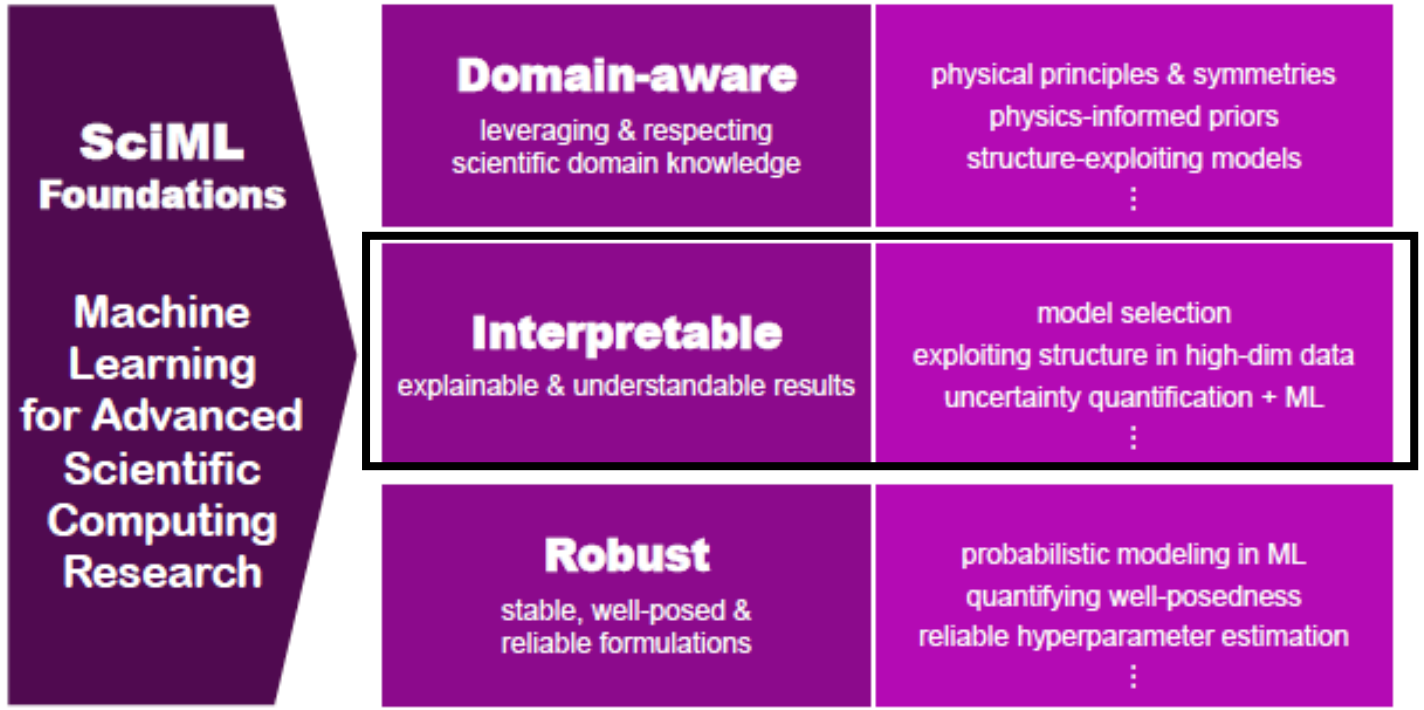
Uncertainty Quantification for Deep Learning

Focus

- *Uncertainty Quantification*: How to make my machine learning models say “I don’t know”?

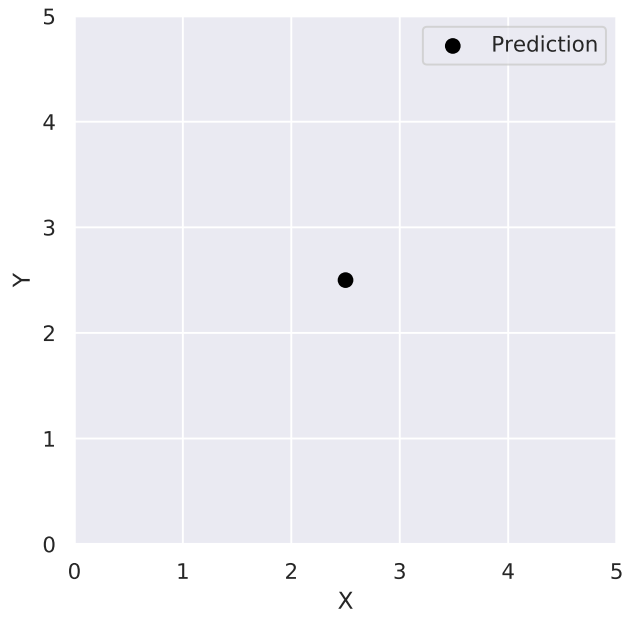
- *Interpretability*: In addition to telling me “What”, how can I make my machine learning models tell me “Why”?
  Answers & *Insight*.

My Research Focus



[1]Workshop report on Basic Research Needs for Scientific Machine Learning: Core technologies for artificial intelligence. USDOE Office of Science, (2019)

A Thought Experiment



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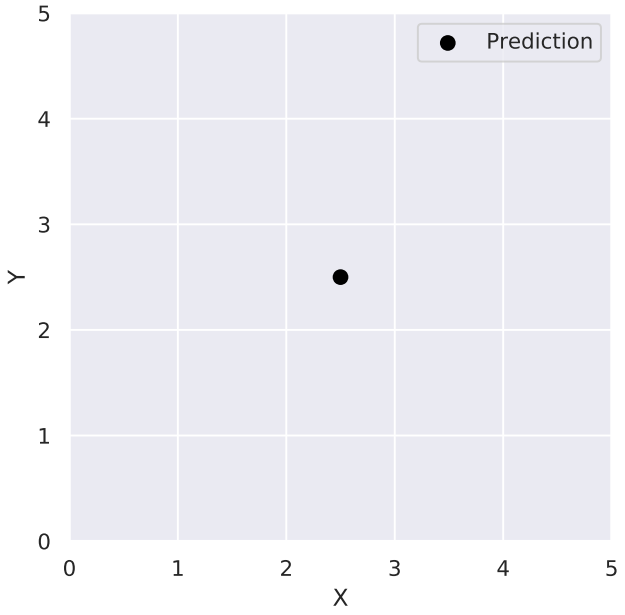

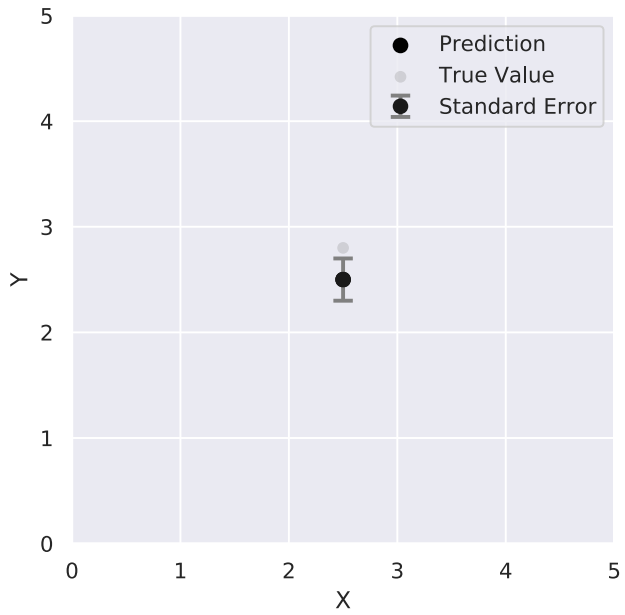

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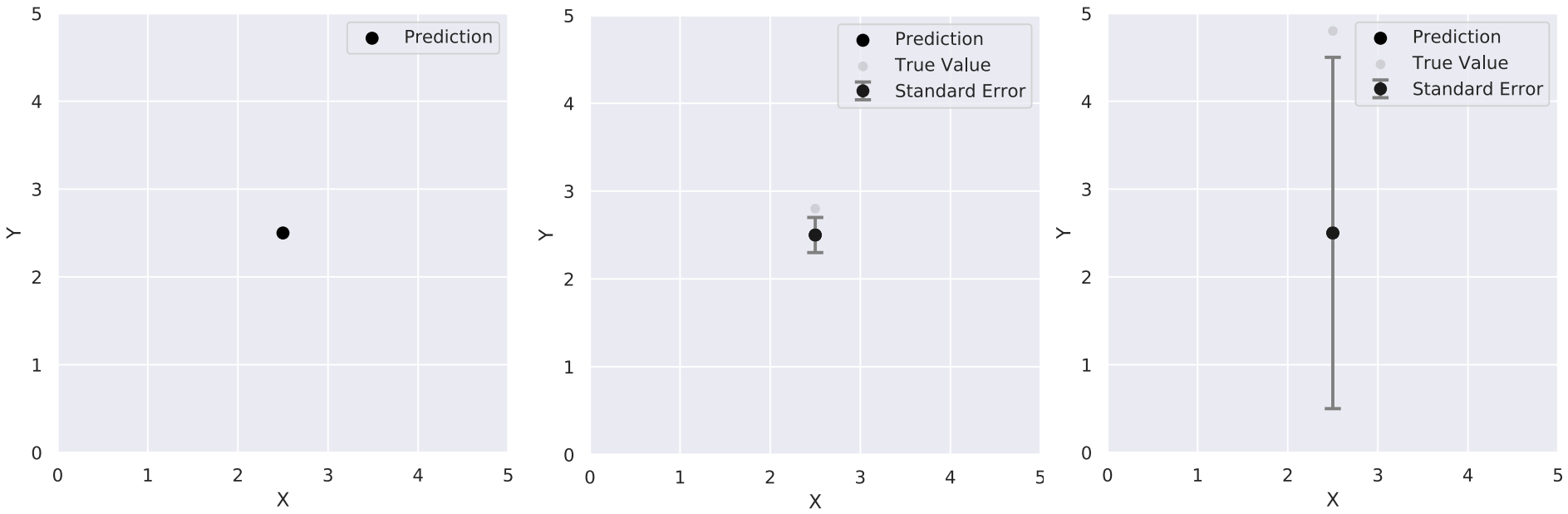

