Qualcomm Amsterdam

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Bayesian Model Selection
in Deep Learning

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Outline

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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1. The promises of Bayesian Model Selection
2. Difficulties with Bayesian Inference in Deep Learning

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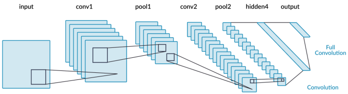
Talk outline:

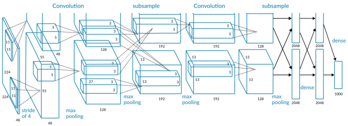
1. The promises of Bayesian Model Selection
2. Difficulties with Bayesian Inference in Deep Learning
3. Other approaches: Ensembles and Architecture Search

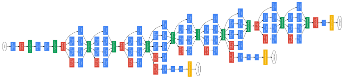
Model Selection

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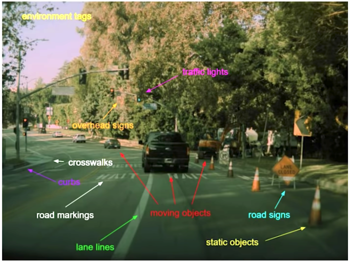
As architectures get more complex, so does design! E.g. multitask.

- 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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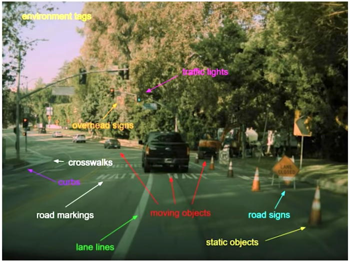

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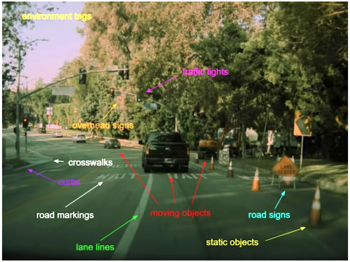

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Main tool is **crossvalidation**.

Goal: Make it as easy as learning weights.

Overview

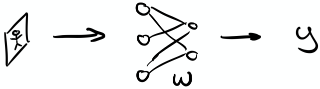
The Promises of Bayesian Model Selection

Difficulties with Bayesian Inference in Deep Learning

Ensembles and Architecture Search

Conclusion

Bayesian Inference



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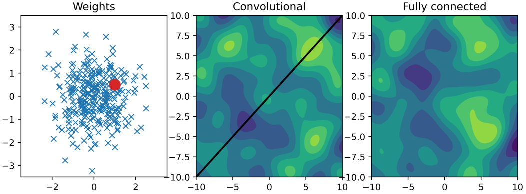

- A prior on parameters leads to a prior on functions
- Architectural **hyperparameters** influence prior on functions
- BDL focusses mostly on uncertainty in the function:

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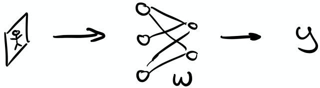

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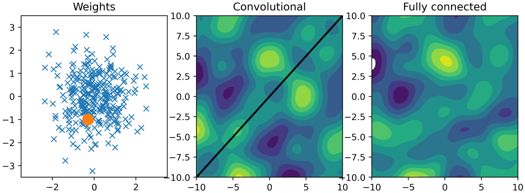

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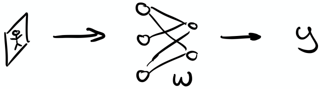

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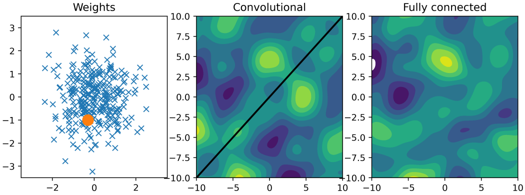

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But we want to determine the hyperparameters θ too!

