"Thinking Hour" @ UvA

Imperial College London

Inductive Biases, Input Densities, and Predictive Uncertainty

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I could have spoken about actual research

I'm excited about **learning** invariances/equivariance.
I didn't finish this slide in time...

Questions

- How do uncertainty and inductive bias interact?
- What is good behaviour of predictive error bars?
- Should we be uncertain ”far away” from the training data?
- Can we use input density as a metric for predictive uncertainty?

How should we measure uncertainty quality?

In particular when there is domain shift.

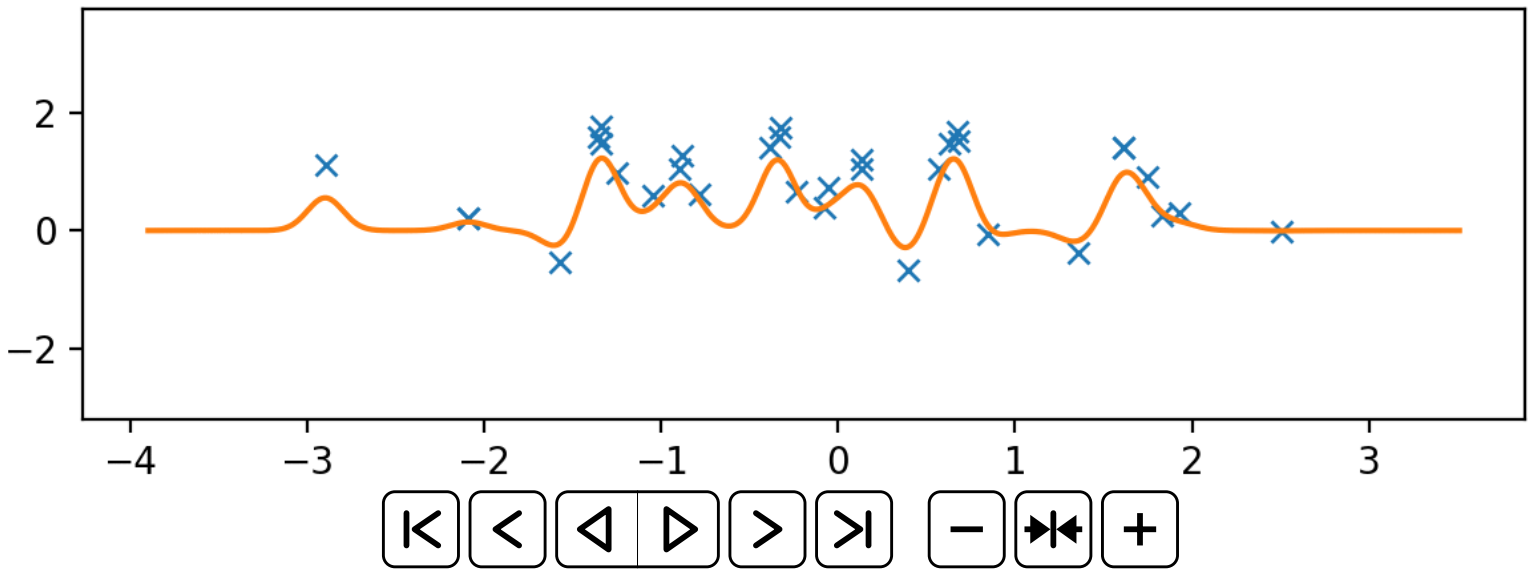
- Toy examples to illustrate what it looks like when it **works**
- Inspiration for new ways to measure and probe behaviour?
- Let’s look at some pictures (need Acrobat for animations)

Minimising training loss

We're looking for a fit that will **generalise** to new unseen test data.
Let's minimise the training loss of the posterior mean.

$$\mathcal{L}(\theta, \sigma) = \sum_{n=1}^{N} \left[k_\theta(\mathbf{x}_n, X) \left(\mathbf{K}_\theta + \sigma^2 \mathbf{I} \right)^{-1} \mathbf{y} - y_n \right]^2 \tag{1}$$

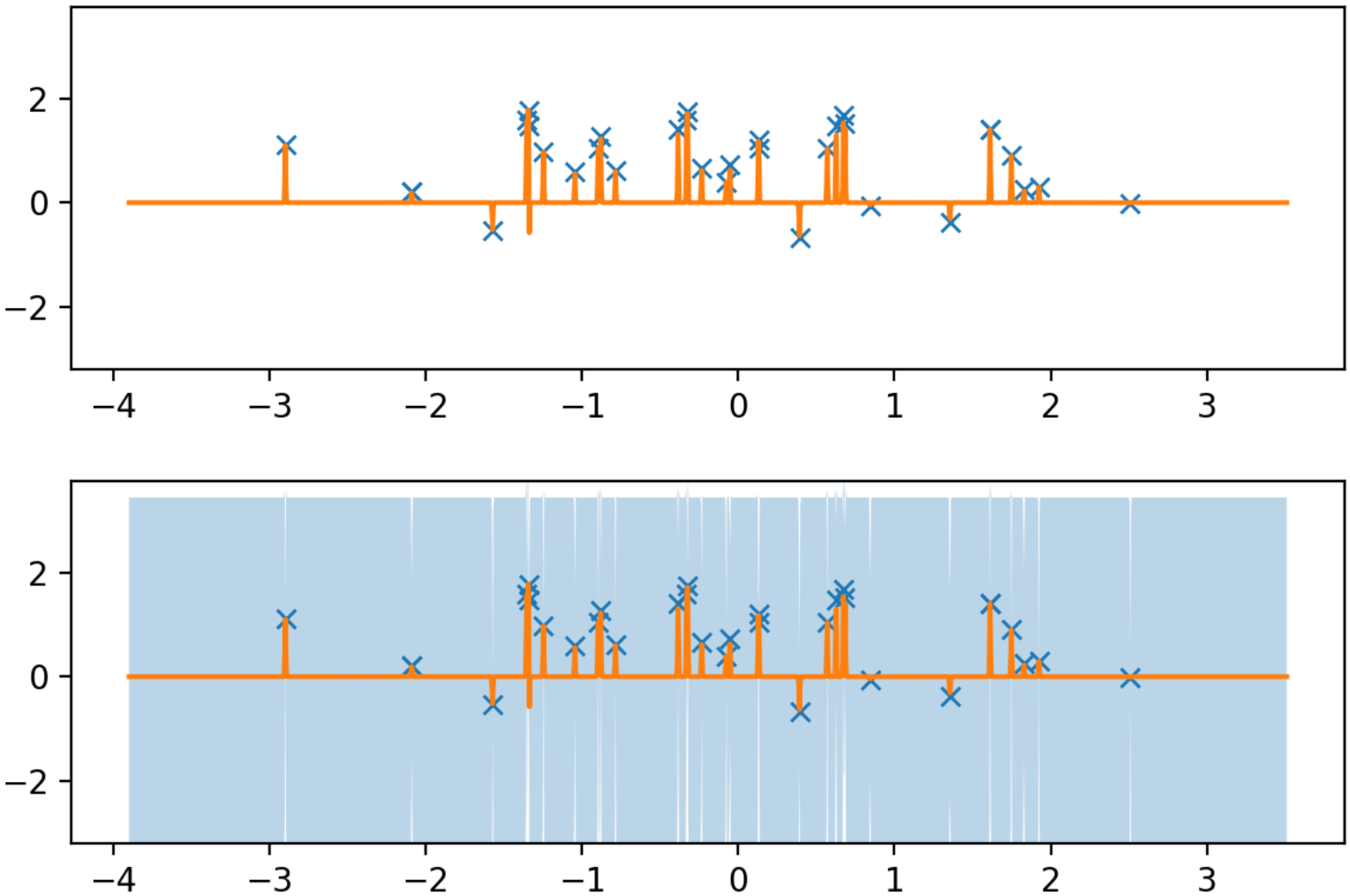
$$\{\theta^*, \sigma^*\} = \underset{\theta, \sigma}{\operatorname{argmin}}\, \mathcal{L}(\theta, \sigma) \tag{2}$$



