# Machine Learning

## Bayesian Optimisation

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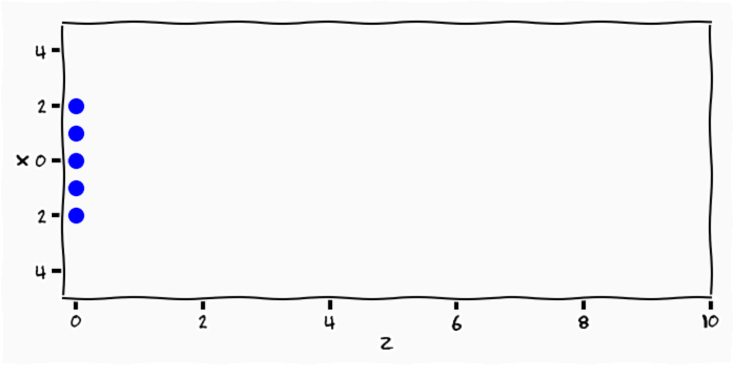
# Introduction

## Unsupervised Learning



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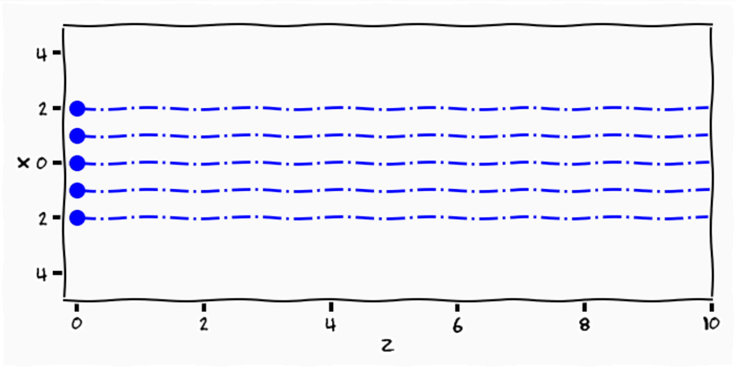

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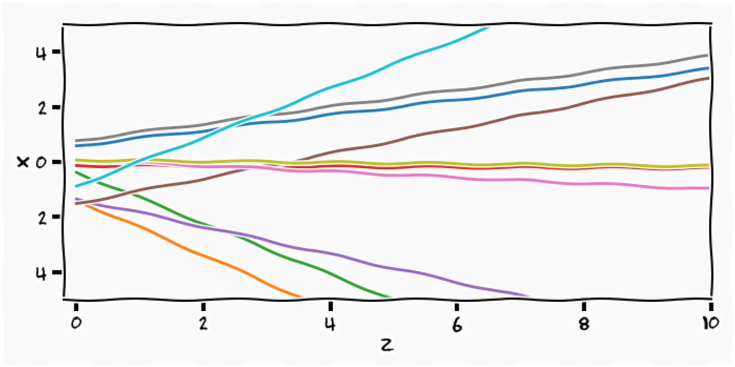

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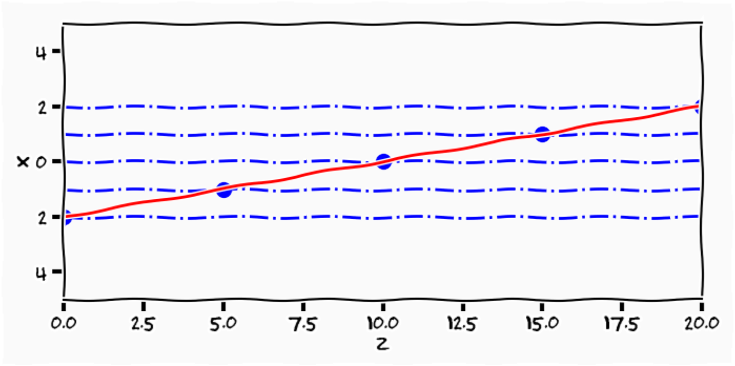

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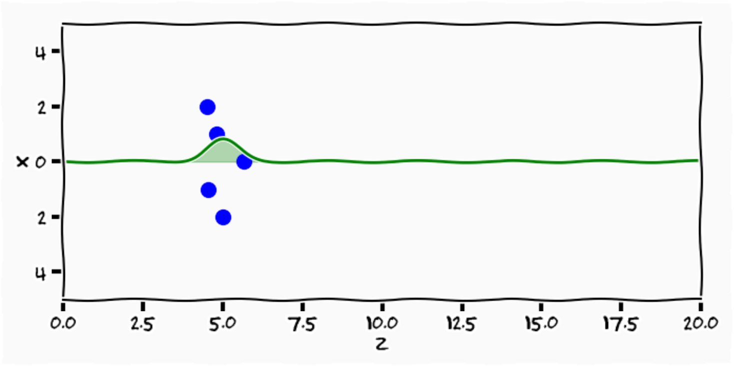

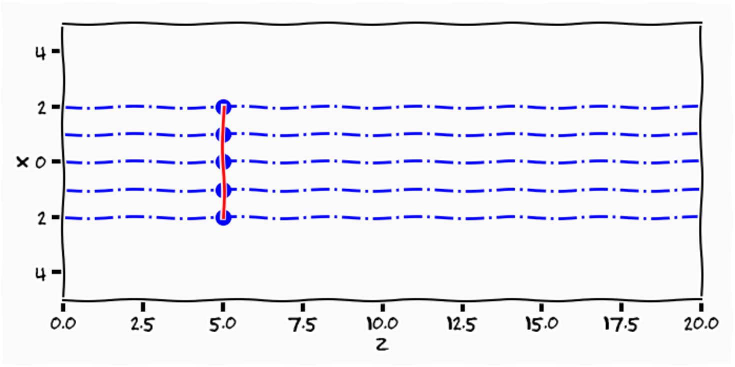
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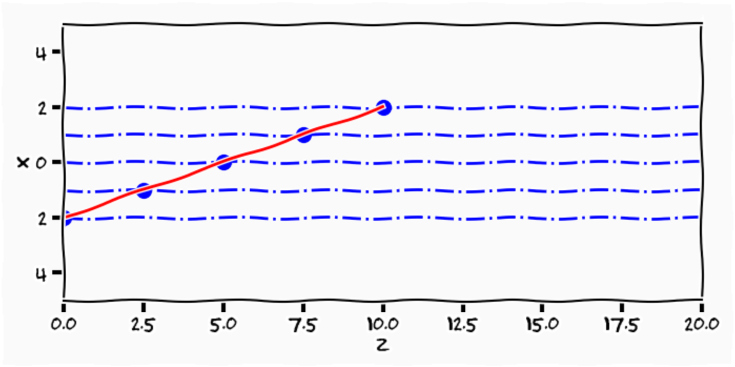

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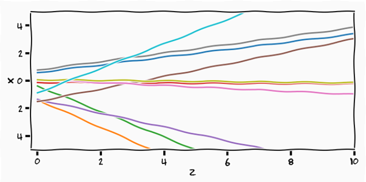


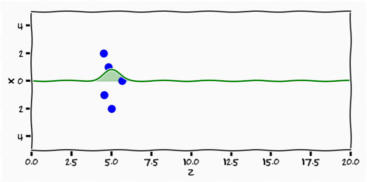


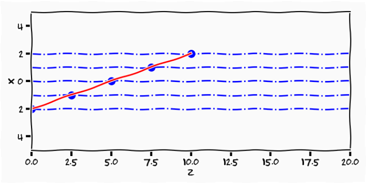

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- Linear Regression

$$p(\mathbf{W}|\mathbf{t}, \mathbf{X}) \propto p(\mathbf{t}|\mathbf{W}, \mathbf{X})p(\mathbf{W})$$

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- Actually formulating the posterior over both $\mathbf{W}$ and $\mathbf{z}$ is intractable

