UNIVERSITY OF CAMBRIDGE

Machine Learning and the Physical World

Lecture 6 : Sequential Decision Making - Bayesian Optimisation

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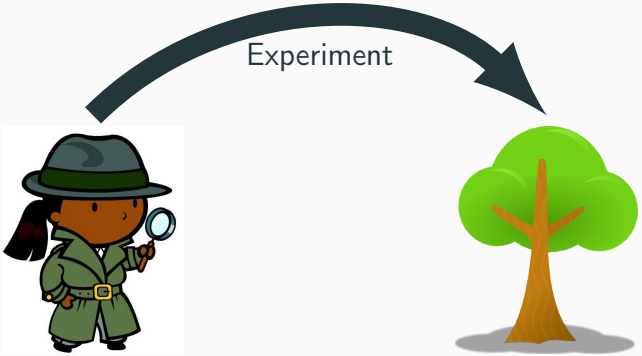
$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \int \ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y) p(x, y) \mathrm{d}x \mathrm{d}y$$

- $\mathcal{F}$ space of functions
- $\mathcal{A}$ learning algorithm
- $\mathcal{S} \sim P(\mathcal{X} \times \mathcal{Y})$
- $\ell(\mathcal{A}_{\mathcal{F}}(\mathcal{S}), x, y)$ loss function

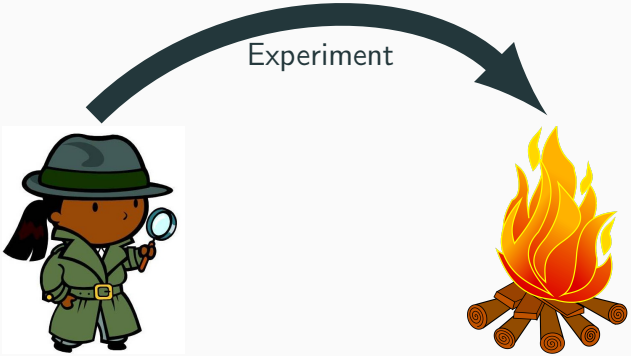
Active Learning

Active Learning

Active Learning



Active Learning



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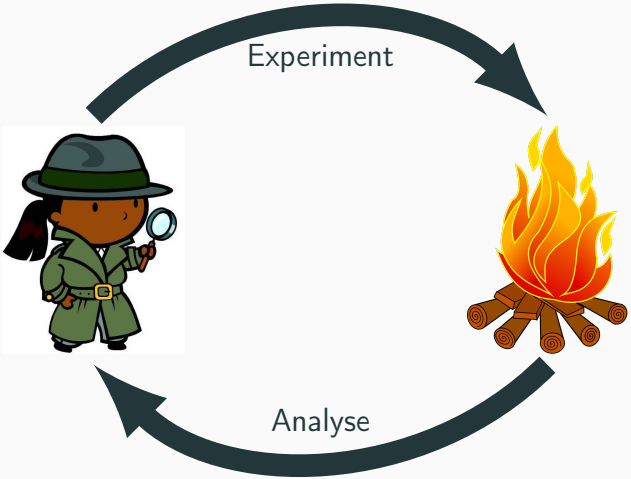
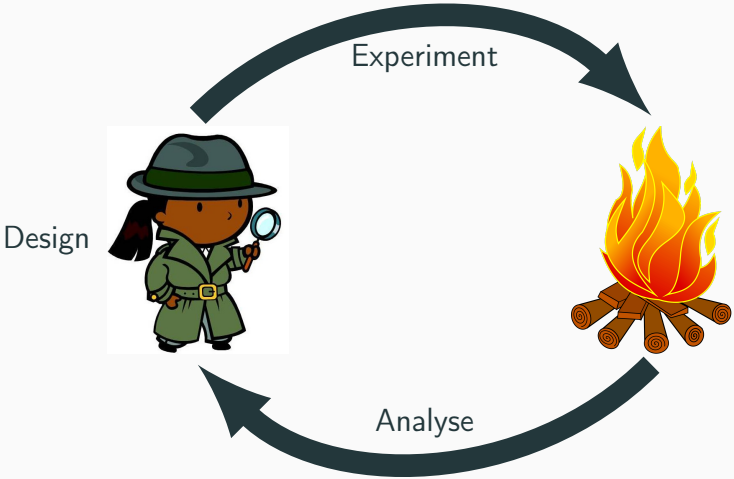
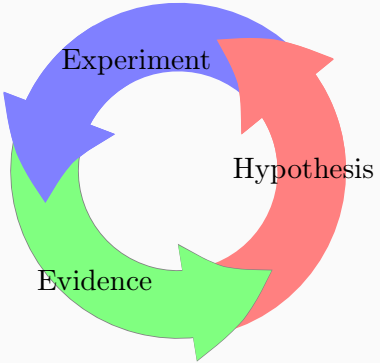