We can fit anything with a tiny lengthscale and noise variance!

How does uncertainty help?

Does uncertainty help against the overfitting?



Model Selection according to Bayes

Model selection from a Bayesian point of view:

$$
\begin{aligned}
p(f, \boldsymbol{\theta} \mid \mathbf{y}) &= \frac{p(\mathbf{y} \mid f) p(f \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{p(\mathbf{y})} \\
&= \underbrace{\frac{p(\mathbf{y} \mid f) p(f \mid \boldsymbol{\theta})}{p(\mathbf{y} \mid \boldsymbol{\theta})}}_{p(f \mid \mathbf{y}, \boldsymbol{\theta})} \underbrace{\frac{p(\mathbf{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{p(\mathbf{y})}}_{p(\boldsymbol{\theta} \mid \mathbf{y})}
\end{aligned}
$$

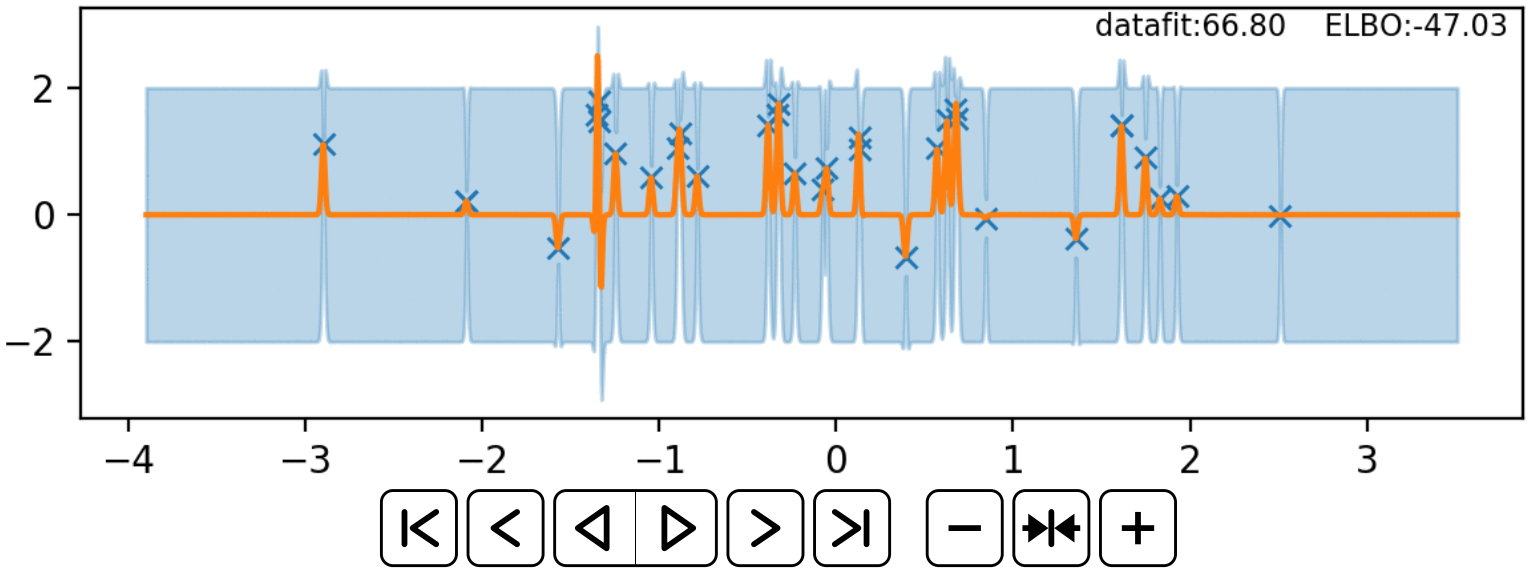
Key quantity for model selection is the **marginal likelihood**

$$
p(\mathbf{y} \mid \boldsymbol{\theta}) = \int p(\mathbf{y} \mid f) p(f \mid \boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta}
$$

By handing our uncertainty on $f(\cdot)$ in a Bayesian way, we also get the marginal likelihood for model selection.

Marginal likelihood fixes things

Instead, choose hyperparameters by maximising marginal likelihood:



In above $\mathcal{L}$ is indicated by 'datafit', while 'ELBO' indicates the marginal likelihood.

- More sensible fit as the marginal likelihood rises
- Datafit gets worse!

Marginal likelihood trades off
data fit and **model complexity**.

Why does marginal likelihood work?

We have seen

- Minimising training error doesn't work
- Uncertainty doesn't necessarily help, but does make us more cautious
- Marginal likelihood seems to trade-off complexity and data fit

But **why** does the marginal likelihood lead to models that generalise well?

