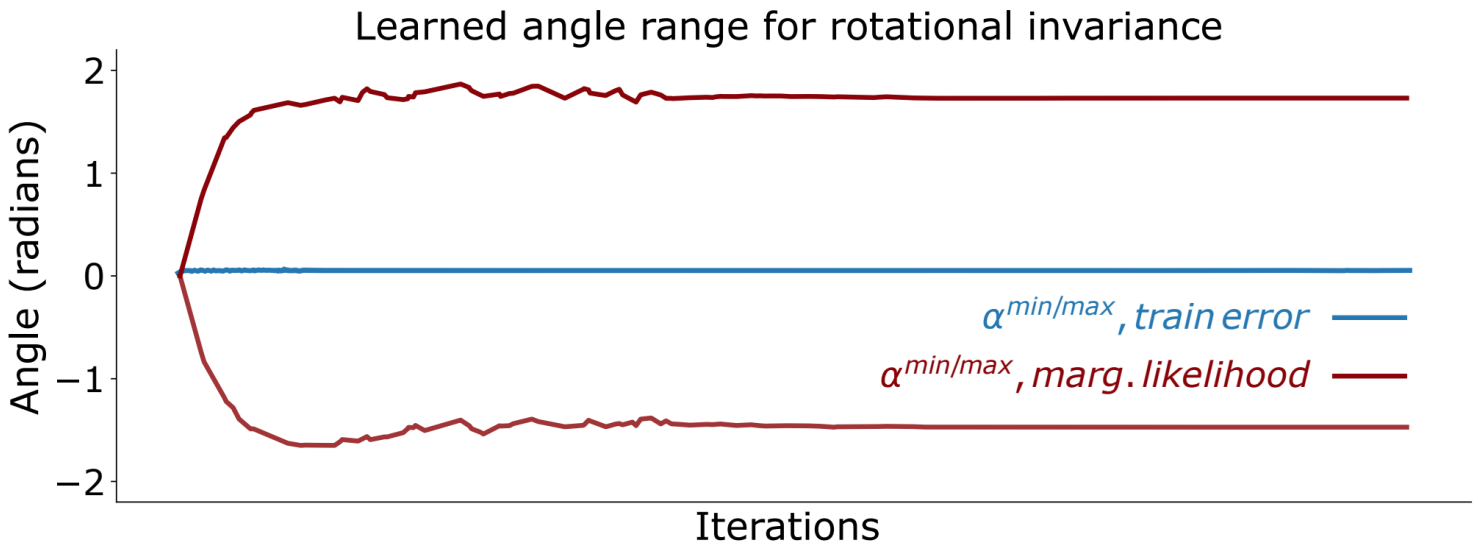

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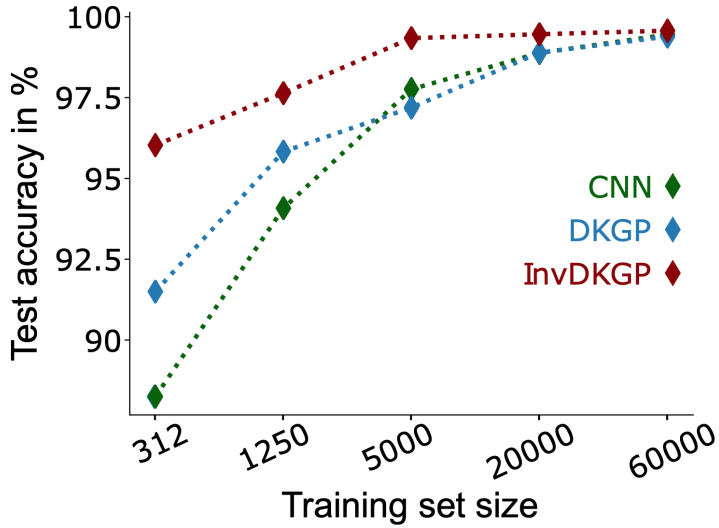

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- New methods make DGPs easier to use, and look remarkably similar to DNNs. **Convergence?**