# Type II Maximum Likelihood

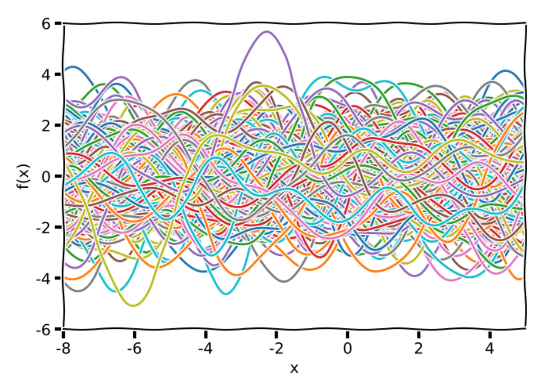
$$\hat{\mathsf{W}} = \text{argmax}_{\mathsf{W}} p(\mathsf{x}|\mathsf{W}) = \int p(\mathsf{x}|\mathsf{W}, \mathsf{z}) p(\mathsf{z}) \mathrm{d}\mathsf{z}$$

1. Intractable to reach posterior of both
2. Integrate out one variable, marginalise, expectation
3. Take point-estimate of the remaining

# Principal Component Analysis

- You might have seen this explained in a different way
  - *Retain variance*
  - *Error minimisation*
- These provides the same solution as the maximum likelihood but solved by an eigenvalue problem
- Do not provide intuition as it doesn't state assumptions

# Non-linear latent variable model




$$p(\mathsf{x}, \mathsf{z}|\theta) = \int p(\mathsf{x}|\mathbf{f})p(\mathbf{f}|\mathsf{z}, \theta)p(\mathsf{z})\mathrm{d}\mathbf{f}$$

# Unsupervised Learning

- Unsupervised learning is a misnomer, there is no such thing, you have to have beliefs in order to learn.
- Think about unsupervised learning as "less supervised" learning, you have to have stronger beliefs

# Machine Learning

1. Specify your statistical model over sample space $\mathcal{Y}$, relationship between "parameters" and observations

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3. Formluate your belief in the "setting" of the model

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4. Aquire data
5. Derive your updated belief, derive knowledge from data

$$p(\theta|\mathbf{Y}) = \frac{p(\mathbf{Y}|\theta)p(\theta)}{\int p(\mathbf{Y}|\theta)p(\theta)}$$

# Next lectures

| | |
|---|---|
| **Today** | Bayesian Optimisation |
| **Tuesday** | Evidence and Graphical Models |
| **Monday** | Dirichlet Processes |
| **Tuesday** | Topic Models |
| **Monday** | Neural Networks |
| **Tuesday** | Reinforcement Learning |

The aim is for you to connect these things to what you have learnt so far and see that what the methodology allows you to do and different tools following the same methodology. Try to see that it is all the same thing.

# Bayesian Optimisation

# Uncertainty

- Deterministic world

$$x = 4$$

- Point estimate world

$$\text{argmax}_x p(x) = 4$$

- Stochastic world

$$p(x) = \mathcal{N}(4, 10^2)$$

# Uncertainty

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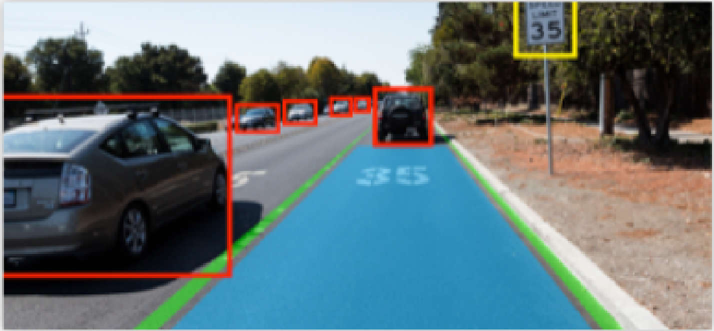


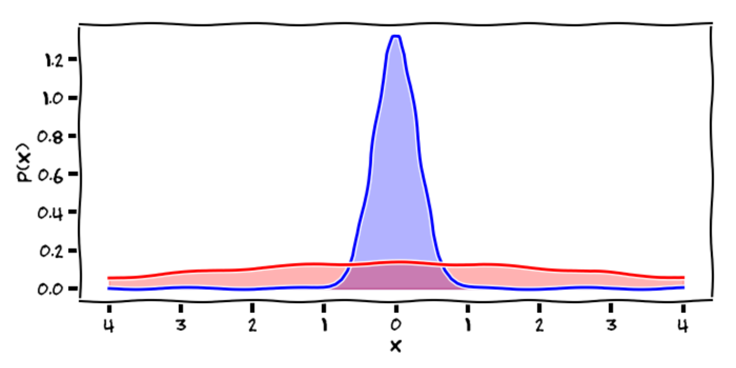
# The Uber Crash

# The Uber Crash[1]

*..the system first registered radar and LIDAR observations of the pedestrian about 6 seconds before impact, when the vehicle was traveling at 43 mph. As the vehicle and pedestrian paths converged, the self-driving system software classified the pedestrian as an unknown object, as a vehicle, and then as a bicycle with varying expectations of future travel path.*

[1] Link to report

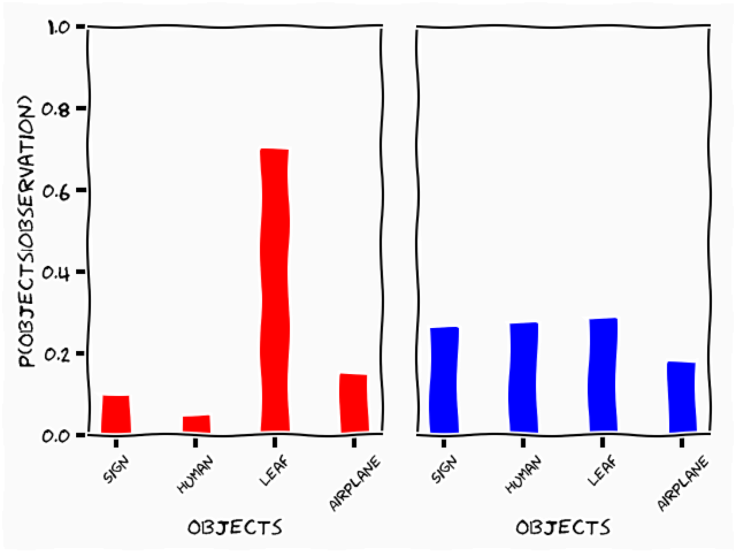
# The importance of uncertainty




$$\hat{x} = \mathrm{argmax}_x \, p(x) = \mathrm{argmax}_x \, p(x)$$

$$p(\hat{x}) \neq p(\hat{x})$$

# The importance of uncertainty



# The Uber Crash[1]

*According to Uber, emergency braking maneuvers are not enabled while the vehicle is under computer control, to reduce the potential for erratic vehicle behavior. The vehicle operator is relied on to intervene and take action. The system is not designed to alert the operator.*

# Real Doctors

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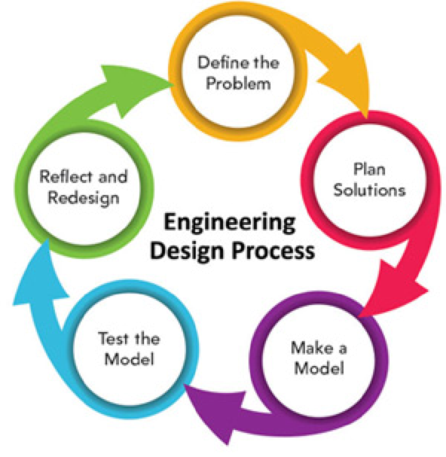
# Medicine