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

Variational Bayesian Model Selection

Bayes tells us what to do, but not how to do it. Variational inference actually does it, and gives us

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

The Ingredients

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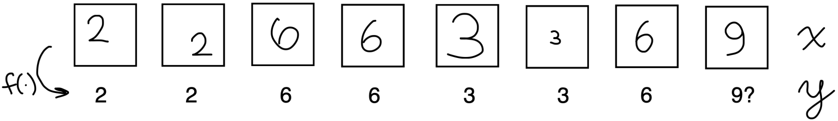
1. A way to **constrain** our learnable function to be invariant



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

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

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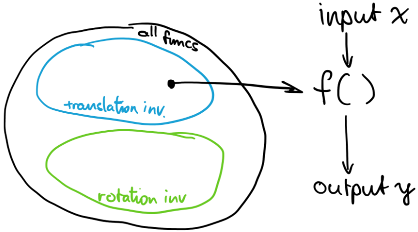

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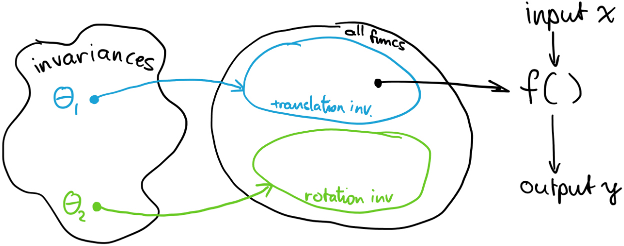

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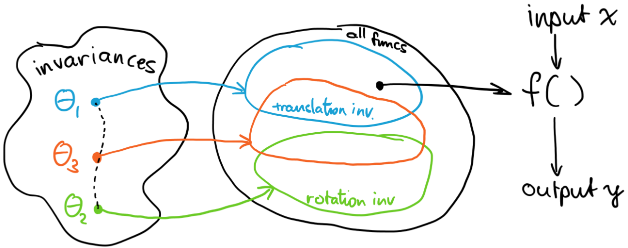

The Ingredients

We need

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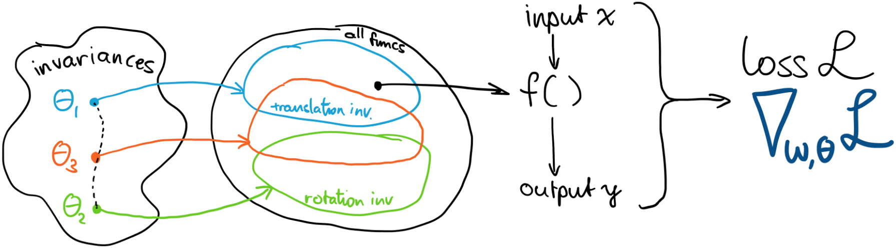
2. A way to **parameterise** different sets of invariant functions. **Differentiably**.
3. An objective function for learning **both** the function (i.e. weights), and invariance (i.e. θ).



Invariant functions

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

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 $f(\mathbf{x})$:

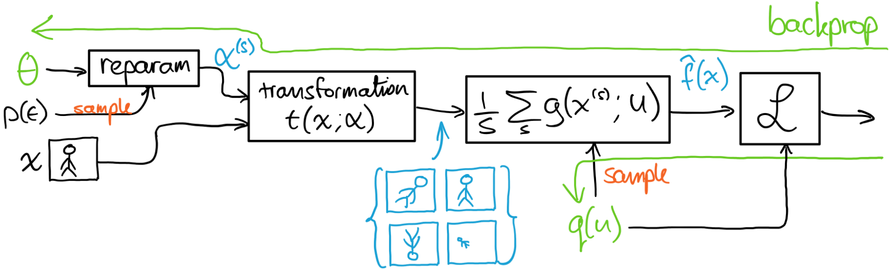
$$\hat{f}(\mathbf{x}) = \frac{1}{S} \sum_{s=1}^{S} g(\mathbf{x}^{(s)}; \mathbf{u})$$

