No Free Lunches in Machine Learning

Neill Campbell

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Department of Computer Science, University of Bath

Slide input credits: Carl Henrik Ek, Javier González, Simon Prince, Julian Faraway

AI Talks: AI & ML Research Group, Department of Computer Science

11 Oct 2023	Prof Simon Prince	Understanding Deep Learning: The Technology Behind Modern AI
15 Nov 2023	Prof Nello Cristianini	The Shortcut: How Machines Became Intelligent Without Thinking in a Human Way
13 Dec 2023	Prof Mike Tipping	The Irresistible Rise of Machine Learning
28 Feb 2024	Prof Neill Campbell	No Free Lunches in Machine Learning
20 Mar 2024	Prof Özgür Şimşek	Reinforcement Learning and the Pursuit of Artificial Intelligence
17 Apr 2024	Dr Harish Tayyar Madabushi	Emergent Abilities of Language Models: Do they pose an existential threat?
8 May 2024	Prof Darren Cosker	AI for Human Sensing: Research, Productisation and Ethics
TBD	Prof Mike Tipping	Bayesian Inference in Machine Learning: Indistinguishable from Magic?


THIS IS THE WAY
makeameme.org

Overview

Common Questions?

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- Can I use ML to solve x?

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- Can any of this be used for science/engineering?

Things to consider..

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Overview...

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No Free Lunch

Uncertainty / Error Bars

Model Selection

Causality

Conclusions

No Free Lunch

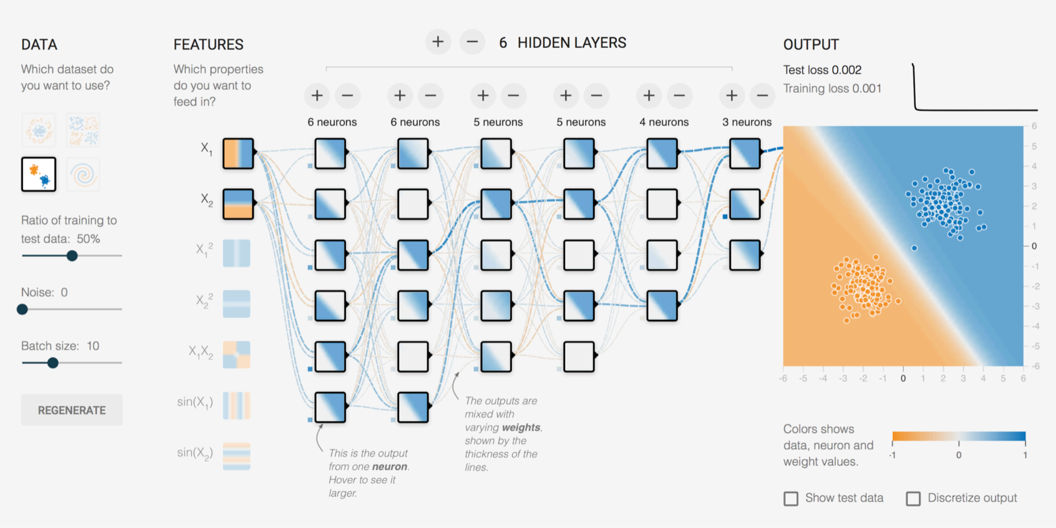
Overview...

Machine Learning illustration

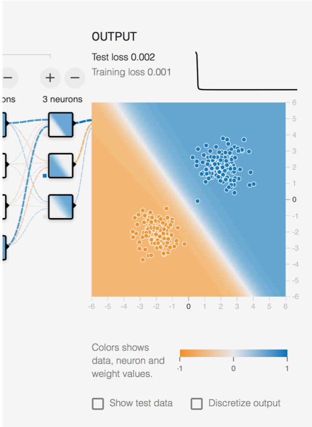
Neural Network Playground:

- https://playground.tensorflow.org/

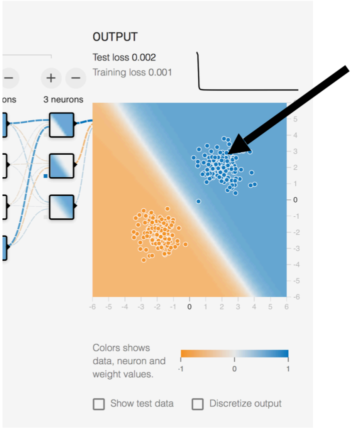
Machine Learning illustration



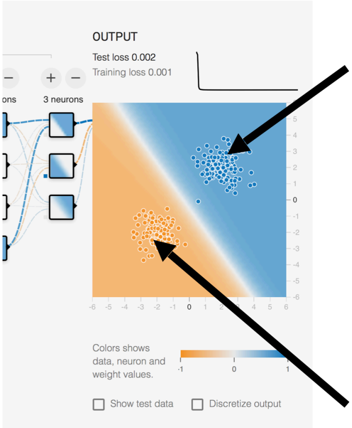
Machine Learning illustration

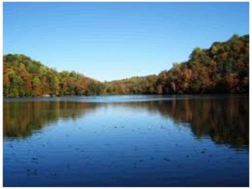


Machine Learning illustration



Machine Learning illustration





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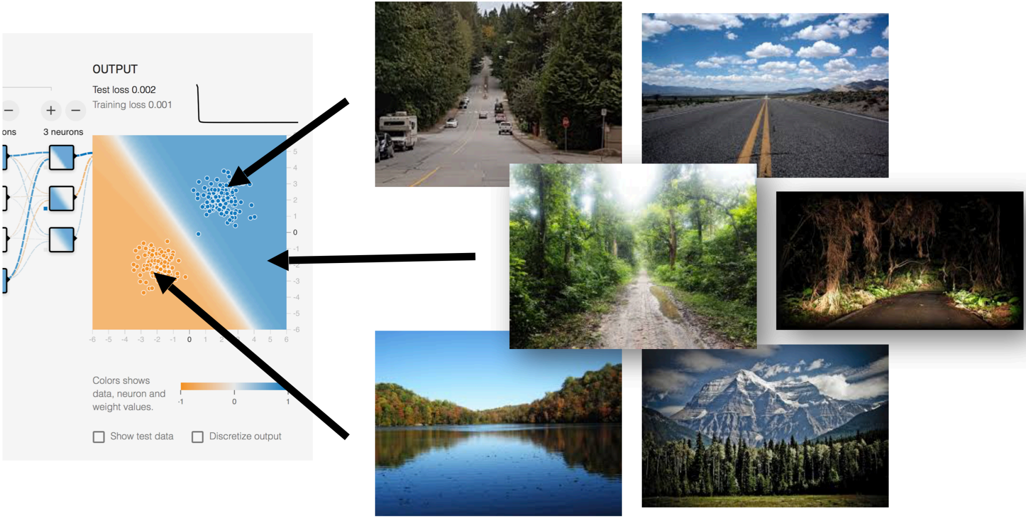

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What if we use a probabilistic approach?

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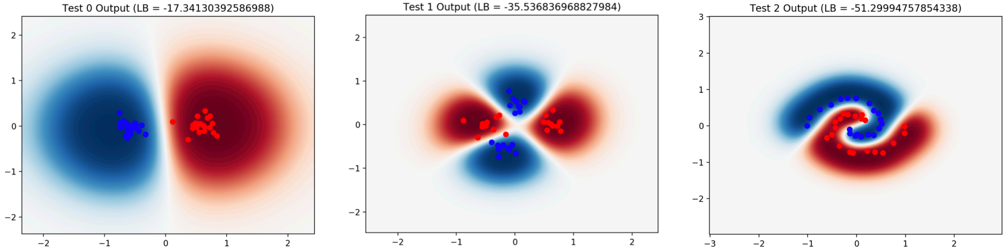

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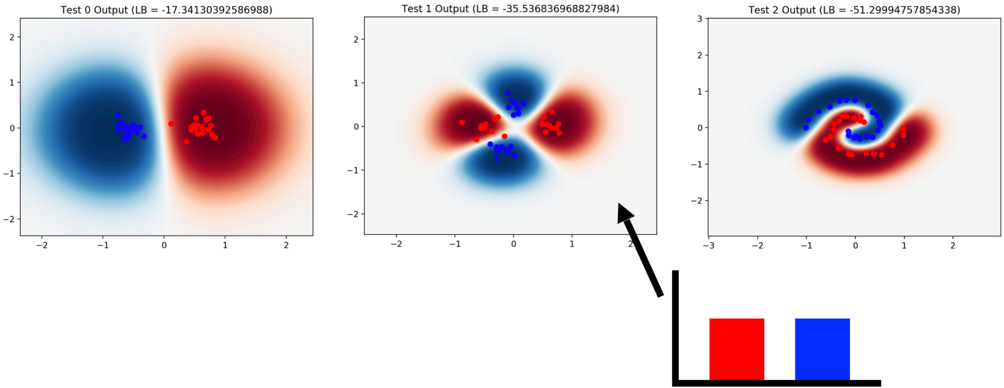

We need to consider properties of Machine Learning approaches

What happens between the dots?