# Data science

# Design


Define the Problem
Plan Solutions
Make a Model
Test the Model
Reflect and Redesign
Engineering Design Process

# Optimisation

- All problems above can be seen as optimisation problems
- Classic optimisation

$$\hat{x} = \mathrm{argmin}_x f(x)$$

- Much more common

$$\hat{x} = \mathrm{argmin}_x \text{black-box}(x)$$

# Optimisation

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- in most cases we have an objective function that we do not know
- we can test something and see how it works, i.e. evaluate the function
- the number of parameters, possible tests are huge
- the cost of each test is expensive
- the test is noisy
- *can we use machine learning to do this for us?*

# Global Optimisation

$$x_M = \text{argmin}_{x \in \mathcal{X}} f(x)$$

- $\mathcal{X}$ is a bounded domain
- $f$ is explicitly unknown
- Evaluations of $f$ may be noisy
- Evaluations of $f$ is expensive

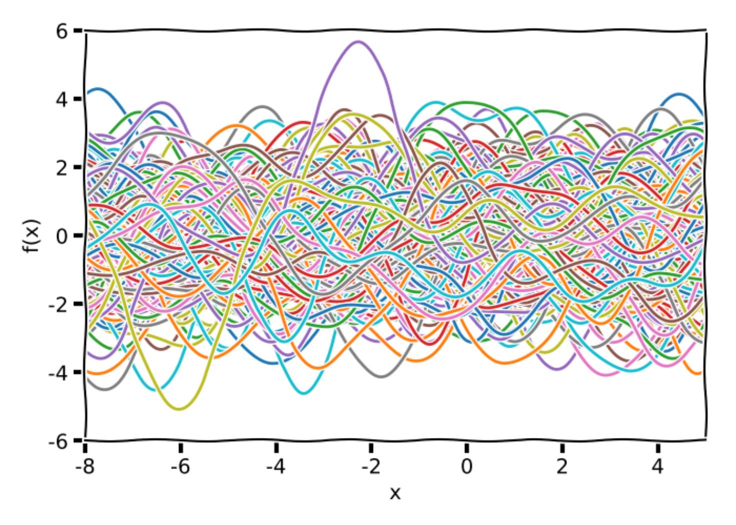
# Strategies

- Implicit knowledge
- Grid search

$$f(x_M) - f(x'_M) \leq \epsilon$$

  we need $(L/\epsilon)^D$ evaluations (if f is L-Lipschitz)
- Random sampling

# BO in practice



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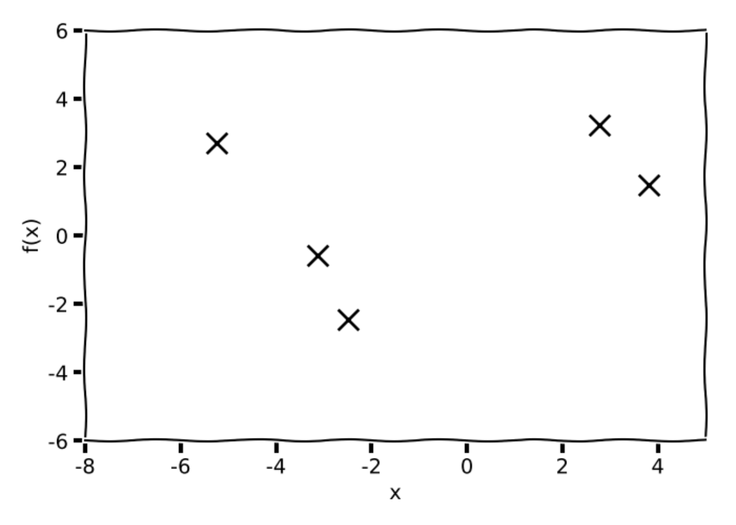

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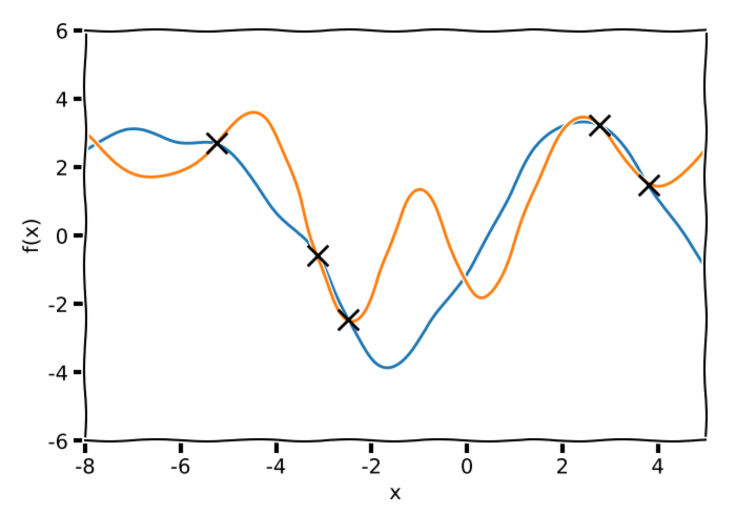

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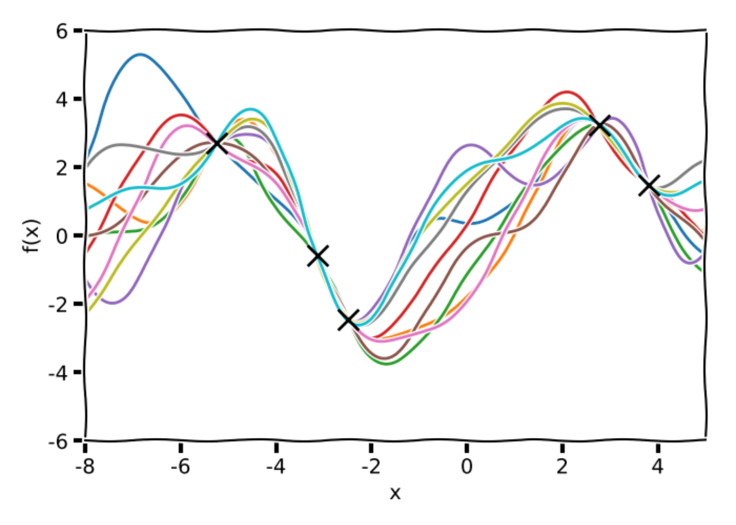

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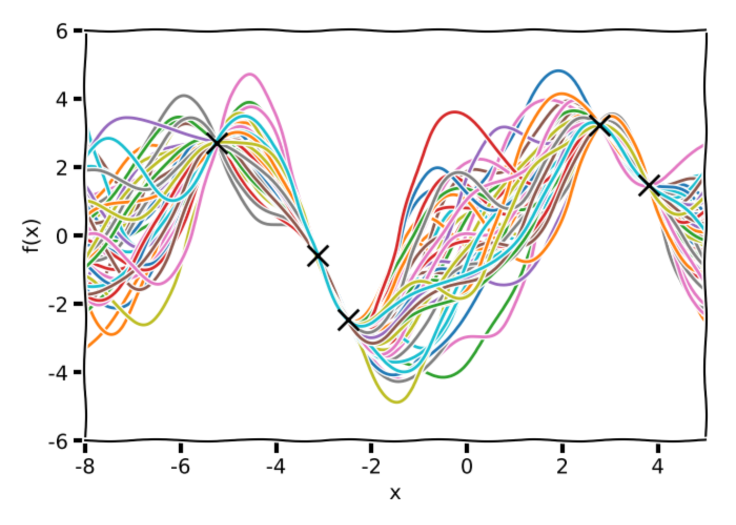