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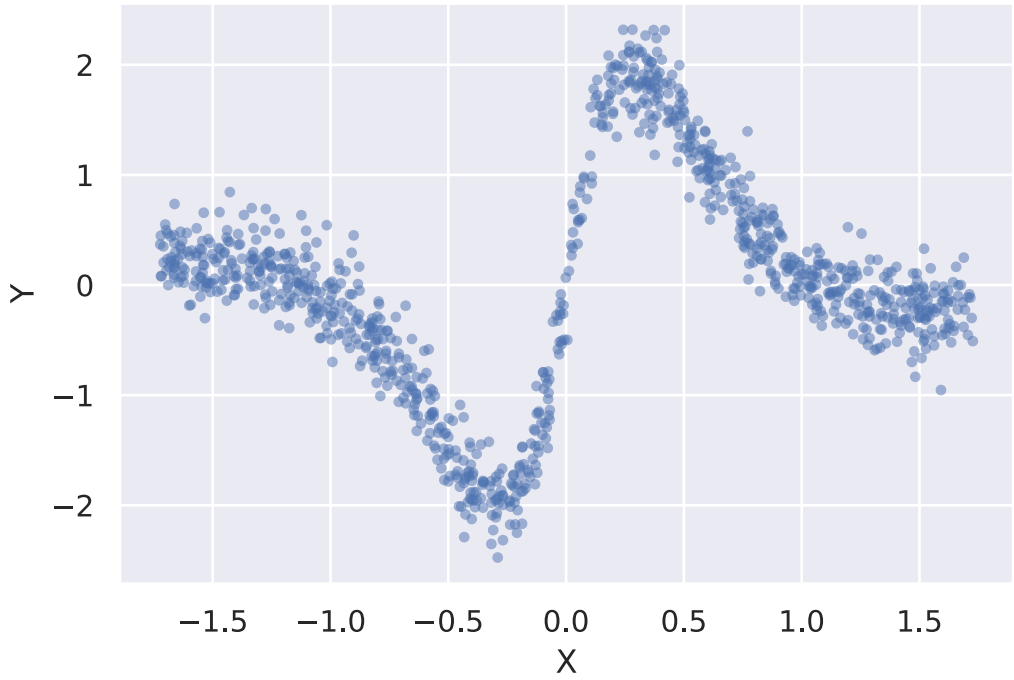
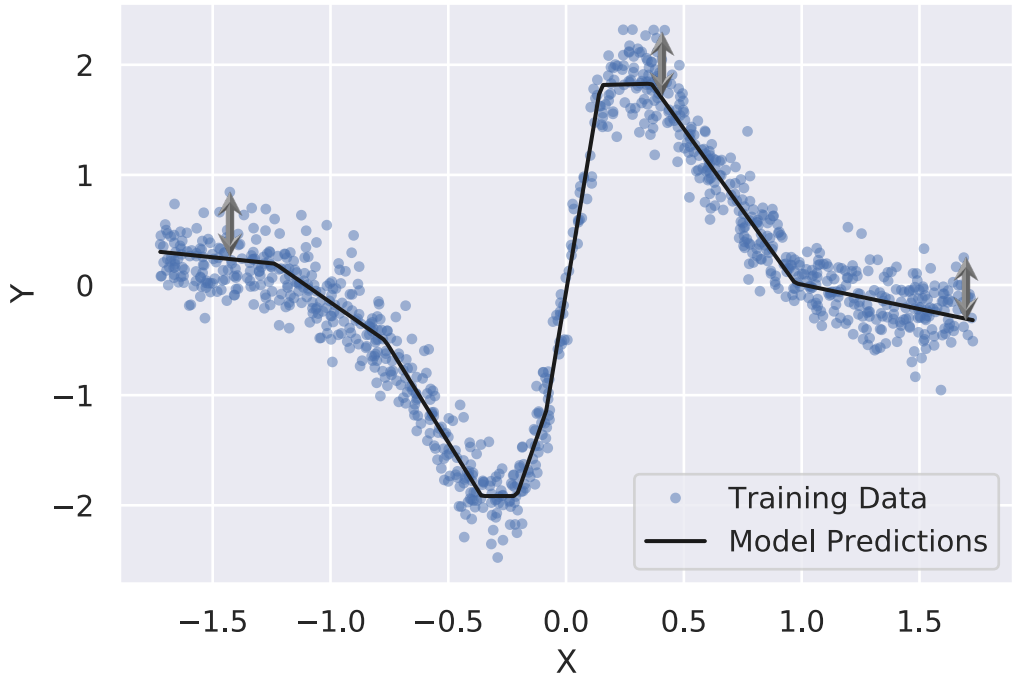


$$f(x) = \frac{\sin x}{1 + x^2} + \varepsilon$$

A Thought Experiment



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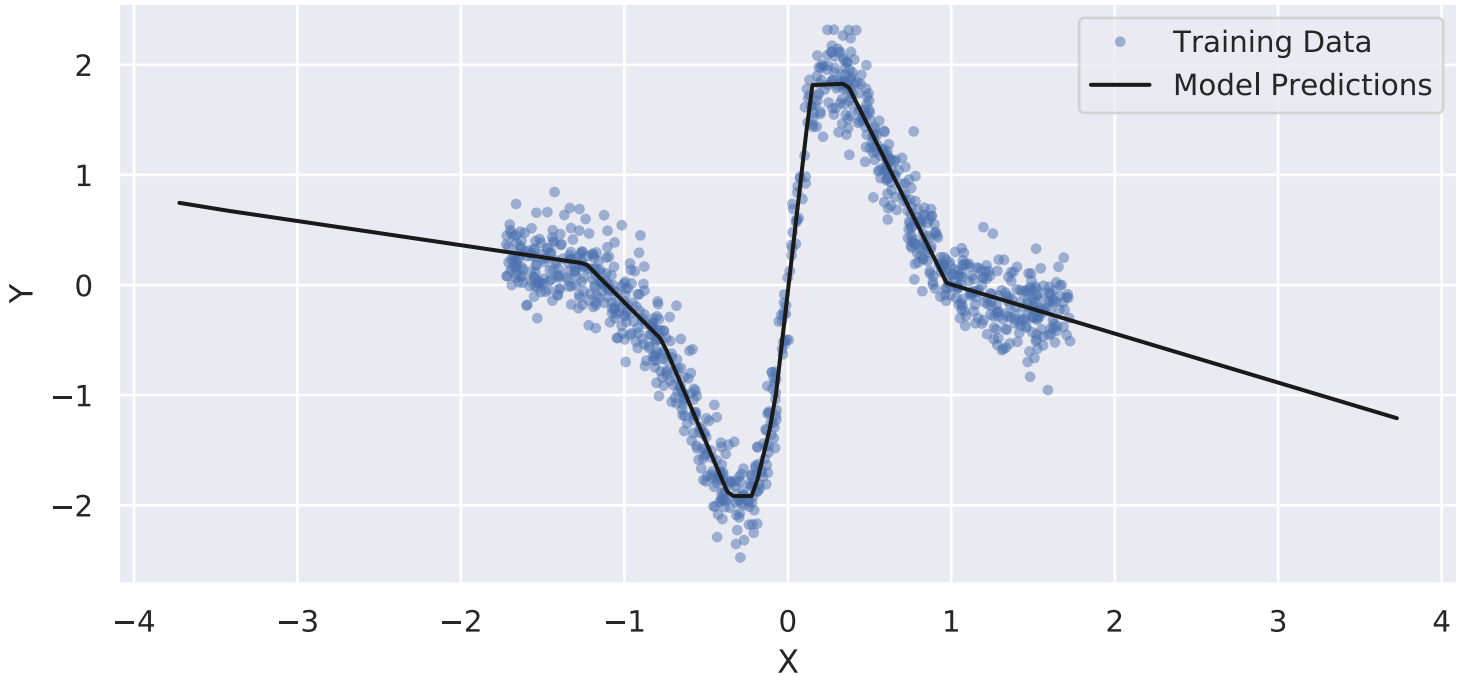

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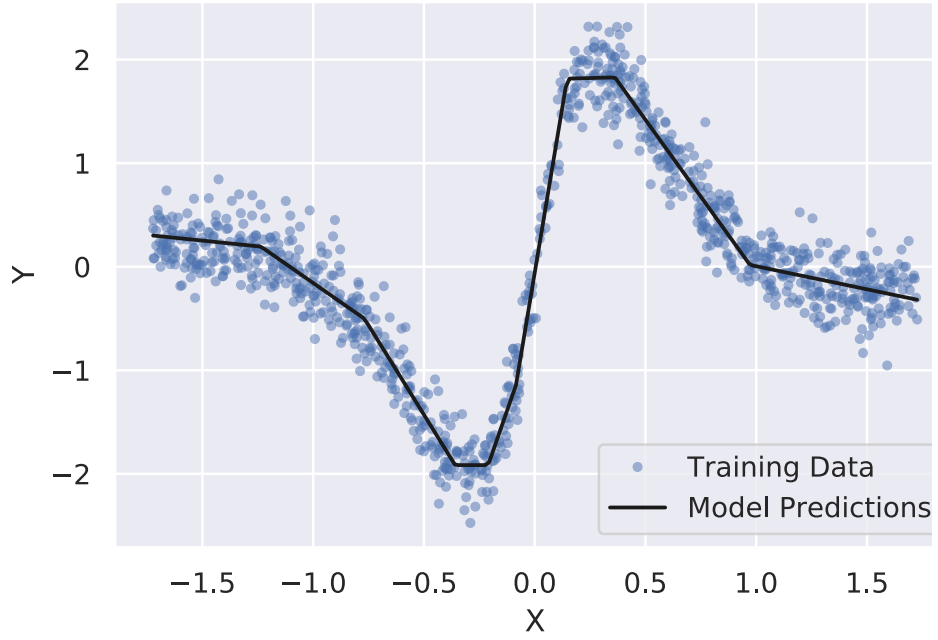