Overview

Ensembles and Posteriors

For linear models, ensembles and posteriors can be identical (Matthews et al., 2017):

$$\mathbf{w}^{(k)} \overset{\text{iid}}{\sim} \mathcal{N}(0, \boldsymbol{I}) \tag{9}$$

$$\mathbf{w}_p^{(k)} := \text{GradDesc}(\mathbf{w}^{(k)}, ||\mathbf{y} - \Phi(X)\mathbf{w}||^2) \tag{10}$$

$$\implies \mathbf{w}_p^{(k)} \overset{\text{iid}}{\sim} p(\mathbf{w}|\mathbf{y}) \tag{11}$$

where $p(y_n|\mathbf{w}) = \mathcal{N}\left(y_n; \boldsymbol{\phi}(\mathbf{x}_n)^\top \mathbf{w}, \sigma^2\right)$, with $\sigma^2 \to 0$.

Can optimisation do Bayesian Model Selection?

$$\log p(\mathbf{y}) = \sum_{i=1}^{n} \log p(y_i \mid \mathbf{y}_{<i}) = \sum_i \log \mathbb{E}_{p(\mathbf{w}|\mathbf{y}_{<i})}[p(y_i|\mathbf{w})]$$
$$\geqslant \sum_i \mathbb{E}_{p(\mathbf{w}|\mathbf{y}_{<i})}[\log p(y_i|\mathbf{w})]$$

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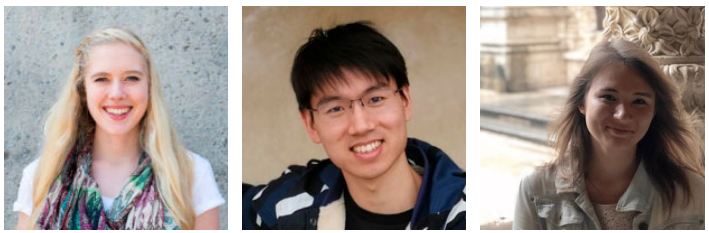

Clare Lyle, Lisa Schut, Binxin Ru, Yarin Gal, MvdW

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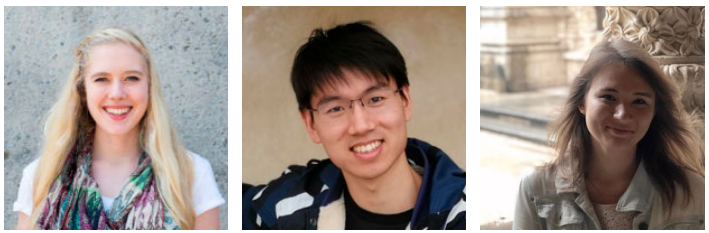

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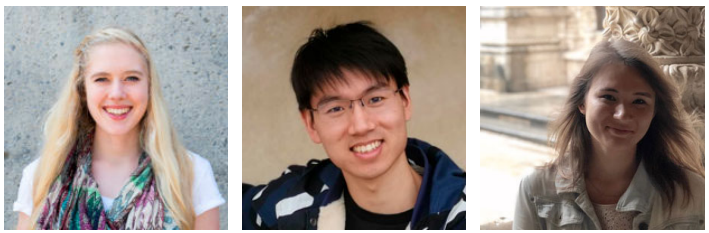