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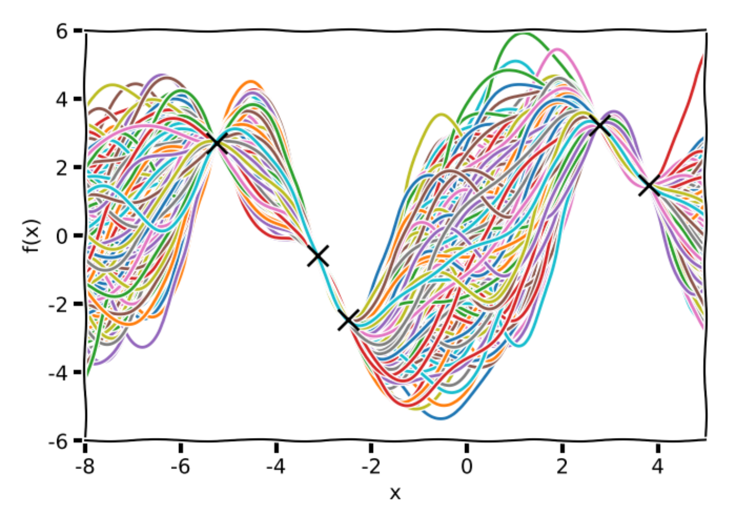
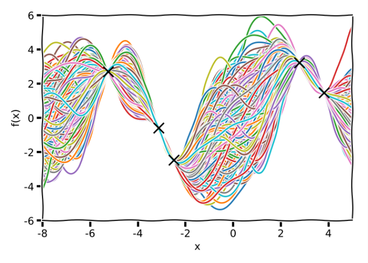
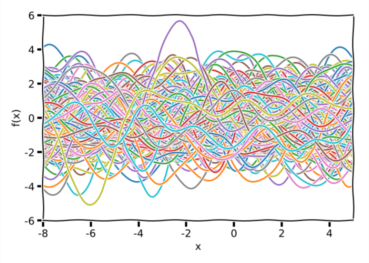


# What did we actually do




$$p(f_*|f, \mathbf{X}, \mathbf{x}_*) = \frac{p(f_*, f|\mathbf{X}, \mathbf{x}_*)}{p(f|\mathbf{X})}$$

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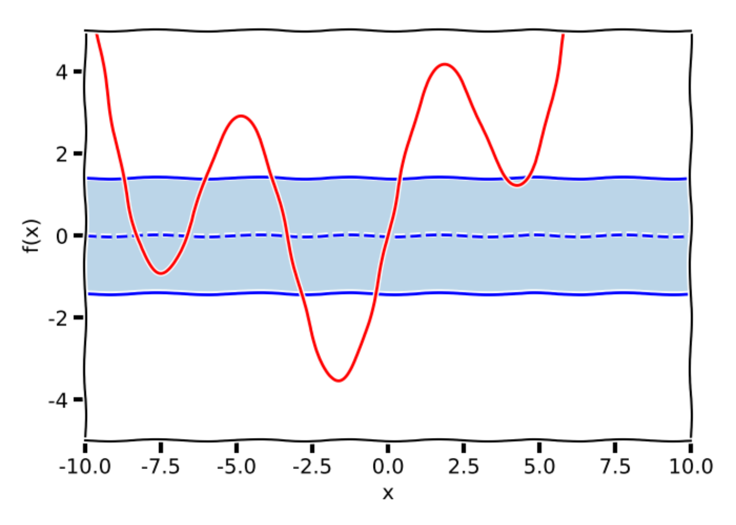

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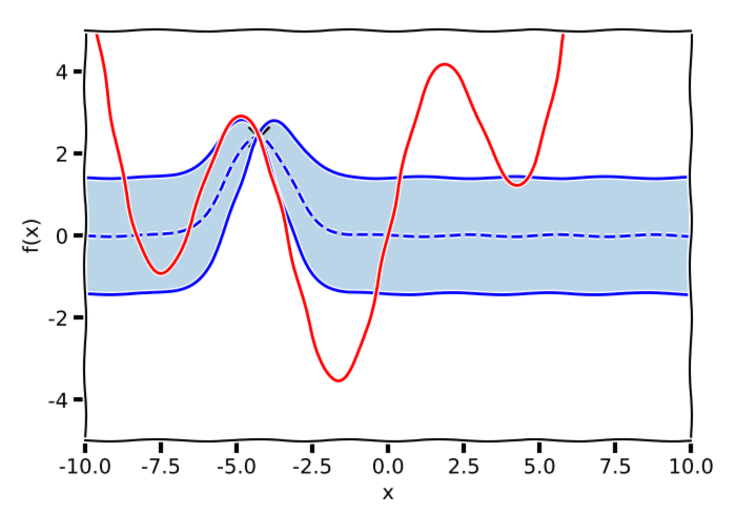

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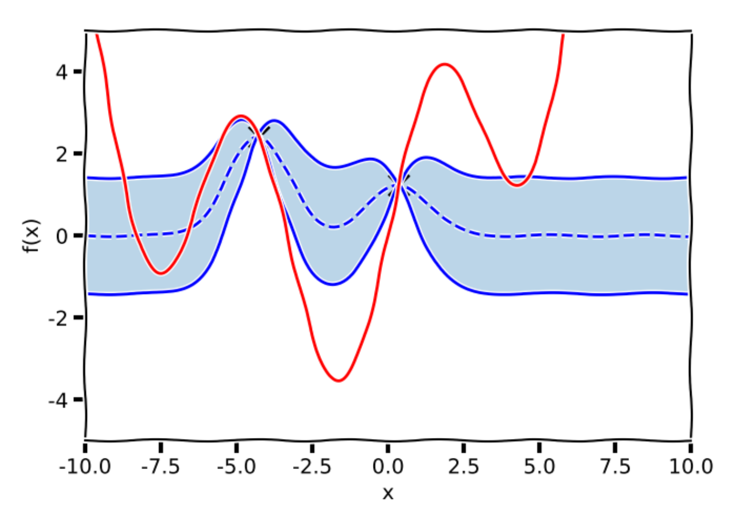

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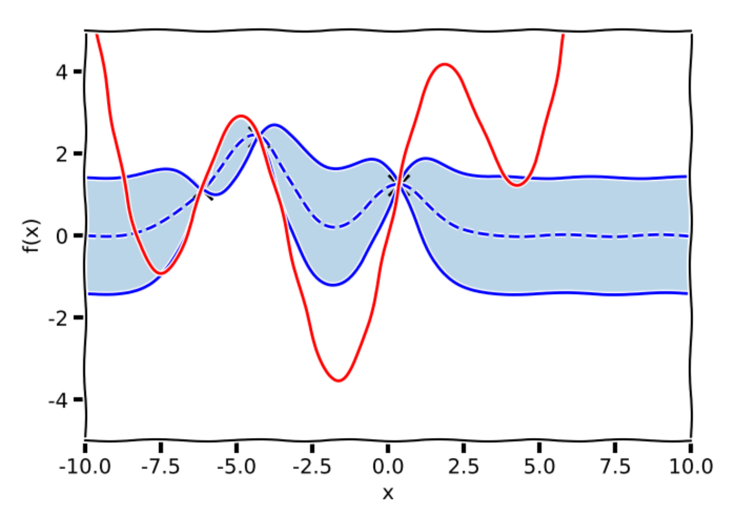