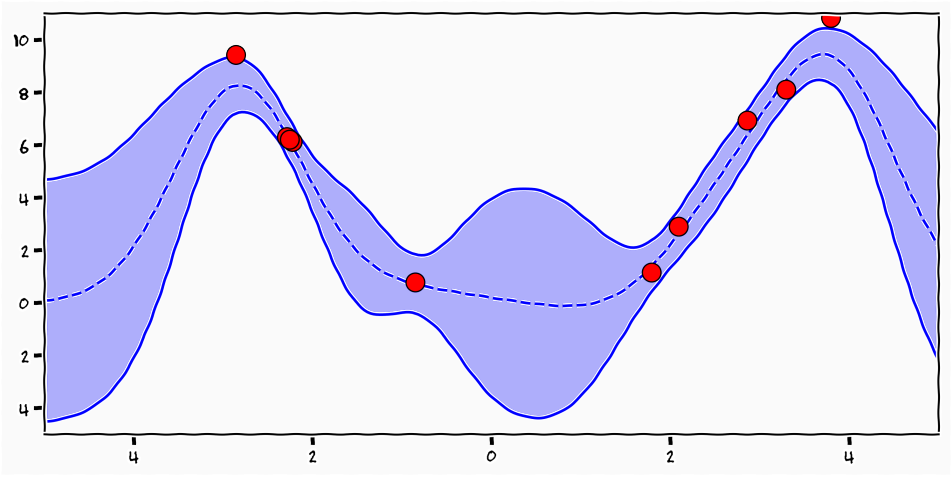
Active Learning



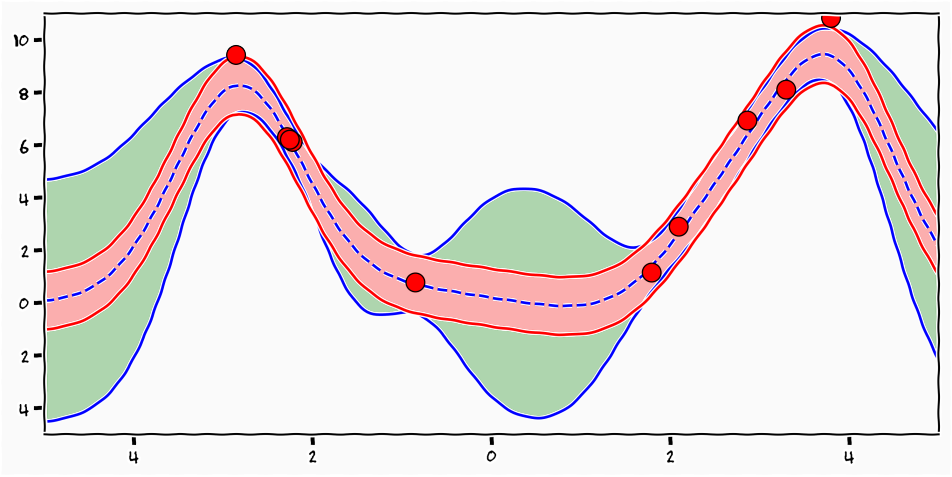
The Role Uncertainty



Functions



Uncertainty Quantification/Factorisation

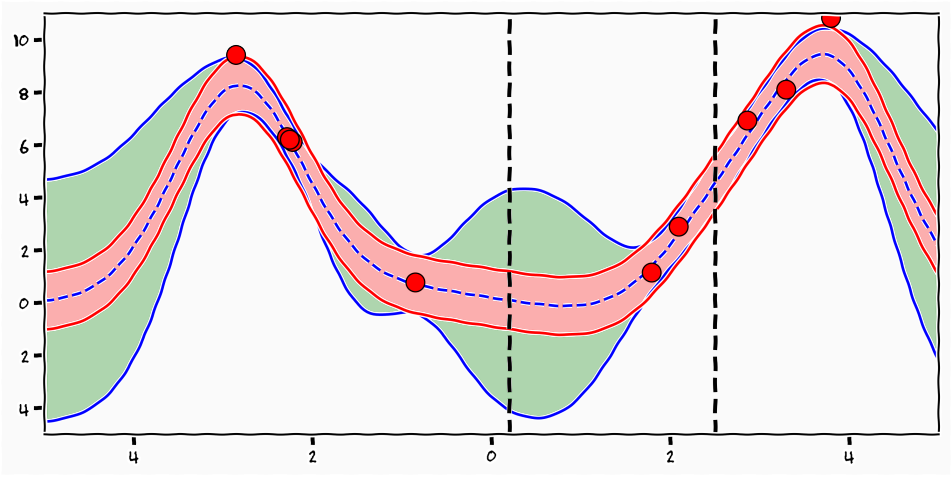


Uncertainty Quantification

Aleatoric/Stochastic "Randomness" inherent in system, or noise in our measurement of system

Epistemic Uncertainty related to our ignorance of a the underlying system

Uncertainty for Decision Making



Today

Black-Box Optimisation how can we find the minima of an explicitly unknown function?

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Surrogate Models how can we build a model as a surrogate for the unknown function?