Marginal likelihood as incremental prediction

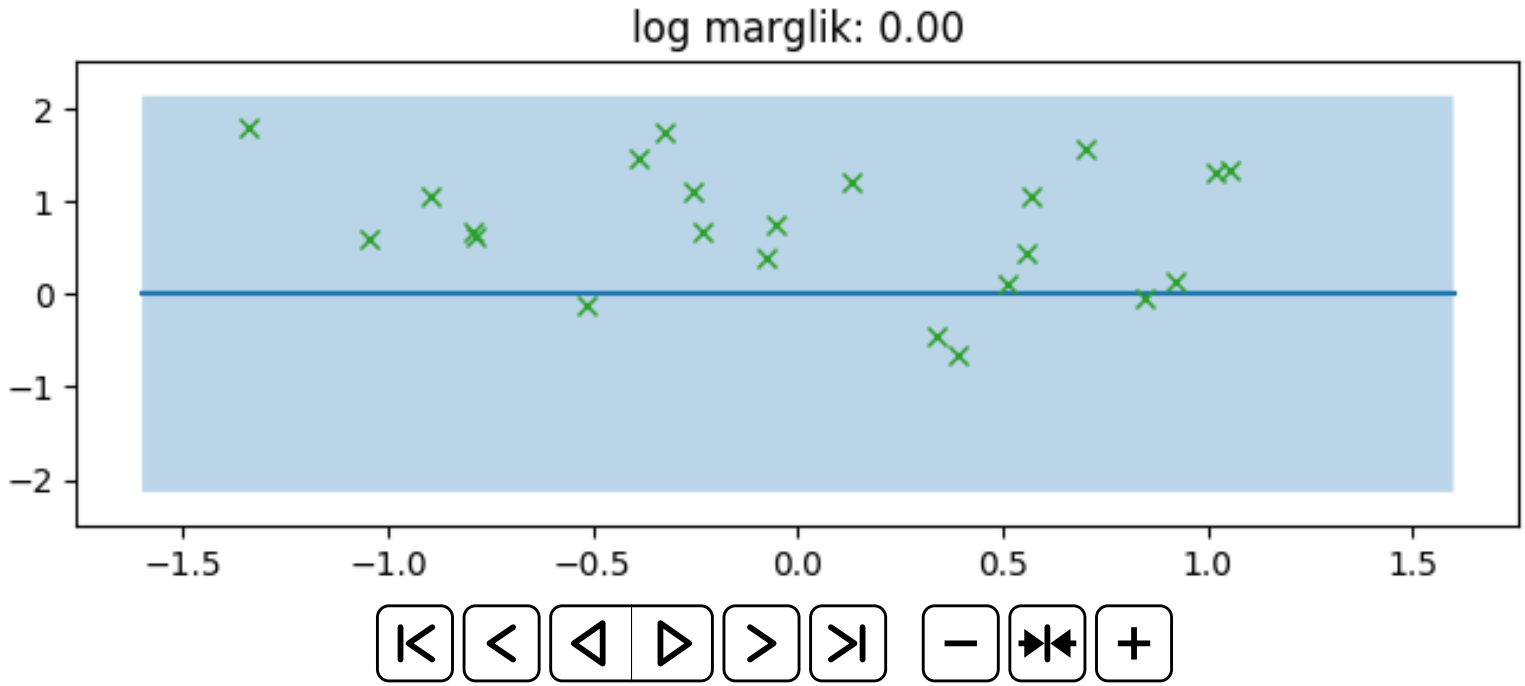
We can split the marginal likelihood up using the **product rule**:

$$p(\mathbf{y}) = p(y_1)p(y_2|y_1)p(y_3|\{y_i\}_{i=1}^{2})\dots \tag{3}$$

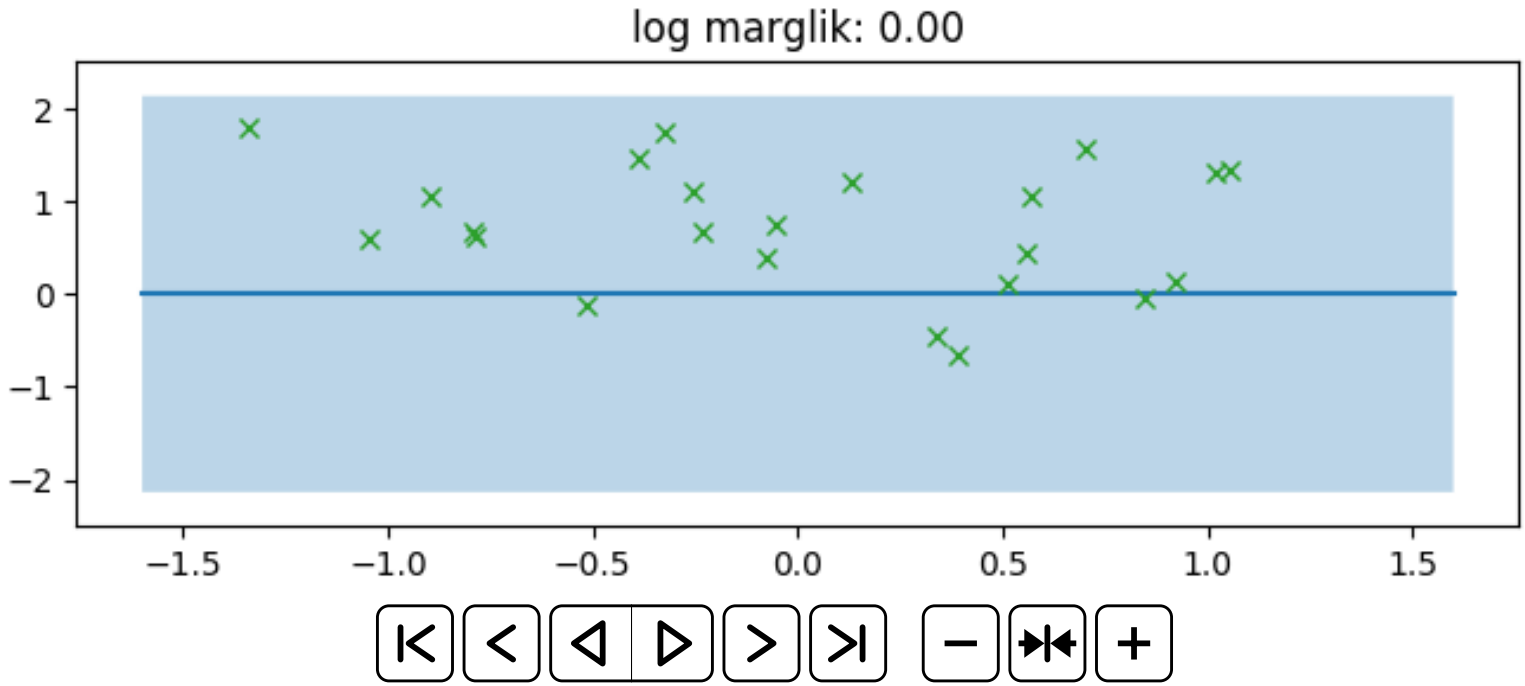
$$= \prod_{n=1}^{N} p(y_n|\{\mathbf{x}_i, y_i\}_{i=1}^{n-1}) \tag{4}$$

- The marginal likelihood measures how well previous training points predict the next one
- If it continuously predicted well on all N points previously, it probably will do well next time