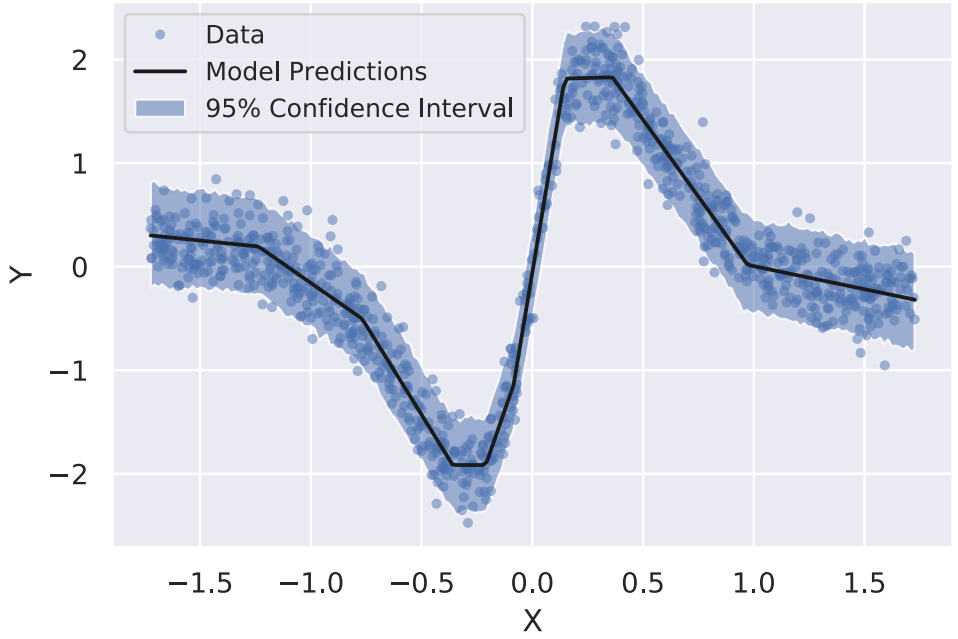

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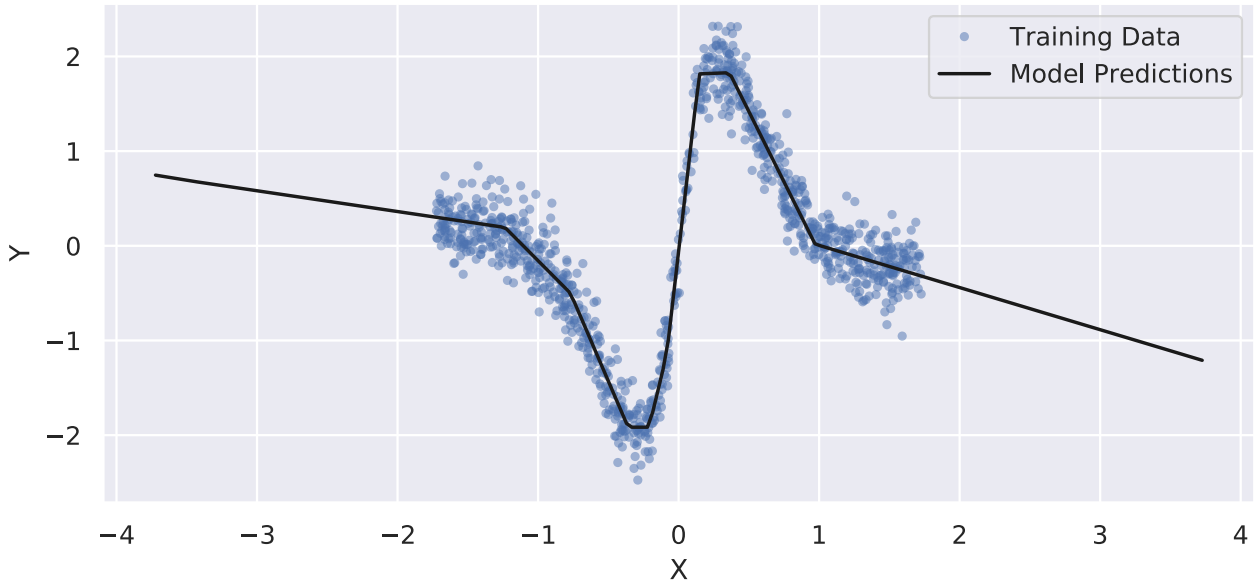
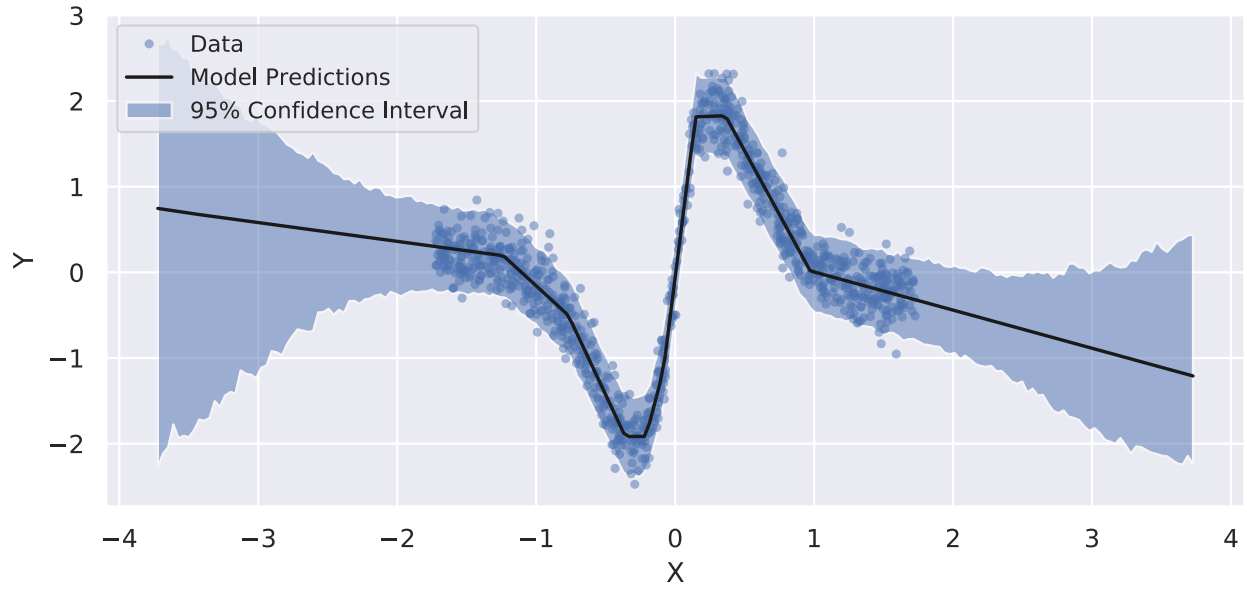




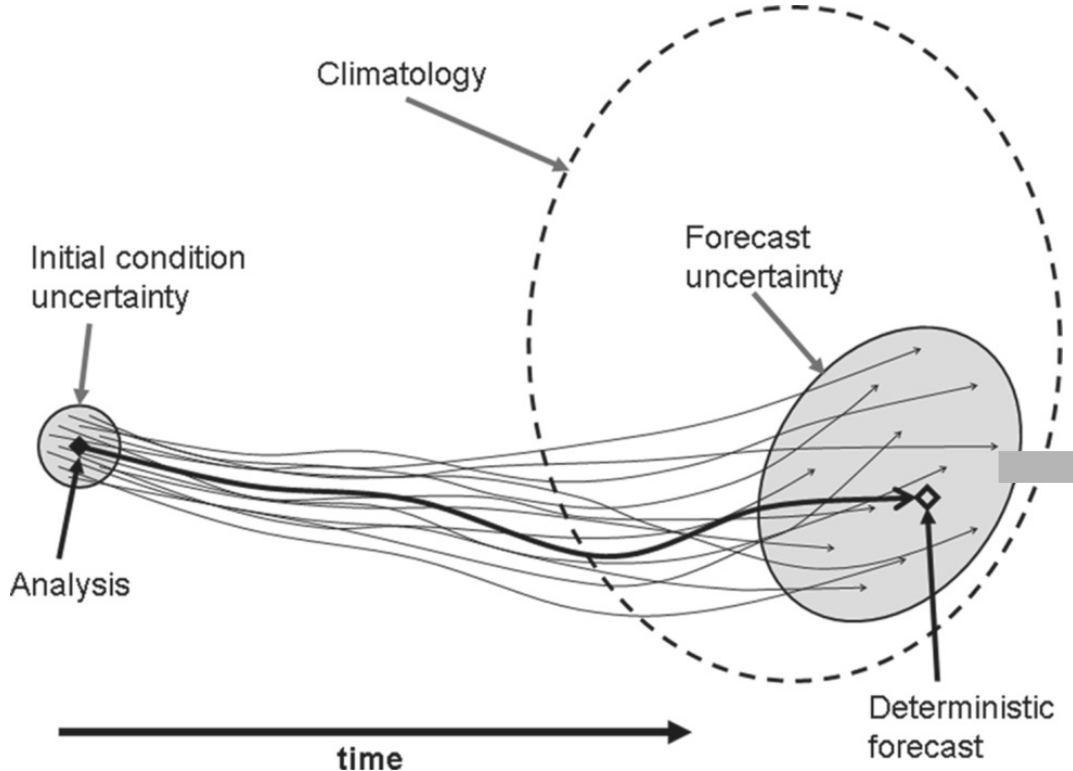
Uncertainty Quantification: Introduction

- Science of identifying, estimating and reducing errors & uncertainties and their propagation in models, algorithms, experiments and their predictions.