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Black-Box Optimisation how can we find the minima of an explicitly unknown function?

Surrogate Models how can we build a model as a surrogate for the unknown function?

Sequential decision making how can we come up with a strategy for sequentially exploring the function?

Bayesian Optimisation

Black-box Optimisation

$$x^{(*)} = \operatorname*{argmin}_{x \in \mathcal{X}} f(x)$$

- $\mathcal{X}$ is a bounded domain

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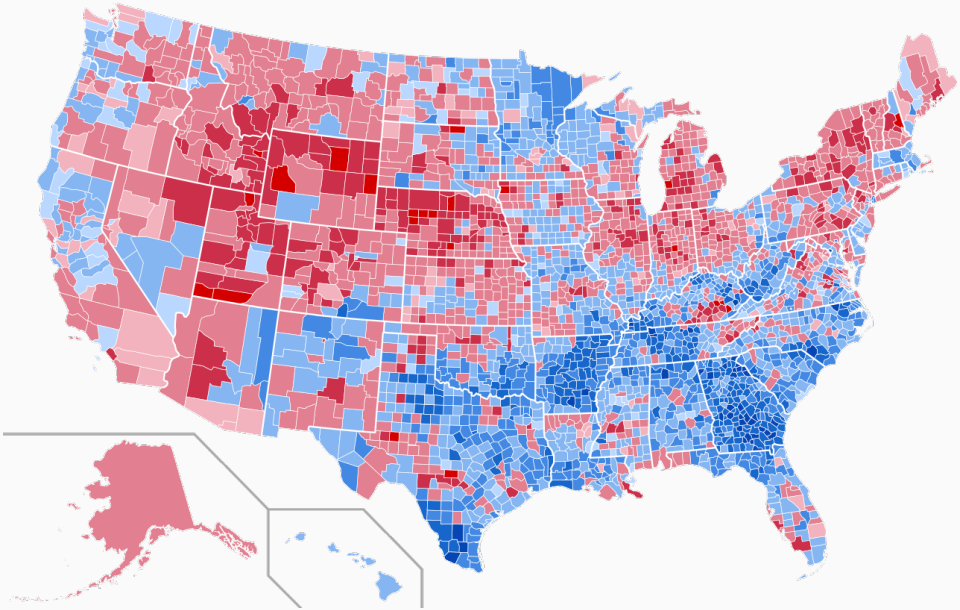
- Evaluations of f may be noisy
- Evaluations of f is expensive



