OoD Generalisation, Predictive Uncertainty, and Continual Learning

Mark van der Wilk
LASR Reading Group, University of Oxford

Department of
COMPUTER
SCIENCE

https://mvdw.uk
@markvanderwilk

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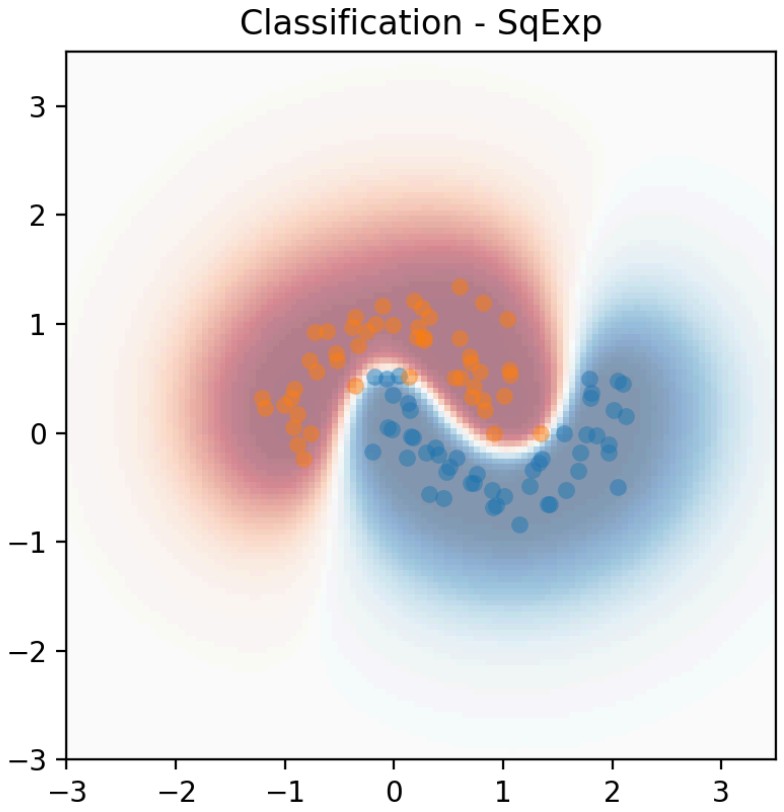

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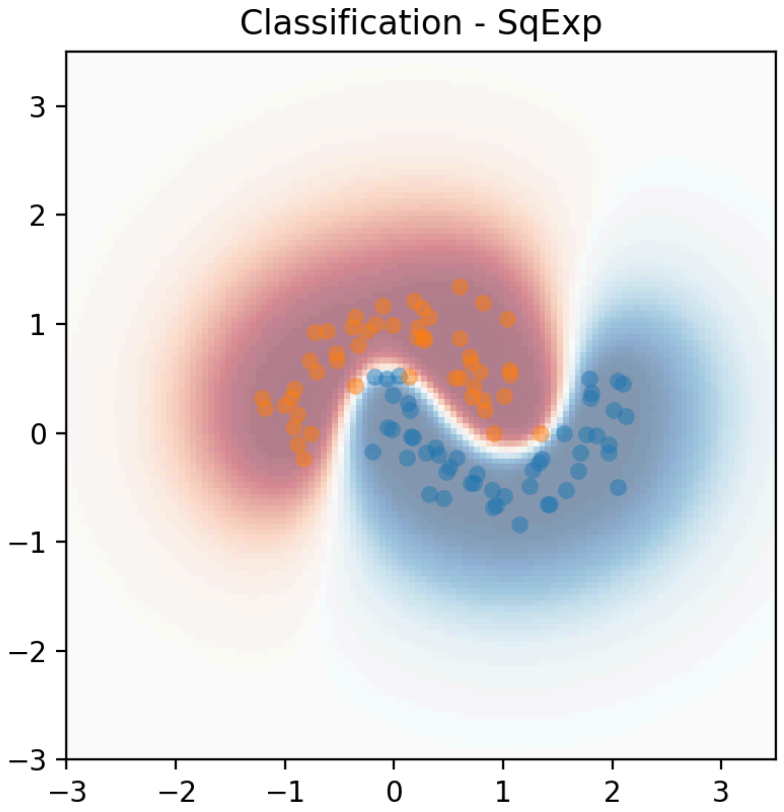

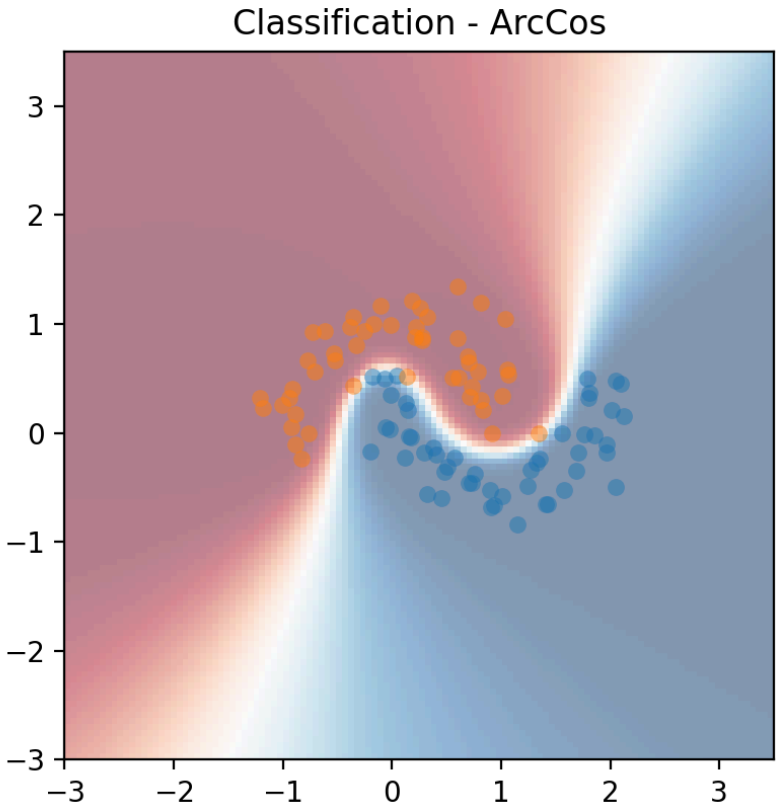

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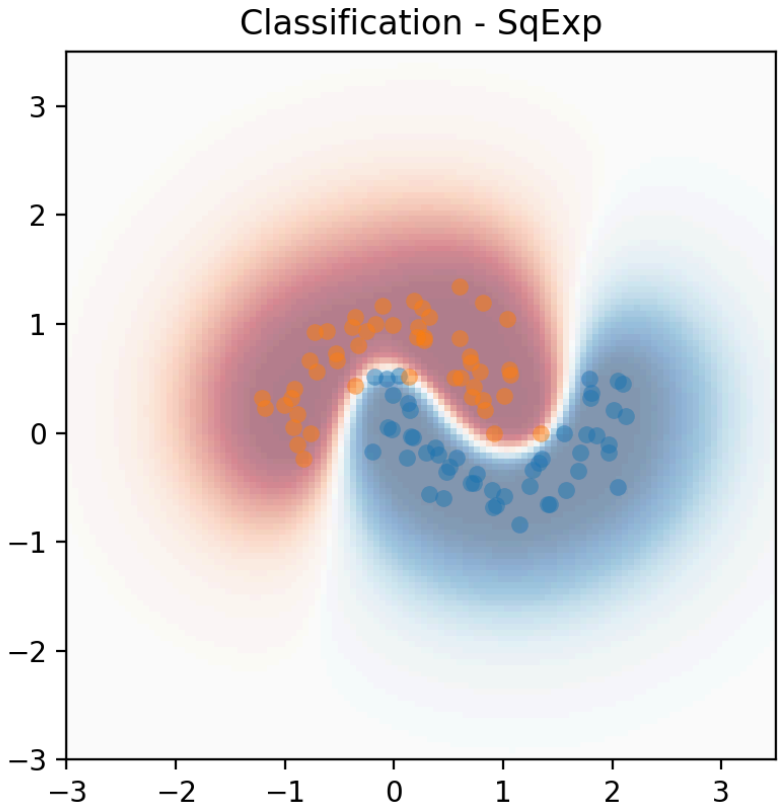

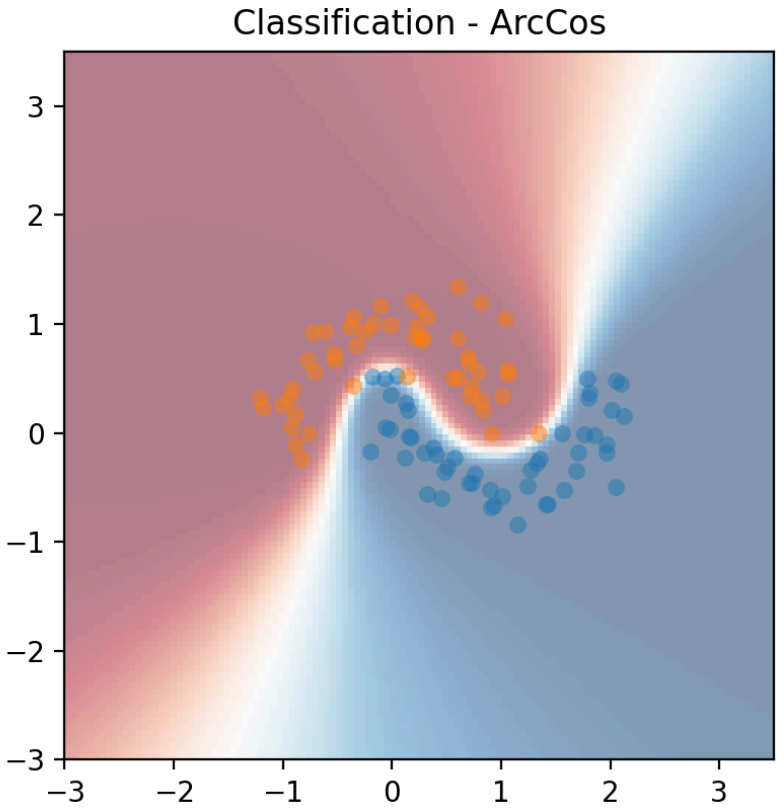

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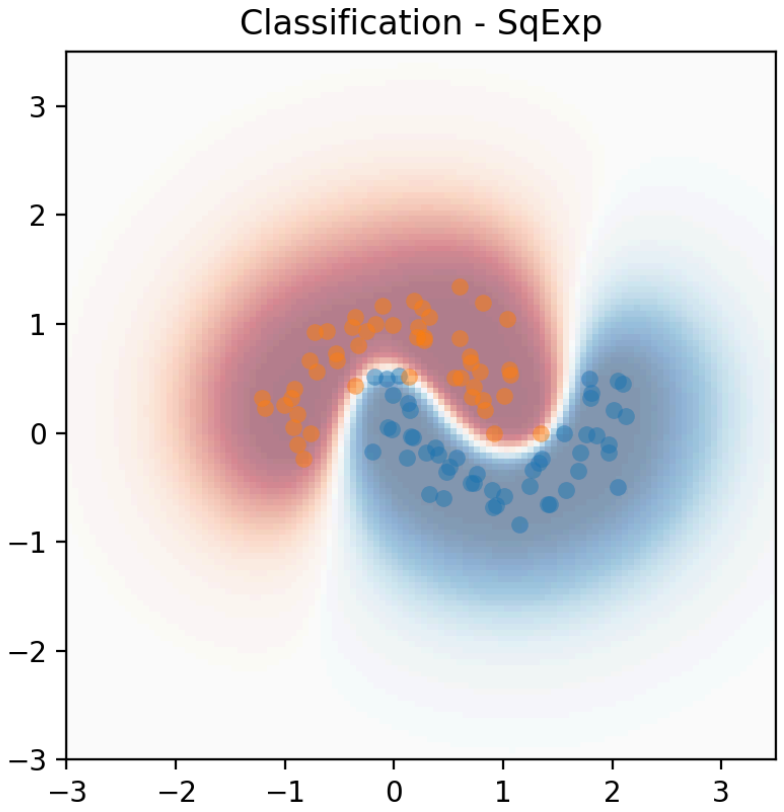