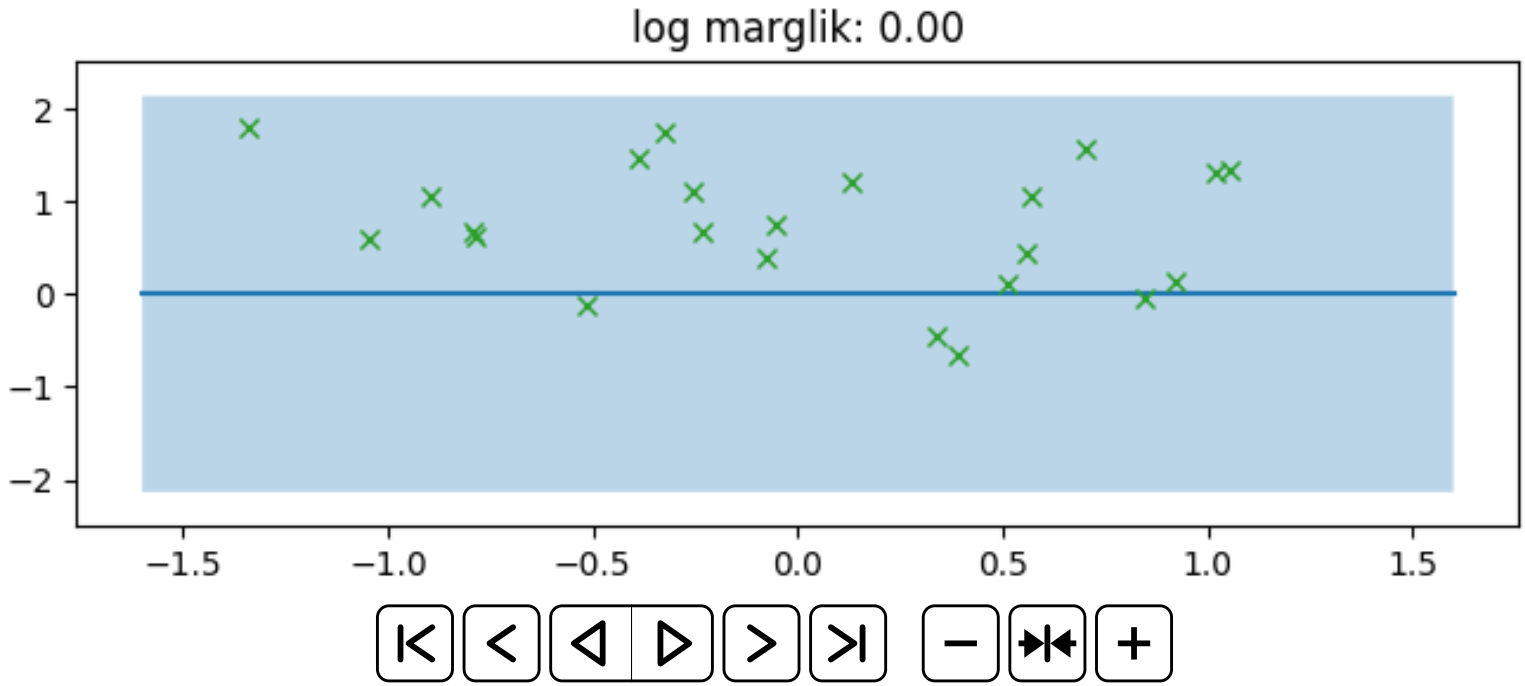
Marginal likelihood computation in action



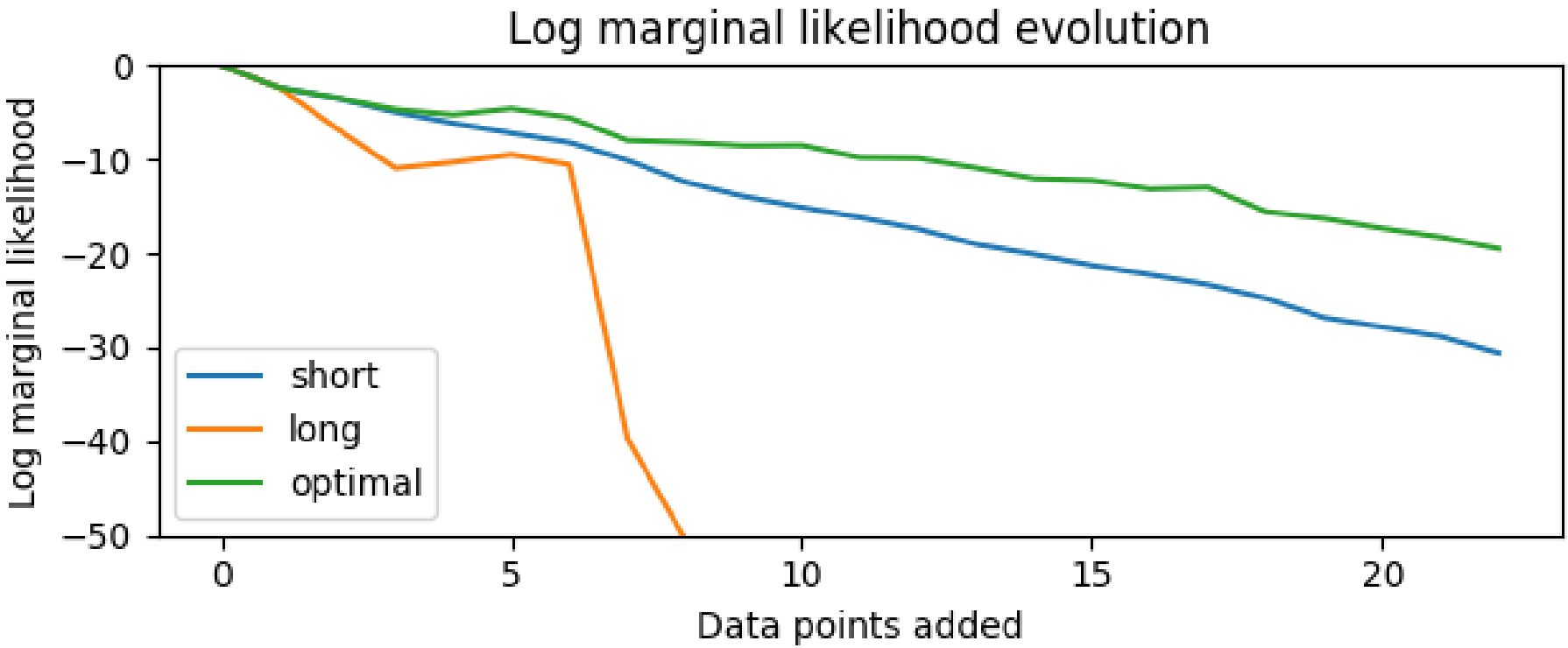
Marginal likelihood computation in action