Random Search [Brochu et al., 2010]

- Random Search

$$f(x^{(-)}) \leq f(x^{(*)}) - \epsilon$$

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- Lipschitz Continuity

$$\|f(x_1) - f(x_2)\| \leq C\|x_1 - x_2\|$$

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- Requires $\left(\frac{C}{2\epsilon}\right)^d$ evaluations on a d -dimensional hypercube

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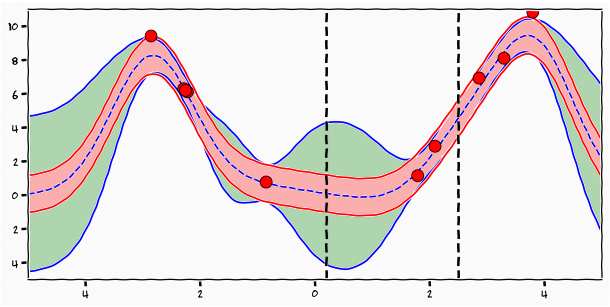
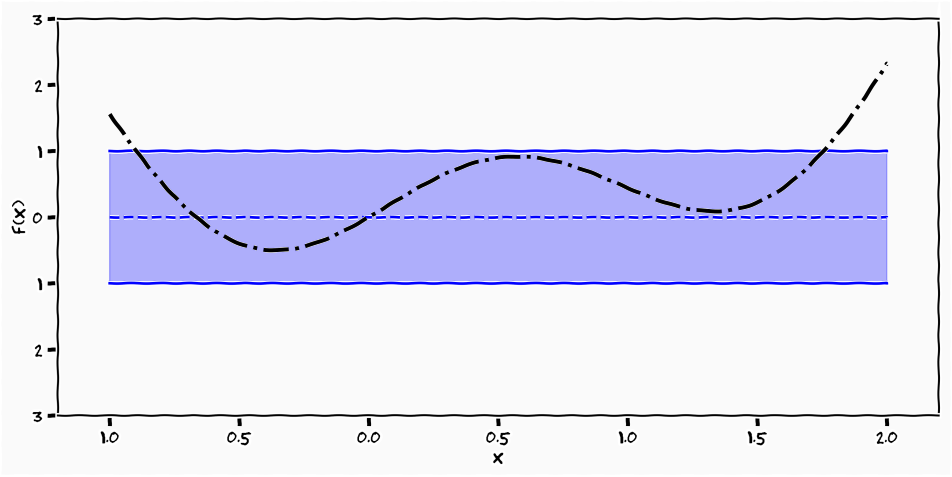
- Requires $\left(\frac{C}{2\epsilon}\right)^d$ evaluations on a d -dimensional hypercube
- Surrogate model $p(f)$

Gaussian Process Surrogate



- allows for principled priors and narrow priors
- provides belief over the whole domain

Posterior Search



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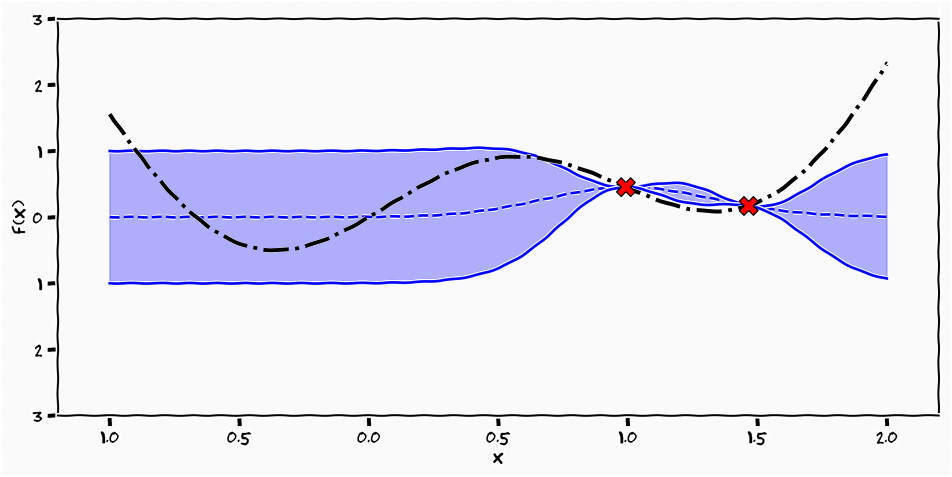