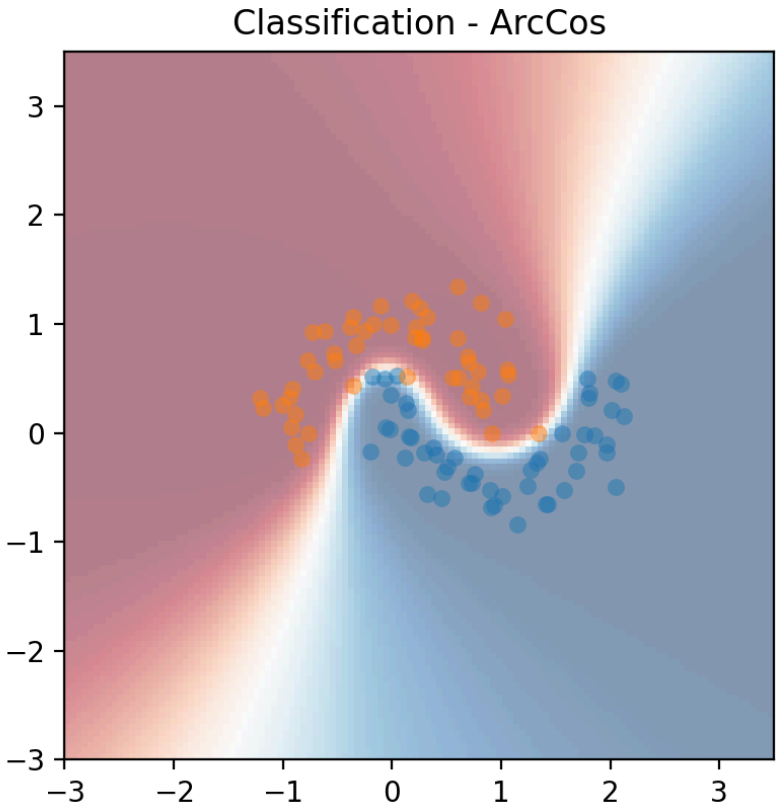

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- Which solution generalises “Out of Distribution”?
- Which solution has “correct”/“better” uncertainty?

Observations

You cannot distinguish generalisation from training loss

- Both solutions fit the training data equally well.
- Different prior assumptions: “function can move anywhere” vs “only one decision boundary”

You cannot generalise while *also* being uncertain

- Prediction specificity and uncertainty are a trade-off
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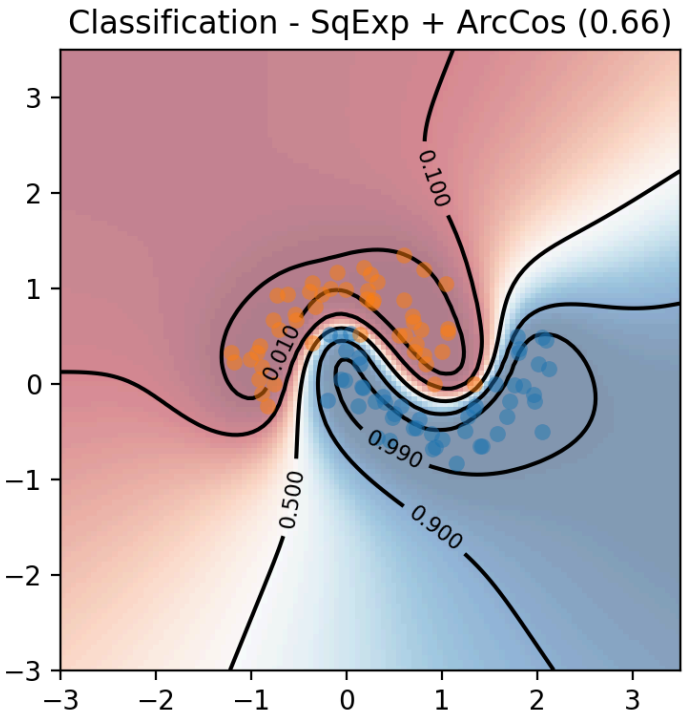

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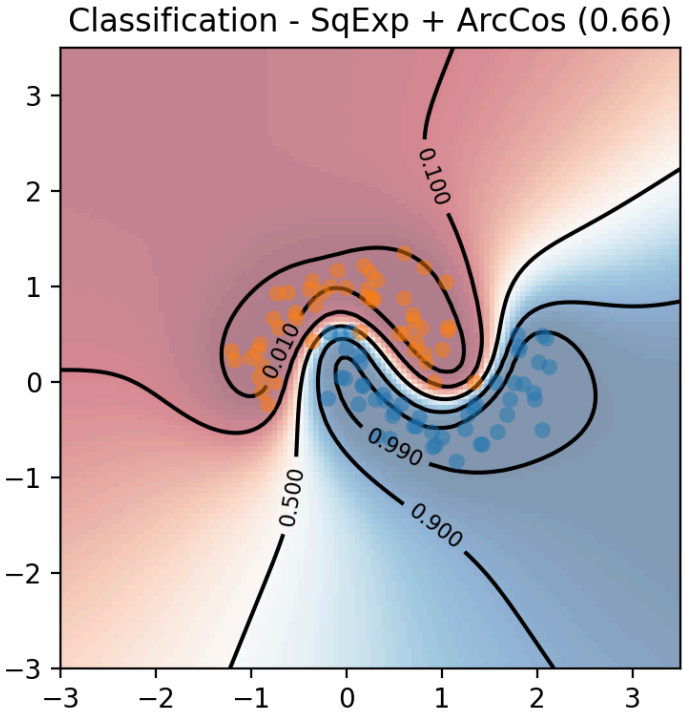

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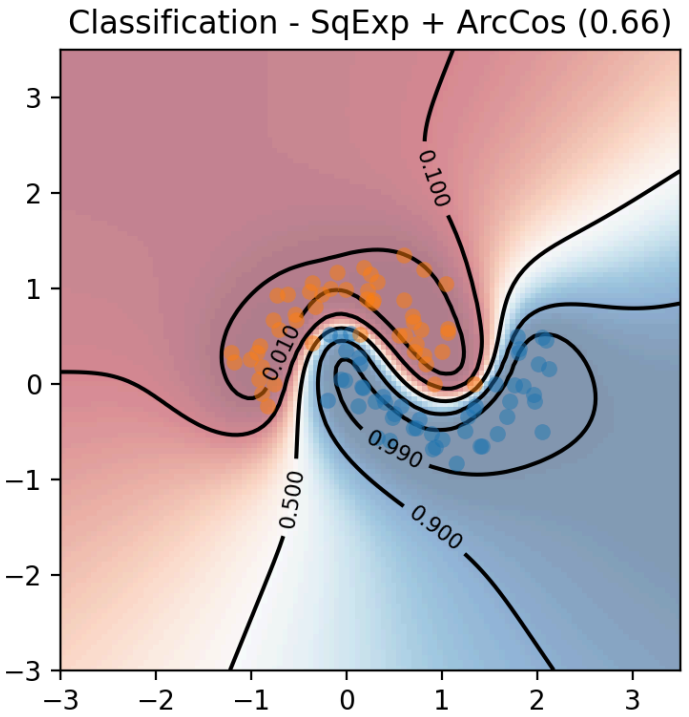

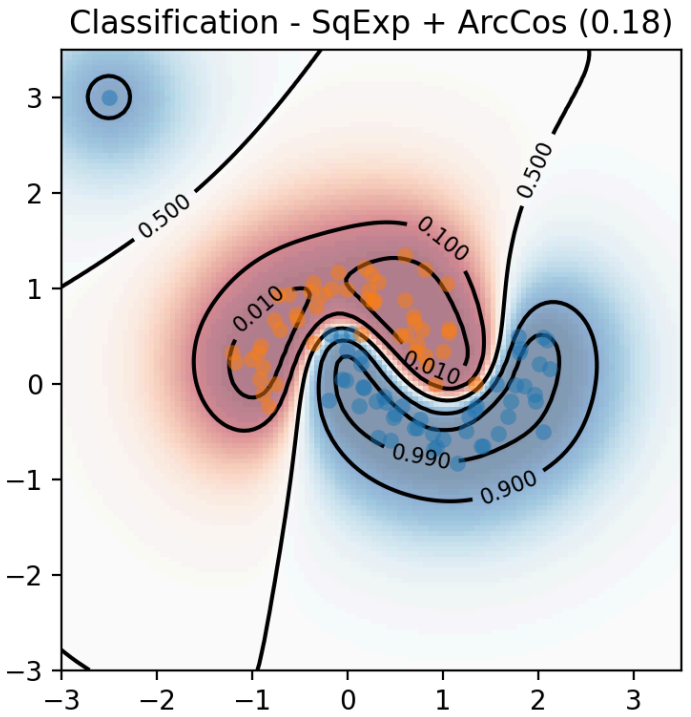

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We need working continual learning methods to mitigate the risk of making strong OoD generalisations

Model Size & Continual Learning

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From Kepler to Newton:
Inductive Biases Guide Learned World Models in Transformers

Ziming Liu [1] **Sophia Sanborn** [1] **Surya Ganguli** [1] **Andreas Tolias** [1]

Inductive Bias 3: Temporal Locality

Failure mode: A regression transformer fails to learn the Newtonian model when the context length is too large.
Solution: Reducing the context length to 2 induces a Newtonian model. Short context lengths induce the Newtonian model, while long context lengths induce the Keplerian model.

Goals

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- 🎯 **We need working continual learning methods to mitigate the risk of making strong OoD generalisations**
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All these problems are interconnected!

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Ideas from Bayesian Nonparametrics may help with new capabilities in deep learning

A Method for Finding
Inductive Bias, **Weights**, and **Model Size**
with a single objective function

🎯

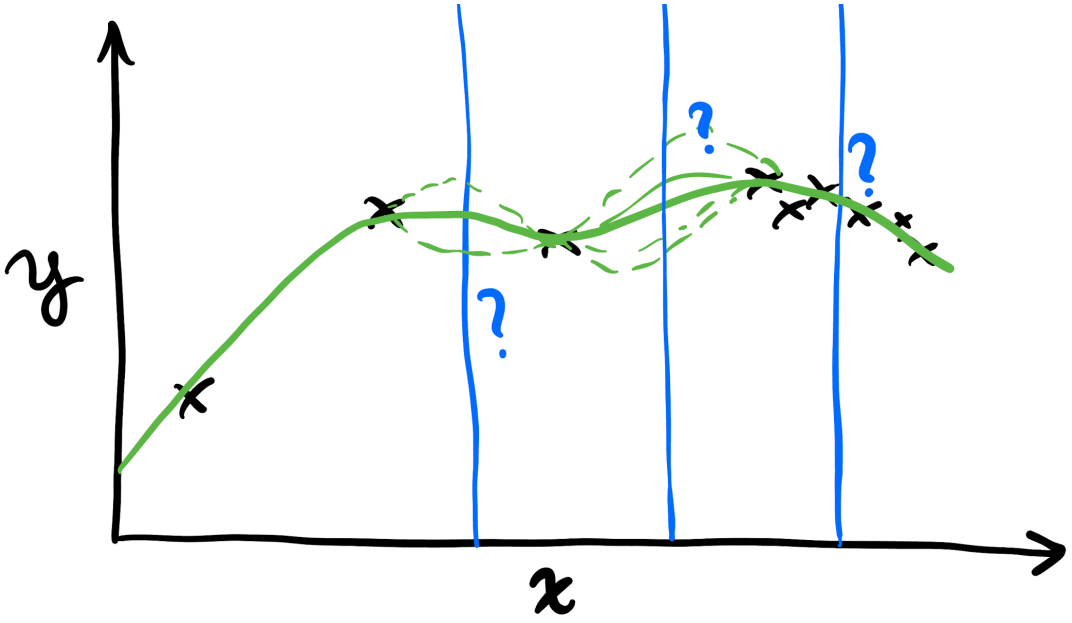
Minimise model size,
while maintaining near-optimal predictions.

Most of Machine Learning is just *Curve Fitting*

Dataset: $(x_n, y_n)_{n=1}^N$.

Inputs $x_n \in \mathcal{X}$, outputs $y_n \in \mathcal{Y}$.

Goal: Find $f : \mathcal{X} \to \mathcal{Y}$, that predicts well for new x.



Neural networks just parameterise functions $f_w(x)$.