Marginal likelihood computation in action

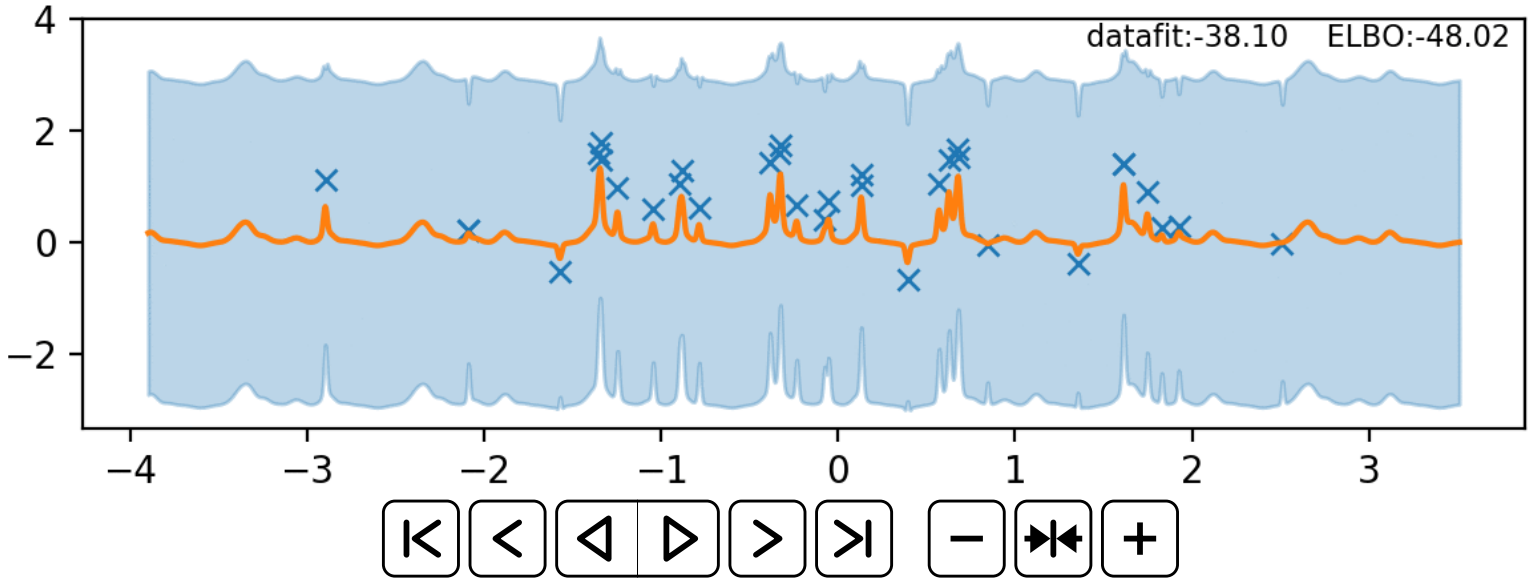


Marginal likelihood evolution



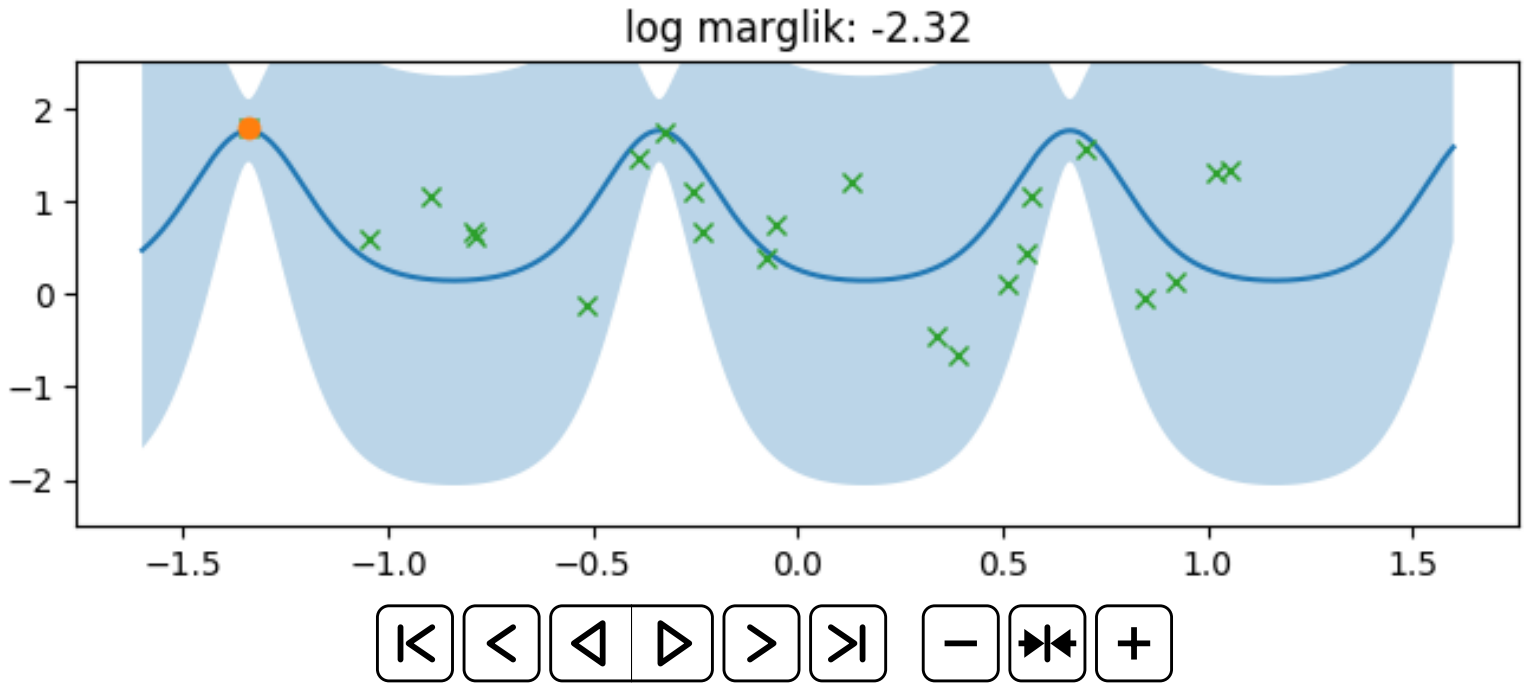
- **Short** lengthscale consistently **over-estimates variance**, so **can't get a high density** even with the observation in the error bars
- **Long lengthscale** consistently **under-estimates variance**, so gets a low density because the **observations are outside error bars**
- Optimal lengthscale **trades off** these behaviours... well.

Marginal likelihood in action



- We chose the prior: $f(\mathbf{x}) = \theta_s f_{\text{smooth}}(\mathbf{x}) + \theta_p f_{\text{periodic}}(\mathbf{x})$, with smooth and periodic GP priors respectively.
- Marginal likelihood learns **how** to generalise not just to fit the data.
- Amount of periodicity vs smoothness is automatically chosen by selecting hyperparameters θ_s, θ_p.

Marginal likelihood in action



Marginal likelihood as a prior probability

A complementary view

- Marginal likelihood is the probability of the data under the prior.

$$p(\mathbf{y}|\theta, X) = \int p(\mathbf{y} \mid f(X), \theta) p(f \mid \theta) \mathrm{d}f \tag{5}$$

- For zero-mean GP regression models it has the explicit form:

$$\begin{aligned} \log p(\mathbf{y}|\theta, X) &= \log \mathcal{N}\left(\mathbf{y}; 0, \mathbf{K} + \sigma^2 \mathbf{I}\right) \\ &= -\frac{N}{2} \log 2\pi - \underbrace{\frac{1}{2} \log \left|\mathbf{K} + \sigma^2 \mathbf{I}\right|}_{\text{Complexity penalty}} - \underbrace{\frac{1}{2} \mathbf{y}^\intercal \left(\mathbf{K} + \sigma^2 \mathbf{I}\right)^{-1} \mathbf{y}}_{\text{Data fit}} \end{aligned} \tag{6}$$

- Laplace approximations in Neural Networks look similar
- Pretty amazing that you can estimate updating behaviour from the shape of the loss function (ELBOs give lower bound!)