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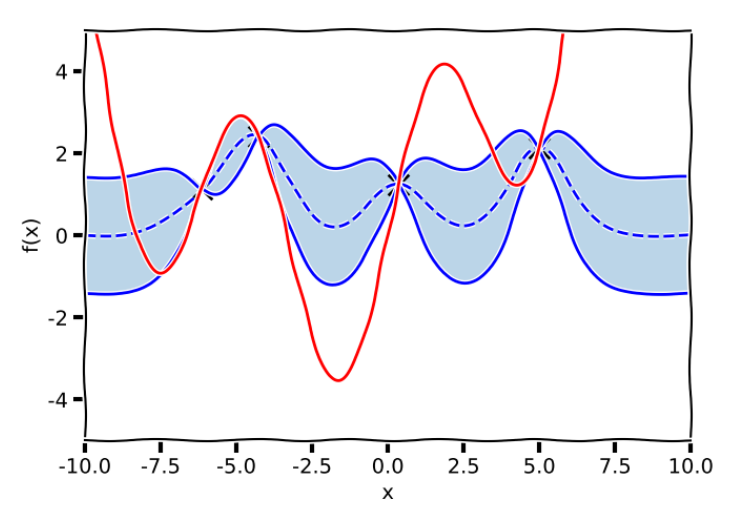

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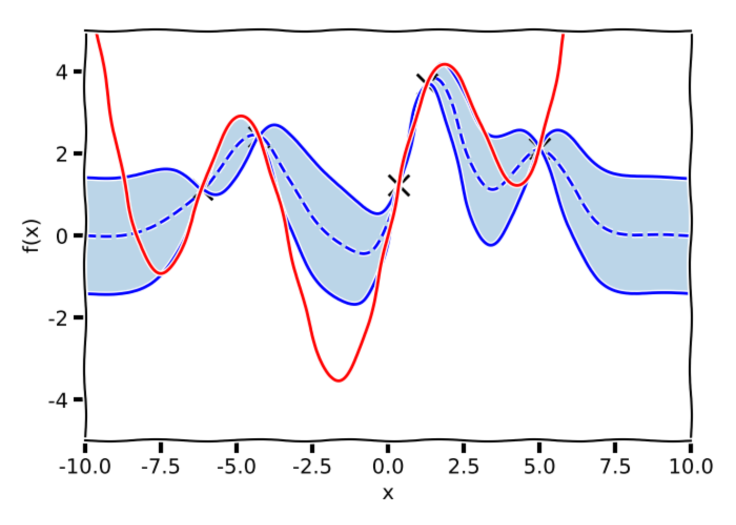

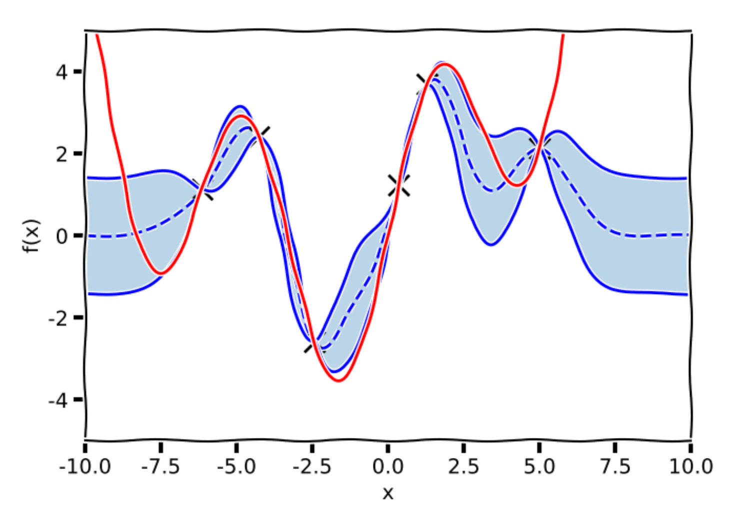
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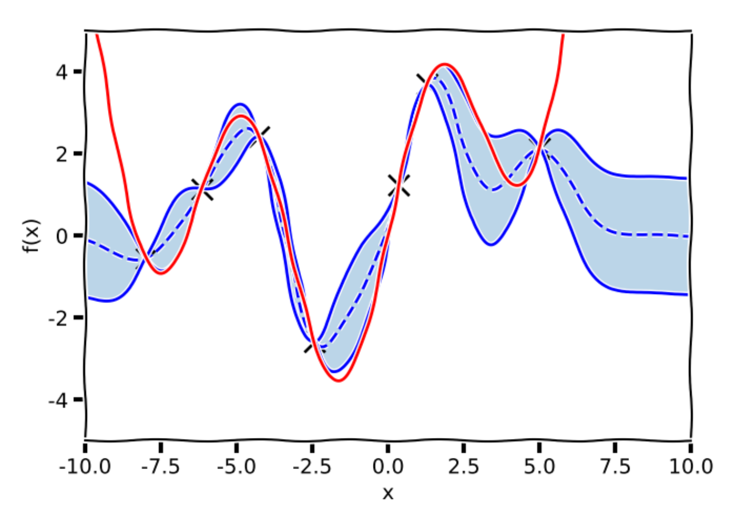

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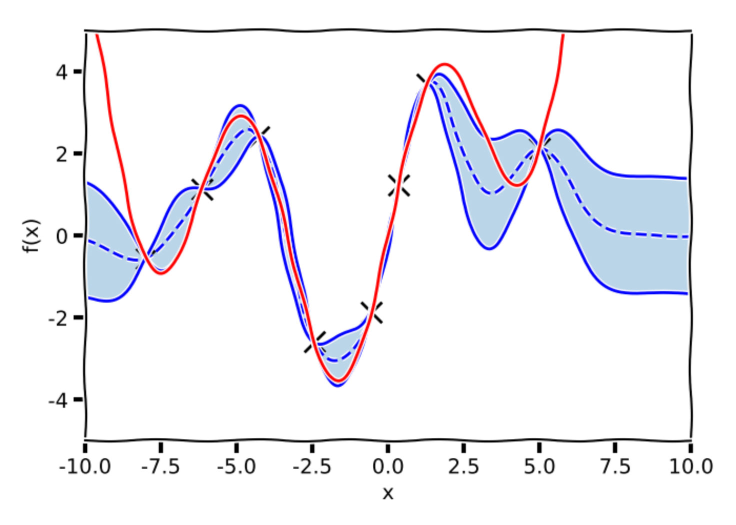

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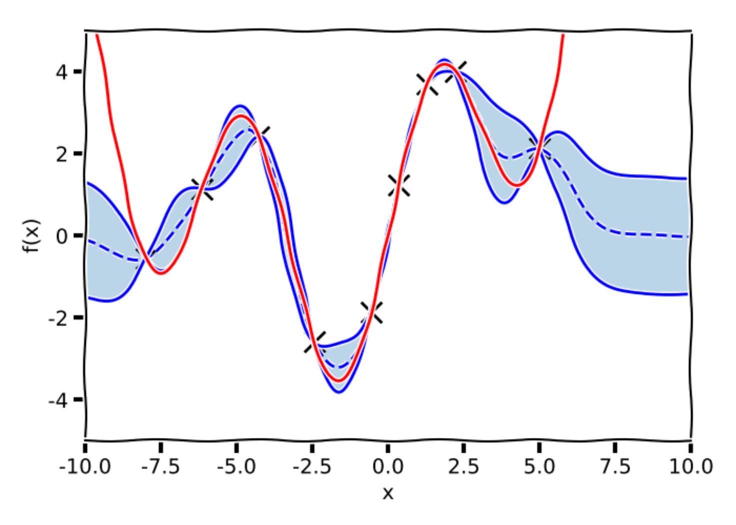