Designing a Neural Network

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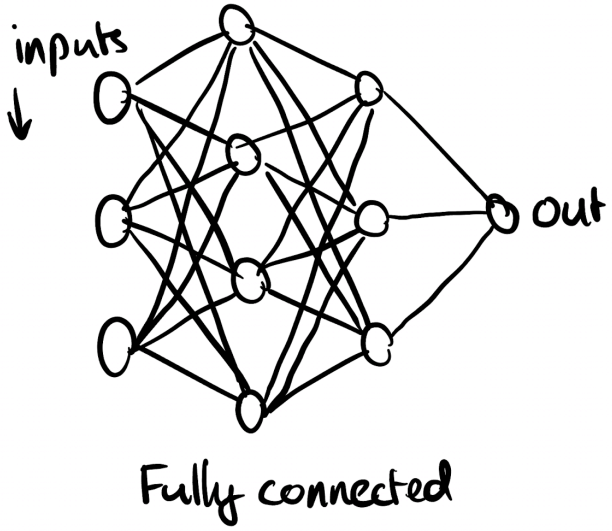

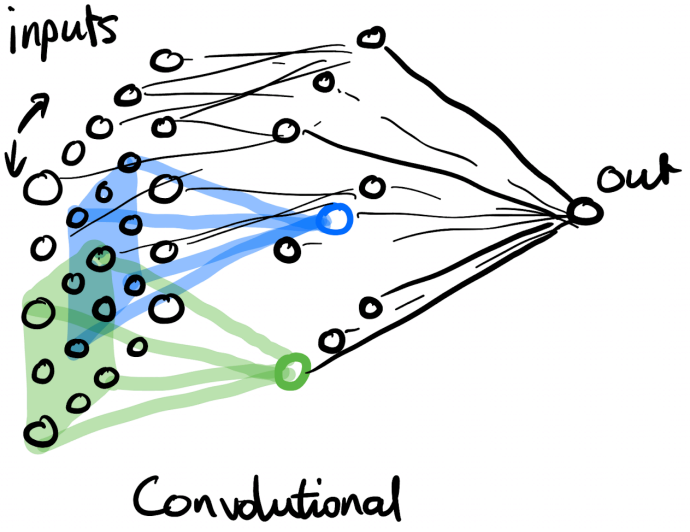

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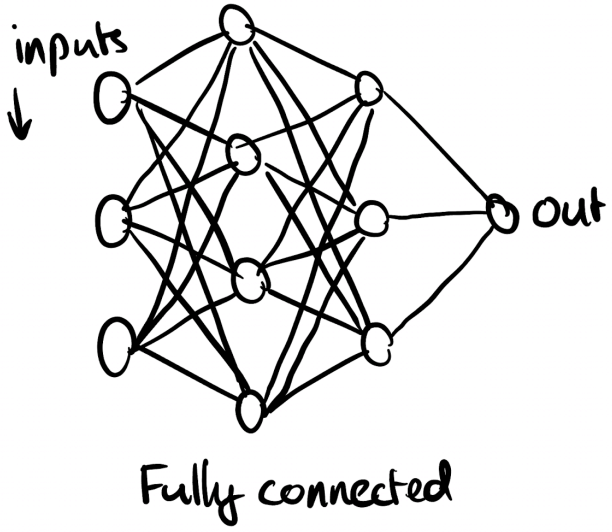

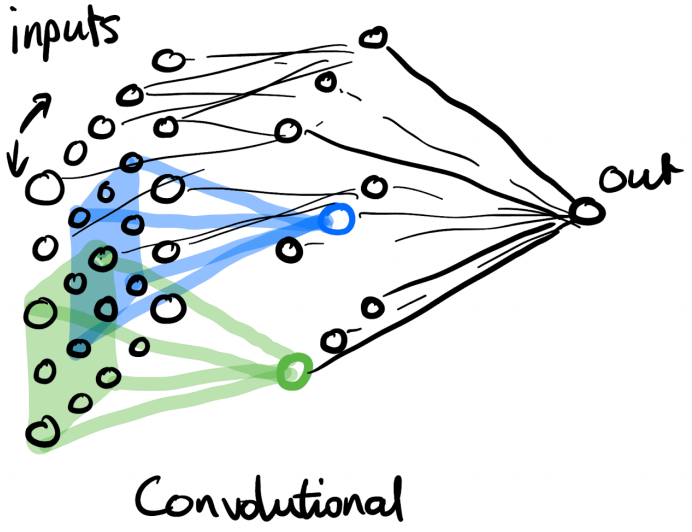

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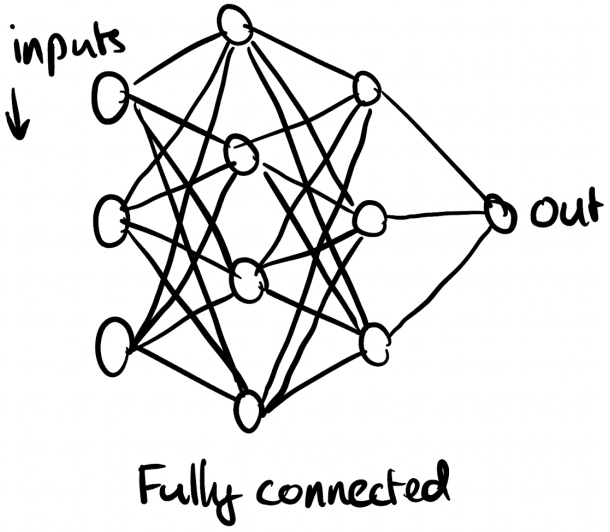

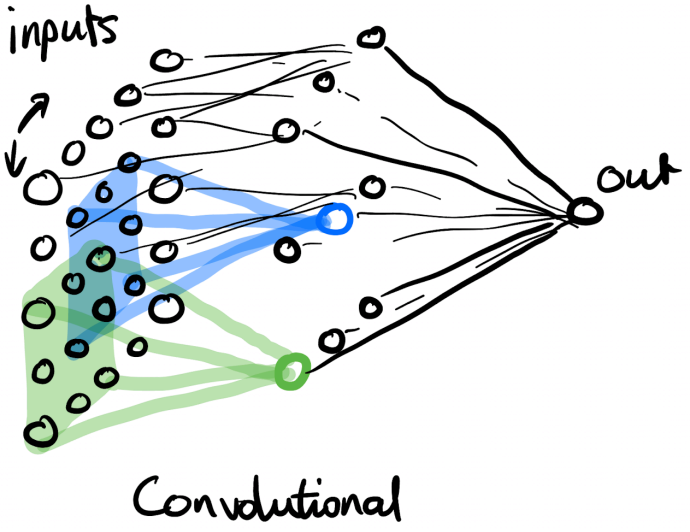

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- Choose **weights**, using *backpropagation*

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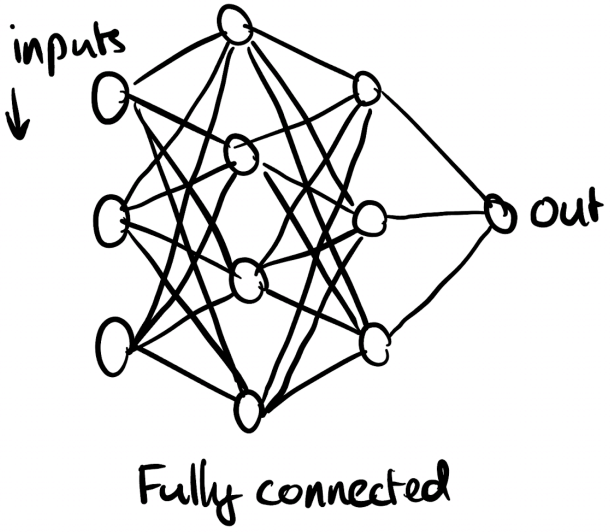

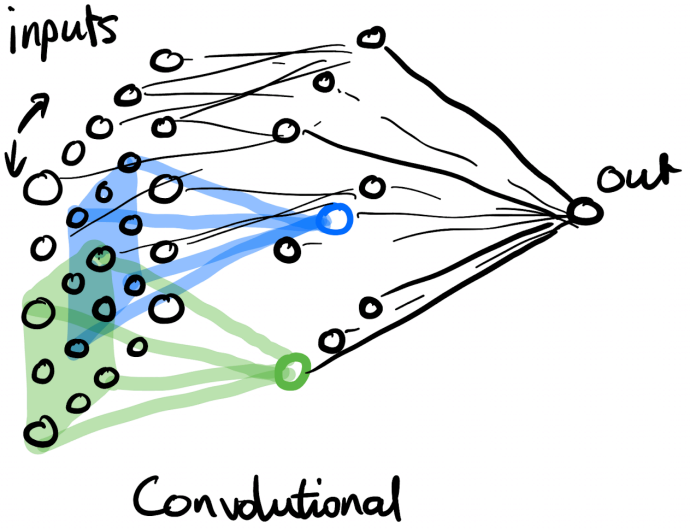

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These problems should be tackled *together*.

Problem Formulation (let's walk before we run)

Predictor is a *single layer* neural network:

$$f(x) = \sum_{m=1}^{M} \varphi(x; Z_m, \theta) w_m$$

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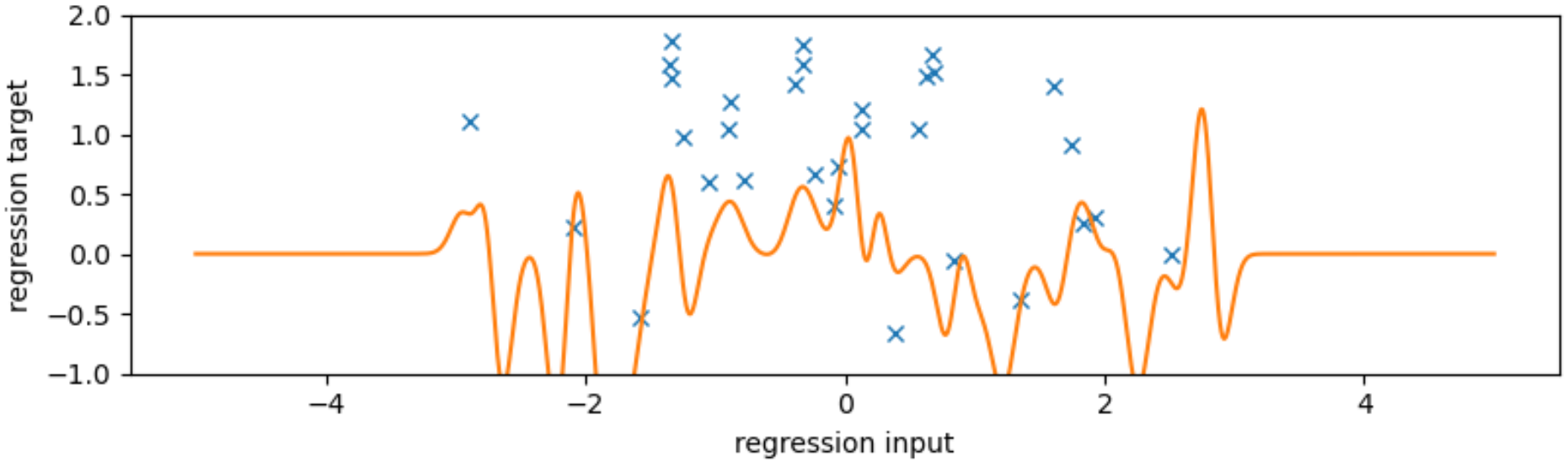
🎯 **Start by finding *clear* answers for single-layer NNs.**

1. **What is wrong with minimising losses?**
2. Bayesian Model Selection
2. Model Selection over Model Size? Or Nonparametrics?
3. A principle for selecting size