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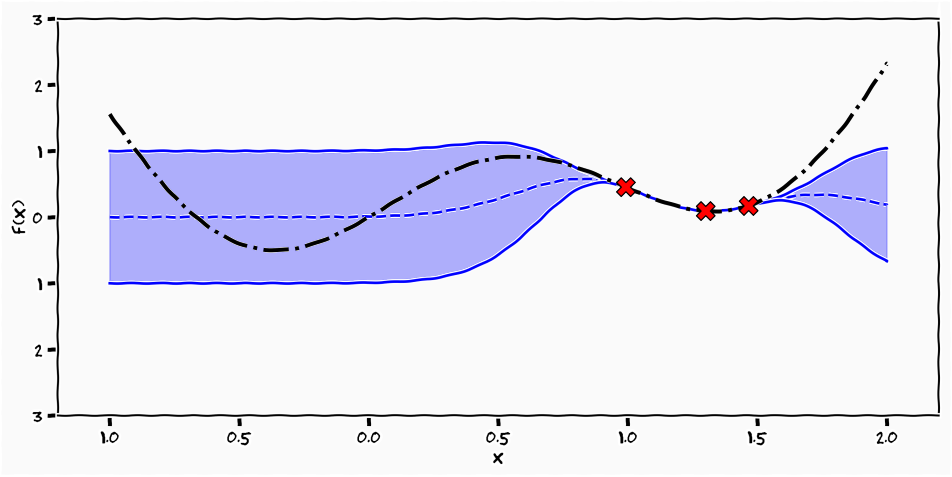

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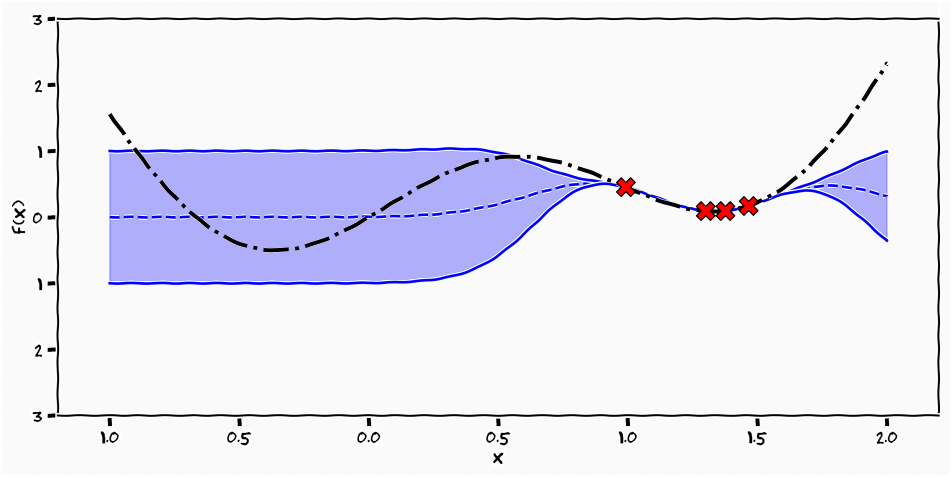