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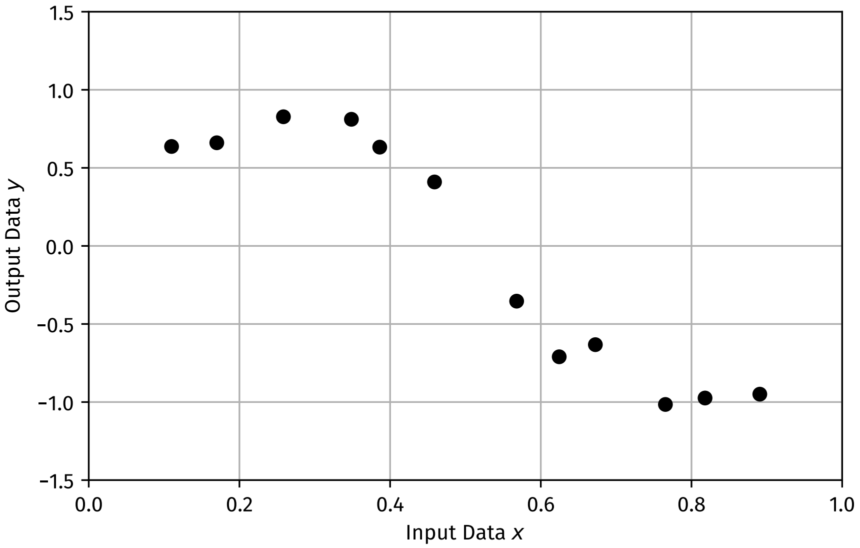

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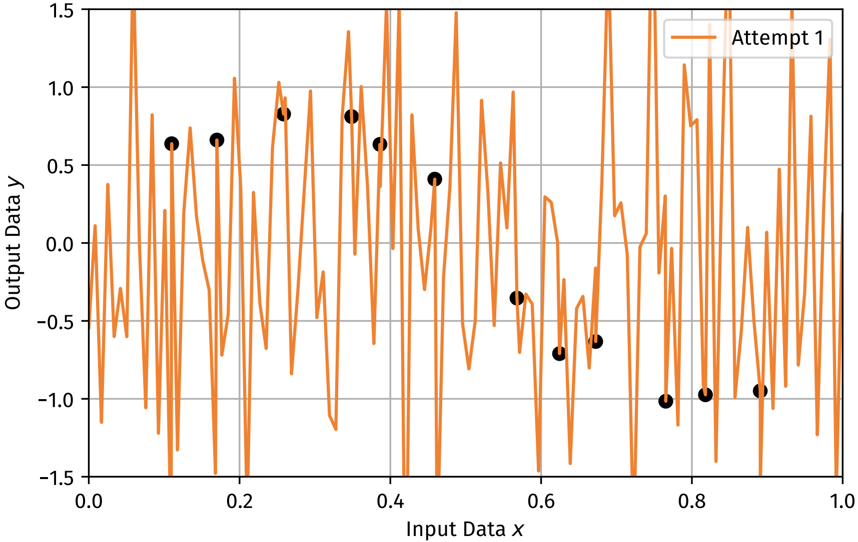

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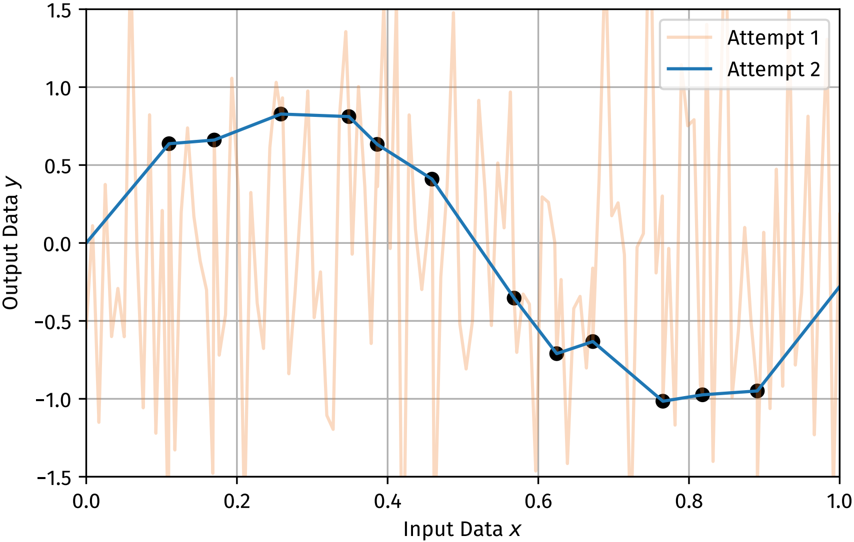

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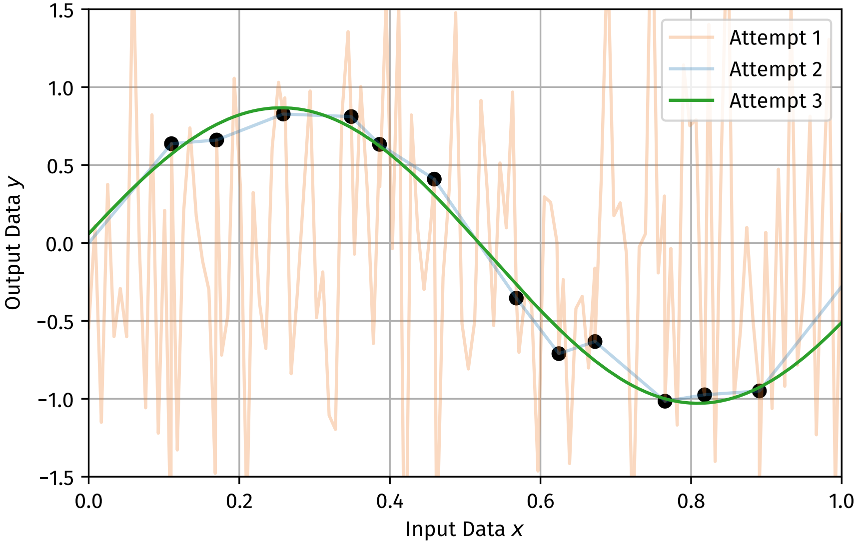

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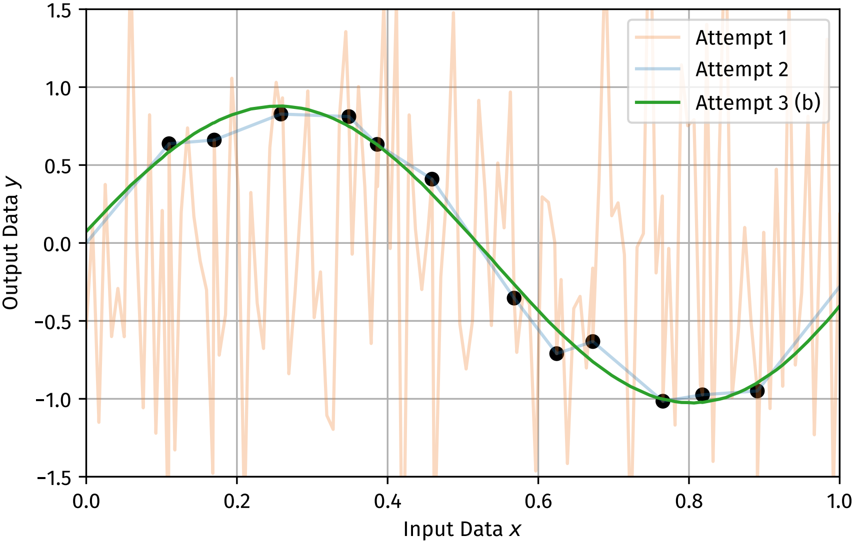

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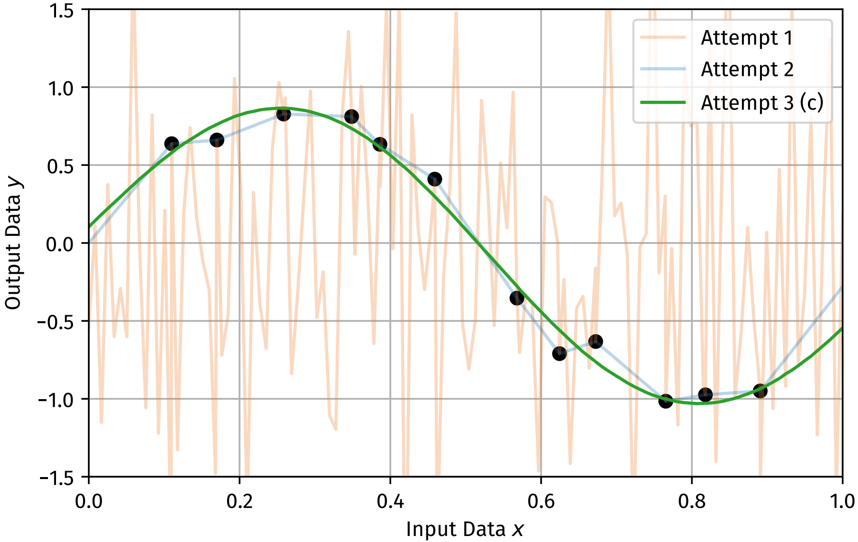