Training Loss / MaxLik is not sufficient

If we train weights W only, *given* (θ, M) by

$$f^* = \operatorname*{argmin}_W \ \text{const} + \sum_n (f(x_n) - y_n))^2$$



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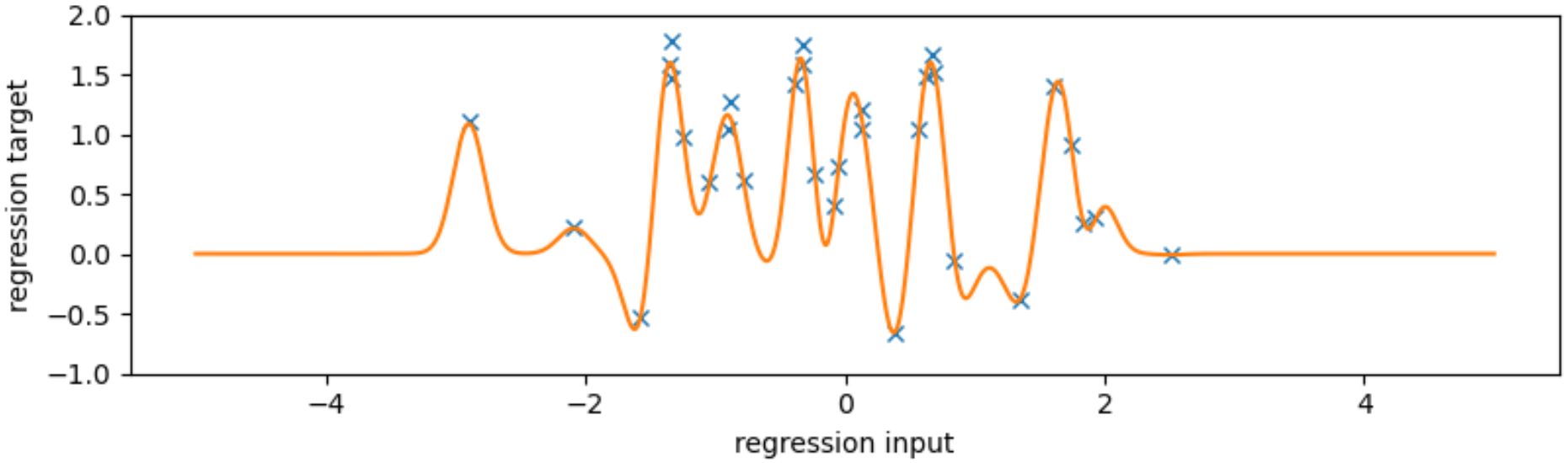

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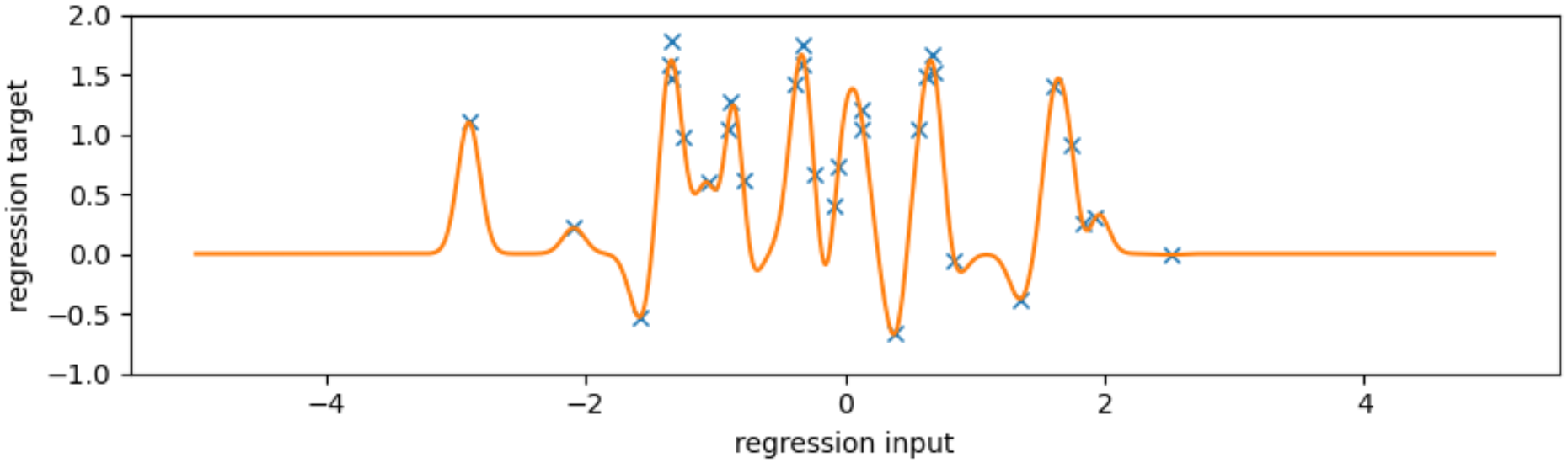

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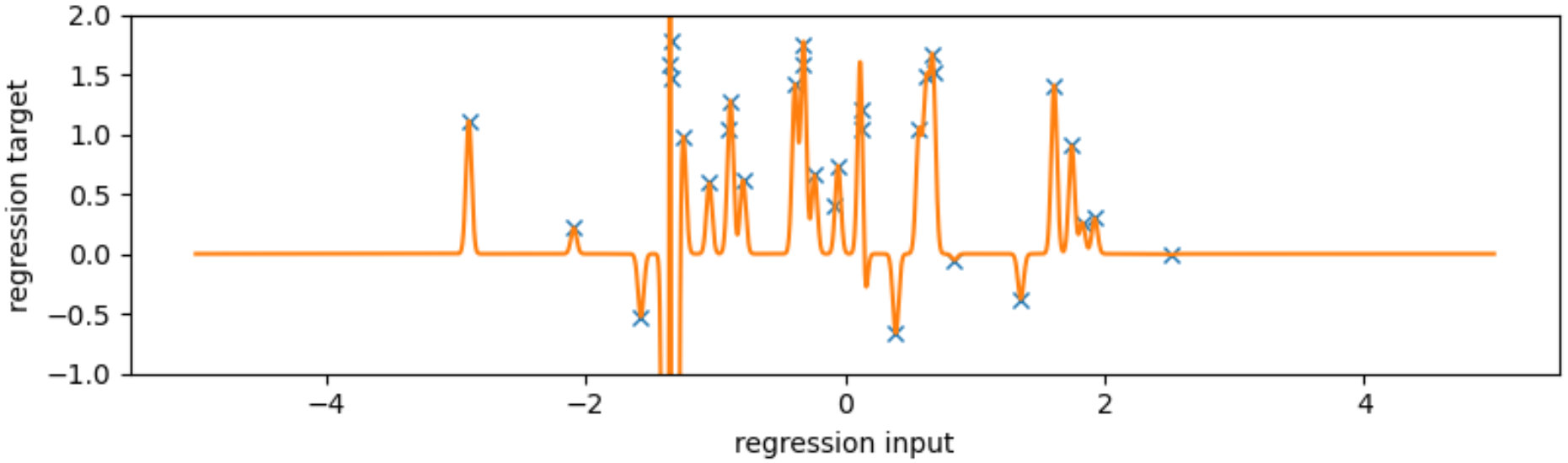

- Restricting model size never improves loss $\Rightarrow M \to N$
- Narrower basis functions to allow more flexible functions
- "Overfitting"

1. What is wrong with minimising losses.
2. **Bayesian Model Selection?**
2. The Bayesian answer to model size: Nonparametrics.
3. A principle for selecting size

The Bayesian Answer

Let's accept the "large" number of basis functions for now, and solve the overfitting problem.

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

$$p(\mathcal{D}|\theta) = \int p(\mathcal{D}|W, \theta)p(W|\theta)\,\mathrm{d}W$$

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Bayesian computations are often intractable. $\Rightarrow$ Approximating $p(\mathcal{D}|\theta)$ is hard enough, let alone for many different values of θ!

$$\theta^* = \operatorname*{argmin}_{\theta} \log p(\mathcal{D} \mid \theta)$$

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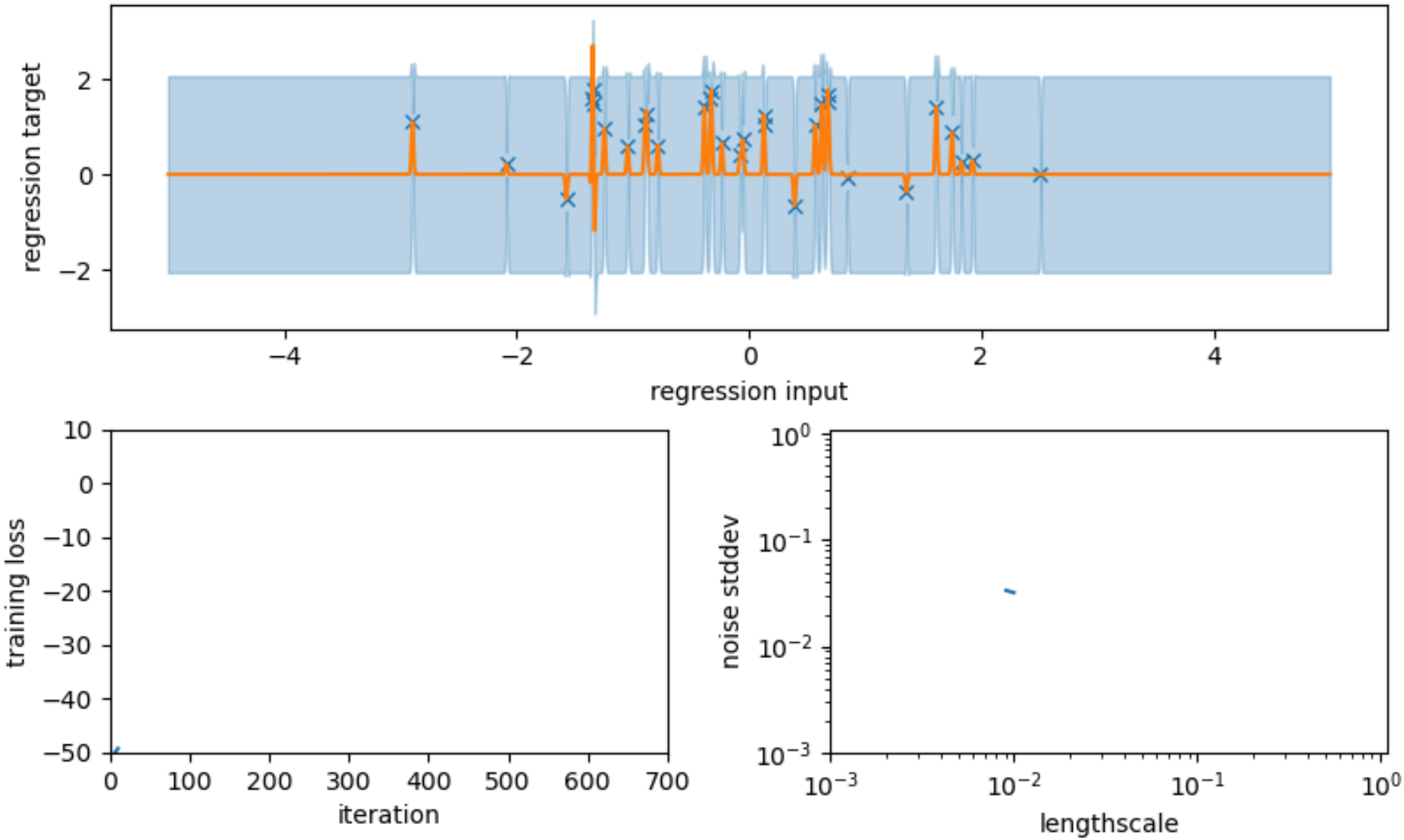
The Pragmatic Bayesian Answer