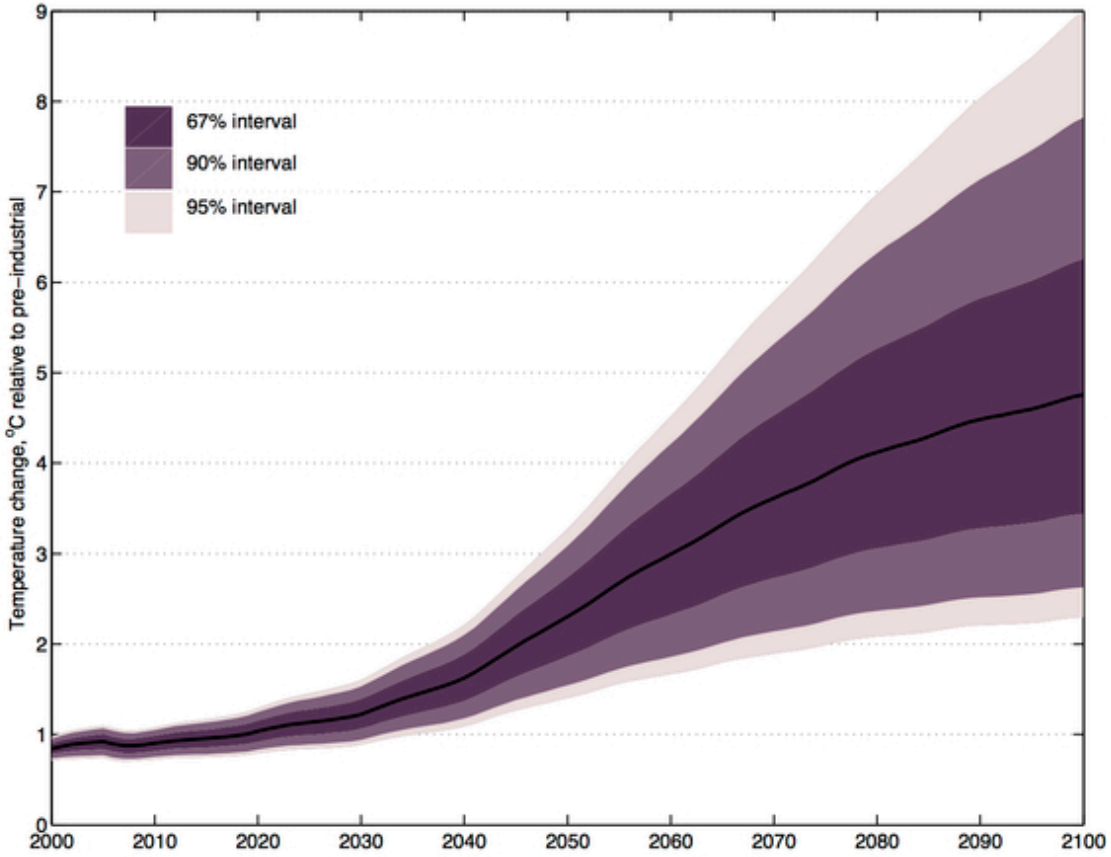
- How different uncertainties interact and affect the predictions,
  how they propagate in a model,
  How to make informed decisions under uncertainty?

UQ Illustration: Weather Forecasts

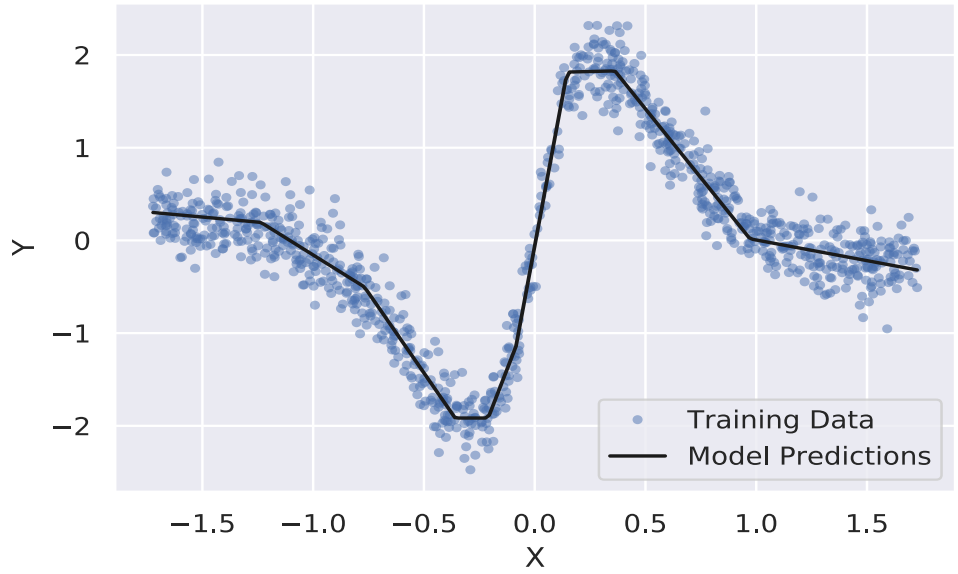
- Solar+Earth+Atmosphere+Ocean system.
- Aleatoric uncertainty: Location of weather balloons.
  Epistemic uncertainty: Limitations of model to represent radiation, convection, turbulent mixing.
- Numerical Weather Prediction- Ensemble forecasts.