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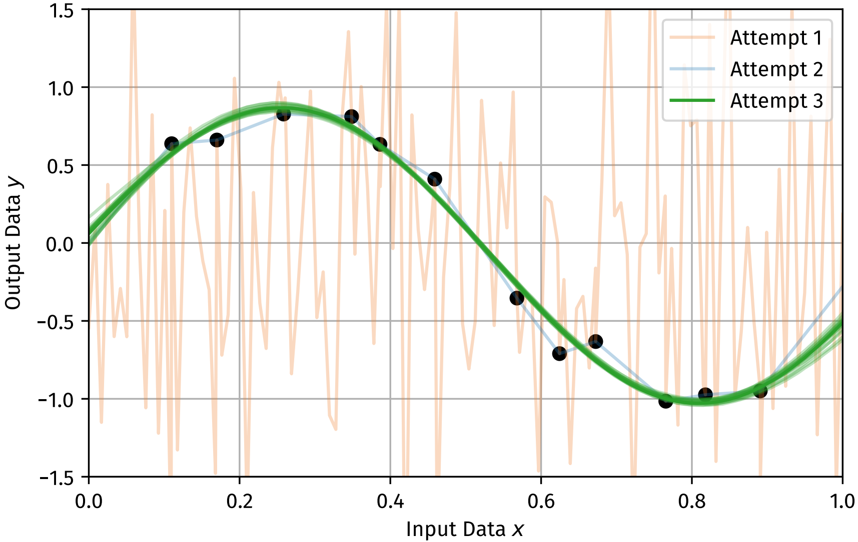
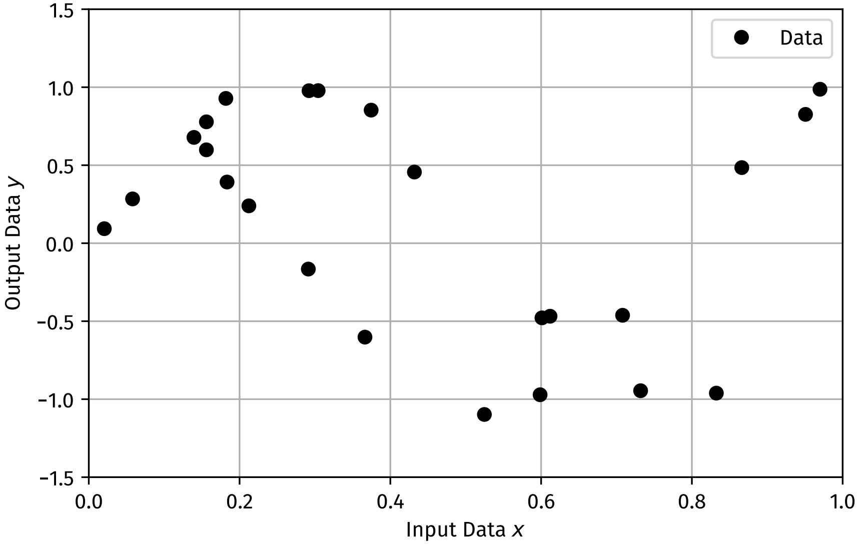
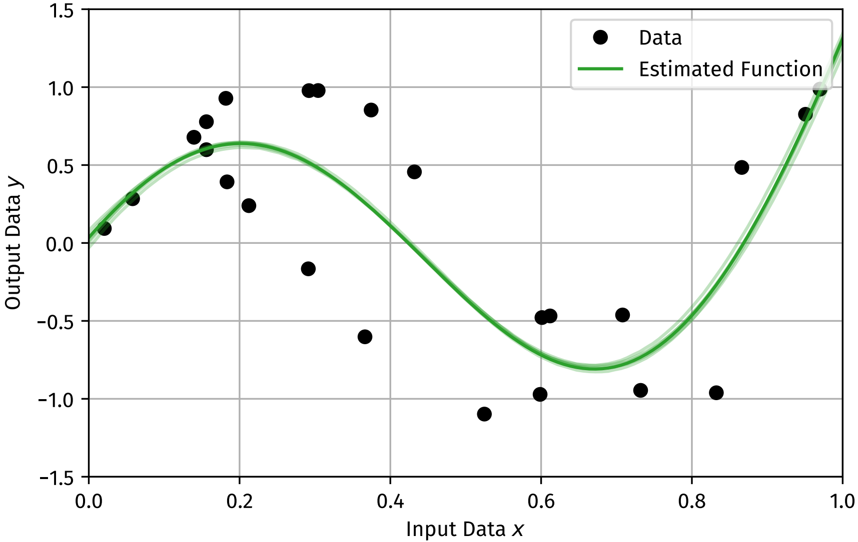


Ambiguity..



Data
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
Output Data y
0.0
0.2
0.4
0.6
0.8
1.0
Input Data x

Ambiguity..



Data
Estimated Function
Output Data y
Input Data x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0.0
0.2
0.4
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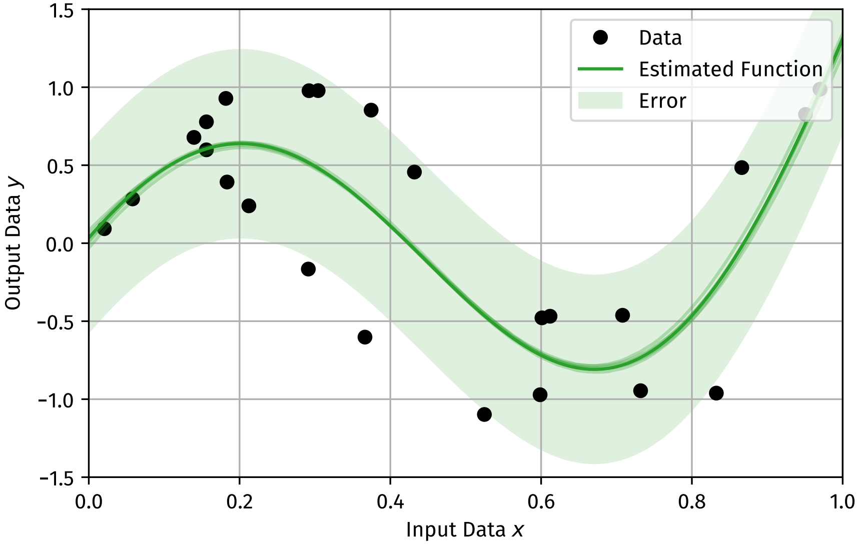
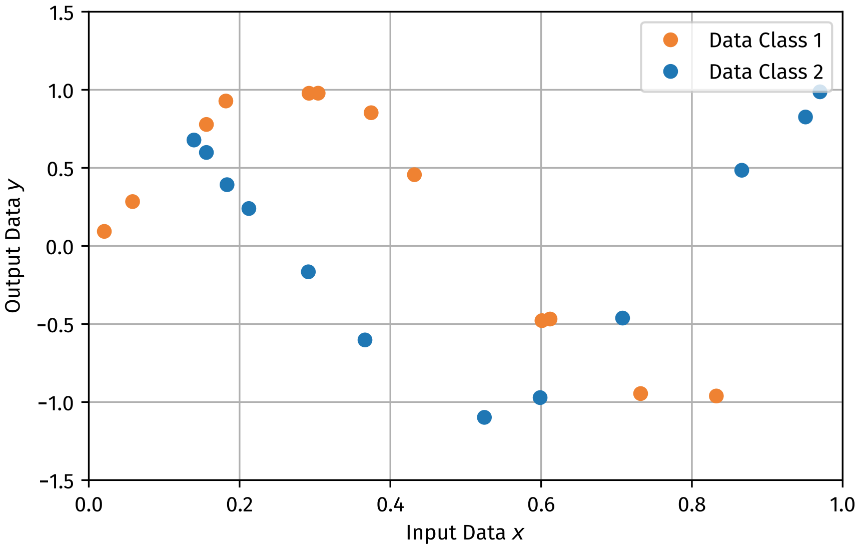
Ambiguity..



Data
Estimated Function
Error
Output Data y
Input Data x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0.0
0.2
0.4
0.6
0.8
1.0

Ambiguity..


Data Class 1
Data Class 2
1.5
1.0
0.5
0.0
−0.5
−1.0
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0.2
0.4
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1.0
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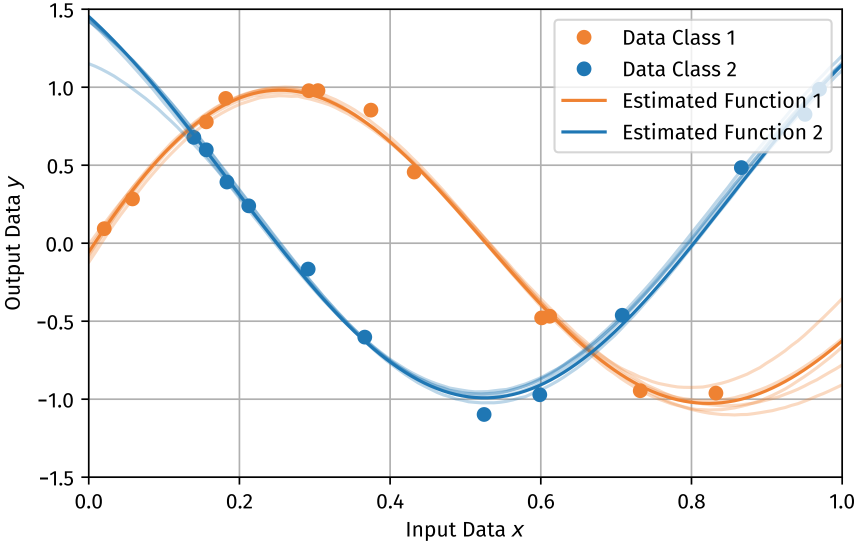
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1.5
1.0
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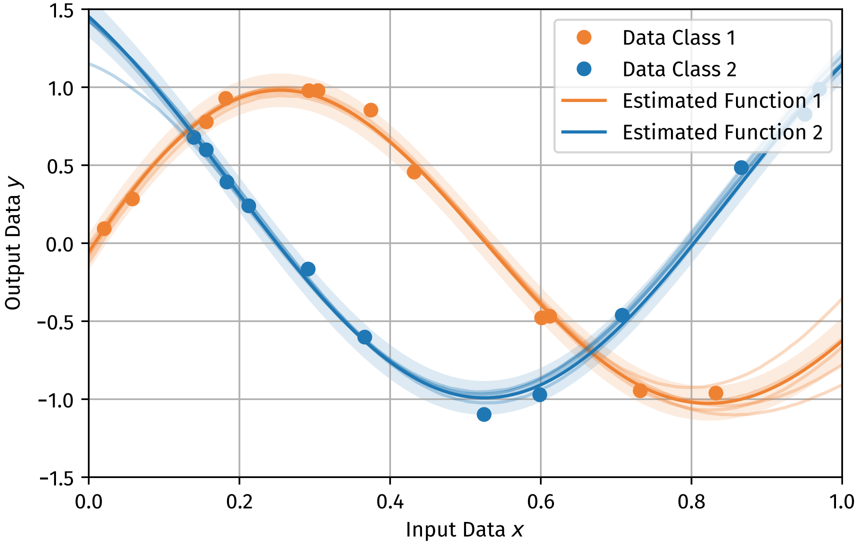
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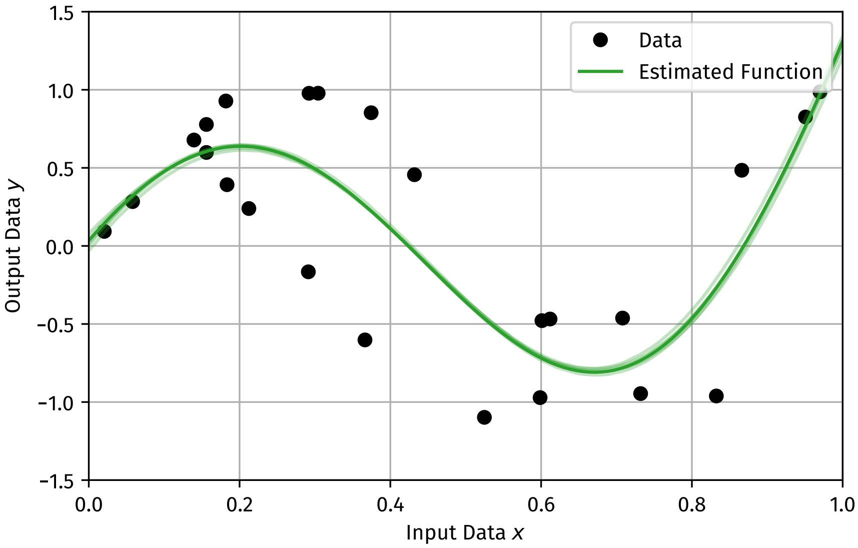