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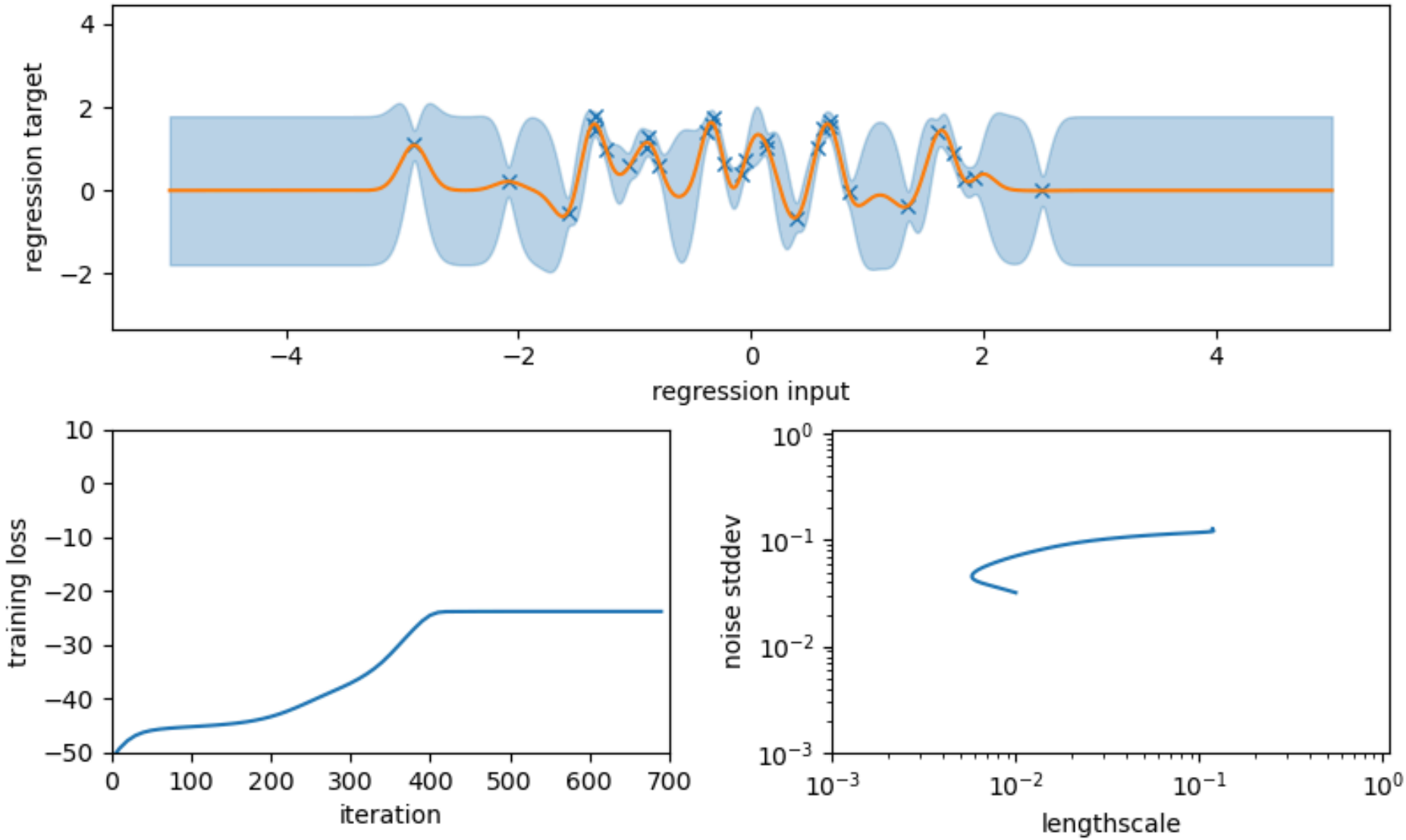

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- You may have noticed this was a Gaussian process.
- Interestingly, form of predictor is still single-layer NN:

$$f(x) = \sum_{m=0}^{N} \varphi(x;\theta,Z_m)w_m$$

$$\varphi(x;\theta,Z_m) = k_\theta(x,X_m) \qquad\qquad \boldsymbol{w} = \left(K(X,X) + \sigma^2 I\right)^{-1}\boldsymbol{y}$$

Where are we in our goals?

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- The size of the model M

  Number of neurons. 🤨

Where are we in our goals?

Predictor is a *single layer* neural network:

$$f(x) = \sum_{m=1}^{M} \varphi(x; Z_m, \theta) w_m$$

Goal is to find:

- Hyperparameters θ

  Inductive bias. ✅
- Parameters ("weights") $W = \{w_m, Z_m\}_{m=1}^{M}$

  Control the function. ✅
- The size of the model M

  Number of neurons. 😒

⚠ **Our model grows, but by memorising *all* data!**

1. What is wrong with minimising losses.
2. Bayesian Model Selection?
2. **The Bayesian answer to model size: Nonparametrics.**
3. A principle for selecting size

Why use Nonparametric models?

We stumbled into using "large" models, but *why* do we use nonparametric models?

Classic arguments:

1.
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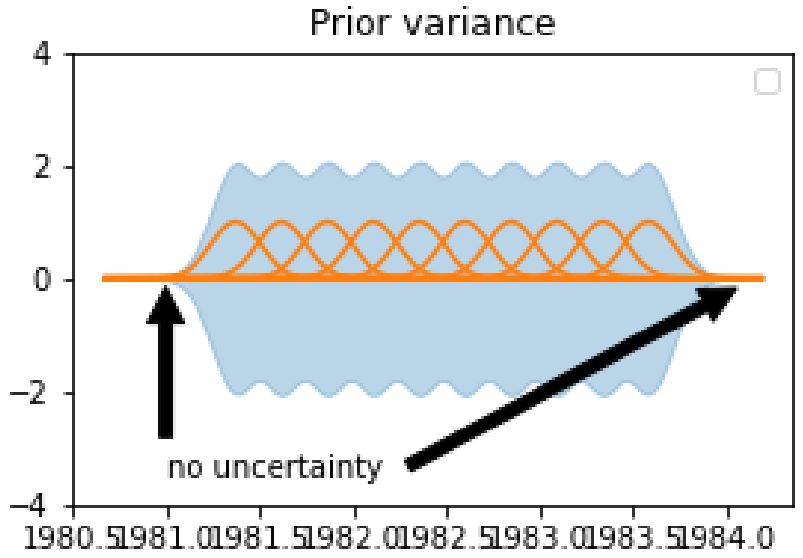

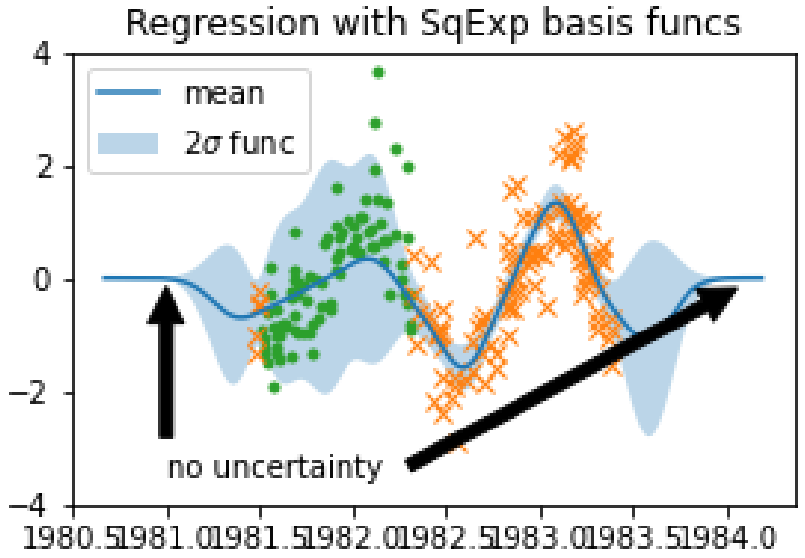

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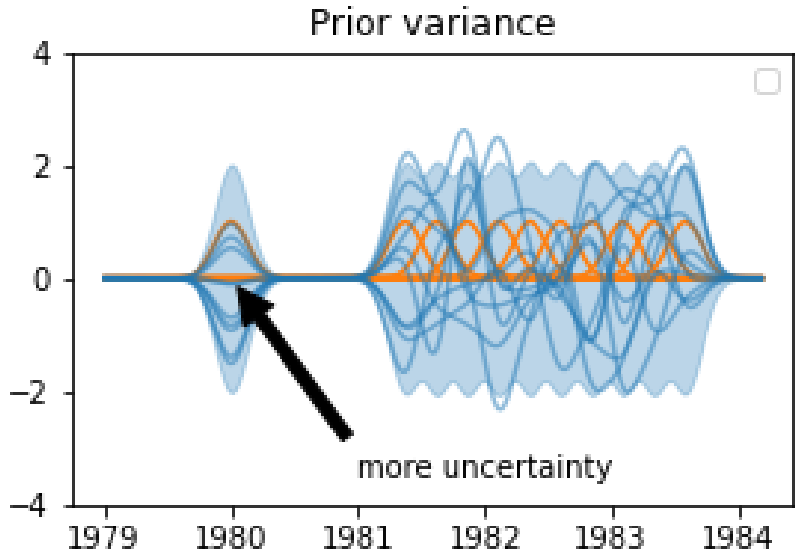

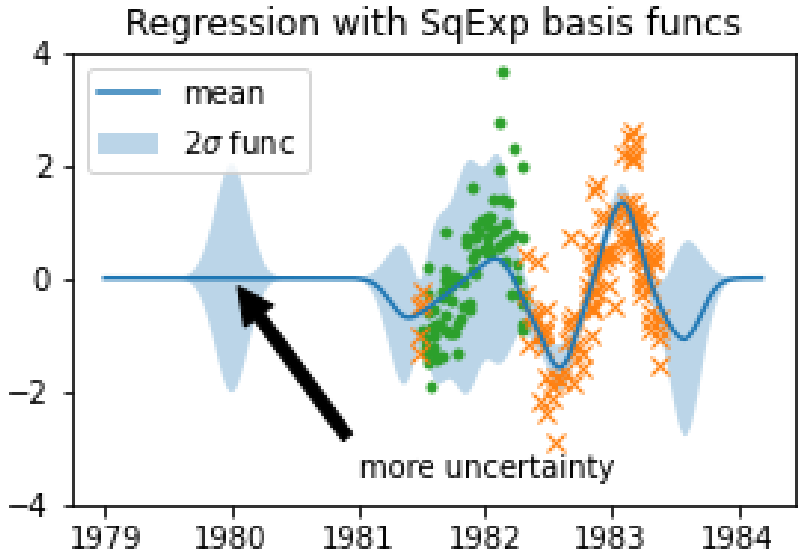

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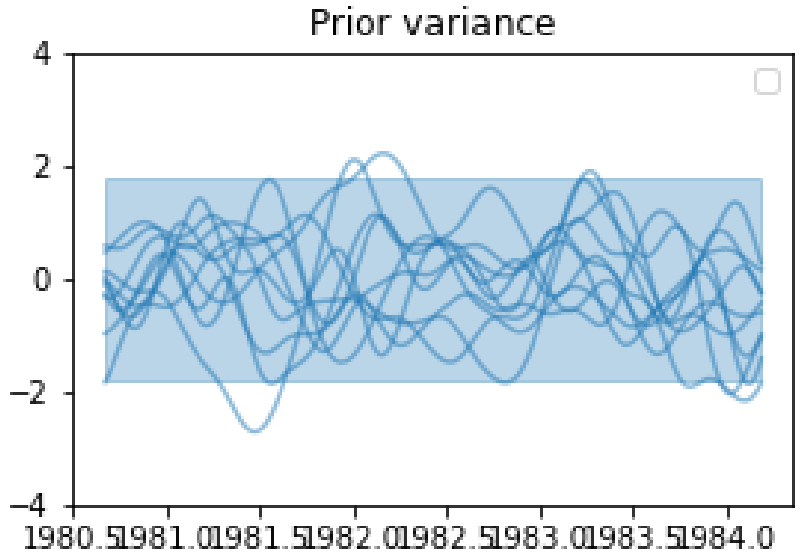

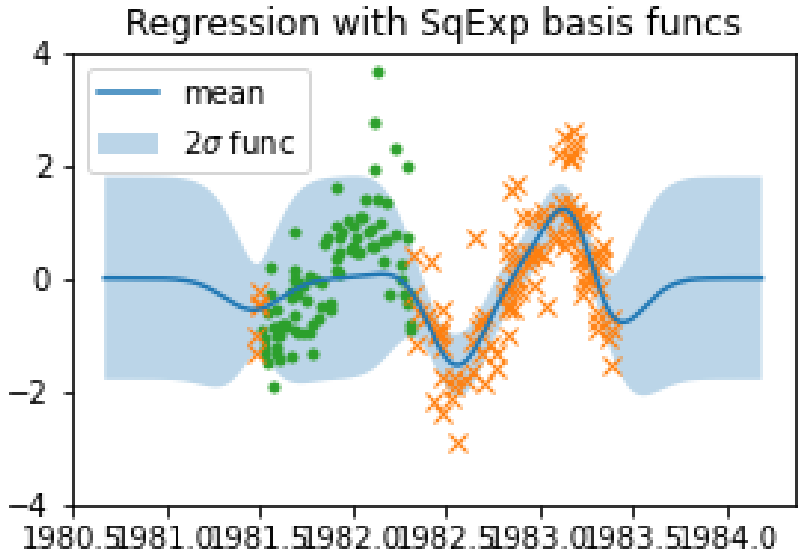

Can Bayes answer the Size Question?