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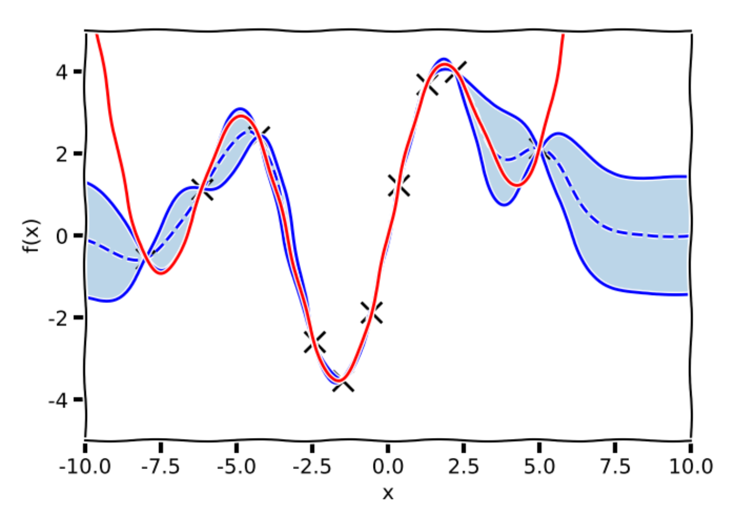

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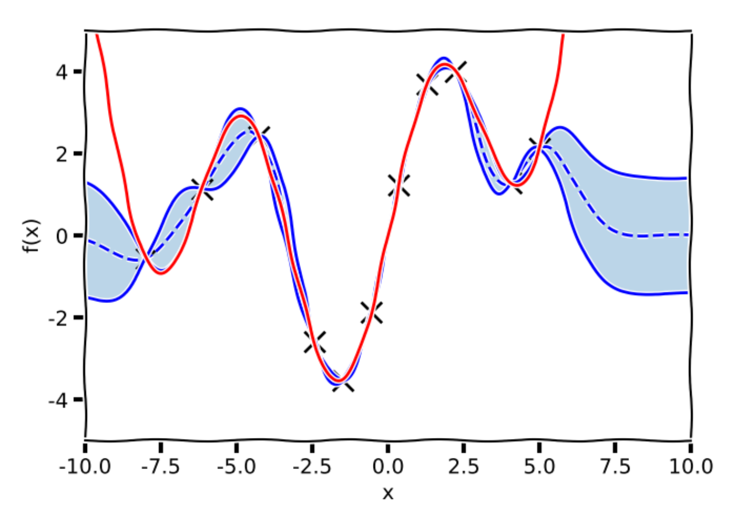

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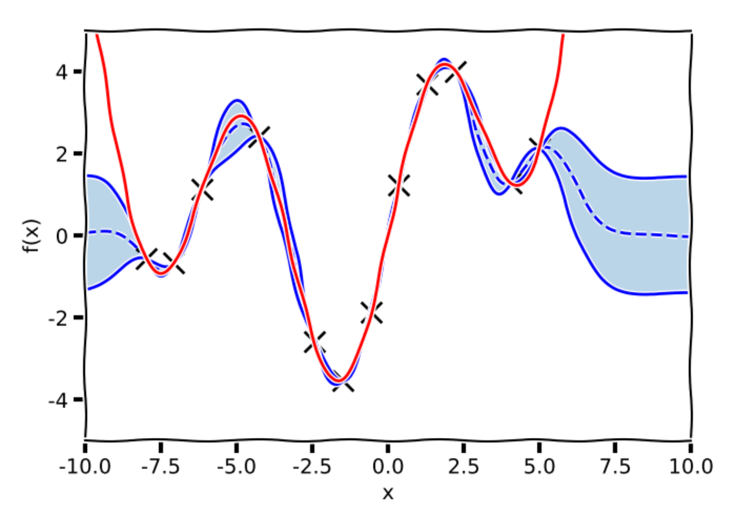

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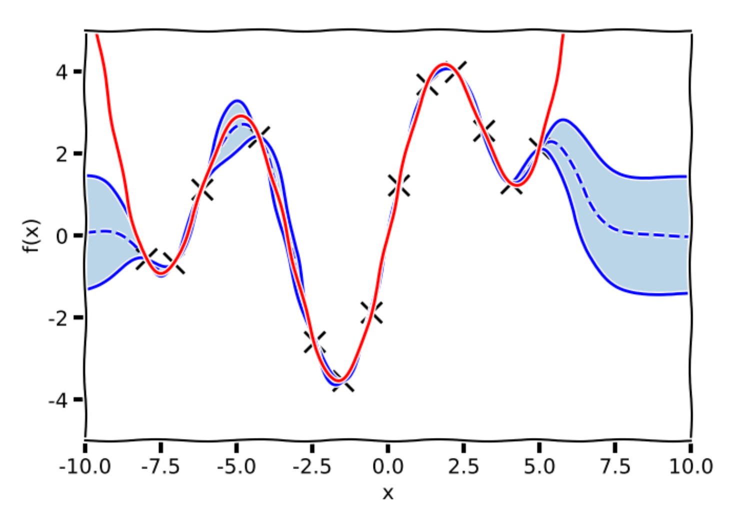

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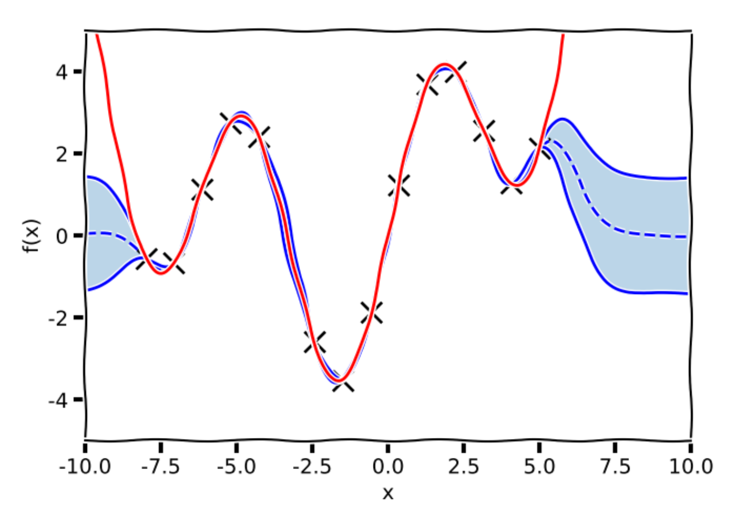

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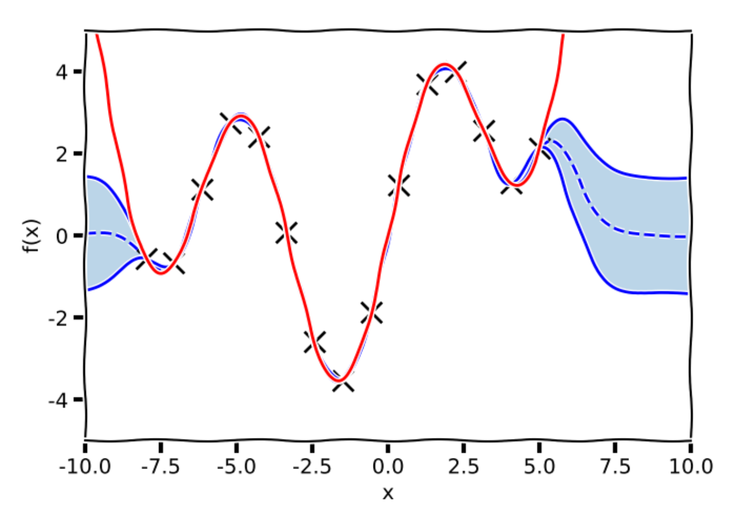

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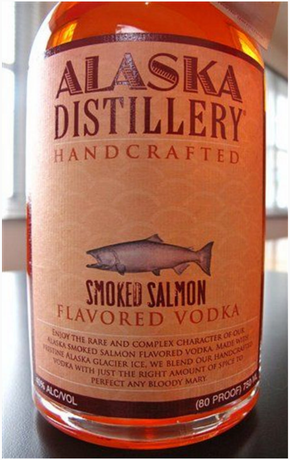
# Exploration vs Exploitation