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

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

4. Backpropagate to get gradients!

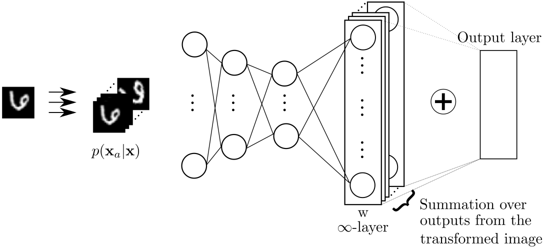
Training procedure



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

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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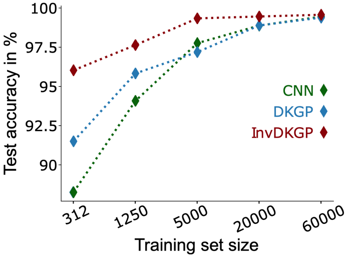

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Next Steps

- Better objective functions that correctly regularise *all* parameters
- Learning convolutions in individual layers
- Decentralising computation

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Variational Bayesian Model Selection in DNNs

How does this work when applied in DNNs?

"Empirically we found optimising the parameters of a prior $p(\mathbf{w})$ *(by taking derivatives of (1)) to not be useful, and yield worse results."*
Weight Uncertainty in Neural Networks, (Blundell et al., 2015)

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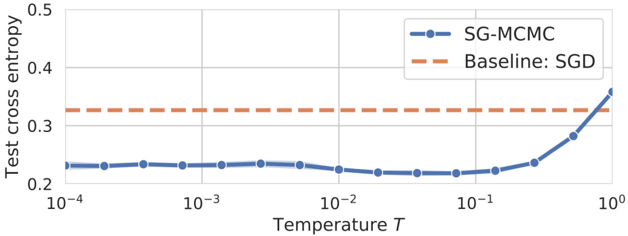
- Does this mean that $\mathrm{KL}[q(f) || p(f|\mathbf{y}, \theta)]$ is large?

Cold Posteriors



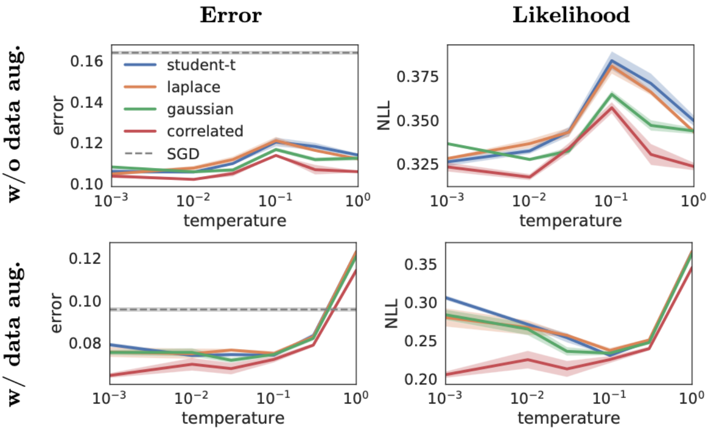
From Wenzel et al. (2020)

$$p_T(\boldsymbol{\theta}|\mathbf{y}) \propto p(\boldsymbol{\theta}|\mathbf{y})^{1/T} \tag{9}$$

- 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†

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We observe:

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Possible explanations:

- Analysis of infinitely wide neural networks shows that independent weights can destroy spatial activation correlation. Correlated weights can recover this (Garriga-Alonso and van der Wilk, 2021).
- Data augmentation should be expressed as an invariance in the prior (v.d.Wilk et al., 2018).

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What makes VI bounds work in deep GPs?

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Ensembles and Posteriors

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

$$\mathbf{w}^{(k)} \overset{\text{iid}}{\sim} \mathcal{N}(0, \boldsymbol{I}) \tag{10}$$

$$\mathbf{w}_p^{(k)} := \text{GradDesc}(\mathbf{w}^{(k)}, ||\mathbf{y} - \Phi(X)\mathbf{w}||^2) \tag{11}$$

$$\implies \mathbf{w}_p^{(k)} \overset{\text{iid}}{\sim} p(\mathbf{w}|\mathbf{y}) \tag{12}$$

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

Can optimisation do Bayesian Model Selection?