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We could do model selection over the model size...

$$p(W, \theta, M|\mathcal{D}) = \frac{p(\mathcal{D}|W, \theta, M)p(W|\theta, M)}{p(\mathcal{D}|\theta, M)} \frac{p(\mathcal{D}|\theta, M)p(\theta)}{p(\mathcal{D})}$$

$$\theta^*, M^* = \operatorname*{argmax}_{\theta, M} \log p(\mathcal{D}|\theta, M)$$

Bayesian Model Selection of Model Size is BAD

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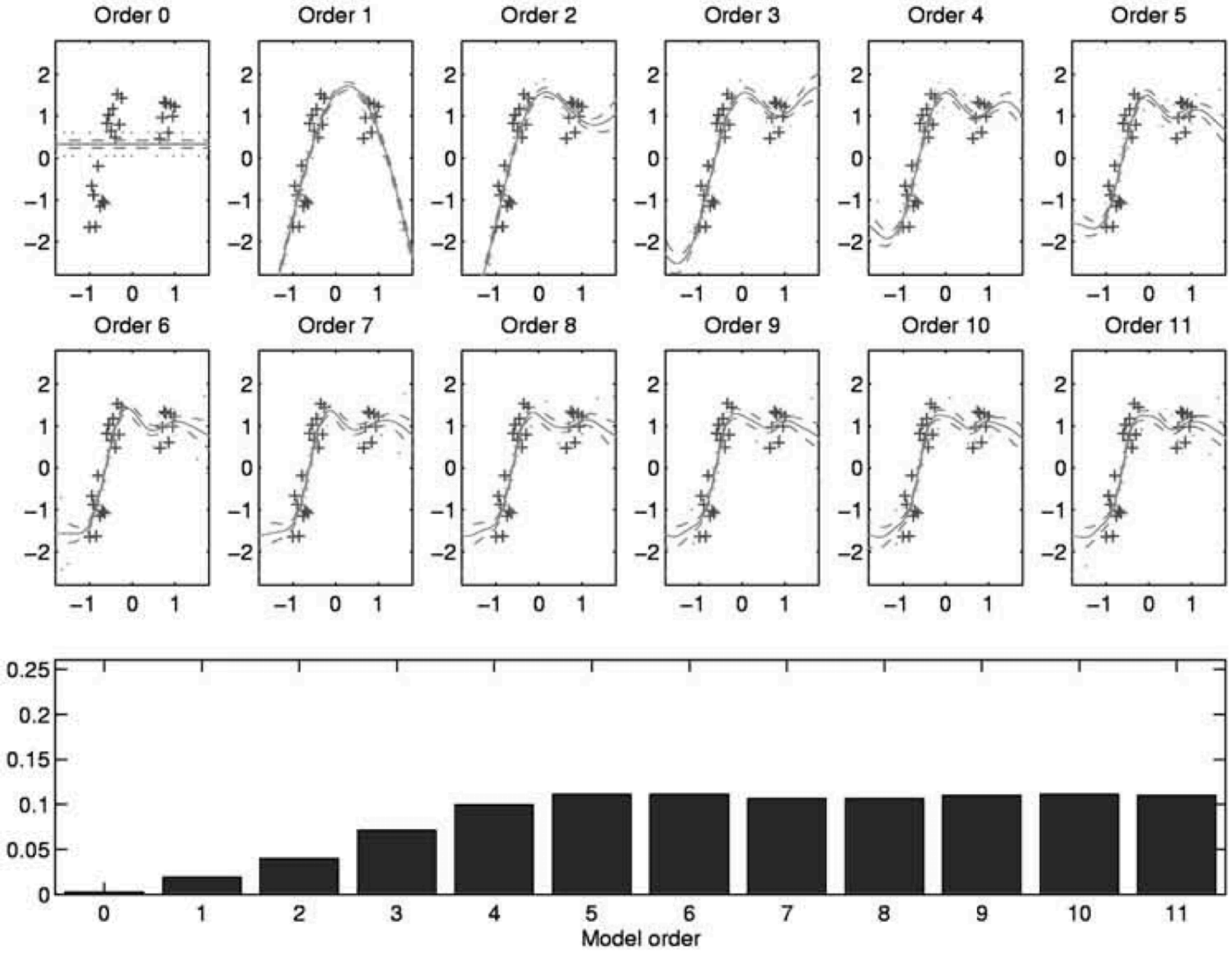
See *Occam's Razor* (Rasmussen & Ghahramani, 2000). One of my favourite papers.


Order 0
Order 1
Order 2
Order 3
Order 4
Order 5
Order 6
Order 7
Order 8
Order 9
Order 10
Order 11
0.25
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7 8 9 10 11
Model order

Bayes selects a nonparametric model!

- Bayes itself is pushing us to use “large” nonparametric models!
- Cannot rely on Bayes to choose a “small” model!

1. What is wrong with minimising losses?
2. Bayesian Model Selection
2. Model Selection over Model Size? Or Nonparametrics?
3. **A Principle for Selecting Model Size**

**What principle can determine a compressed model size,
without removing the benefits of nonparametrics?**

What principle can determine a compressed model size, without removing the benefits of nonparametrics?

Define a nonparametric model, then approximate it with M < N basis funcs.

Approximate GPs (Hensman et al., 2013; Titsias, 2009)

Step 1: Introduce family of approximate predictors

$$q(f(x)) = \mathcal{N}\left(f(x); \sum_{m=1}^{M} \varphi(x; Z_m, \theta) w_m, \ldots \right)$$

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ELBO is a *unified objective* for all our questions!

- Optimising w.r.t. $\boldsymbol{w}, Z$: finds weights (min KL)
- Optimising w.r.t. θ: finds hyperparameters (max $\log p(\mathcal{D}|\theta)$)
- Select M large enough, that more gives diminishing returns!

When Should we Stop Adding Basis Functions?

More basis functions is always better:

$$\mathrm{KL}[q_{M+1}(f) \parallel p(f|\mathcal{D},\theta)] \leq \mathrm{KL}[q_M(f) \parallel p(f|\mathcal{D},\theta)]$$

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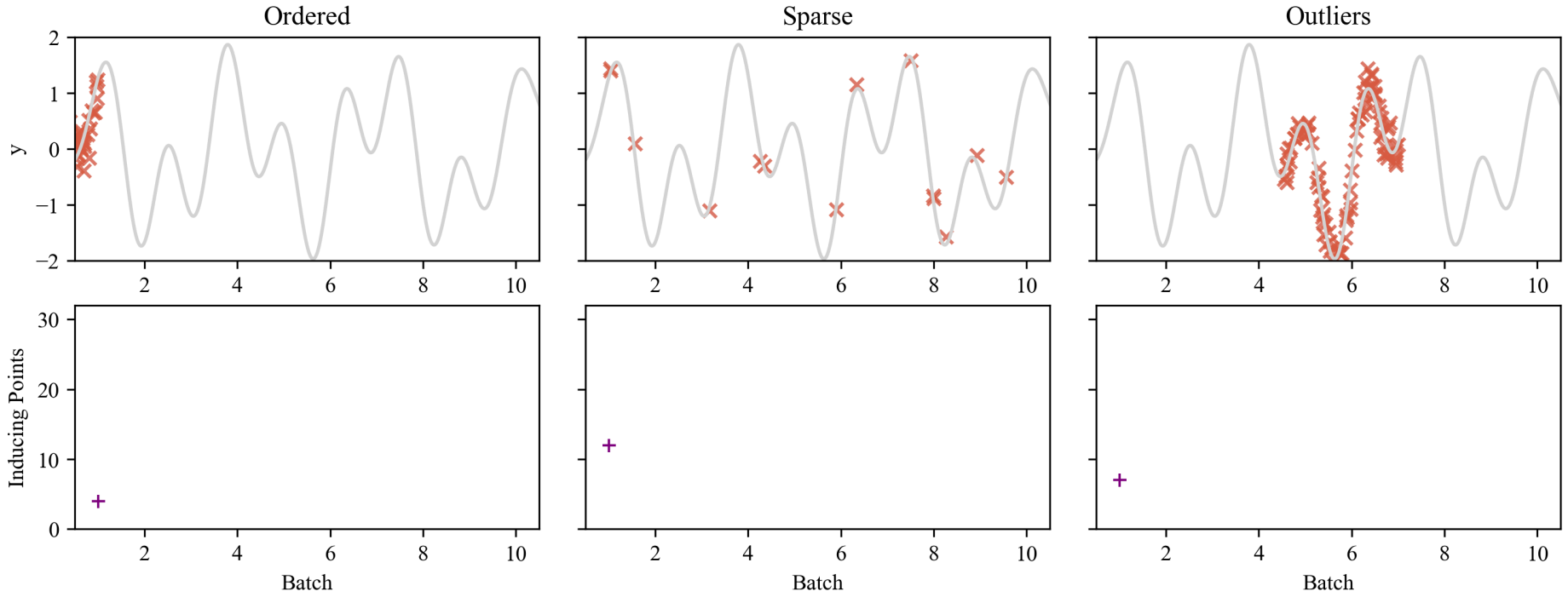
Simple Rule, Interesting Adaptive Behaviour!

Continual Learning (Pescador-Barrios et al., 2024; 2025)



Growth of neurons depends on *novelty* in data.

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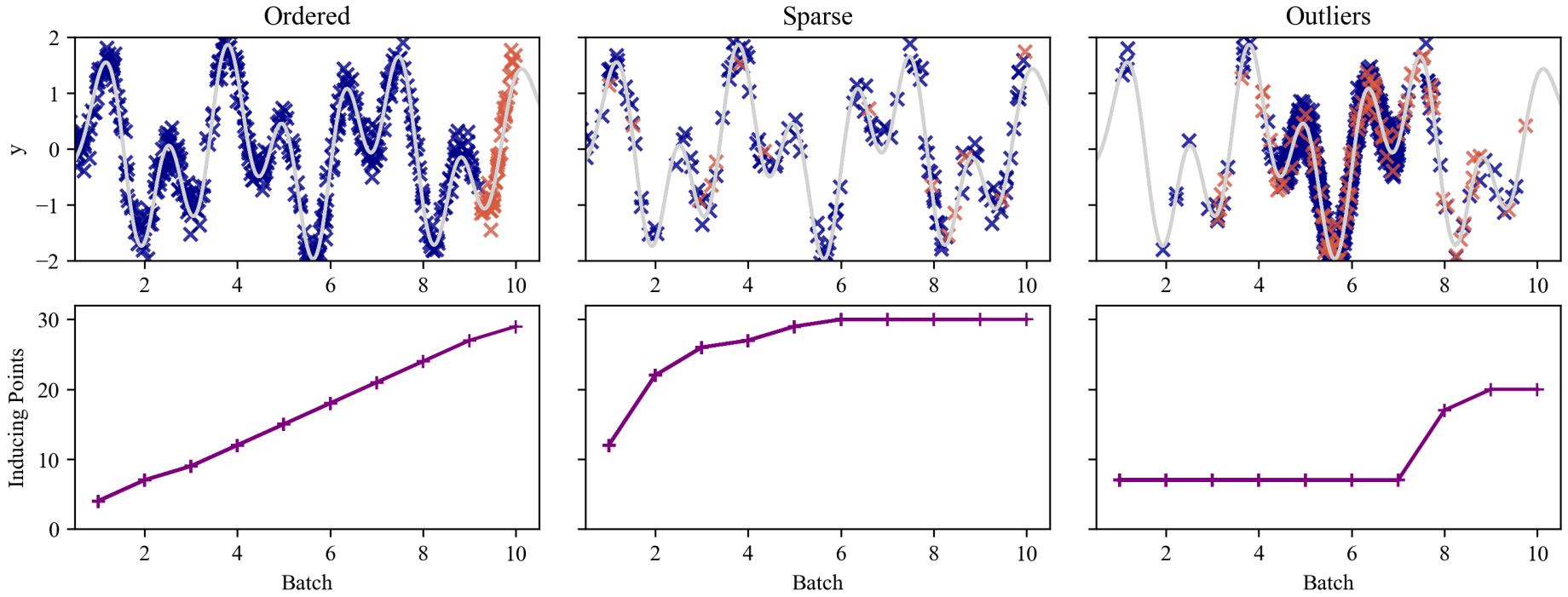