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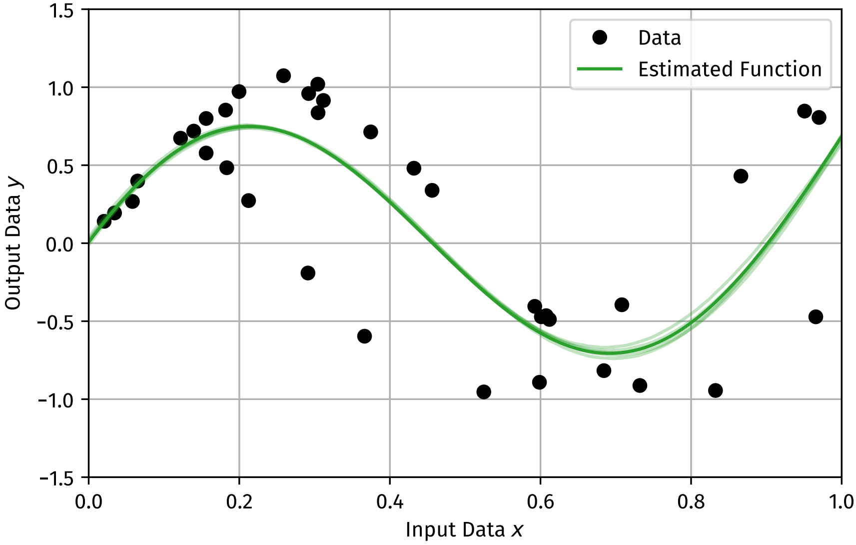

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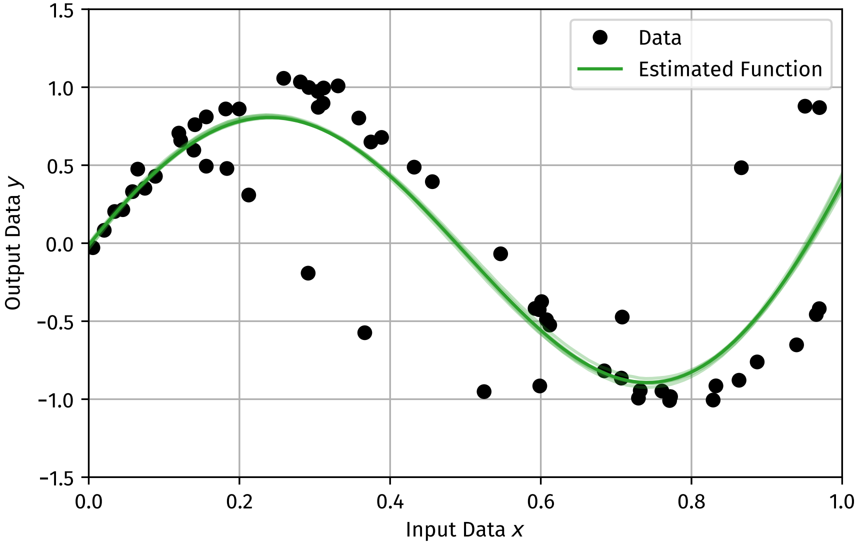

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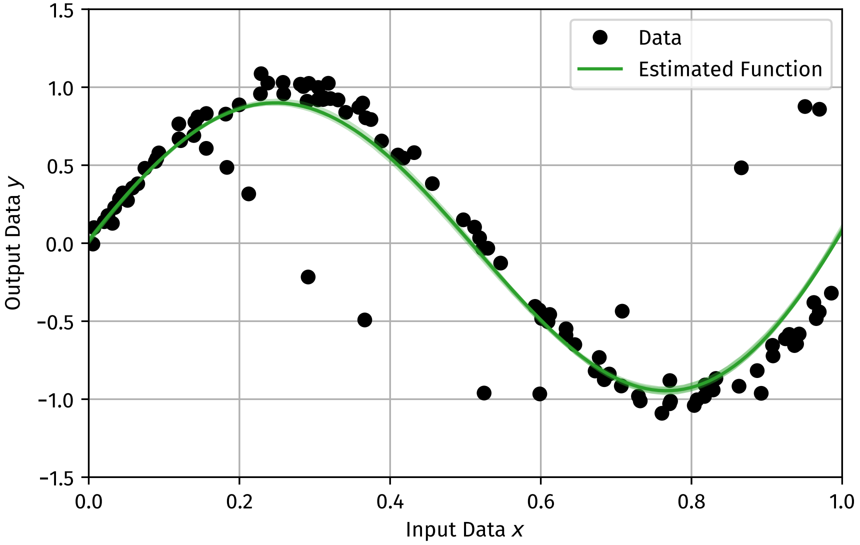
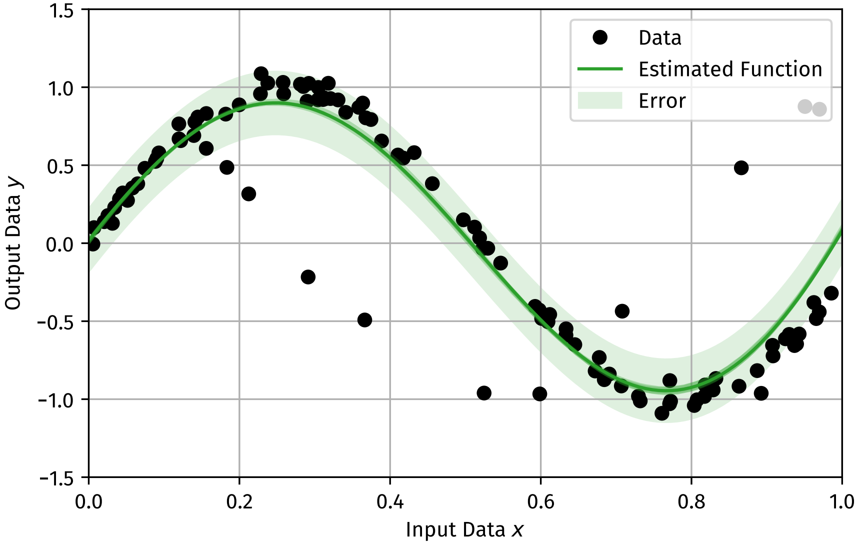
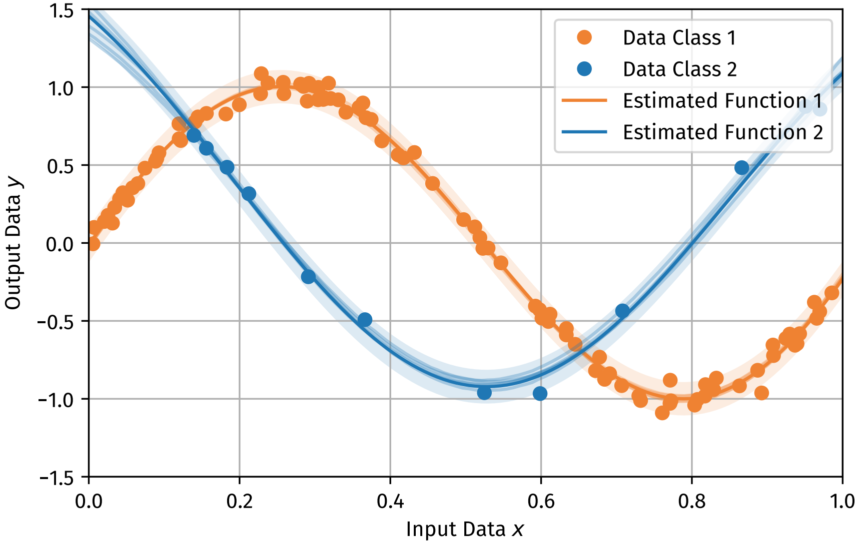


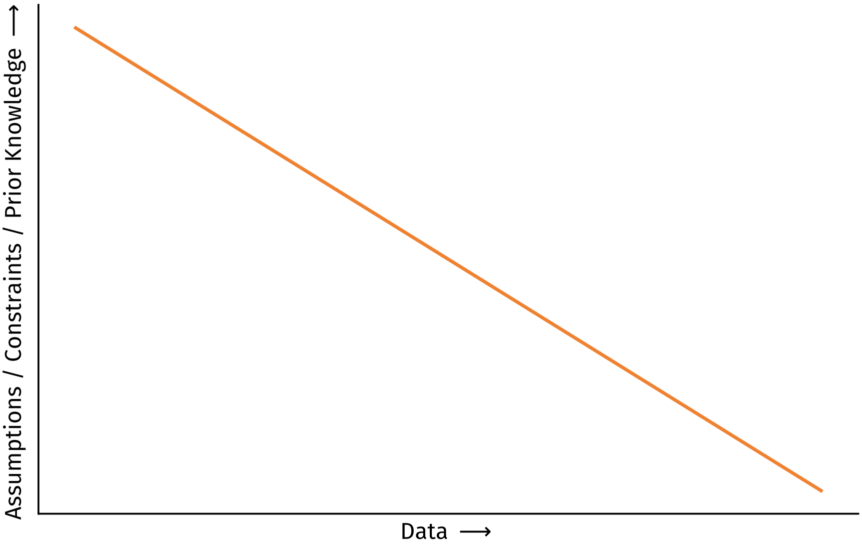
Average vs Worst Case: Failure to model..