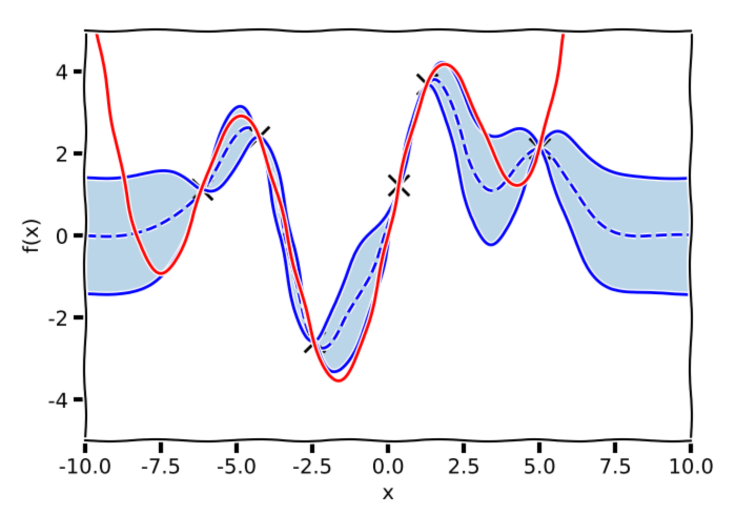
## Exploration vs Exploitation


# Balance is the key



# Aquisition function

- how should we explore the space?
- humans do active search?
    - studying for exam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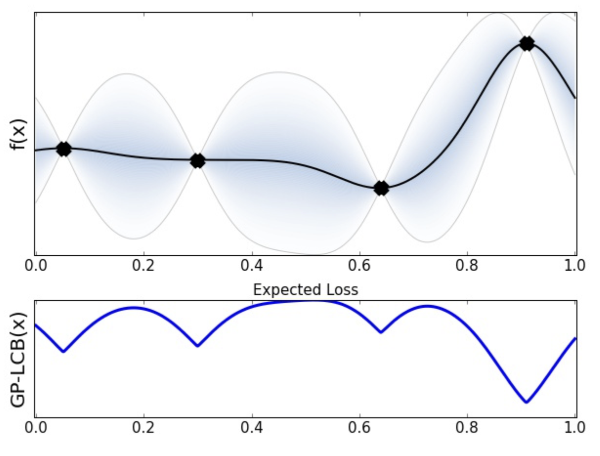
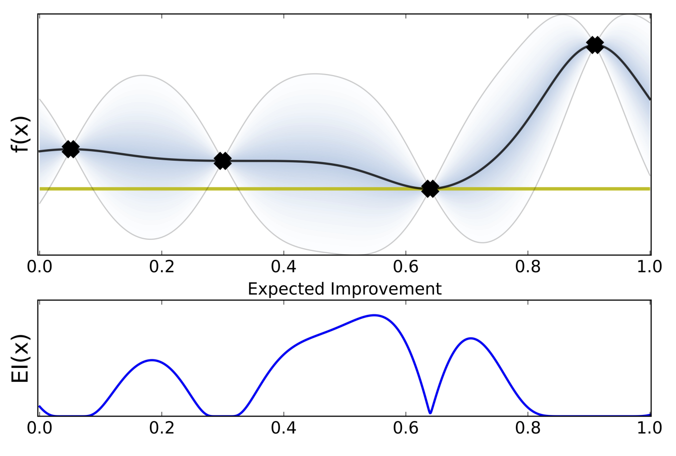
# Confidence



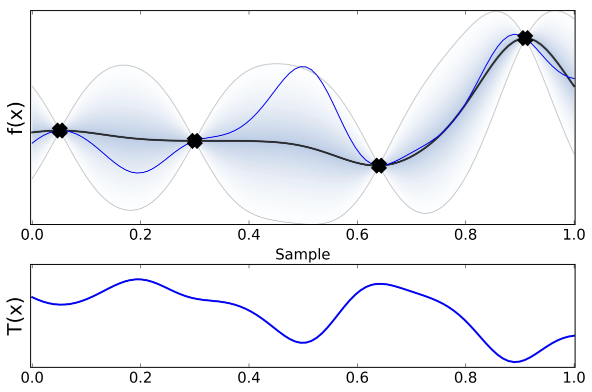

$$\alpha(\mathsf{x}; \theta, \mathcal{D}) = -\mu(\mathsf{x}; \theta, \mathcal{D}) + \beta_t \sigma(\mathsf{x}; \theta, \mathcal{D})$$

# Expected Improvement




$$\alpha(\mathbf{x}; \theta, \mathcal{D}) = \int \max(0, y_{\text{best}} - y) p(y|\mathbf{x}, \theta, \mathcal{D}) \mathrm{d}y$$

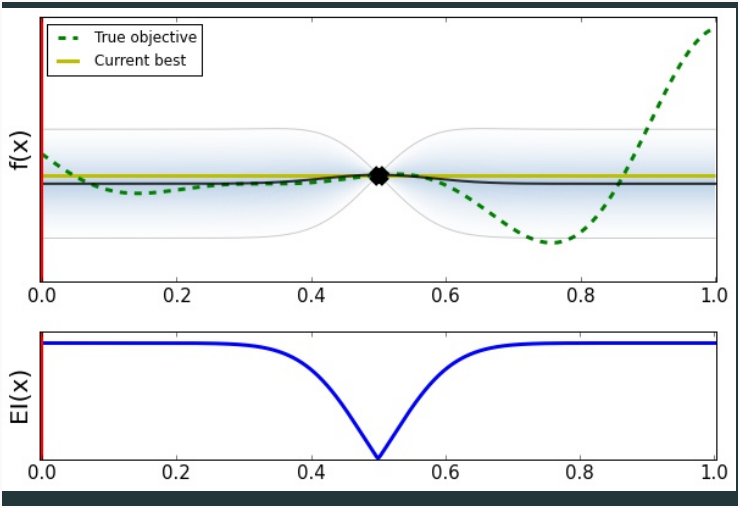
# Thomson Sampling




$$\alpha(\mathbf{x}; \theta, \mathcal{D}) = g(\mathbf{x})$$

$$g(\mathbf{x}) \sim p(y|\mathbf{x}, \theta, \mathcal{D})$$

# Bayesian Optimisation [2]




[2]Slides courtesy of Javier Gonzales

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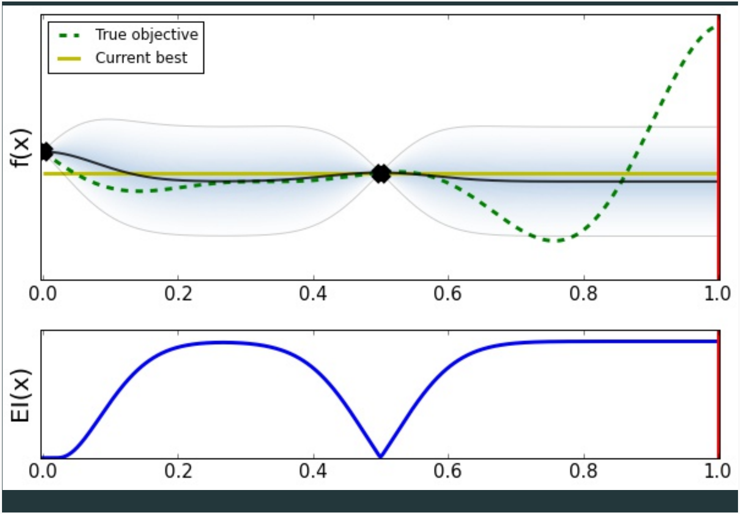