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$$\geqslant \sum_i \mathbb{E}_{p(\mathbf{w}|\mathbf{y}_{<i})}[\log p(y_i|\mathbf{w})]$$

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- Bayesian Perspective on Training Speed and Model Selection

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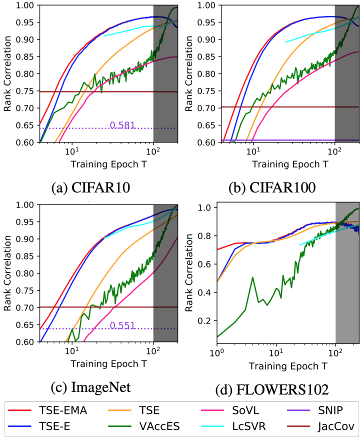
Neural Architecture Search

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



(a) CIFAR10 (b) CIFAR100

(c) ImageNet (d) FLOWERS102

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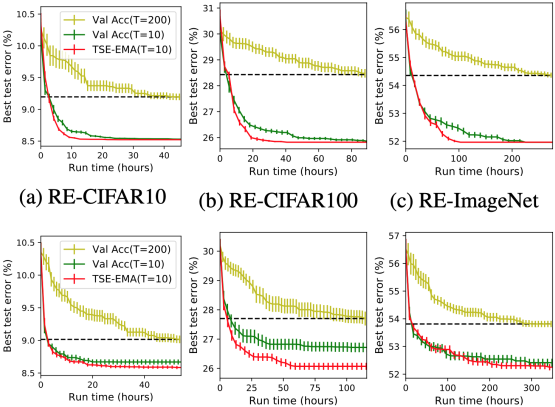

(a) RE-CIFAR10 (b) RE-CIFAR100 (c) RE-ImageNet

(d) TPE-CIFAR10 (e) TPE-CIFAR100 (f) TPE-ImageNet

Overview

The Promises of Bayesian Model Selection

Difficulties with Bayesian Inference in Deep Learning

Ensembles and Architecture Search

Conclusion

Conclusion & Ways Forward

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Possible ways forward:

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- Perhaps model misspecification is a problem? (Wenzel et al., 2020)
- Perhaps optimization mechanisms can do the same thing? (Lyle et al., 2020)

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!

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
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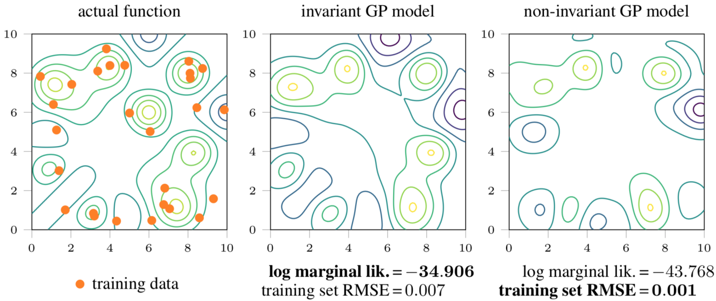

invariant GP model	non-invariant GP model
log marginal lik. = −34.906	log marginal lik. = −43.768
training set RMSE = 0.007	**training set RMSE = 0.001**
test set RMSE = 0.43	test set RMSE = 0.87

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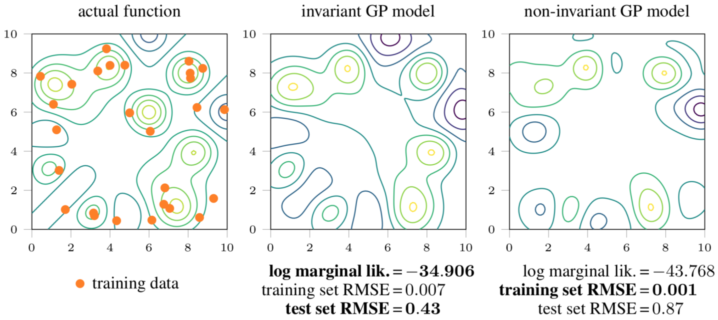

Log marginal likelihood measures **generalisation**:

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

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

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