Average vs Worst Case: Explicitly accounting for imbalance..



No free lunch



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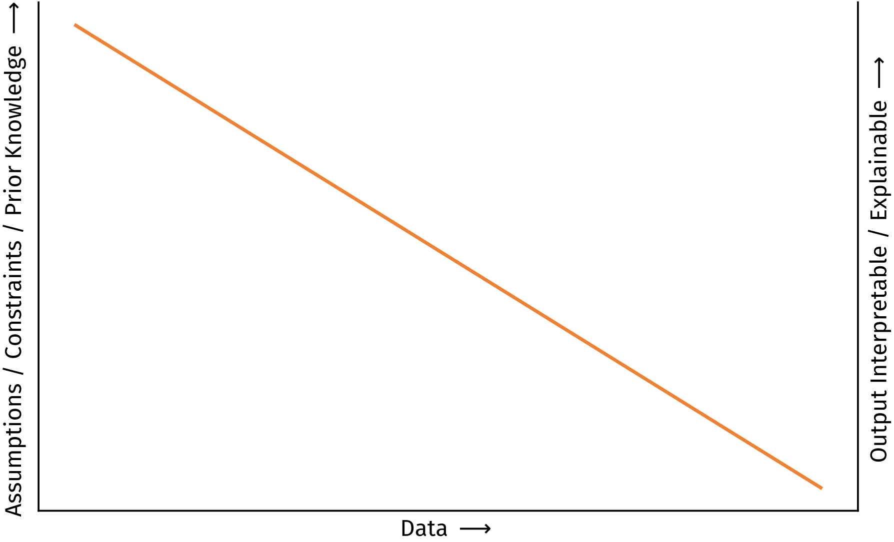
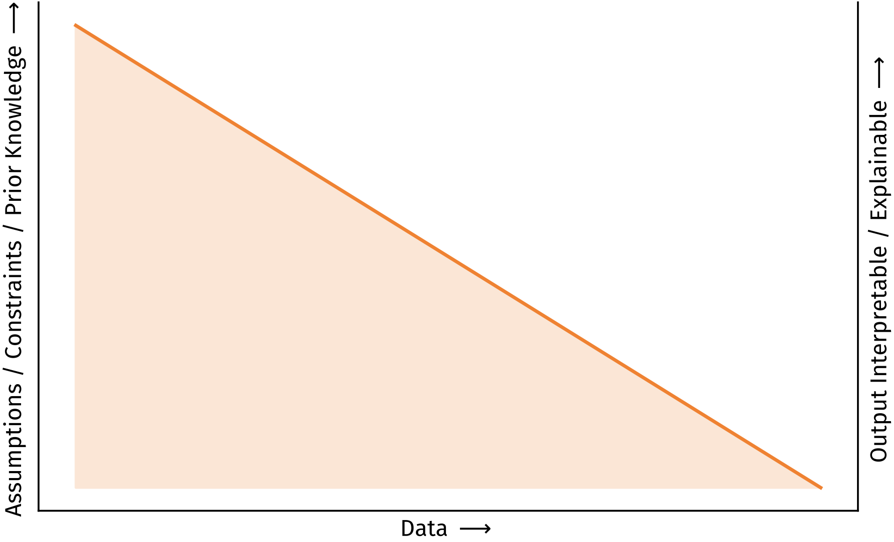
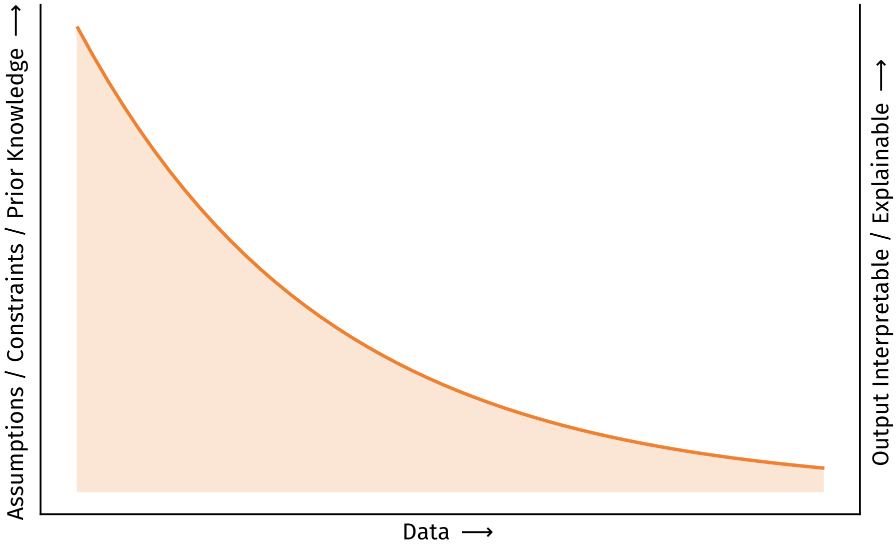


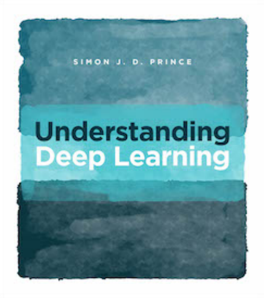
No free lunch



No free lunch (more realistic)



Understanding Deep Learning



Excellent new text book from Simon Prince (visiting Prof in Bath for semester 1):

Understanding Deep Learning, Simon J.D. Prince, MIT Press

Final draft available on the website: `https://udlbook.github.io/udlbook/`

Uncertainty / Error Bars

Overview...

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No Free Lunch

Uncertainty / Error Bars

Model Selection

Causality

Conclusions

- Bayes' Rule

$$\text{Posterior Probability (after)} = \frac{\text{Likelihood (of event)} \times \text{Prior Probability (before)}}{\text{Evidence}}$$

Example of Bayes' Rule..

- Consider a legal trial..

$$\underbrace{p(\text{guilt} \mid \text{observations})}_{\text{Posterior}} = \frac{\overbrace{p(\text{observations} \mid \text{guilt})}^{\text{Likelihood}} \times \overbrace{p(\text{guilt})}^{\text{Prior}}}{\underbrace{p(\text{observations})}_{\text{Evidence}}}$$

$p(A \mid B)$ means "probability of A being the case given that B occurs"

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Monty Hall..

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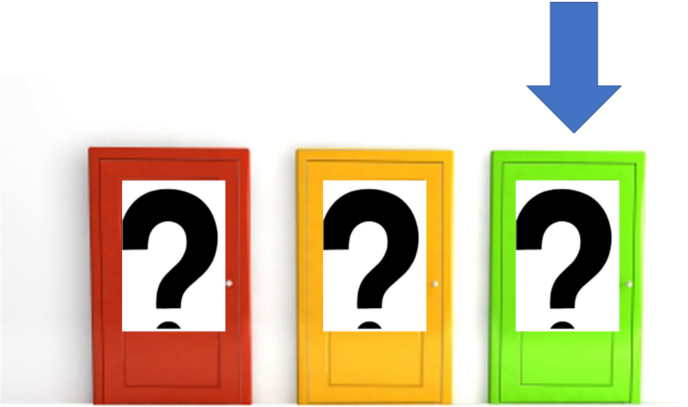

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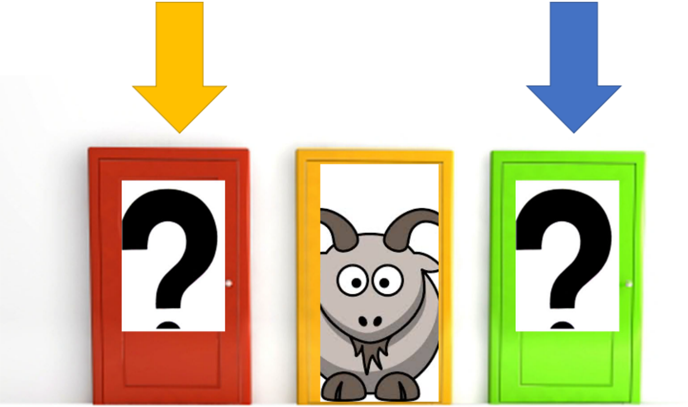

Monty Hall: How would we generate data (or simulate)?