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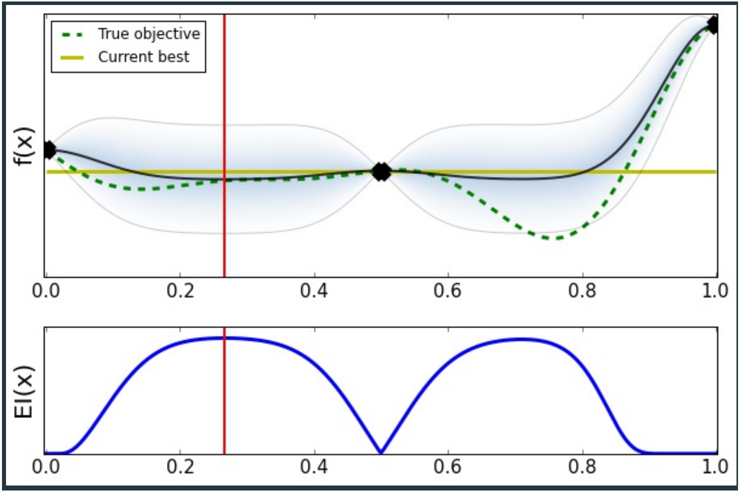


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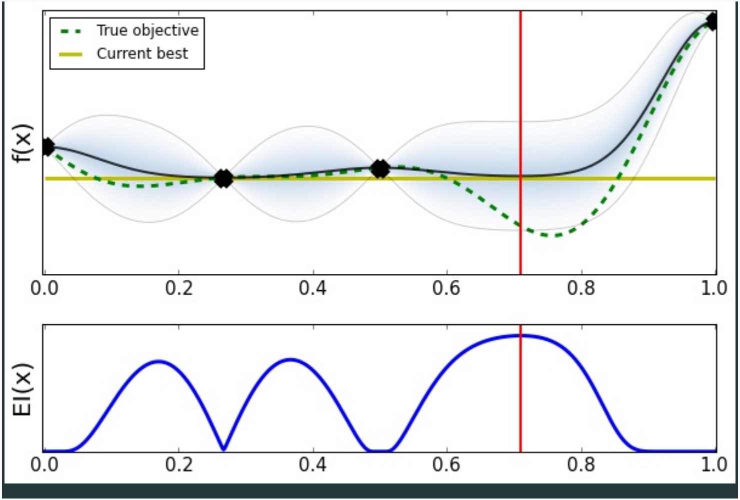


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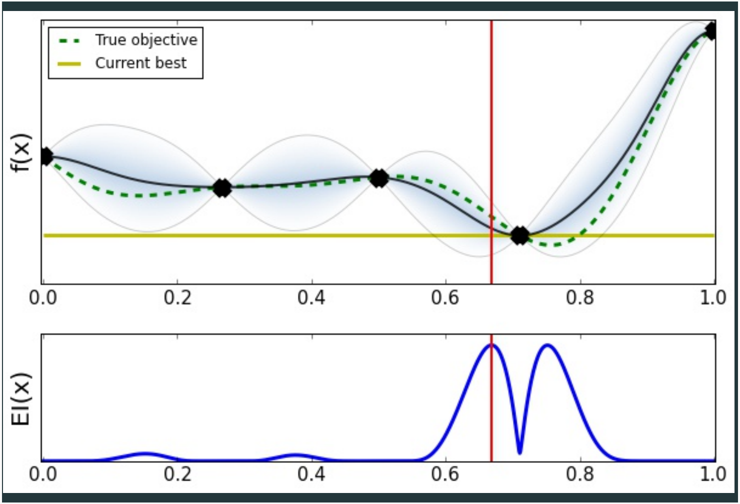


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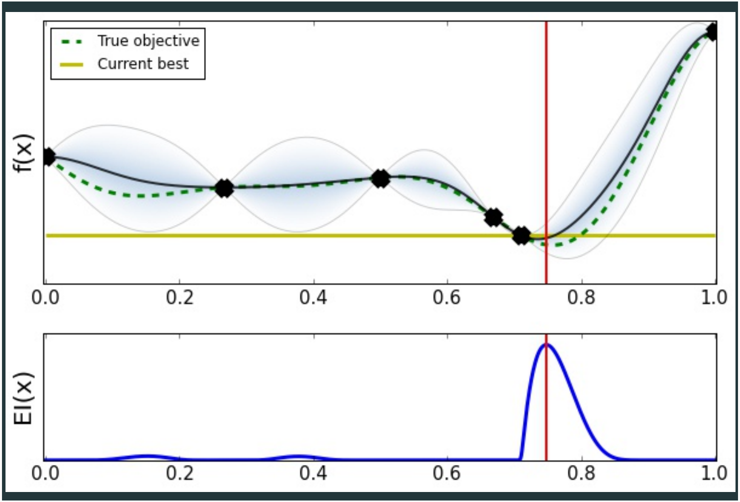


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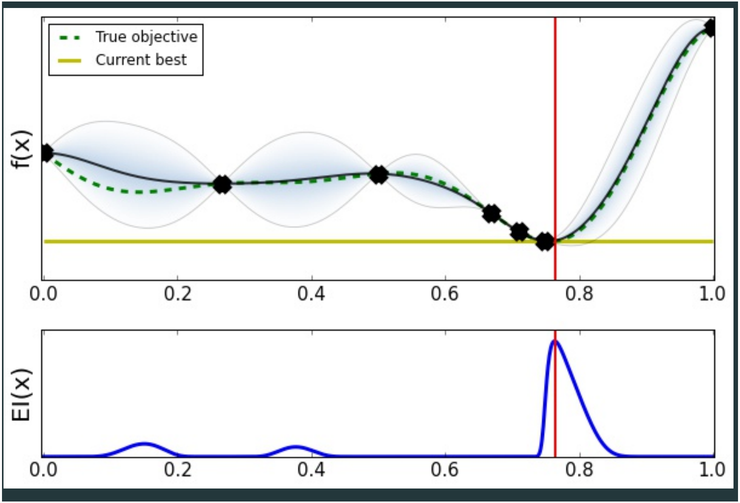


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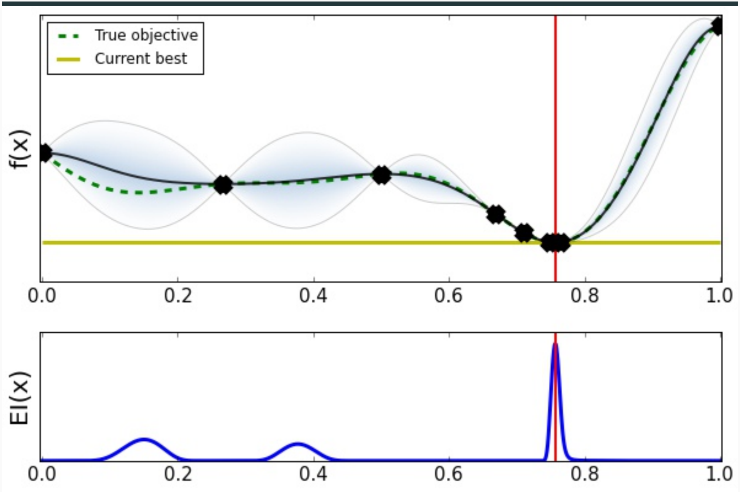


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    - $\alpha(x)$ is cheap to compute

# Bayesian Optmisation

- What assumptions can we make about the function that we are optimising?
  - kernel
  - kernel parameters
  - etc.
- What search strategy should we have
  - exploration vs. exploitation
  - cost of search
- How should we optimise the aquisition function

# Why [3]

| Consumption | $CO_2$ (lbs) |
|---|---:|
| Air travel NY-SF | 1 984 |
| Human life (1 year) | 11 023 |
| American life (1 year) | 36 156 |
| Car life-time | 126 000 |
| Transformers NN | 626 155 |

[3] Strubell, E., Ganesh, A., & McCallum, A., Energy and policy considerations for deep learning in nlp, CoRR, (), (2019).

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    - Aquisition function to model exploration
- Take home message: *uncertainty matters*

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# References

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