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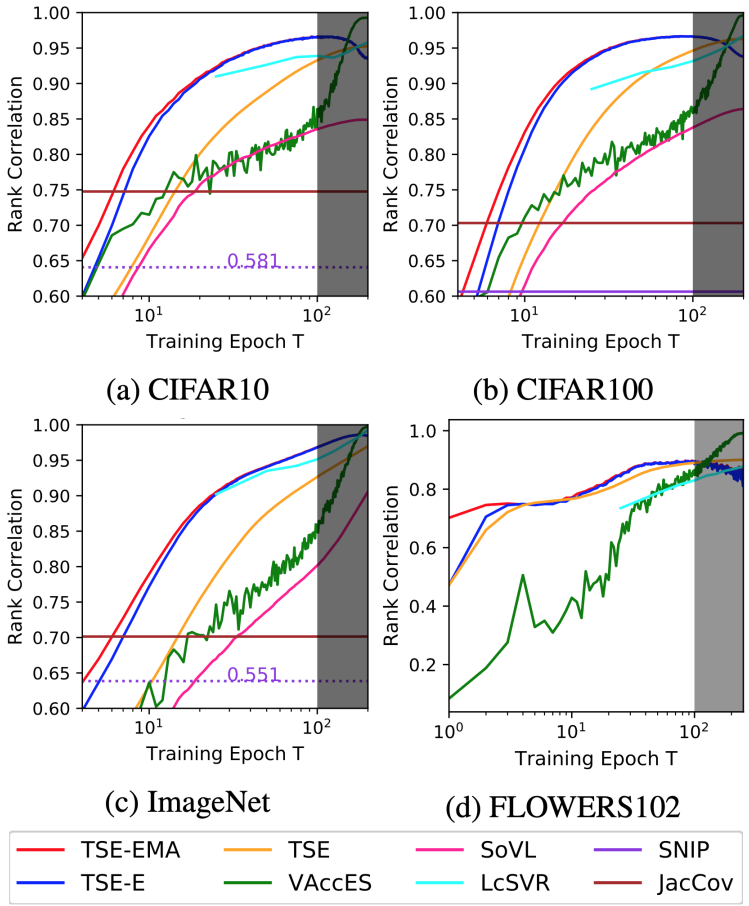
- Bayesian Perspective on Training Speed and Model Selection



Clare Lyle, Lisa Schut, Binxin Ru, Yarin Gal, MvdW

Neural Architecture Search

Inspired by this, we investigated whether training speed could predict testing accuracy of a network.



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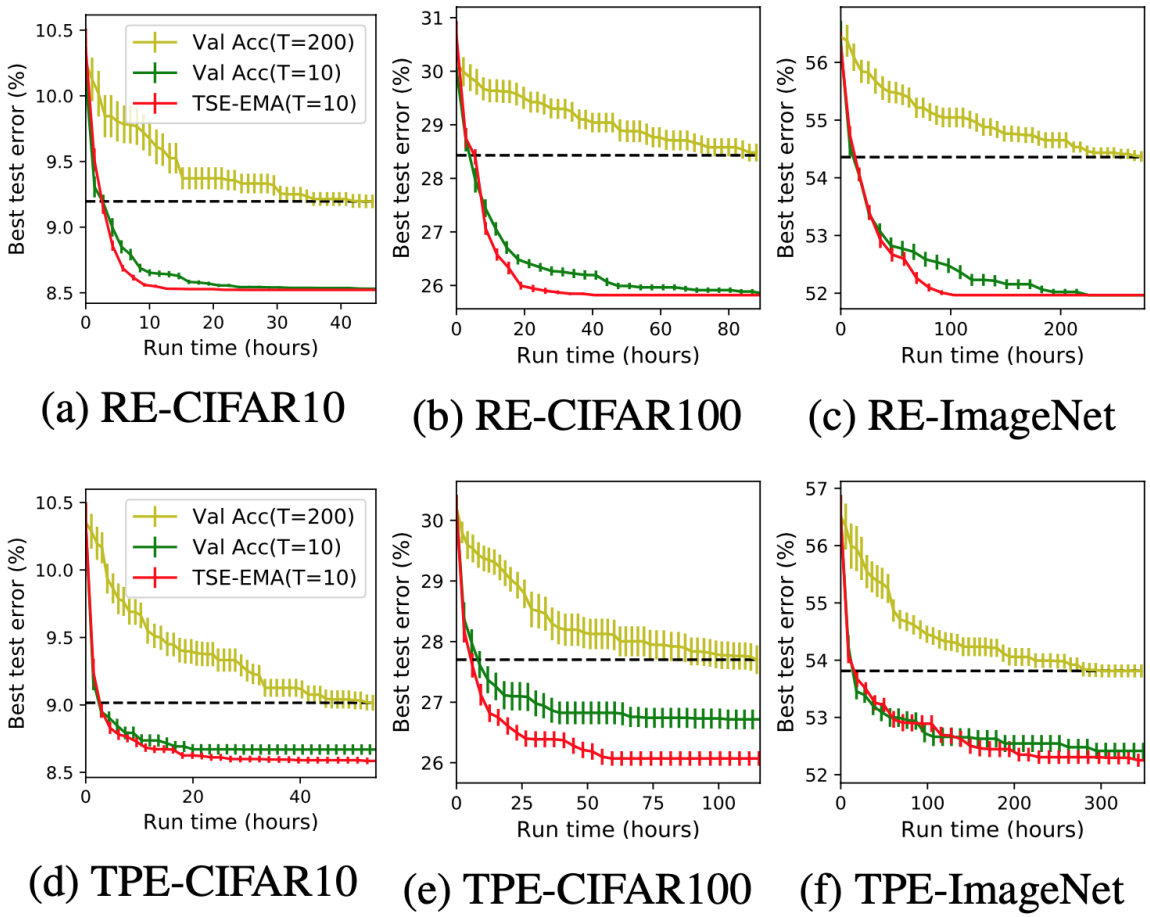