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door_with_car = pick_random({1, 2, 3})
door_with_goat = {1, 2, 3} - door_with_car

door_picked = pick_random({1, 2, 3})

if door_picked == door_with_car:
    door_to_open = pick_random(door_with_goat)
else:
    door_to_open = door_with_goat - door_picked
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door_picked = pick_random({1, 2, 3})            # 1/3 equal chance

if door_picked == door_with_car:
    door_to_open = pick_random(door_with_goat)  # 1 times in 3
else:
    door_to_open = door_with_goat - door_picked # 2 times in 3
```

Consider Modelling and ML as a

Generative Process

Bayes' Rule with models and functions..

$$\underbrace{p(\text{functions} \mid \text{observed data})}_{\text{Posterior}} = \frac{\overbrace{p(\text{observed data} \mid \text{functions})}^{\text{Likelihood}} \times \overbrace{p(\text{functions})}^{\text{Prior}}}{\underbrace{p(\text{observed data})}_{\text{Evidence}}}$$

Bayes' Rule with models and functions..

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$$\underbrace{p(f \mid \mathcal{D})}_{\text{Posterior}} = \frac{\overbrace{p(\mathcal{D} \mid f)}^{\text{Likelihood}} \times \overbrace{p(f)}^{\text{Prior}}}{\underbrace{p(\mathcal{D})}_{\text{Evidence}}} \qquad p(\mathcal{D}) = \sum_f p(\mathcal{D} \mid f)\, p(f)$$

Data $\mathcal{D} = \{X, Y\}$, pairs of inputs $\{x_n\}$ and outputs $\{y_n\}$, and functions f

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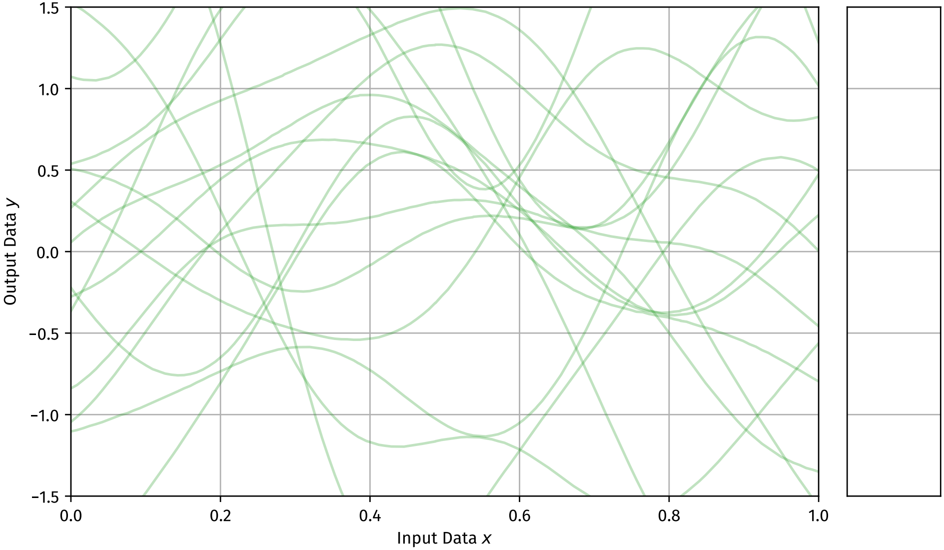
Data $\mathcal{D} = \{X, Y\}$, pairs of inputs $\{x_n\}$ and outputs $\{y_n\}$, and functions f

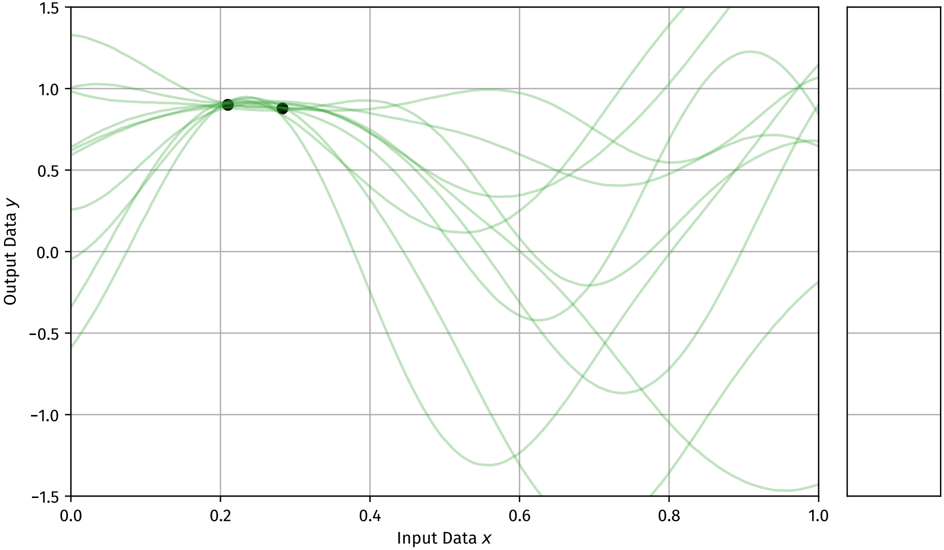
Average over functions to predict unknown output y^* for a **new input** x^*:

$$p(y^* \mid x^*, \mathcal{D}) = \sum_f p(y^* \mid x^*, f)\, p(f \mid \mathcal{D})$$

Prior over functions...



Combine prior with data...



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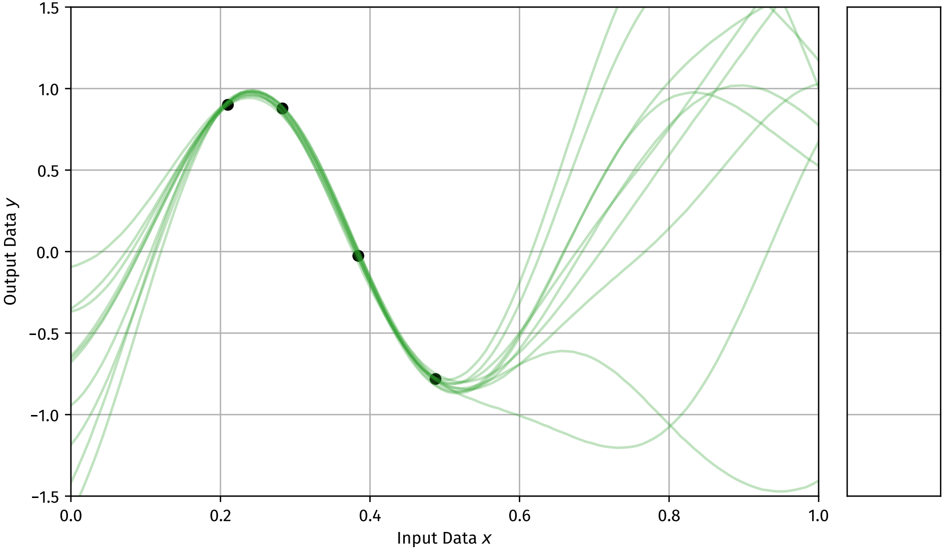

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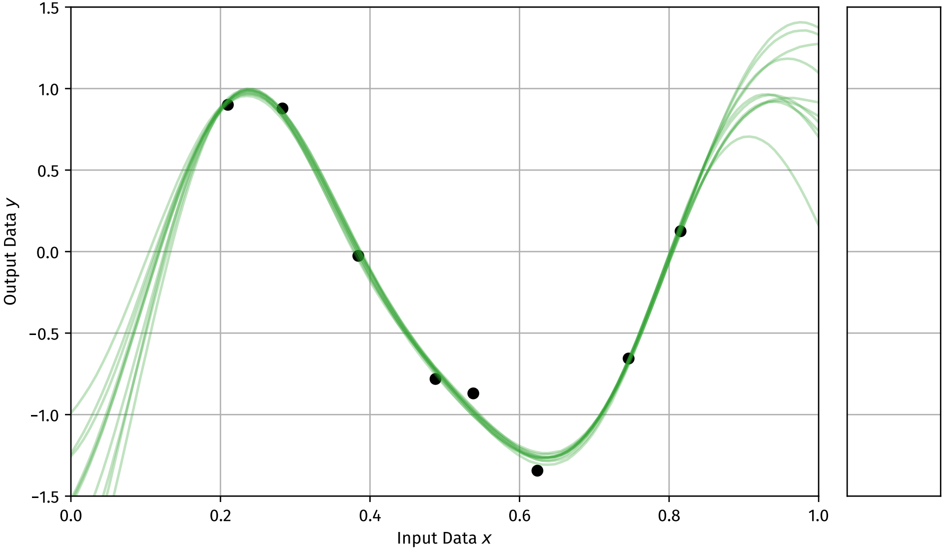
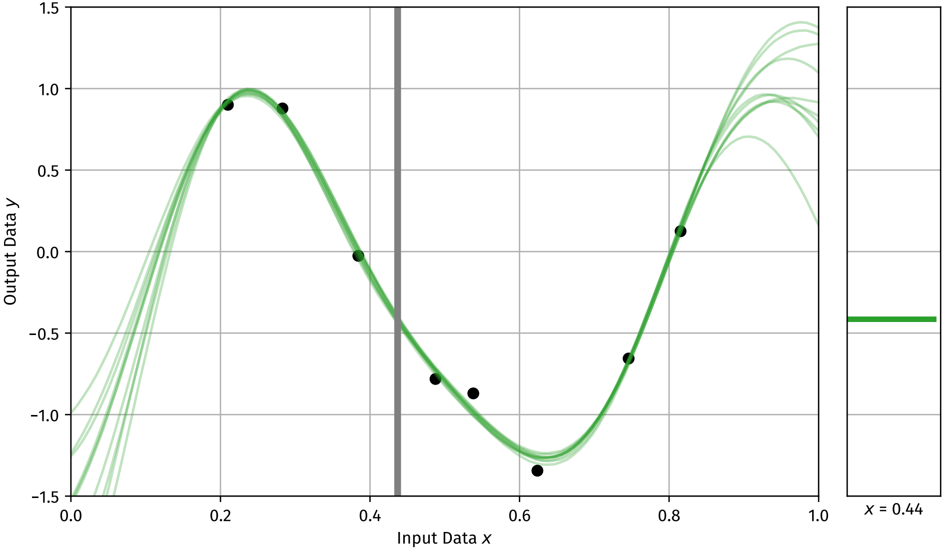
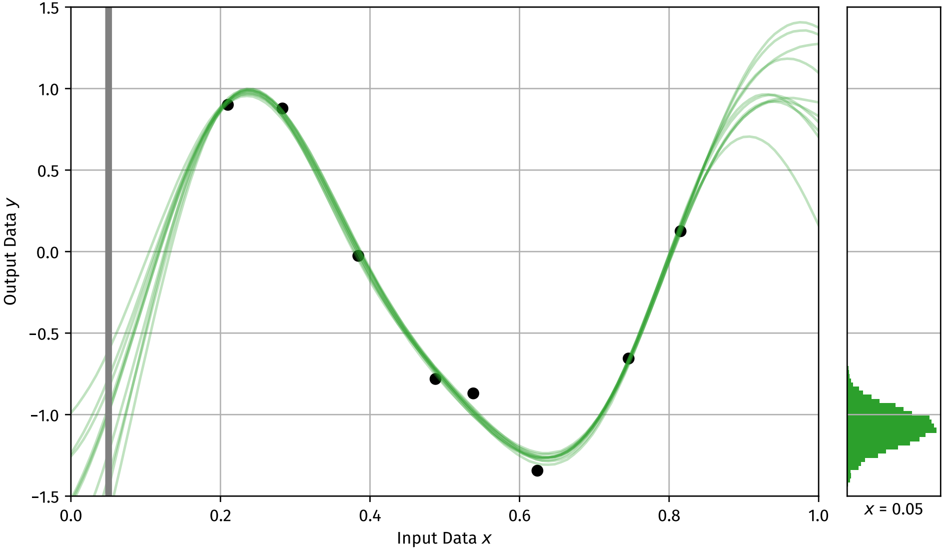


Average over functions to predict...



Averaging over functions gives us (Epistemic) Uncertainty!



Model Selection

- Overview
- No Free Lunch
- Uncertainty / Error Bars
- Model Selection
- Causality
- Conclusions

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we can only demonstrate that things are inconsistent with data

Model selection illustration: Gravity!

Stable Diffusion: *“Drop cannonball and orange off the leaning tower of Pisa.”*

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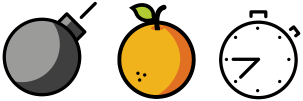
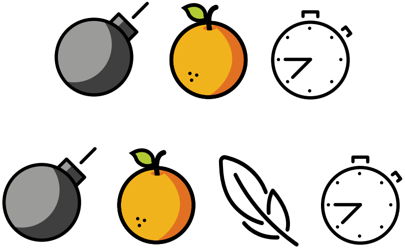


Model selection illustration: Gravity!

Stable Diffusion: *"Drop cannonball and orange off the leaning tower of Pisa."*



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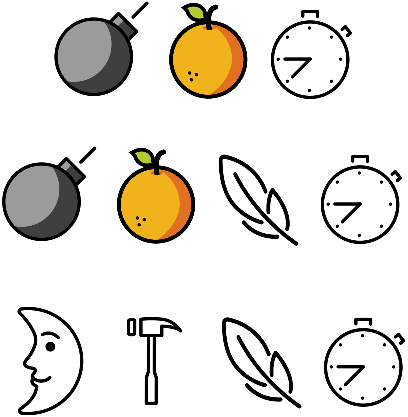

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Apollo 15 Hammer-Feather Drop

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At the end of the last Apollo 15 moon walk, Commander David Scott (pictured above) performed a live demonstration for the television cameras. He held out a geologic hammer and a feather and dropped them at the same time. Because they were essentially in a vacuum, there w ...more

Bayes' Rule for model selection..

$$\underbrace{p(w \mid \mathcal{D})}_{\text{Posterior}} = \frac{\overbrace{p(\mathcal{D} \mid \mathrm{w})}^{\text{Likelihood}} \times \overbrace{p(\mathrm{w})}^{\text{Prior}}}{\underbrace{p(\mathcal{D})}_{\text{Evidence}}}$$