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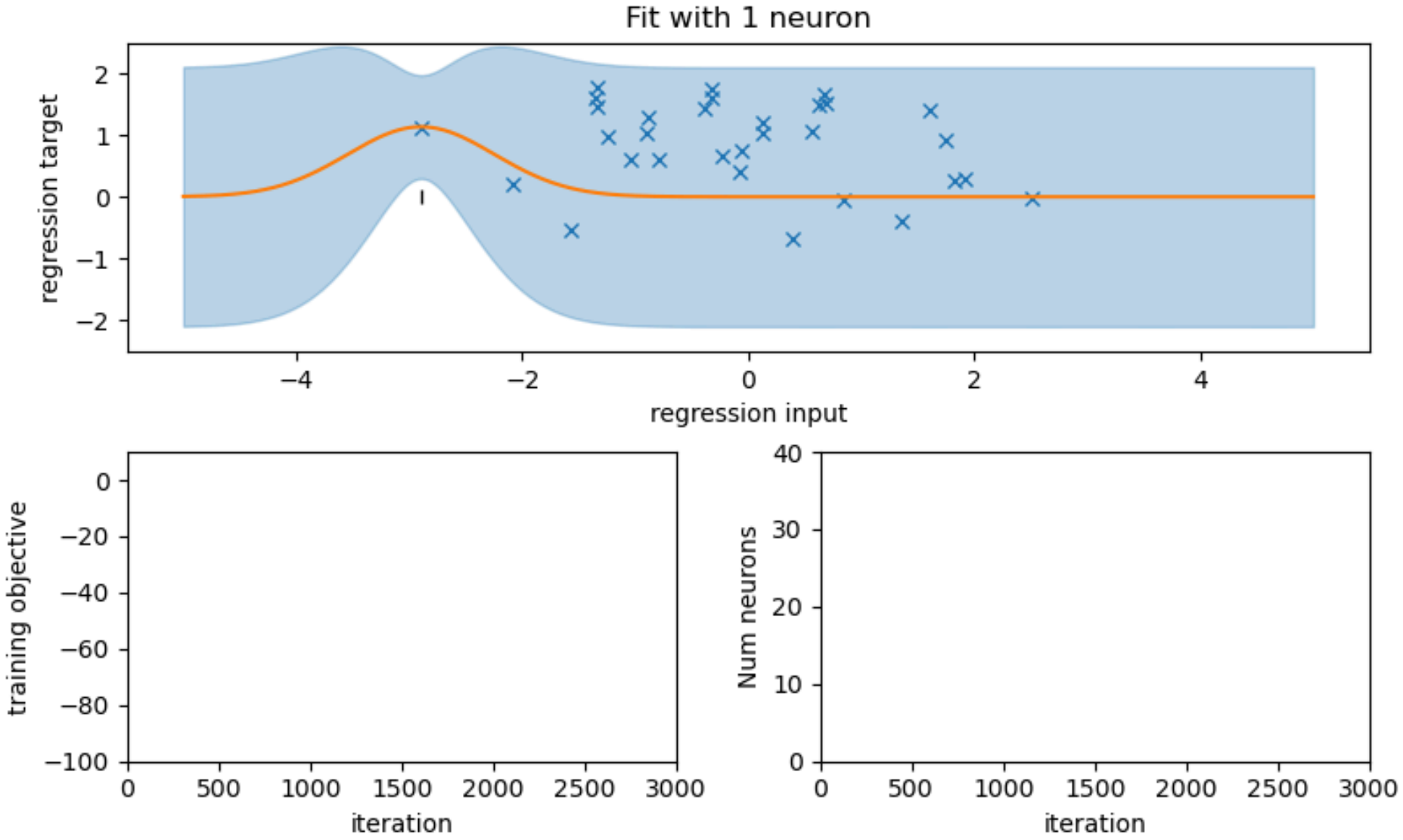

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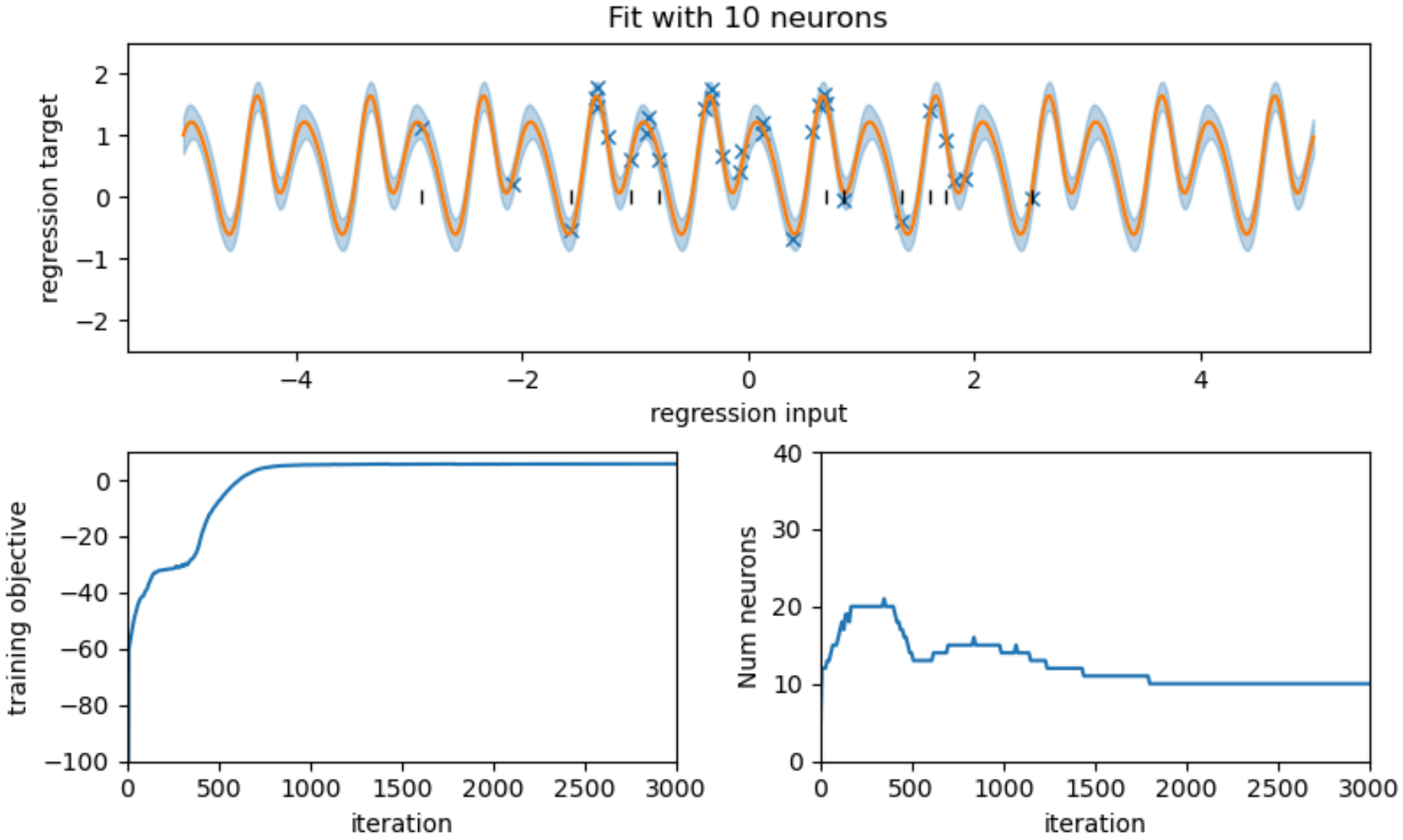
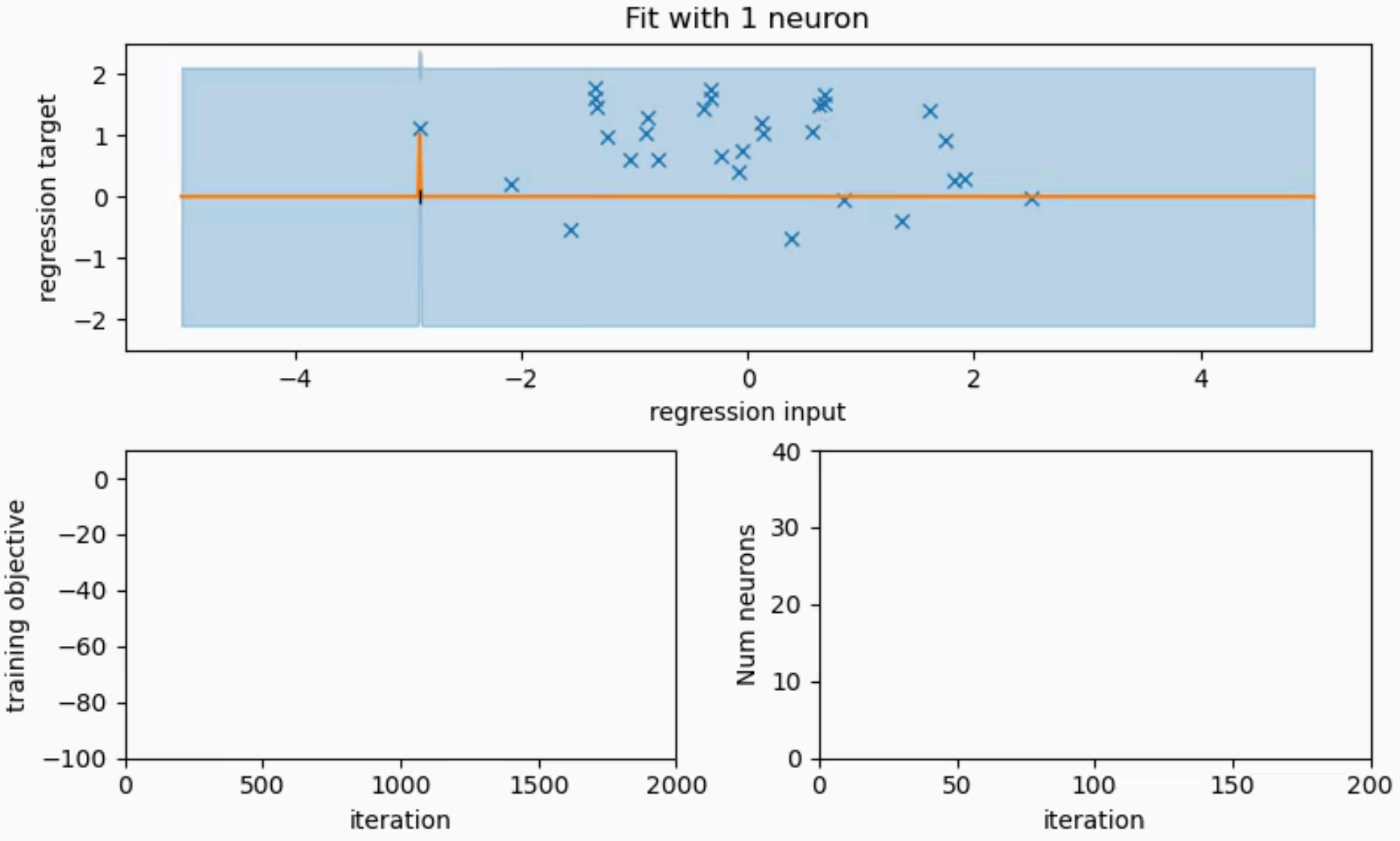