Intermediate take-homes

Q: How do uncertainty and inductive bias interact?

- Prior is super important to getting the right behaviour in uncertainty
- Can't get strong generalisation without low uncertainty

Q: How should we pick our prior?

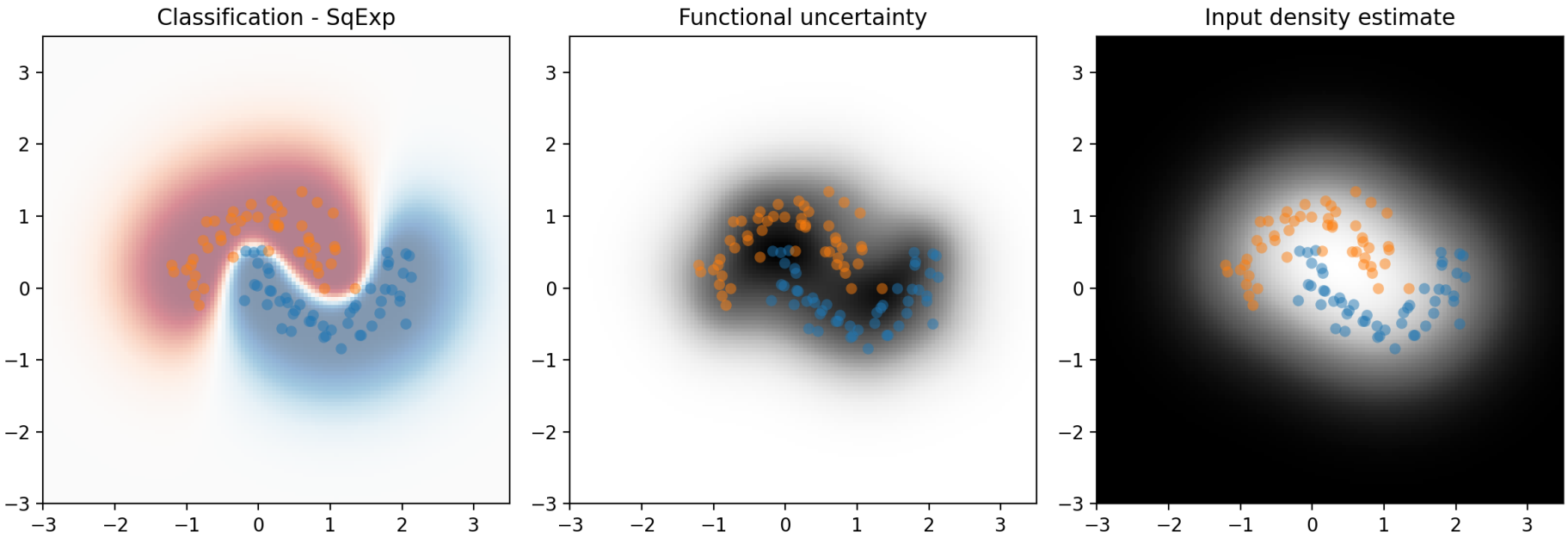
- Marginal likelihood measures incremental predictive performance
- No need for hyperpriors to get good model selection!
- Is the marginal likelihood safe from overfitting?
  $\implies$ It's safe from the kind of overfitting that the normal likelihood exhibits

What is good behaviour of predictive error bars?

Should we be uncertain far from the data?

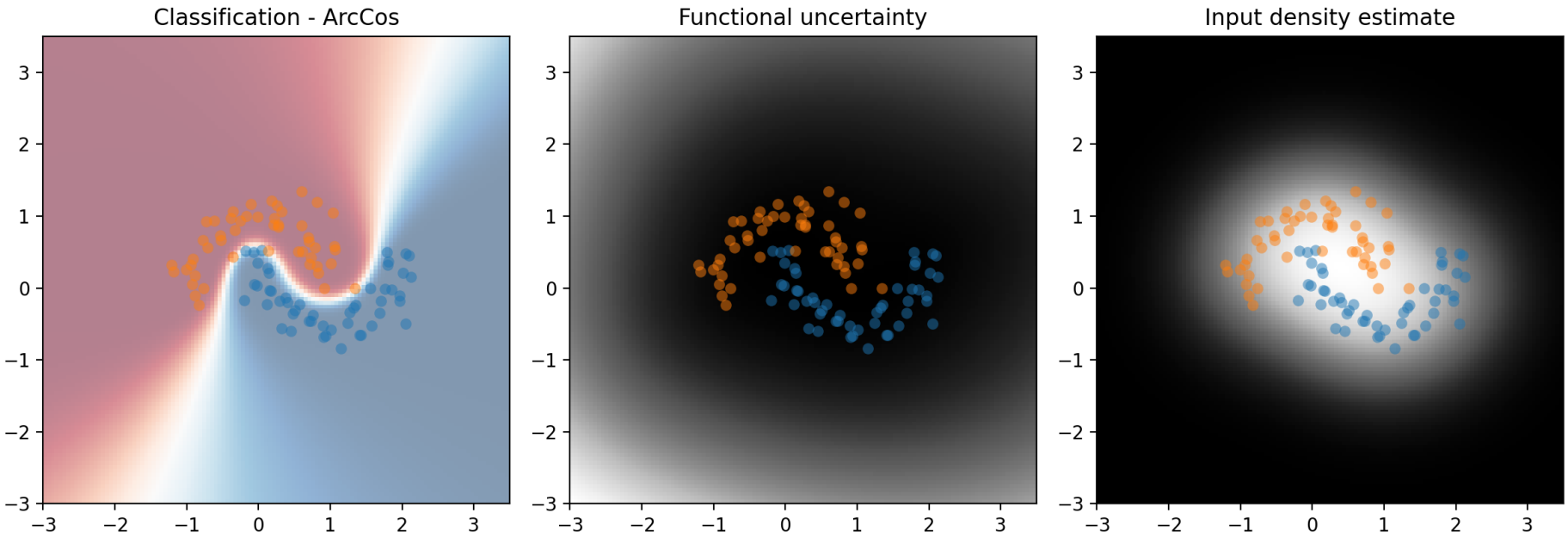
Can we use input density
as a metric for predictive uncertainty?

GPs as a Gold Standard for BNNs



- GPs considered the ”gold standard” model for uncertainty estimation.
- Often in Bayesian Deep Learning, aim is to replicate GP properties in DNNs.
- Though implicitly, a GP with a *Squared Exponential* kernel.

GPs as a Gold Standard for BNNs



- ArcCos kernel is obtained from infinite limit of ReLU NN.
- Still exact inference in a GP. Different inductive bias!
- So what is the right one? What behaviour should BNNs copy?
- Both extrapolations are reasonable.