Data $\mathcal{D} = \{X, Y\}$, input/output pairs, and parameters w

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If prior over models is equal, we compare via the Evidence for the Model: $p(\mathcal{D} \mid \mathcal{M} = m)$

Model selection example

Fitting polynomial models to data under Gaussian noise, $\varepsilon_n \sim \mathcal{N}(0, \sigma^2)$:

$$\text{Model 1} : y_n = a_0 + a_1 x_n + \varepsilon_n$$

$$\text{Model 2} : y_n = a_0 + a_1 x_n + a_2 x^2 + \varepsilon_n$$

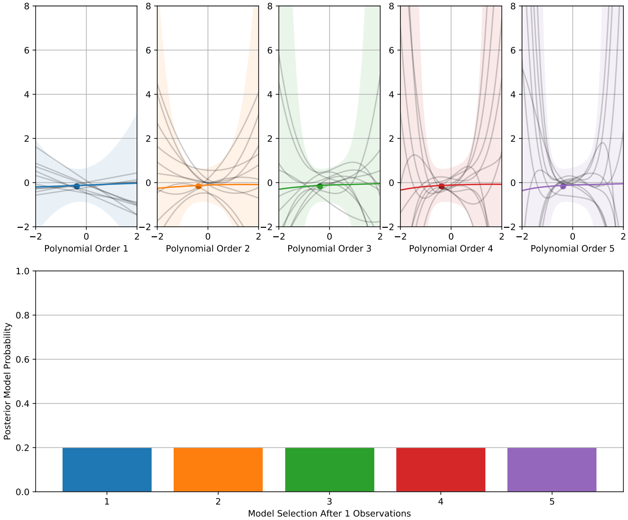
$$\text{Model 3} : y_n = a_0 + a_1 x_n + a_2 x^2 + a_3 x^3 + \varepsilon_n$$

$$\text{Model 4} : y_n = a_0 + a_1 x_n + a_2 x^2 + a_3 x^3 + a_4 x^4 + \varepsilon_n$$

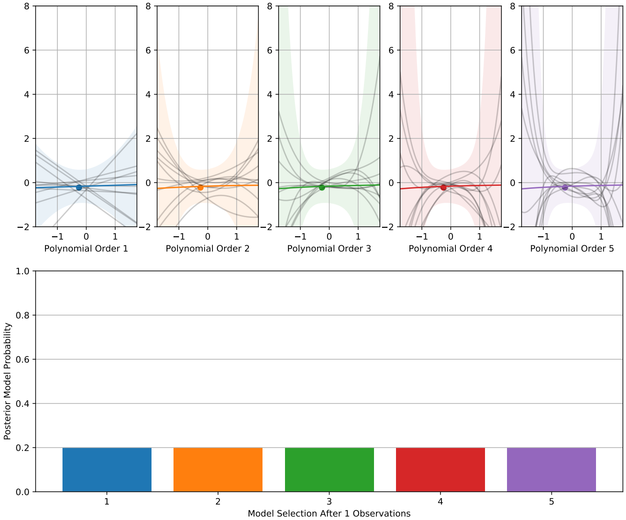
$$\text{Model 5} : y_n = a_0 + a_1 x_n + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + \varepsilon_n$$

Parameters $w_m = [a_0, \ldots, a_m]$ for model m, where $m \in [1, \ldots, 5]$.

Model selection example



Model selection example (more noise)



Causality

Overview...

Overview

No Free Lunch

Uncertainty / Error Bars

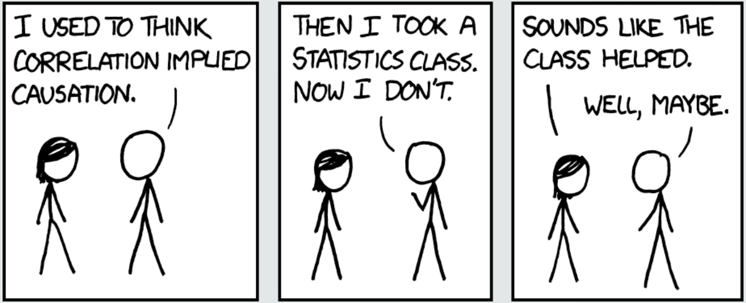
Model Selection

Causality

Conclusions

Correlation is not Causation

Correlation is not Causation



Danger Batman..

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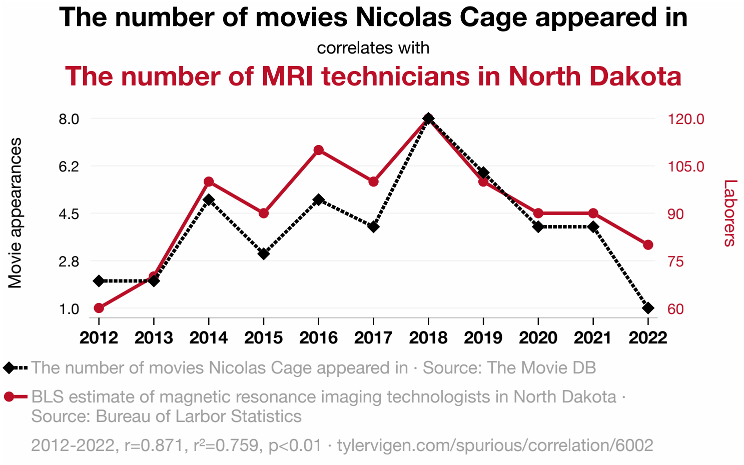

[https://tylervigen.com/spurious-correlations]

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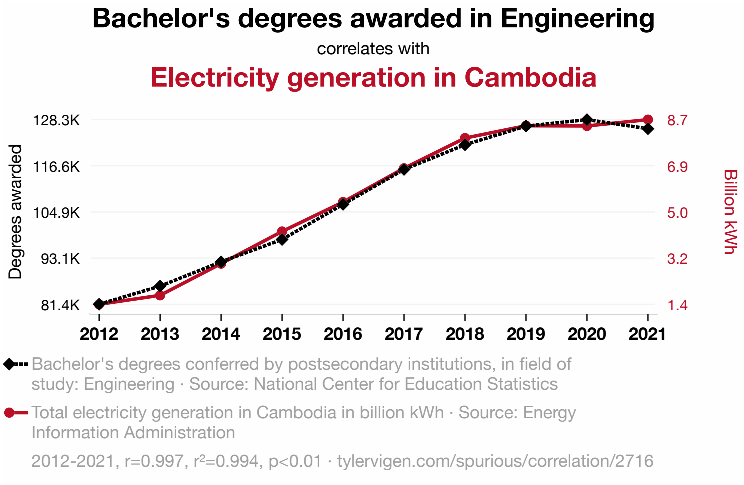

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“Correlation is not Causation”

- Do we need causation?
- Is science not just correlation?

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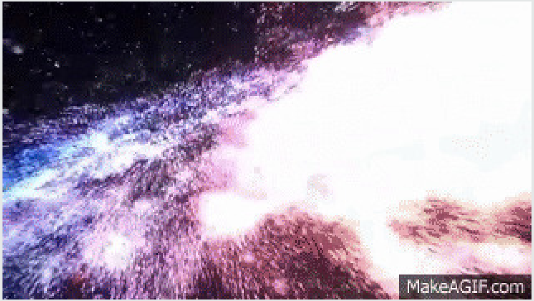
Importance simultaneously undervalued and overestimated?



Objectivity..

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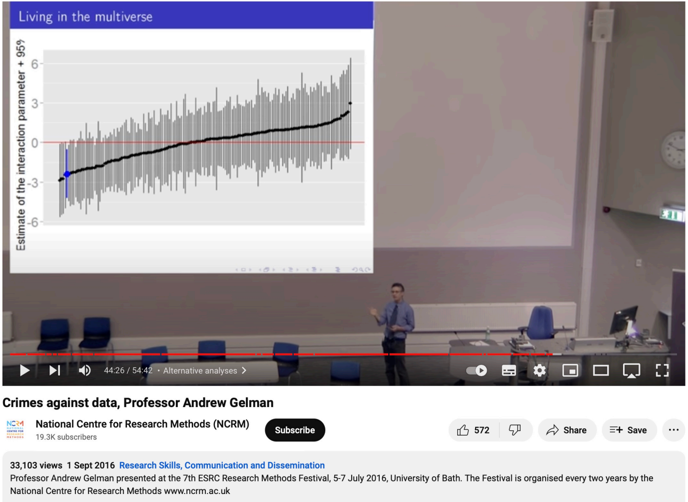

[Andrew Gelman: “Crimes against Data”]

Correlation vs Causation: What’s the difference?

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- Well we all know what the difference is..
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An object is the cause of another …

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- Introduces the idea of a counterfactual

Counterfactuals

- Real world:

$$\textsc{Action} \quad \longrightarrow \quad \textsc{Outcome}$$

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- Difference in outcome $=$ effect of the action!

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ACTION $\longrightarrow$ OUTCOME

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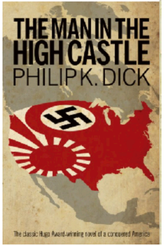
COUNTERFACUTAL ACTION $\longrightarrow$ COUNTERFACTUAL OUTCOME

- Difference in outcome = effect of the action!



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ML for Causation: Pearl's "Ladder of Causation"..

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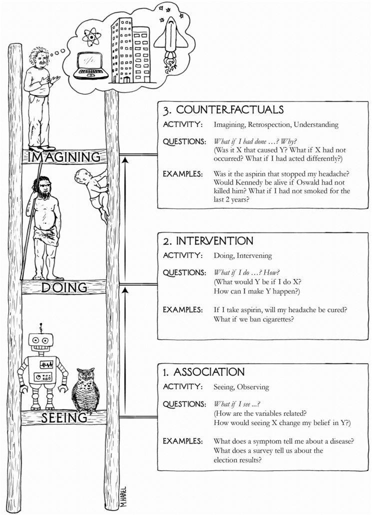

[Pearl and Mackensie 2017]

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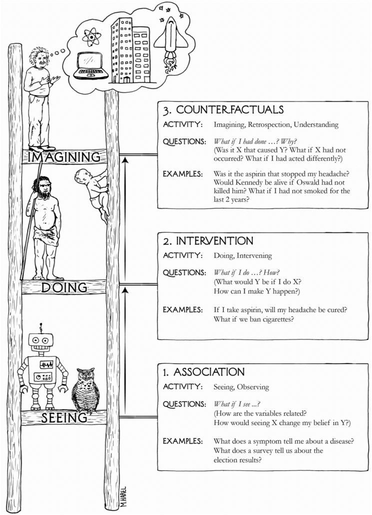

[Pearl and Mackensie 2017]

Causal reasoning cannot be answered by data alone we will need a model as well!

Illustration: Disease treatments

- Two disease treatments (surgical/non-surgival for kidney stones)

	Positive Outcome
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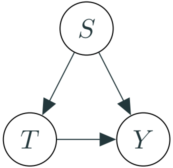

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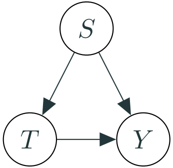

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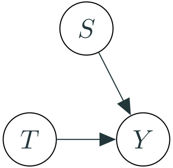