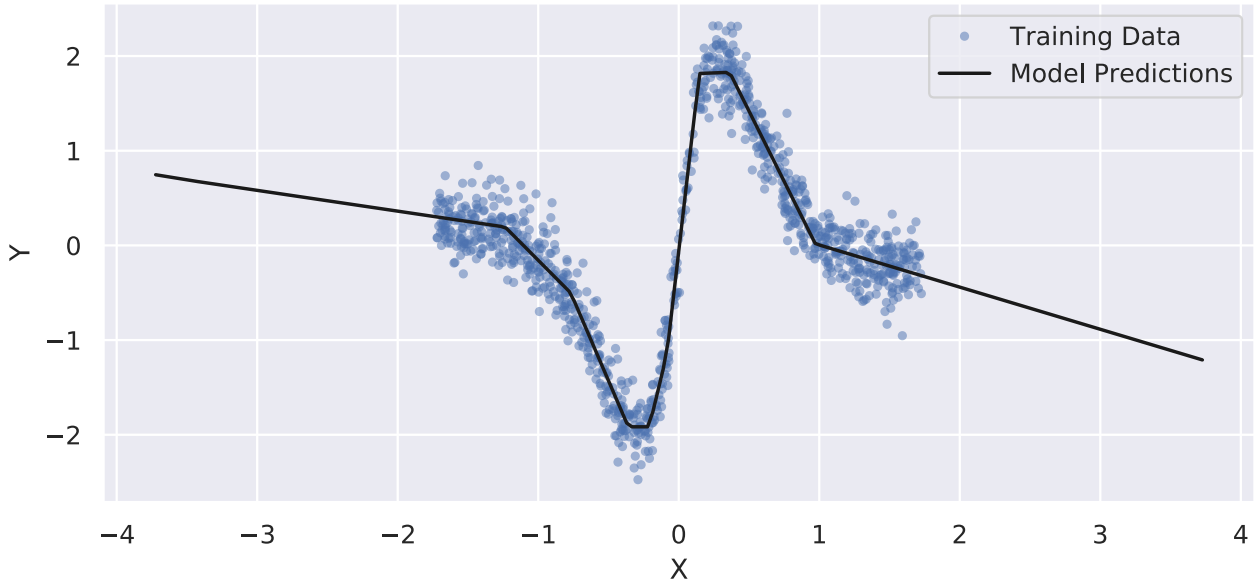


UQ Illustration: Climate Change

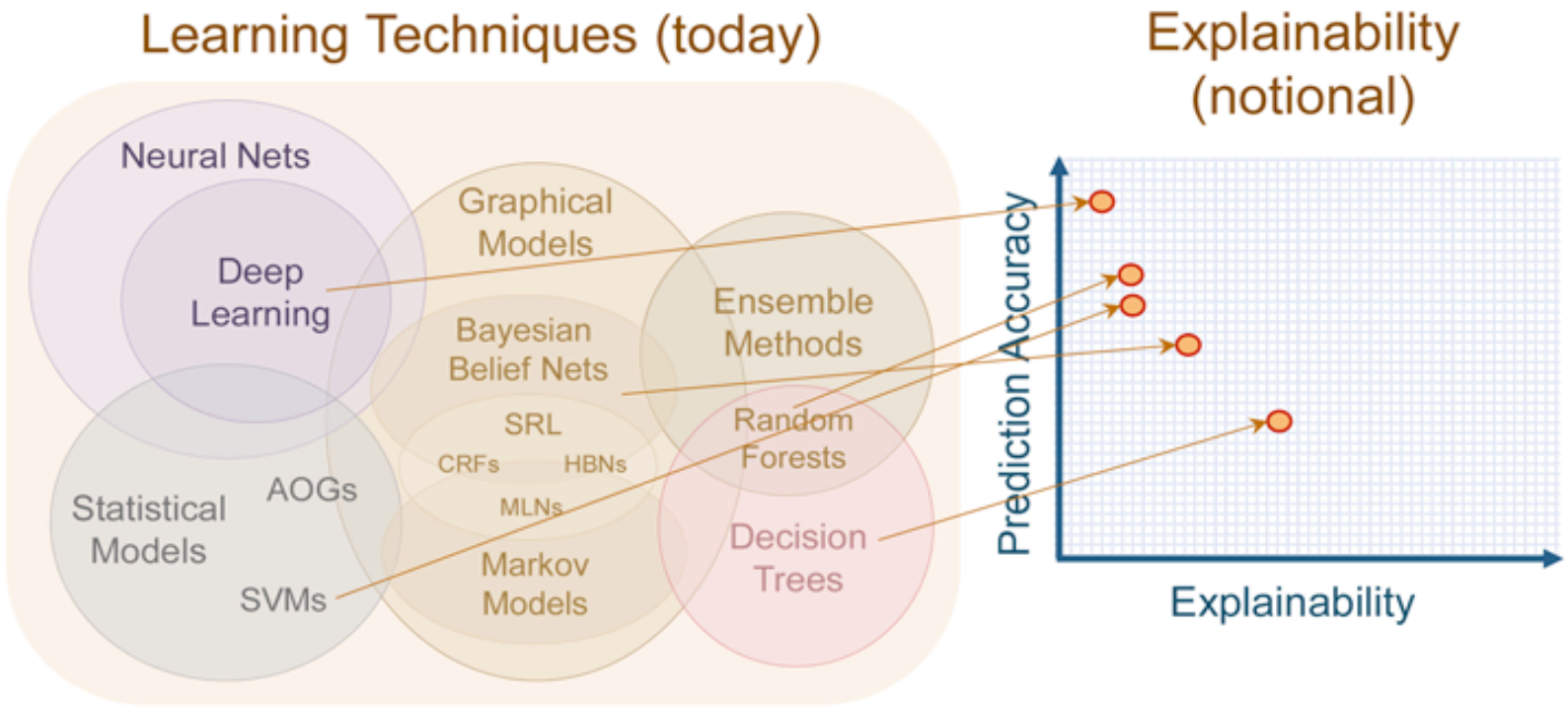


Uncertainty in Neural Network Predictions





Importance of UQ for ML

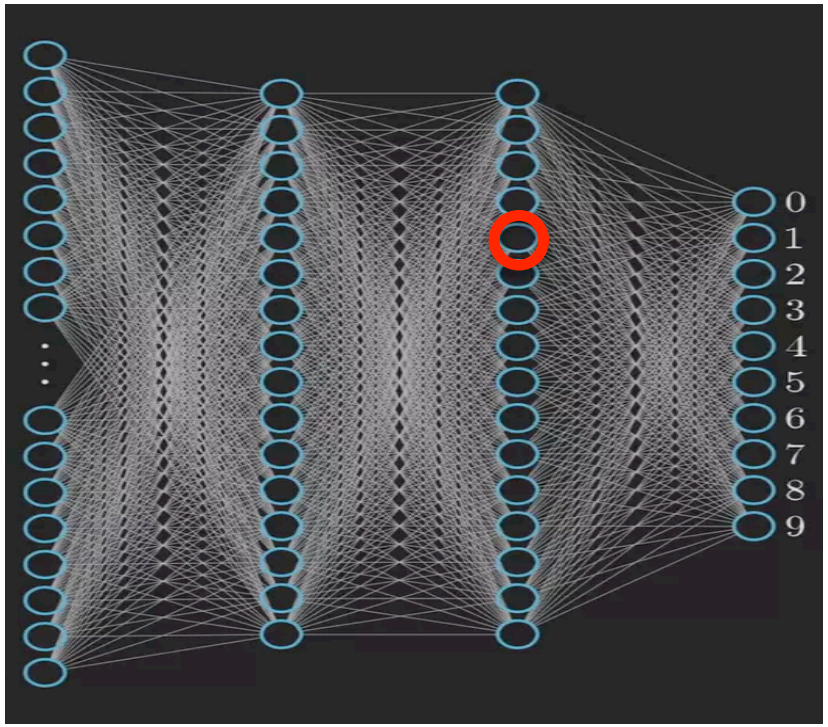


- Neural networks give *answers*, but no *insight*.
- Akin to Black Boxes.

Importance of UQ for ML

$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \rho\vec{g} + \mu\nabla^2\vec{V}$$

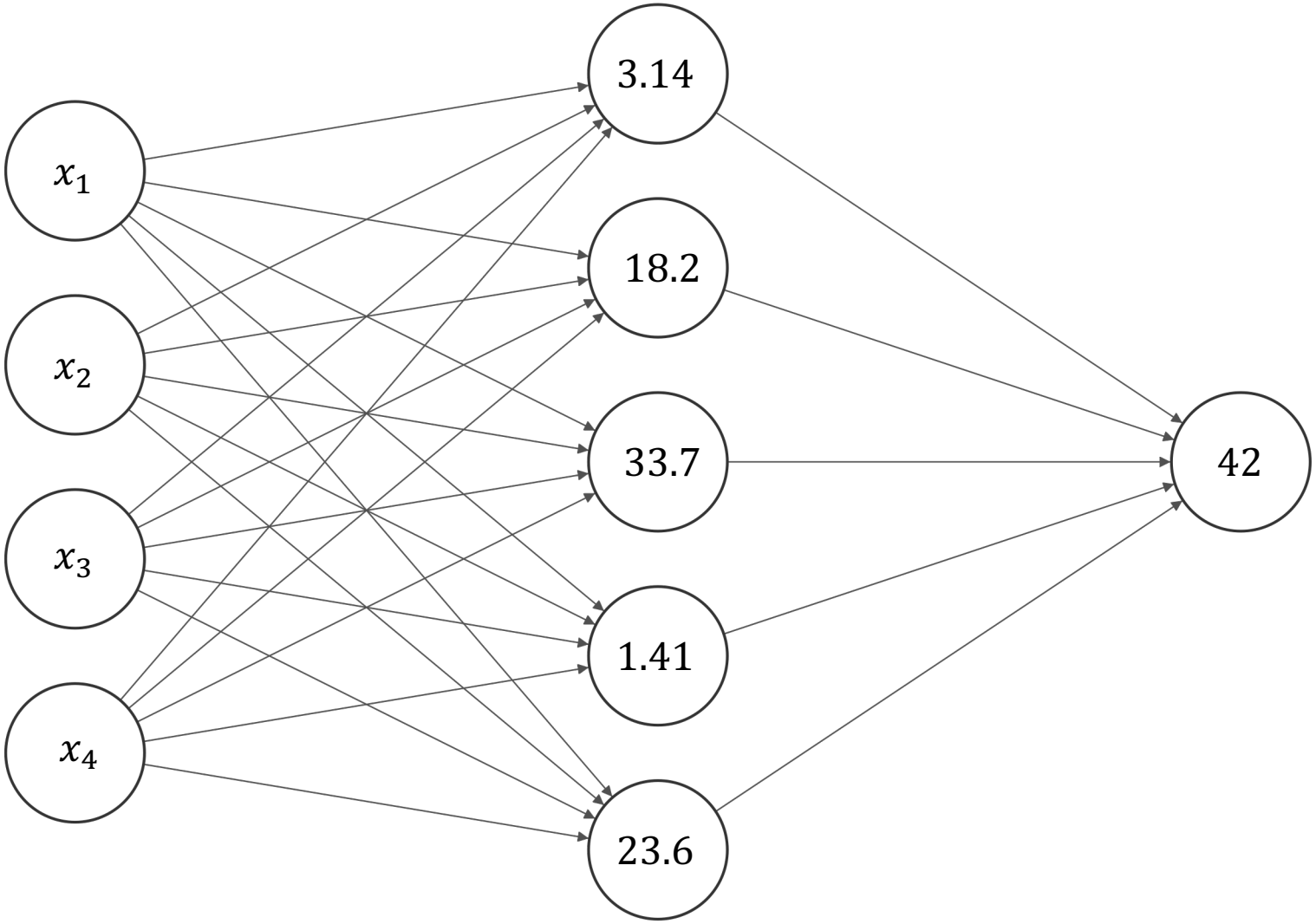
Total derivative | Pressure gradient | Body force term | Diffusion term



Importance of UQ for ML

[1] Yuchi Tian, Kexin Pei, Suman Jana, and Baishakhi Ray. 2018. DeepTest: Automated Testing of Deep-Neural-Network-driven Autonomous Cars. InICSE ’18
[2] https://www.tesla.com/en_GB/blog/tragic-loss