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Summary

Papers we discussed, which I was involved in:

- **Learning Invariance using the Marginal Likelihood**
  v.d.Wilk et al. (2018), NeurIPS
- **Convergence of Sparse Variational Inference in GPR**
  Burt et al. (2019, 2020), ICML, JMLR
- **Software for automatic & robust training of GPs**
  Work in Progress
- **Variational GP Models without Matrix Inverses**
  van der Wilk et al. (2020), AABI, Work in Progress
- **Tighter Bounds on the LML of GPR Using CG**
  Artemev et al. (2021), Preprint
- **Last Layer Marginal Likelihood for Invariance Learning**
  Work in Progress (arxiv soon)
- **Bayesian Image Classification with Deep Convolutional GPs**
  Dutordoir et al. (2020), AISTATS
- **A Bayesian Perspective on Training Speed and Model Selection**
  Lyle et al. (2020), NeurIPS
- **An Efficient Performance Estimator for Neural Architecture Search**
  Ru et al. (2020), Preprint

Conclusion & Ways Forward

Conclusion:

- Bayesian model selection could provide great benefits in DNNs.
- Interesting model selection (invariances) is already possible in GPs.
- Model selection using a marginal likelihood approx already works in deep GPs.

Ways forward:

- GP inference needs to be faster per iteration, and converge faster.
- Alternatively: More accurate marginal likelihood estimates of NNs.
- Deep GPs and DNNs may converge!

Alternative approaches

Two approaches based on back-propagating through a validation set:

- Meta-learning (Zhou et al., 2020)
- Implicit function theorem (Lorraine et al., 2020)
- Straightforward regularization (Benton et al., 2020)

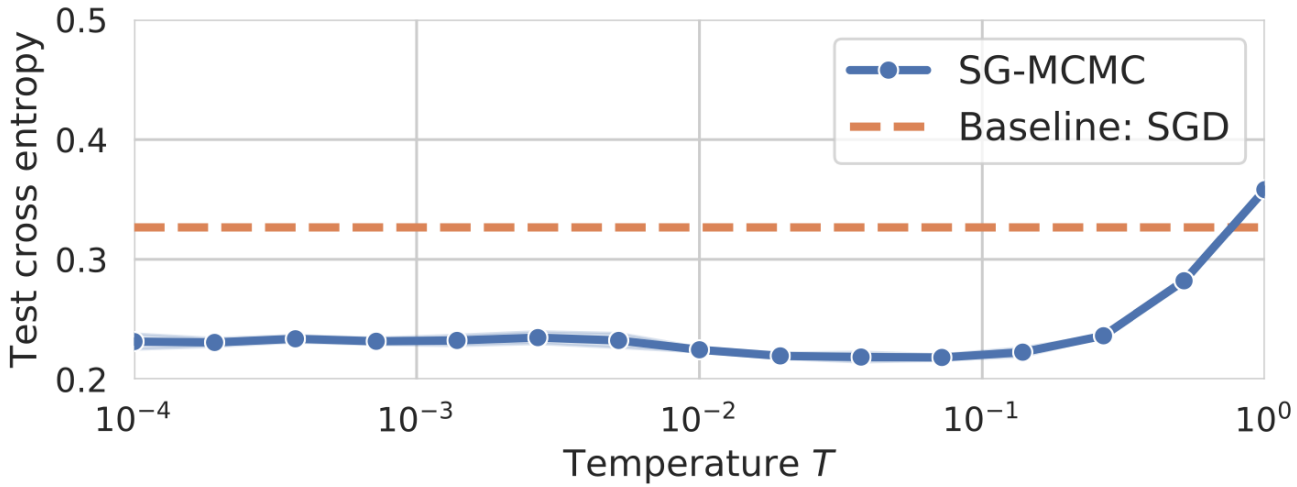
What is going to be best? Only research will tell!