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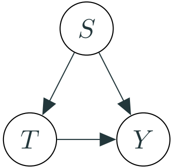

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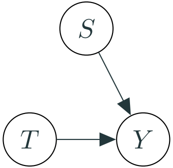

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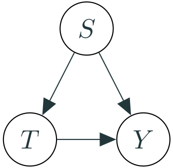

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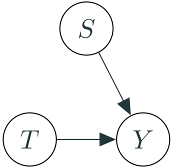

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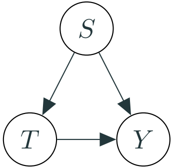

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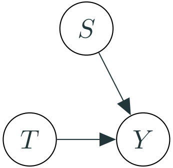

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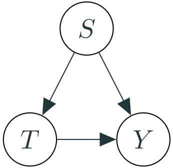

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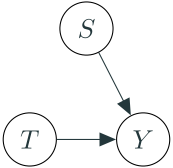

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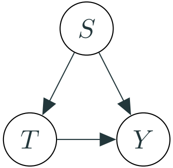

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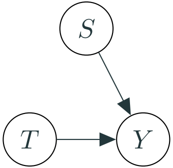

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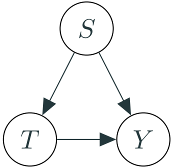

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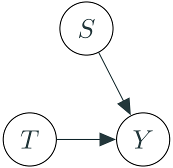

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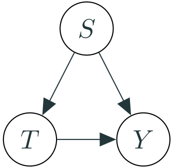

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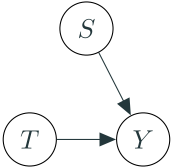

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$$p(Y \mid \mathsf{do}(T{=}b)) = \sum_s p(Y \mid S, \mathsf{do}(T{=}b))\, p(S) = 78\%$$

Causality

- Statistical/Probabilistic reasoning alone cannot support causal inference
- Determining the joint probability distribution of variables says nothing about causation
- Causal Inference: promises to determine the necessary set of (non-data) assumptions sufficient to make a causal conclusion

[Thanks to Julian Faraway for Causal Illustrations]

Conclusions

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Did we answer any of the questions?

- Can I use ML to solve x?
- What does ML actually do?
- Isn't ML just the same as y?
- Can I replace myself/my research team with ML?
- How much data do I need?
- Can I just use Deep Learning/Generative AI/ChatGPT?
- Surely Deep Learning/Generative AI/ChatGPT is all hype?
- Can any of this be used for science/engineering?

Conclusions

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  - Need a Bayesian method
- Want to analyse scientific results
  - e.g. does my new model explain dark matter
  - Need causal inference

Conclusions

Loads of gotchas..

- Availability (using the data you have not the data you need)
- Evaluation measure (is a human baseline sensible?)
- Ignore uncertainty/error bars
- Sample / dataset bias
- Bias / variance trade-off
- Haven't spoken about Decision Theory
- Lots to talk about regarding Causality
- "All models are wrong but some models are useful"
- ...

That’s all folks..

AI Talks: AI & ML Research Group, Department of Computer Science

11 Oct 2023	Prof Simon Prince
	Understanding Deep Learning: The Technology Behind Modern AI
15 Nov 2023	Prof Nello Cristianini
	The Shortcut: How Machines Became Intelligent Without Thinking in a Human Way
13 Dec 2023	Prof Mike Tipping
	The Irresistible Rise of Machine Learning
28 Feb 2024	Prof Neill Campbell
	No Free Lunches in Machine Learning
20 Mar 2024	Prof Özgür Şimşek
	Reinforcement Learning and the Pursuit of Artificial Intelligence
17 Apr 2024	Dr Harish Tayyar Madabushi
	Emergent Abilities of Language Models: Do they pose an existential threat?
8 May 2024	Prof Darren Cosker
	AI for Human Sensing: Research, Productisation and Ethics
TBD	Prof Mike Tipping
	Bayesian Inference in Machine Learning: Indistinguishable from Magic?