Deterministic Versus Bayesian Neural Networks



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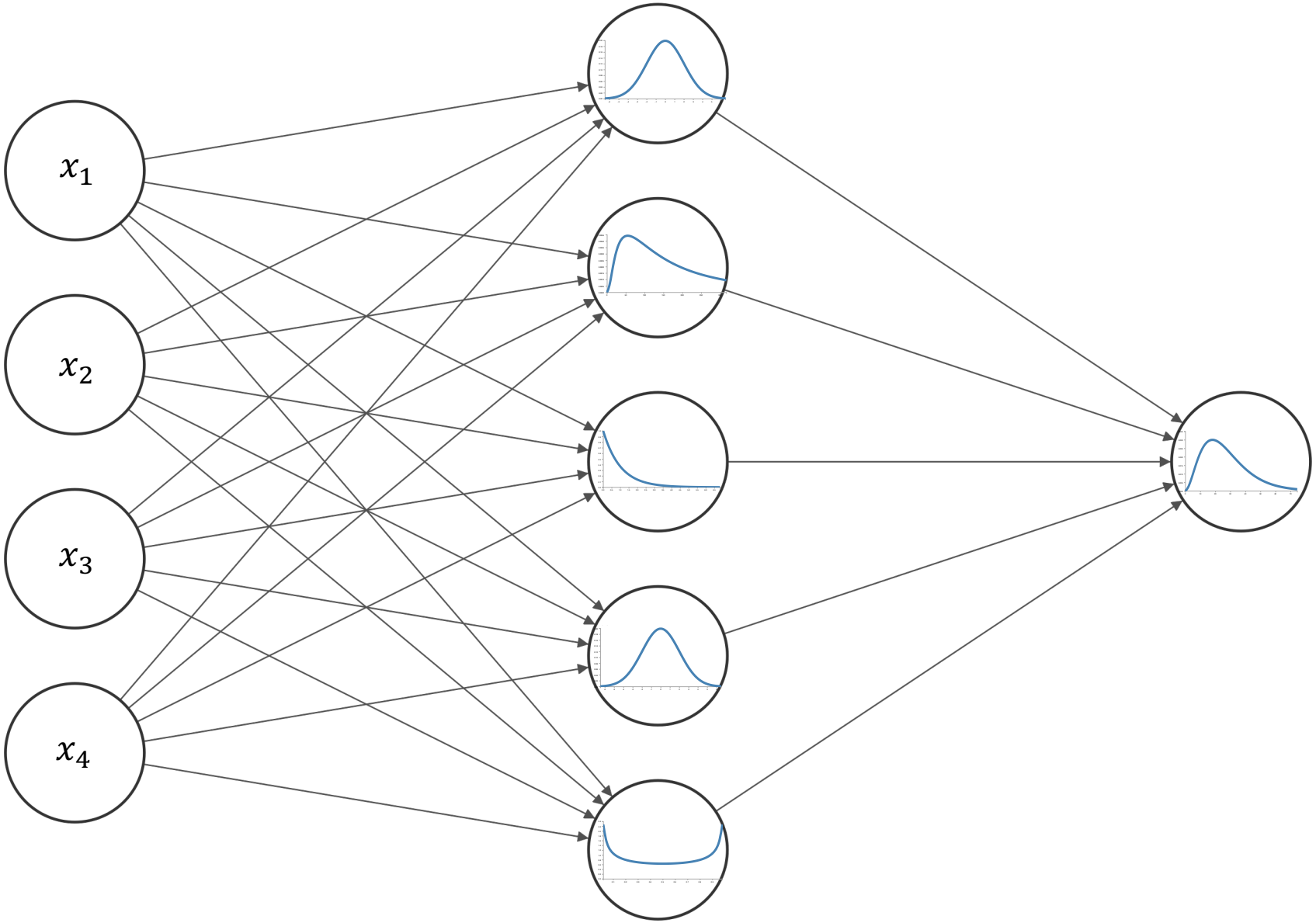

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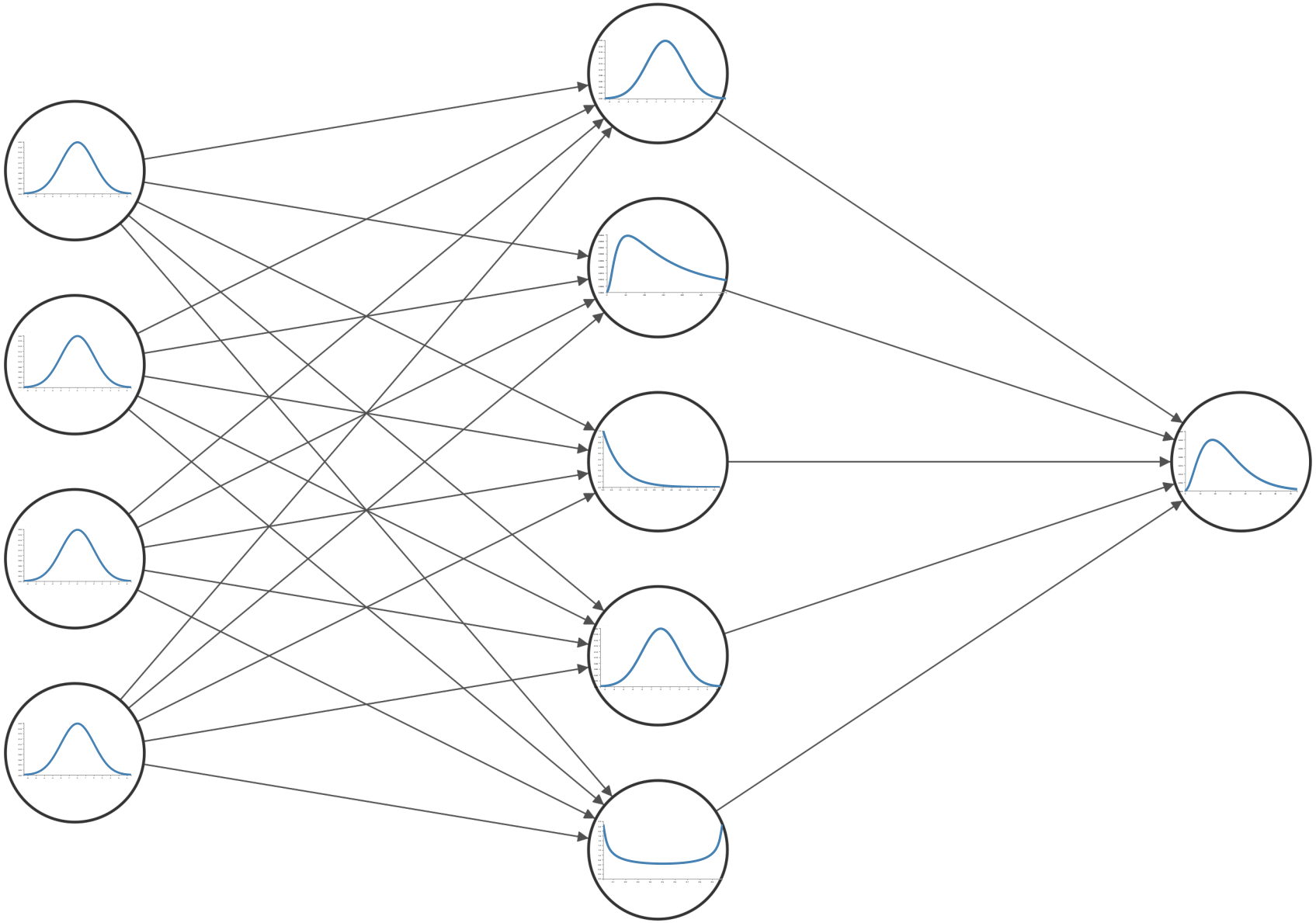

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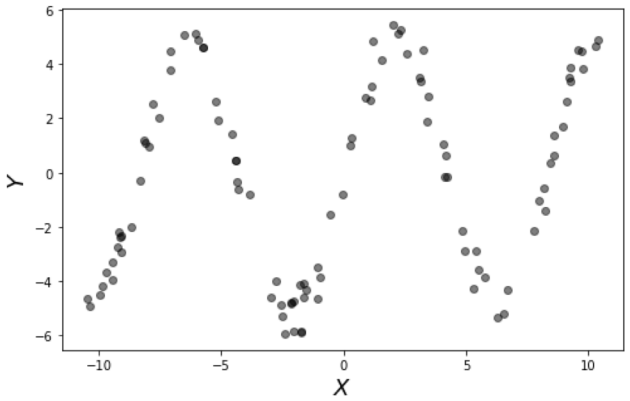
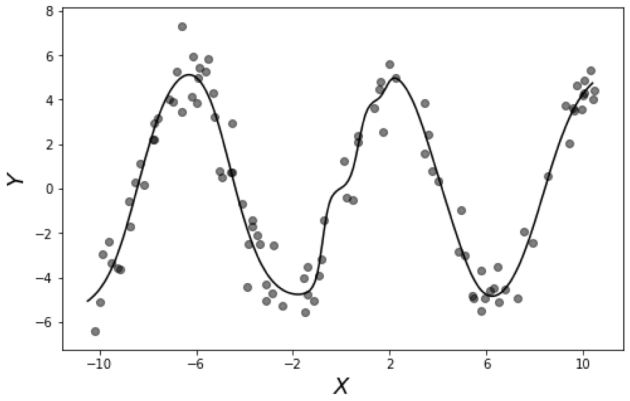
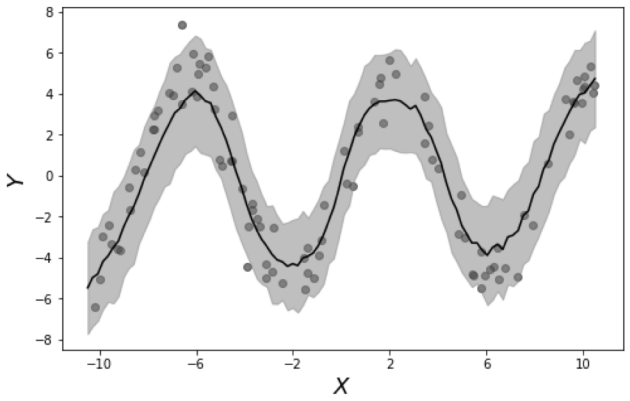