Bonus Content / Directors Cut

Example

TODO: Animations of overfitting, correct fitting, and periodic

Cold Posteriors



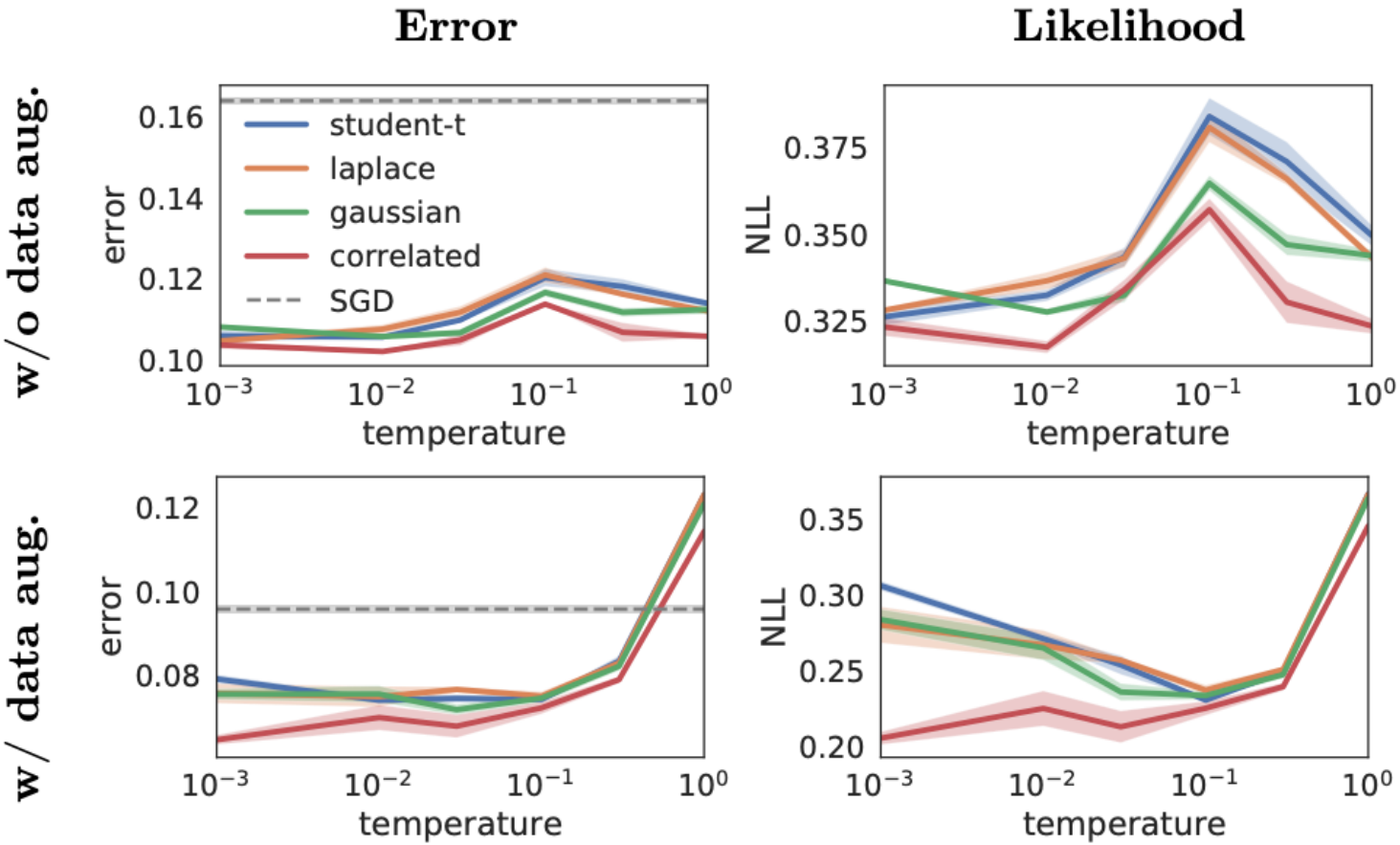
From Wenzel et al. (2020)