Extrapolation: Letting the marginal likelihood decide

As with the periodic example:

$$f(\cdot) = \theta_1 f_{\text{sqexp}}(\cdot) + \theta_2 f_{\text{arccos}}(\cdot)$$

$$f_{\text{sqexp}}(\cdot) \sim \mathcal{GP}\left(0, k_{\text{sqexp}}(\cdot,\cdot')\right), \qquad f_{\text{arccos}}(\cdot) \sim \mathcal{GP}(0, k_{\text{arccos}}(\cdot,\cdot'))$$

- So our marginal likelihood is now a function of $\theta = \{\theta_1, \theta_2\}$, i.e. *how much* each component contributes.
- We *could* consider the full posterior on θ:

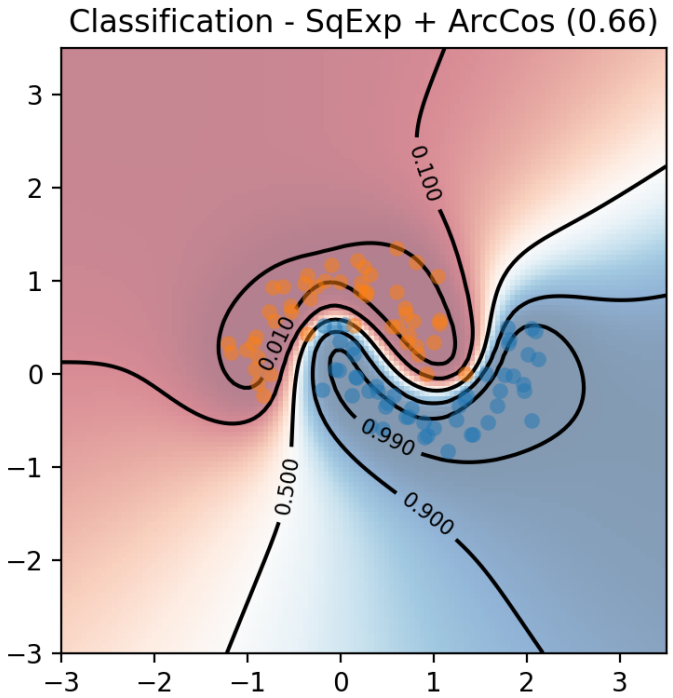
$$p(\theta|\mathbf{y}) = \frac{p(\mathbf{y}|\theta)p(\theta)}{p(\mathbf{y})} \tag{7}$$

  but this takes effort (even just to plot in this simple example).
- As before, we instead take a point estimate:

$$\theta^* = \underset{\theta}{\text{argmax}} \log p(\mathbf{y}|\theta) \tag{8}$$

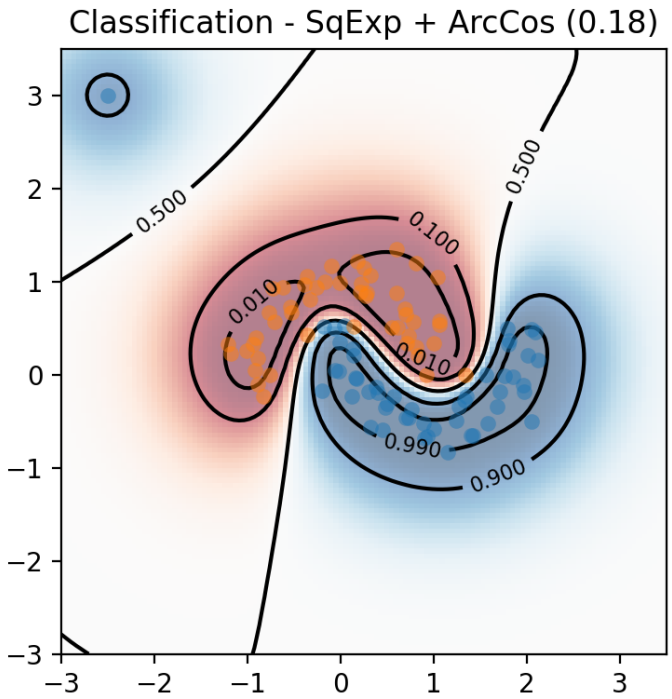
- This is **approximate**, but we'll see it still behaves well.

“Correct” extrapolation with model selection



- Marginal likelihood uses appreciable ArcCos component (0.66!)
- What if it’s wrong?
- Terrible predictive log likelihood if we’re wrong about extrapolation!

Telling the model it's wrong



- Single datapoint is enough to change inductive bias.
- It won't make the same mistake twice!

Evaluating model uncertainty

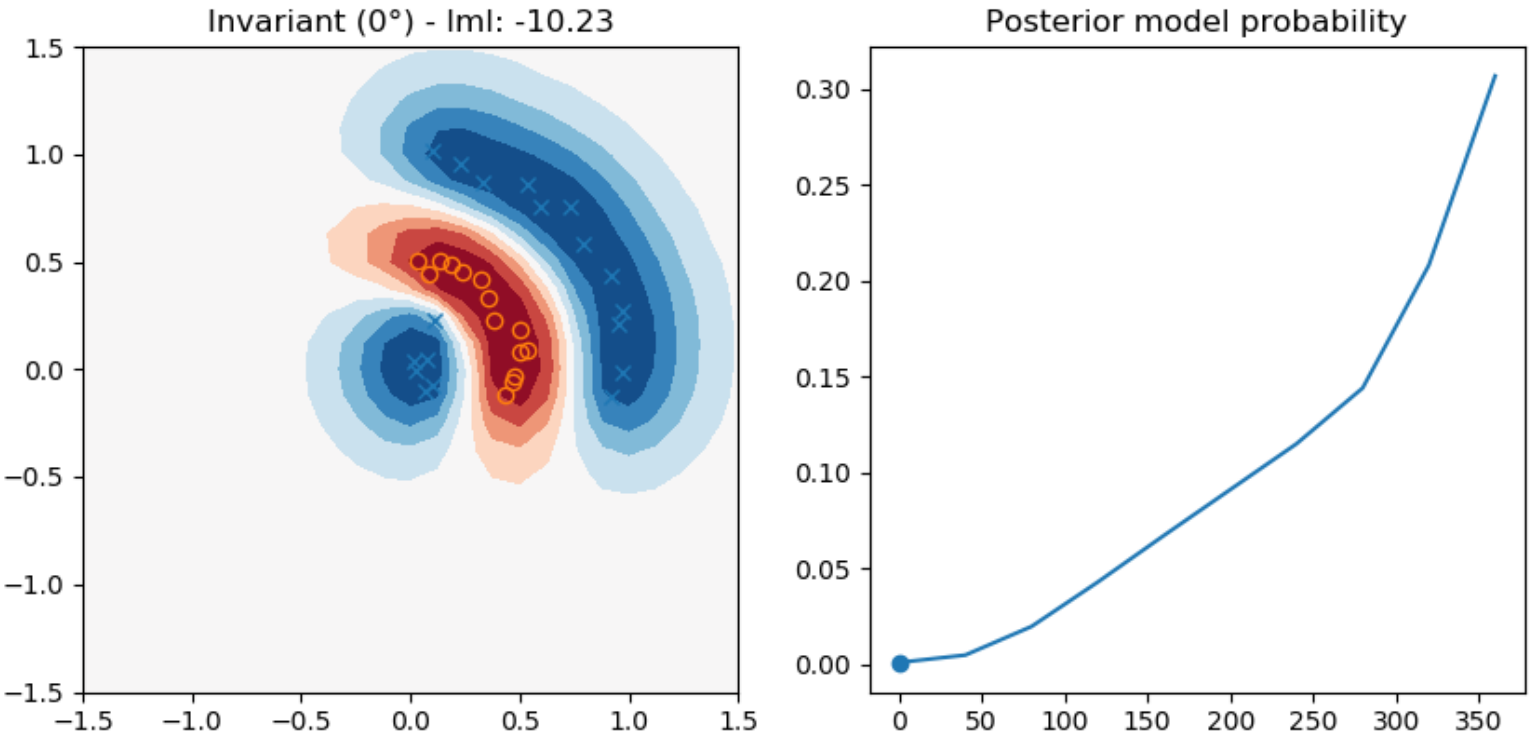
When evaluating uncertainty of models...