Training Data

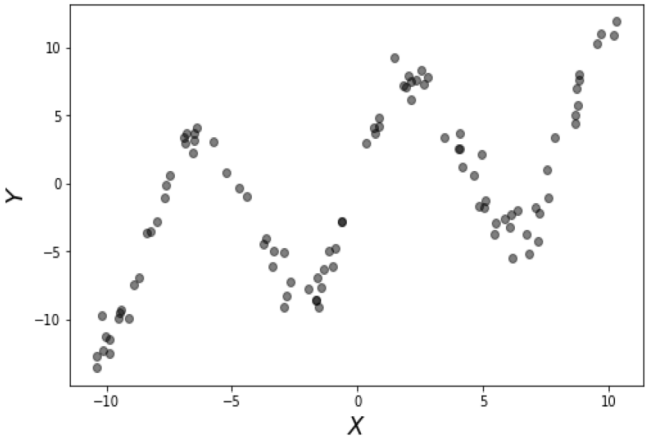


Deterministic Neural Network

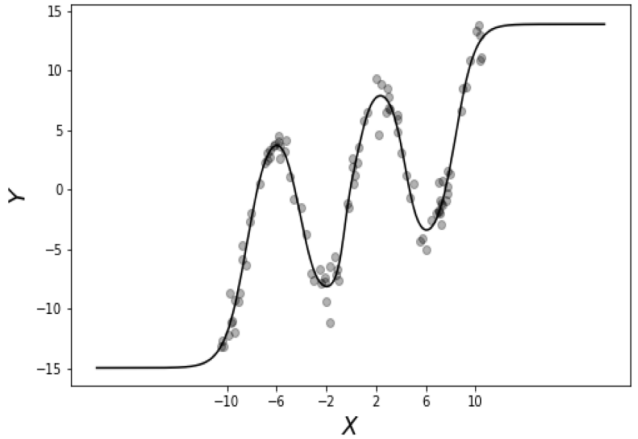


Bayesian Neural Network

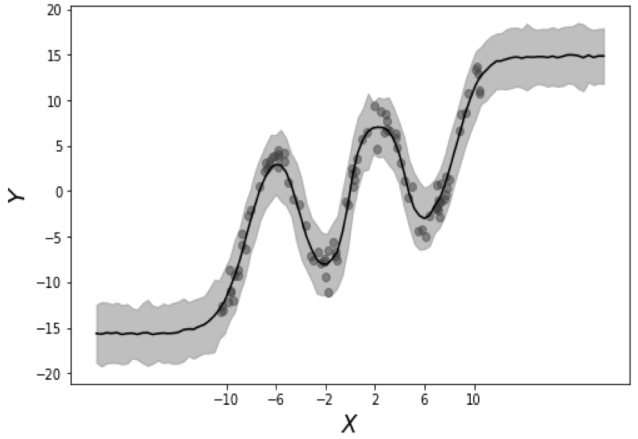
Deterministic Versus Bayesian Neural Networks



Training Data

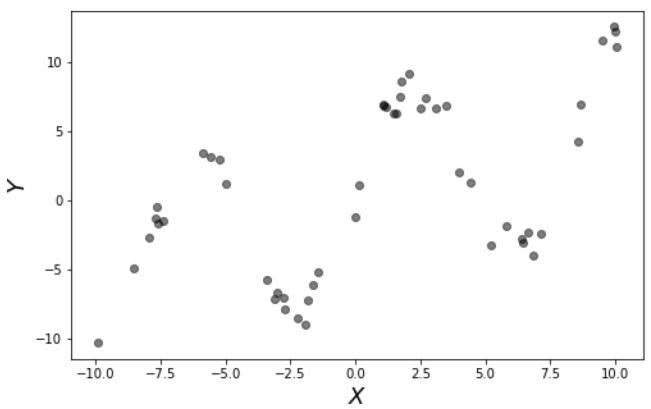


Deterministic Neural Network



Bayesian Neural Network

Deterministic Versus Bayesian Neural Networks



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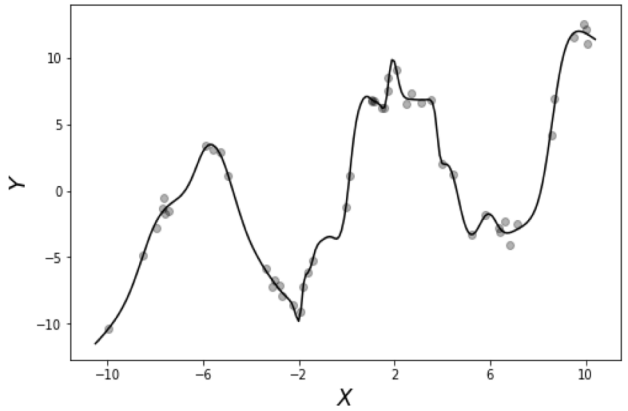

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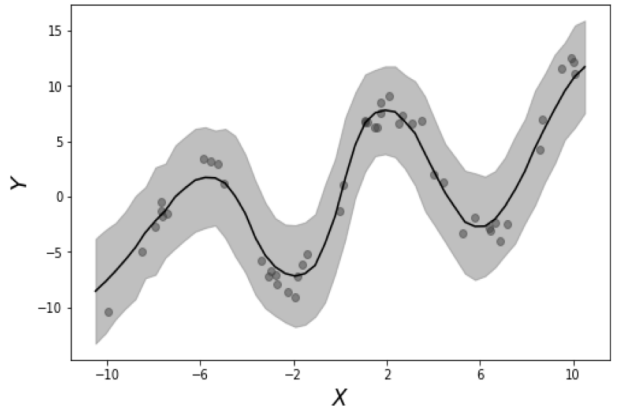
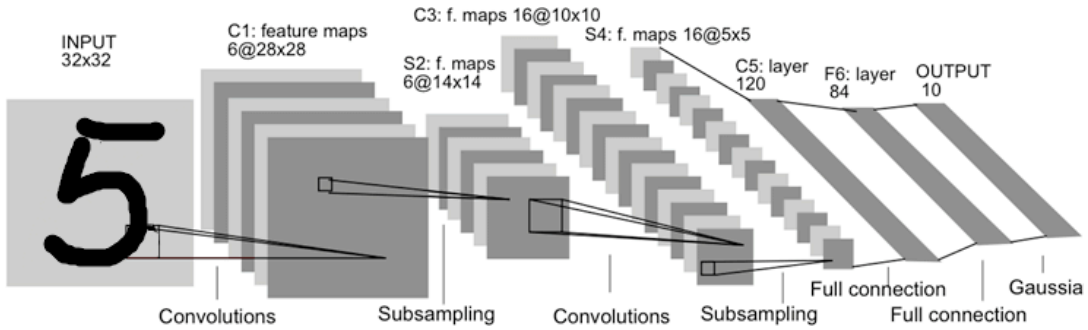


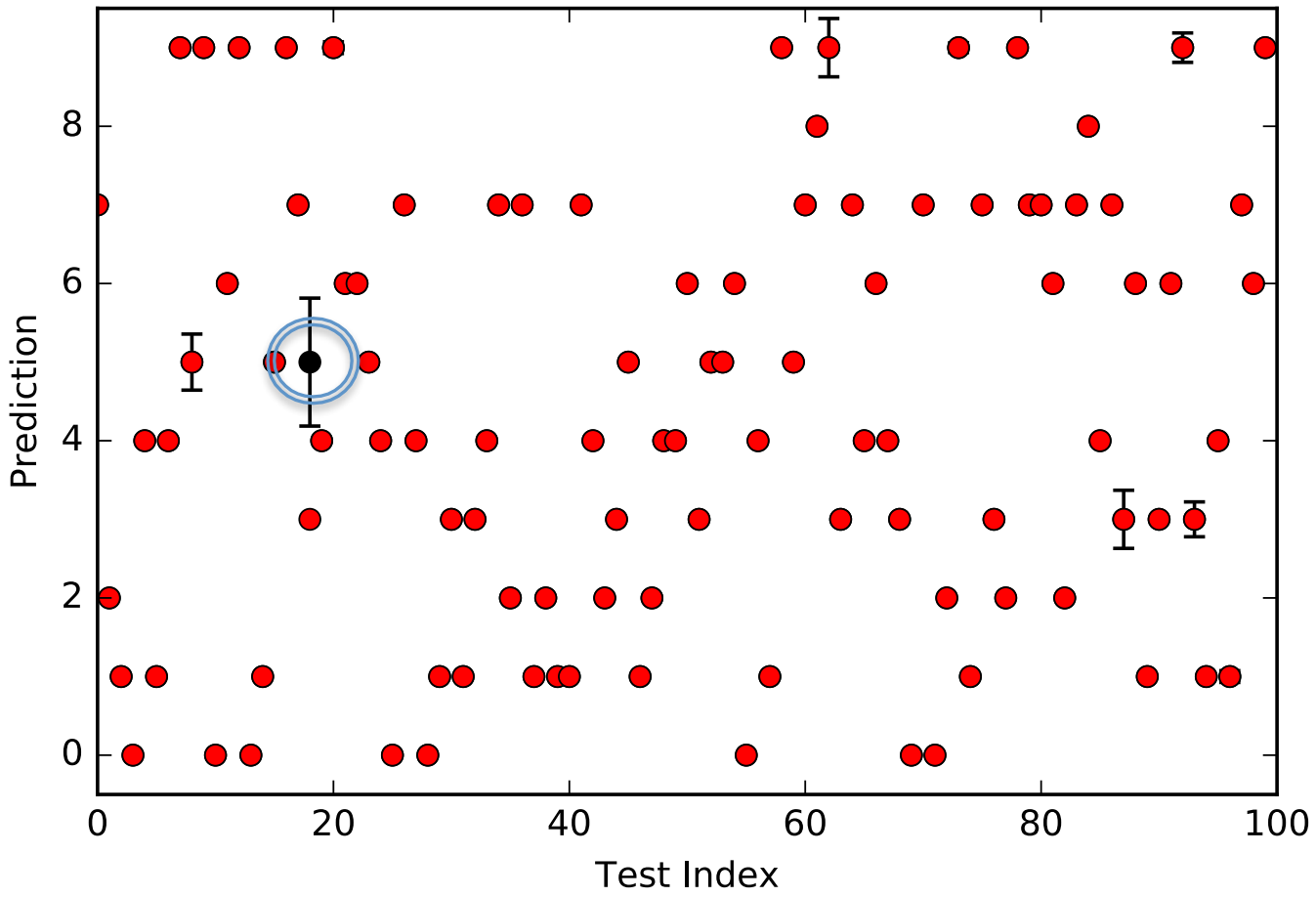
Bayesian Neural Network

Illustrative Application: Handwritten Digit Recognition with MC Dropout

- Convolutional neural network trained to classify handwritten digits.
- Certitude in predictions quantified using MC Dropout.