$$p_T(\boldsymbol{\theta}|\mathbf{y}) \propto p(\boldsymbol{\theta}|\mathbf{y})^{1/T} \tag{12}$$

- Posterior performs worse than point estimate!
- Bayes is sensitive to the prior as well!
- Does the prior make things worse?

Weight Priors

Investigate **different weight priors** in neural networks:



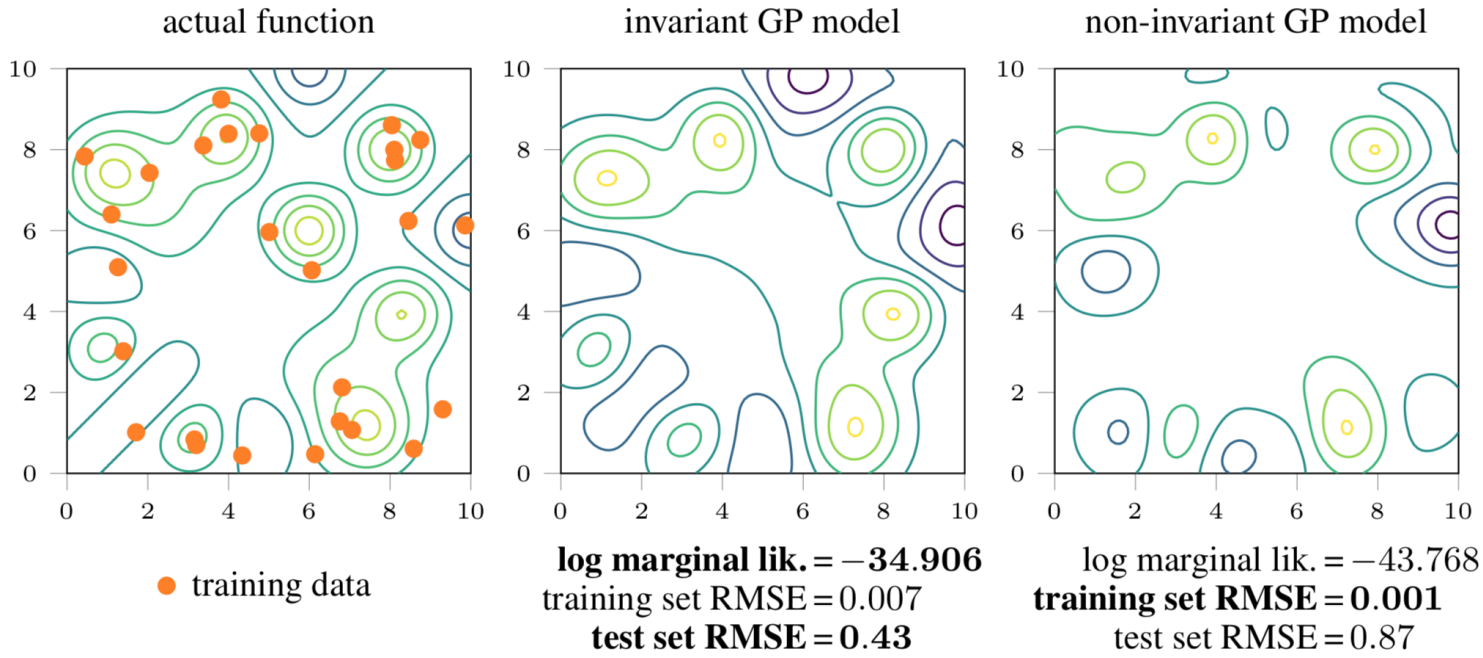
Bayesian Neural Network Priors Revisited

Fortuin*, Garriga-Alonso*, Wenzel, Rätsch, Turner, vdW†, Aitchison†

Why can't we just use training loss?