Memorising first, then pruning



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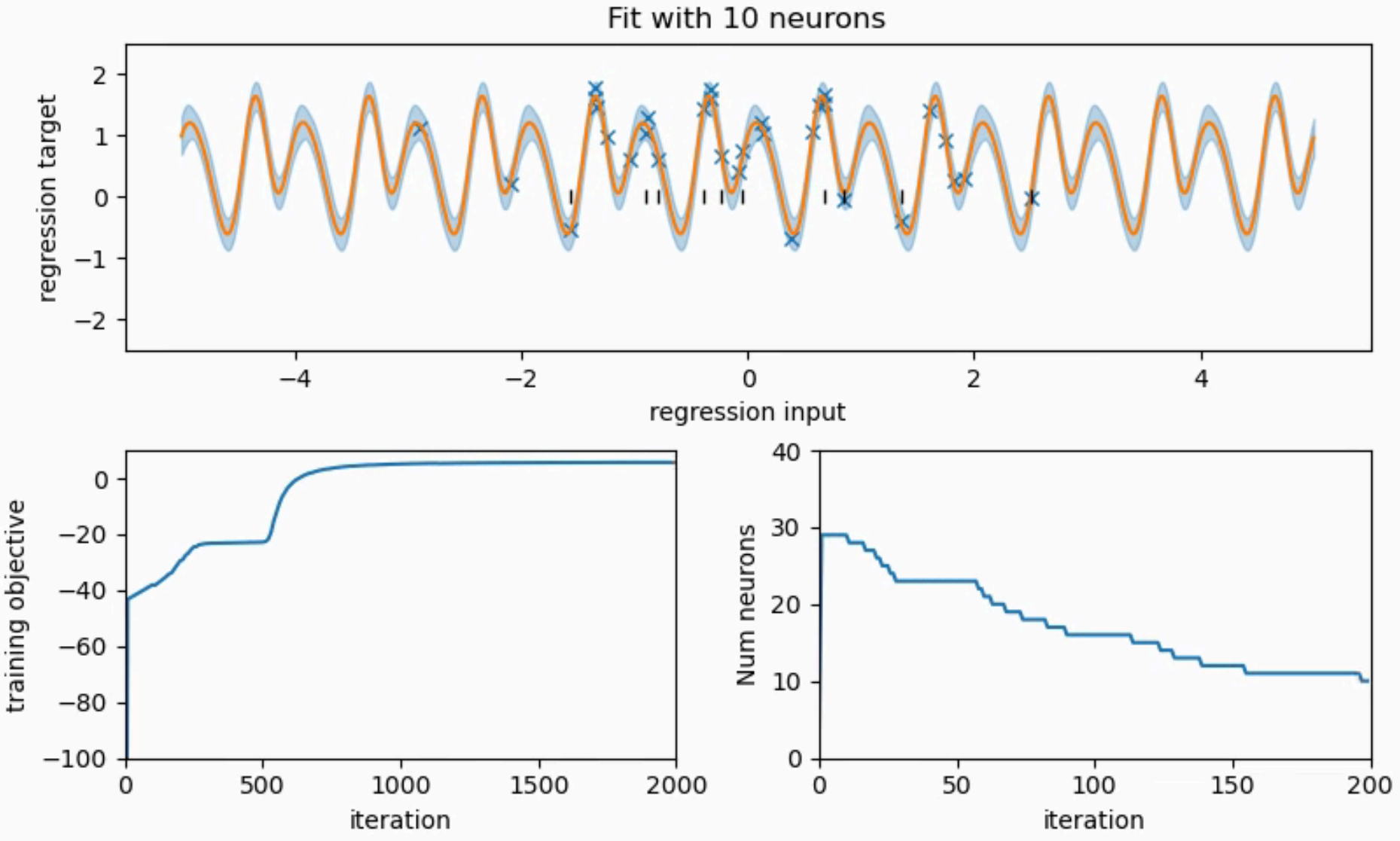

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We can have our cake and eat it

We can *define* an infinite-sized model, but near-perfectly approximate it with *just* the right amount of computational resources!

Designing a Neural Network Training Procedure

🎯 **New procedures for training neural networks!**

Can we automatically find:

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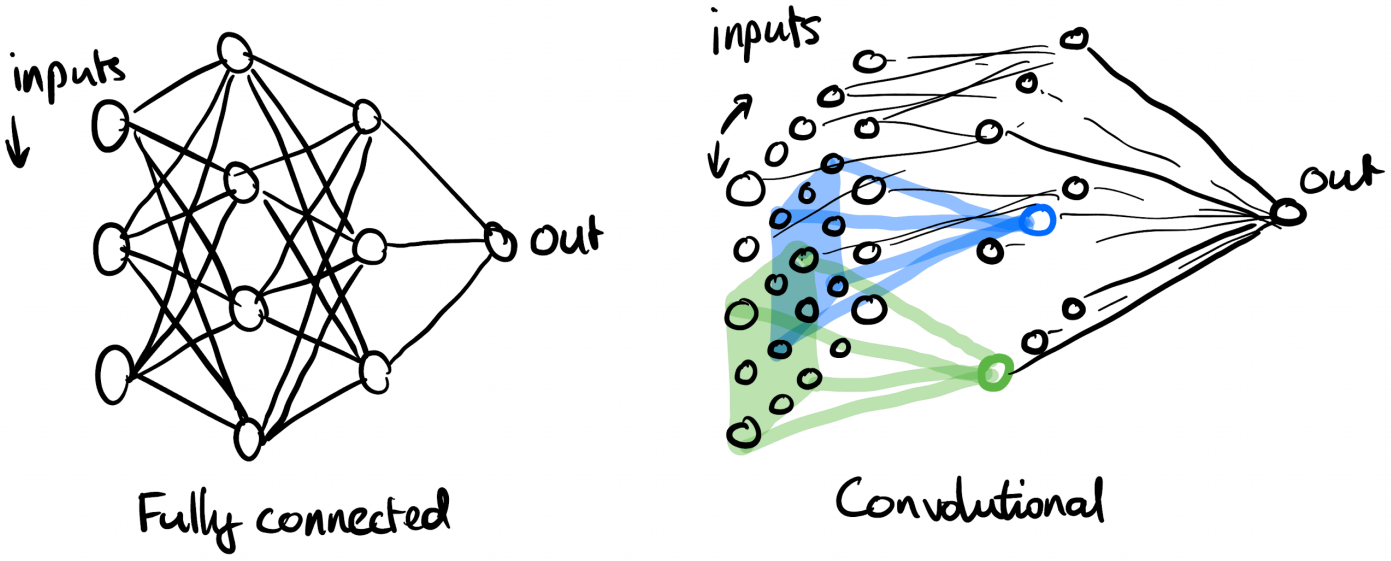

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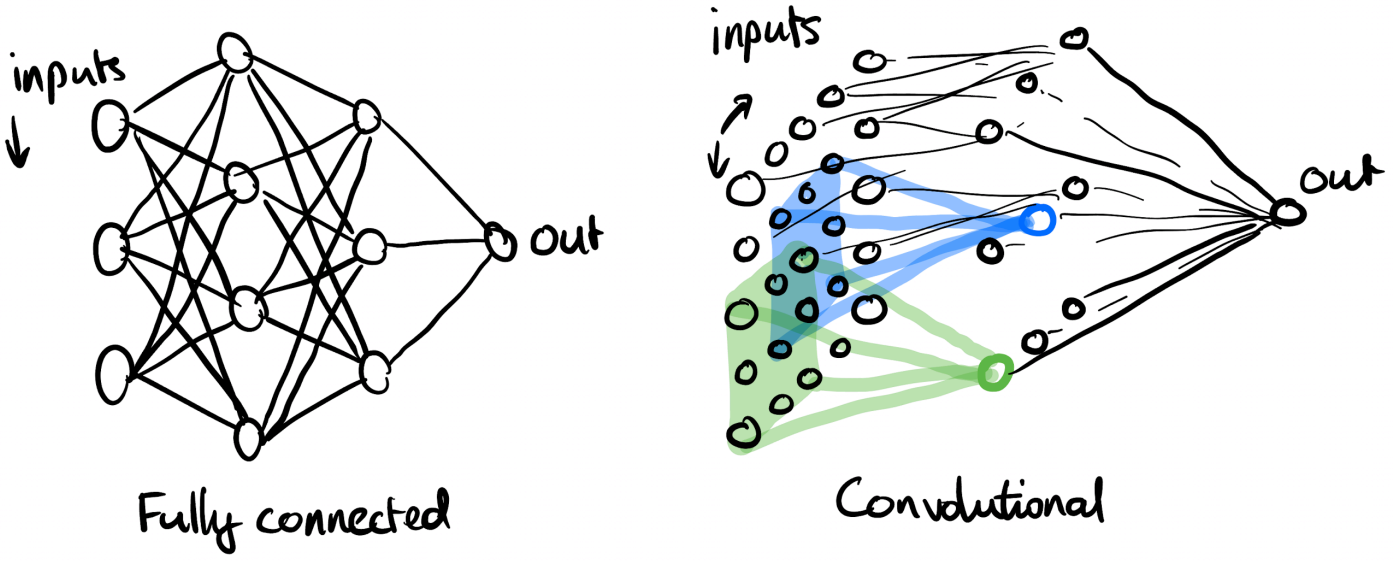

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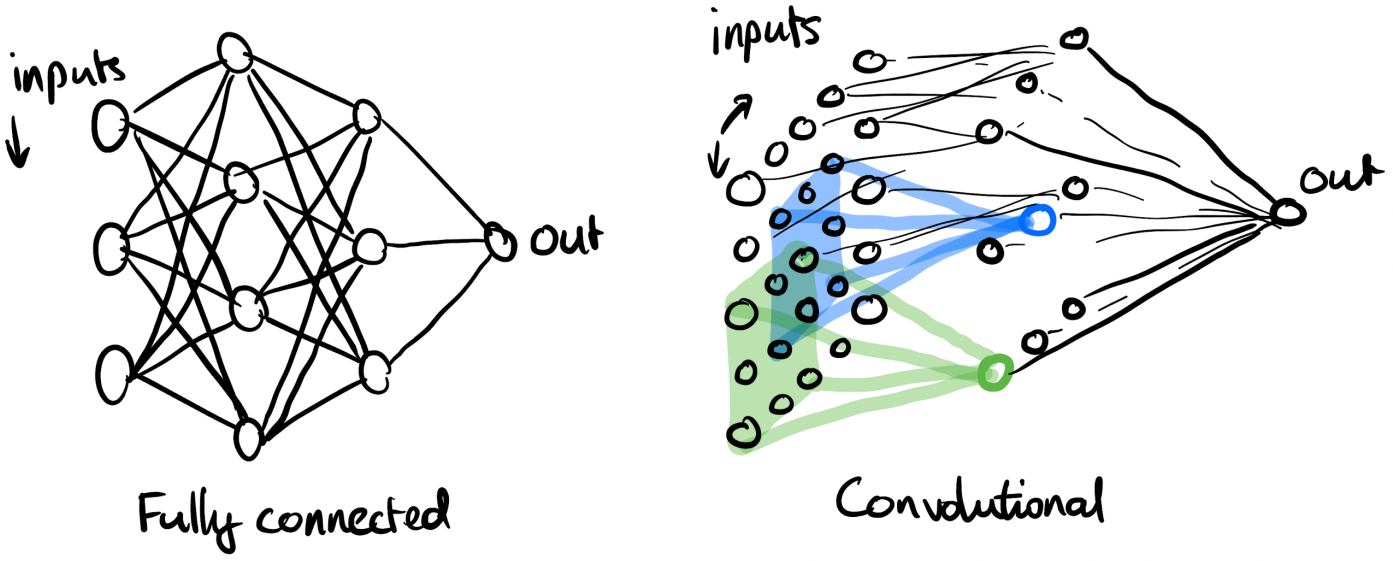

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💡 **More efficient, more adaptive, more automatic!**

Coauthors

From Imperial College London

Guiomar
Pescador-Barrios
PhD candidate

Tycho
van der Ouderaa
PhD candidate

Prof Sarah
Filippi
Co-supervisor

Based on a True Story

Adjusting Model Size in Continual Gaussian Processes: How Big is Big Enough?

Guiomar Pescador-Barrios [1] **Sarah Filippi** [1] **Mark van der Wilk** [2]

Spotlight at ICML 2025.

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A Bayesian Nonparametric View on Adapting Neuron Count During Training

In submission, soon to be on arxiv.

Papers

Gaussian processes:

- For an overview of Titsias/Hensman's (Hensman et al., 2013; Titsias, 2009) method for VI in GPs, see my thesis (van der Wilk, 2019)
- Proof of accuracy of variational approximation (basis for when to stop adding inducing variables / basis functions) (Burt et al., 2019; 2020)
- Adaptive model size for continual learning (Pescador-Barrios et al., 2024)
- Overall narrative of this talk (online soon!)

Bayesian Model Selection in Neural Networks:

- Bayesian Model Selection (Laplace approximation) *recovers* ResNets, without explicit human design (Ouderaa et al., 2023)
- See more by Tycho van der Ouderaa!

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