- In domain adaptation, you basically have to guess, and hope you're lucky (although causality helps you make a good guess).
- How realistic is the train/test split assumption in practice?
- Should we give models a chance to learn under distribution shift?
- We could measure how quickly they adapt?
- Little data can be very informative for OOD / causality

My opinion:

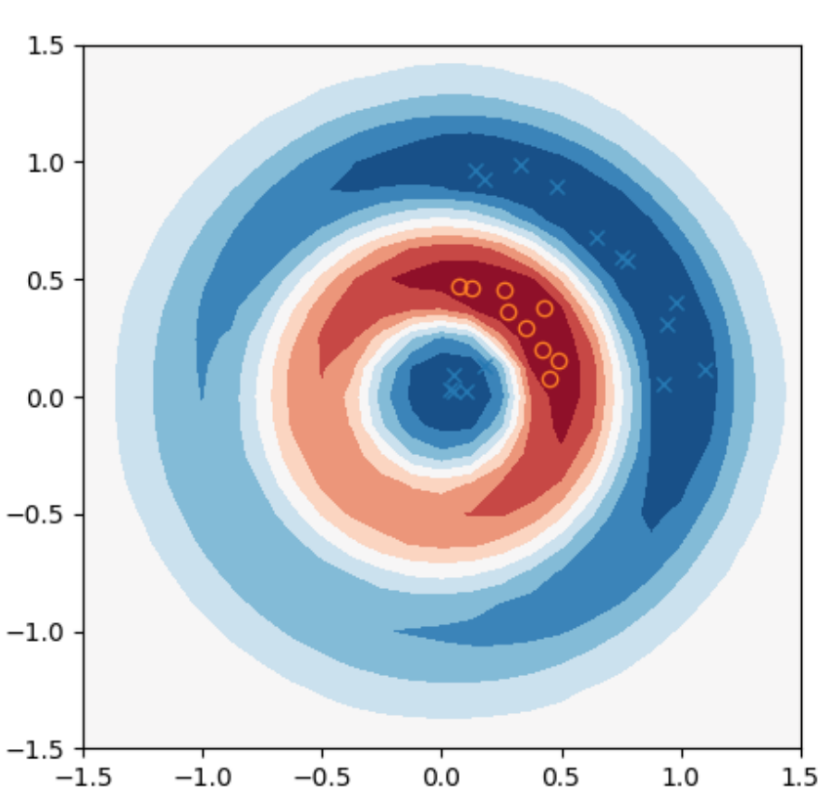
- Continual learning should be the benchmark for uncertainty, and domain adaptation.

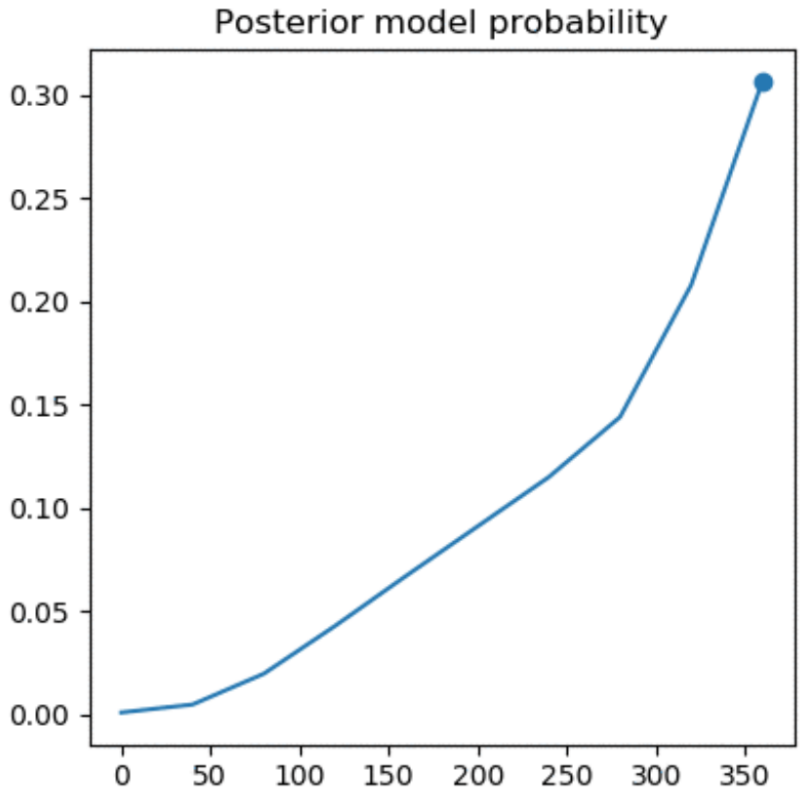
Invariance and Uncertainty



- Another example of strong extrapolation.
- Marginal likelihood prefers really strong predictions

Invariance and Uncertainty: Another solution





- Average over hyperparameters as well!
- More cautious predictions.

$$p(y^*|\mathcal{D}) = \int p(y^*|f)p(f|\theta,\mathcal{D})p(\theta|\mathcal{D})\mathrm{d}f\mathrm{d}\theta \tag{9}$$

Take-homes

- Extrapolation behaviour can be desirable
- This is at odds with being uncertain "far from the data"
- Opinion: We should not rely on input density for uncertainty
- Marginal Likelihood Optimisation can adapt to additional observations
- Full hyperparameter posteriors reduce overconfidence

Discussion points

- Can we use input density for uncertainty estimation?
- We curently force our models to not learn on the job. Is this fair? Should we be assessing uncertainty as part of a continual learning process?
- Causality is often hard because of a lack of data (coloured MNIST). Single example can break a hypothesis used for generalisation!
- How should we implement this behaviour? Bayes? Neural Processes? Meta-learning? Is Bayesian reasoning helpful with this?