For the same reason as why we need cross-validation:

- The training loss is minimised with the most flexible model
- Inductive biases are **constraints**



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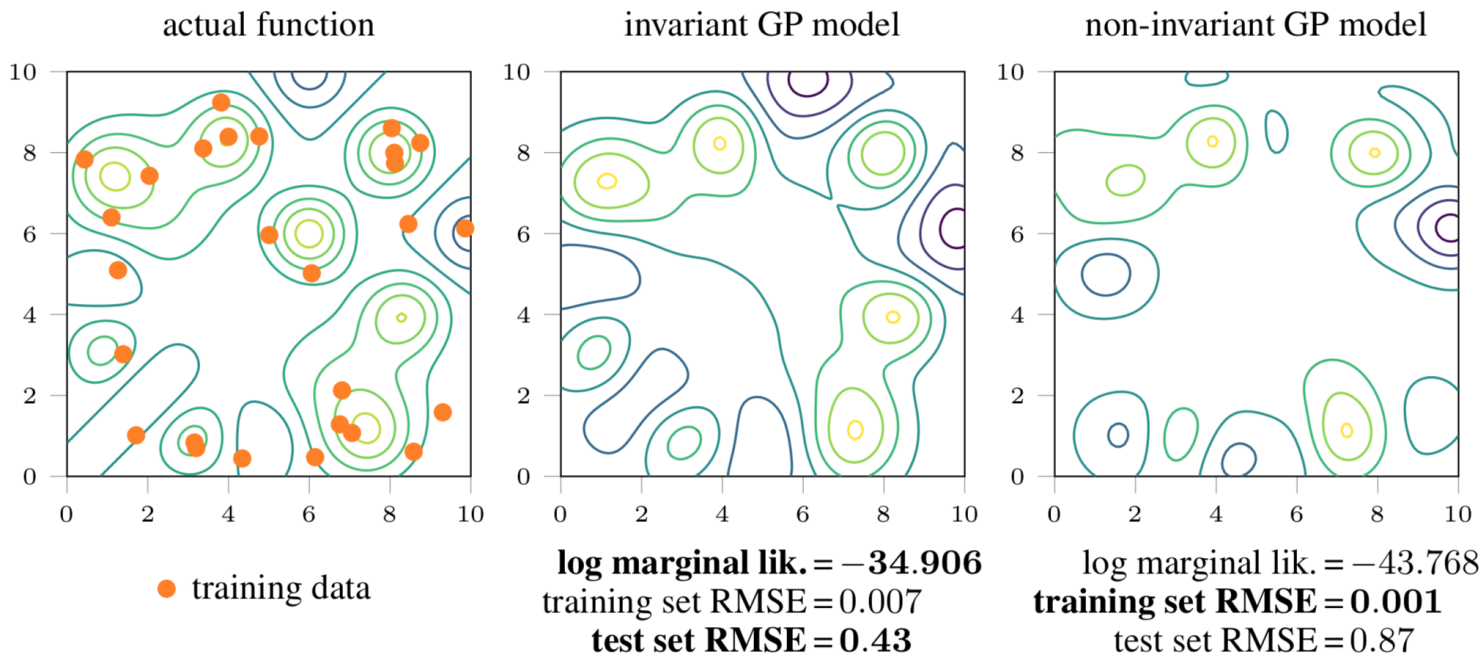

Log marginal likelihood measures **generalisation**:

$$\log p(\mathbf{y} \mid \theta) = \log p(y_1|\theta) + \log p(y_2|\theta, y_1) + \log p(y_3|\theta, \{y_i\}_{i=1}^2) \ldots$$

(It's also related to cross-validation (Fong and Holmes, 2020).)

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