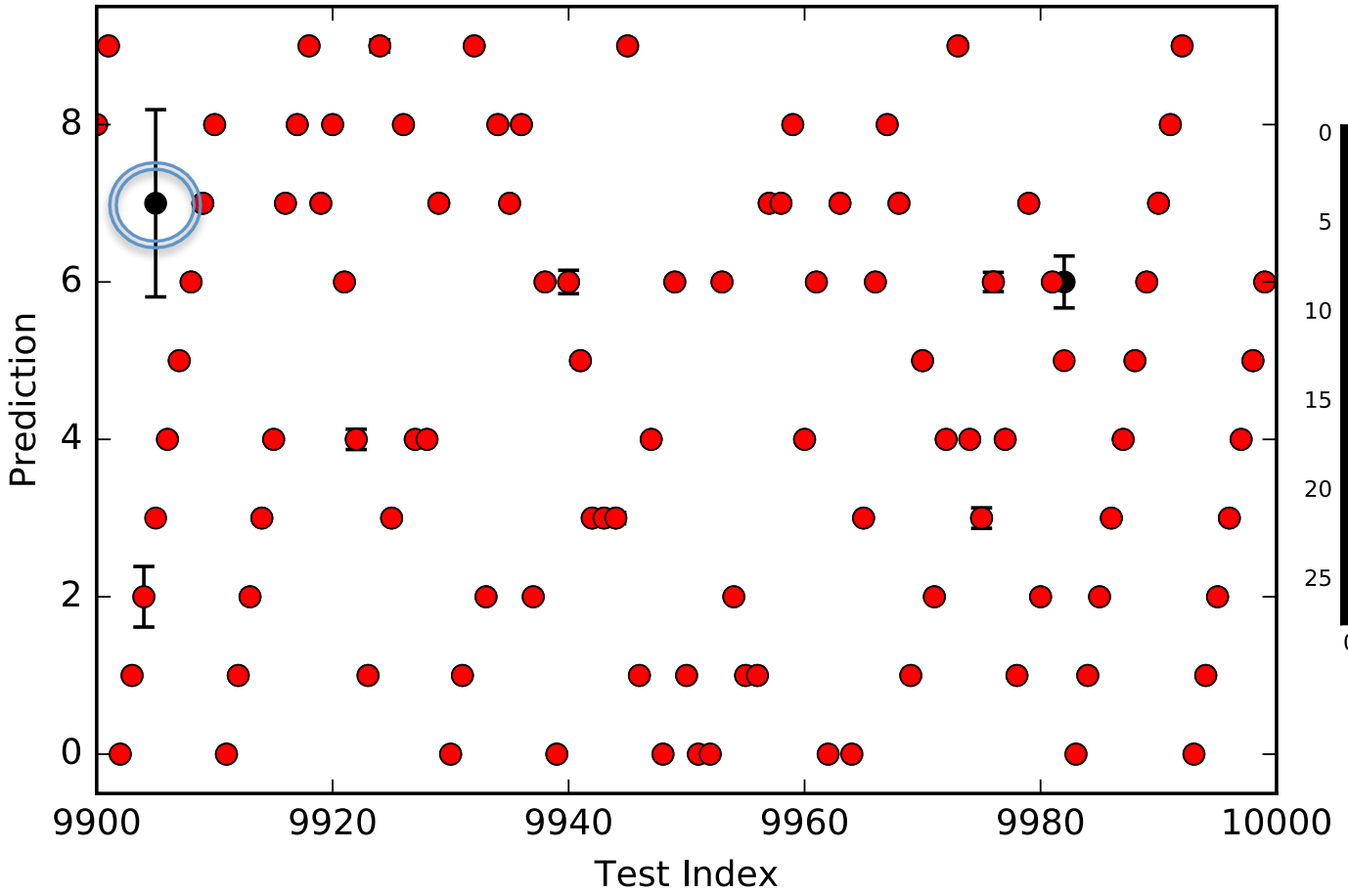


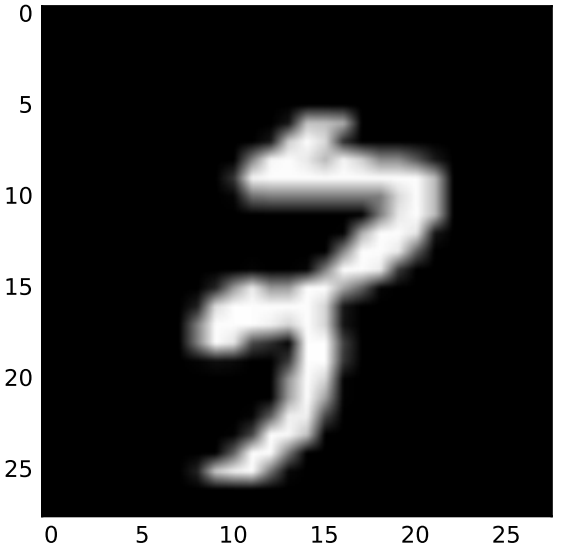
Classification with Quantified Uncertainties-I



3 or 5!

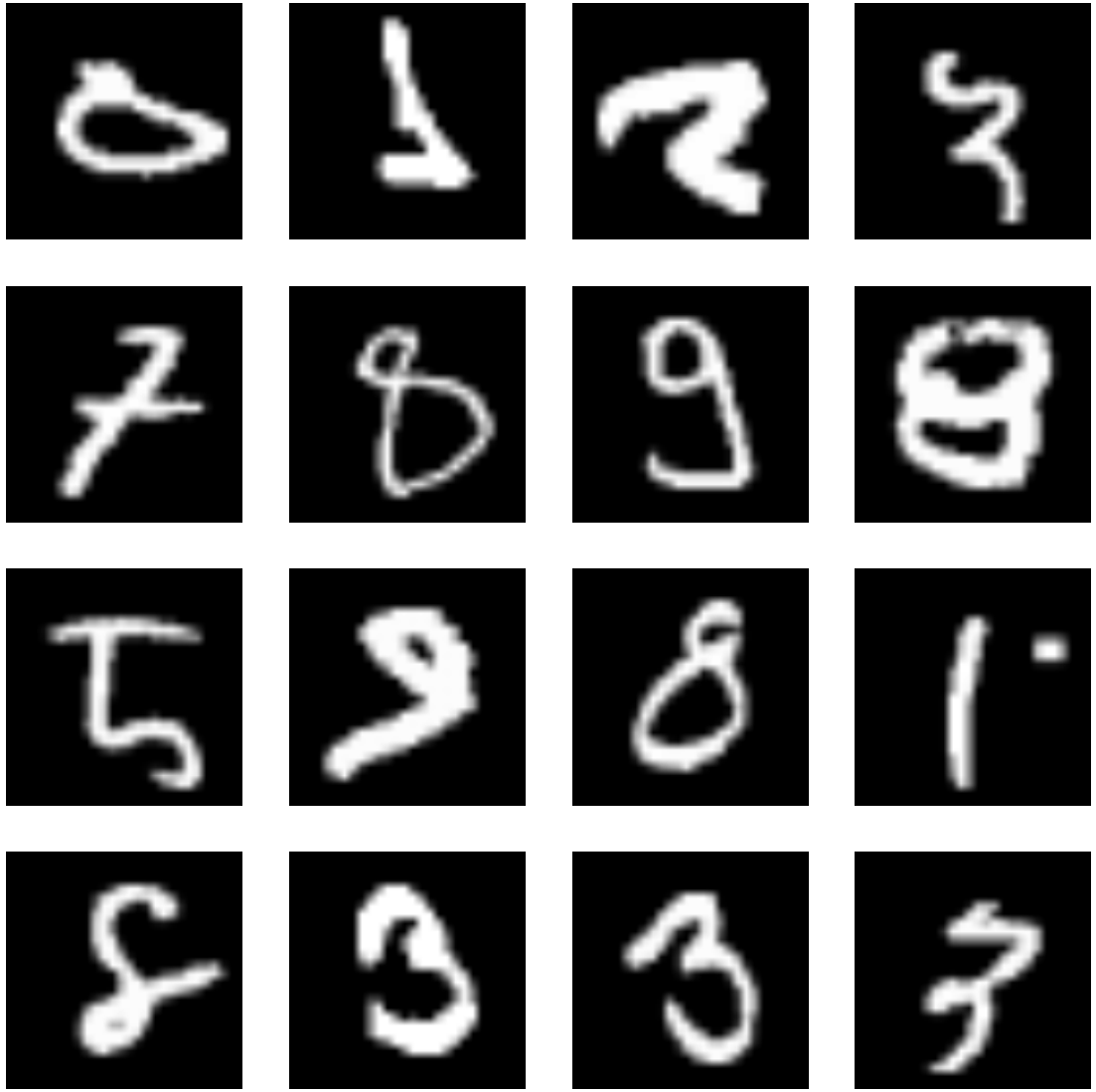
Classification with Quantified Uncertainties-II





3 or 7!

Highest Uncertainties: Unsure Predictions



MC Ensemble Accuracy