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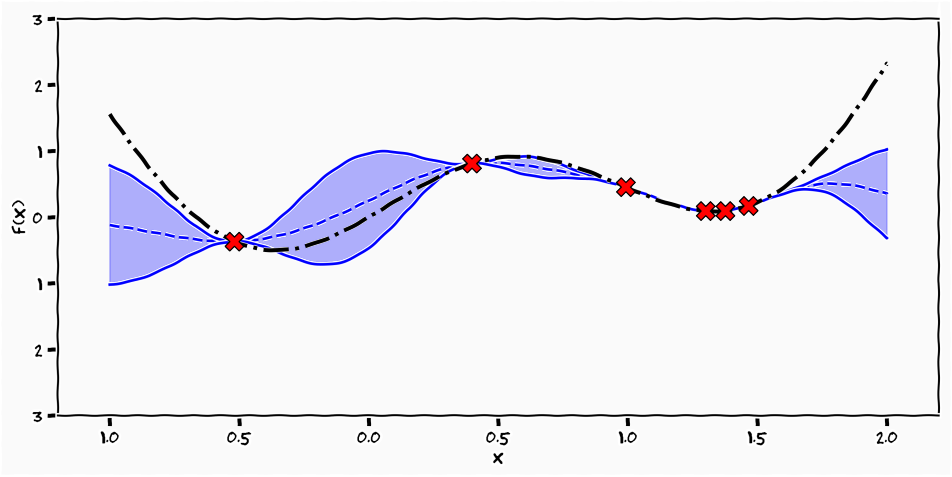

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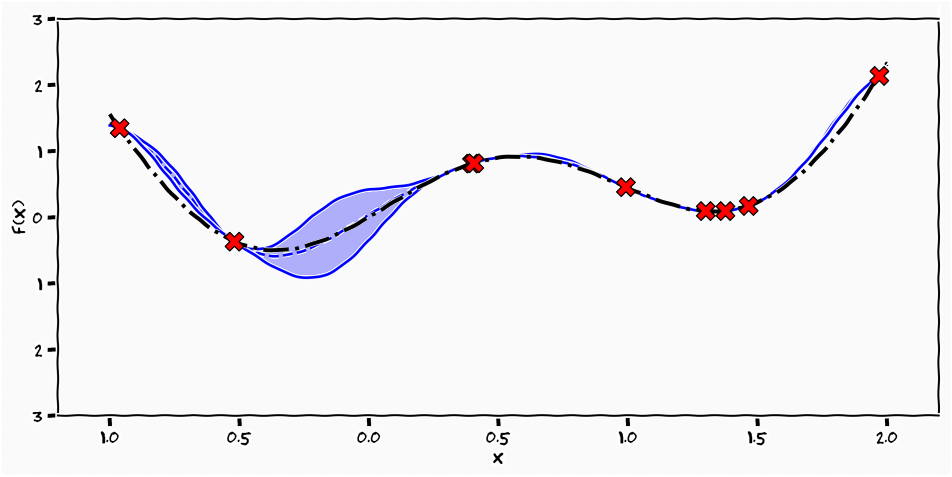

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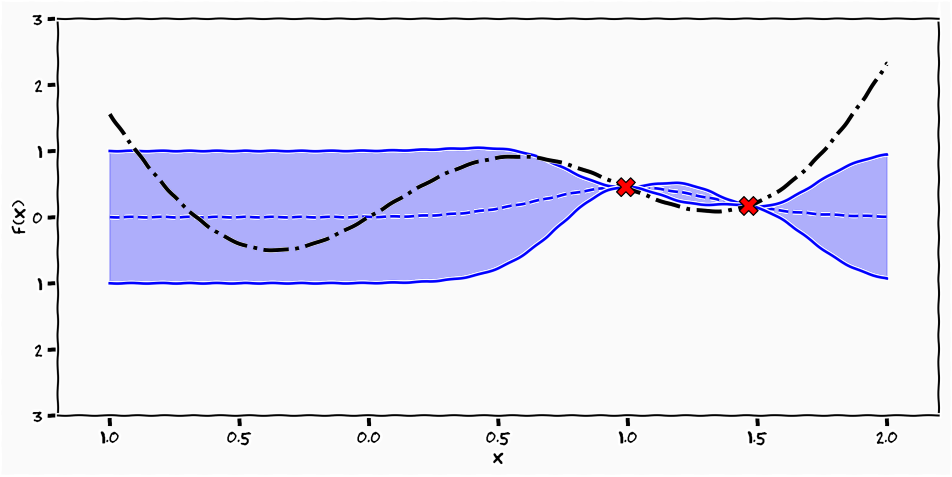

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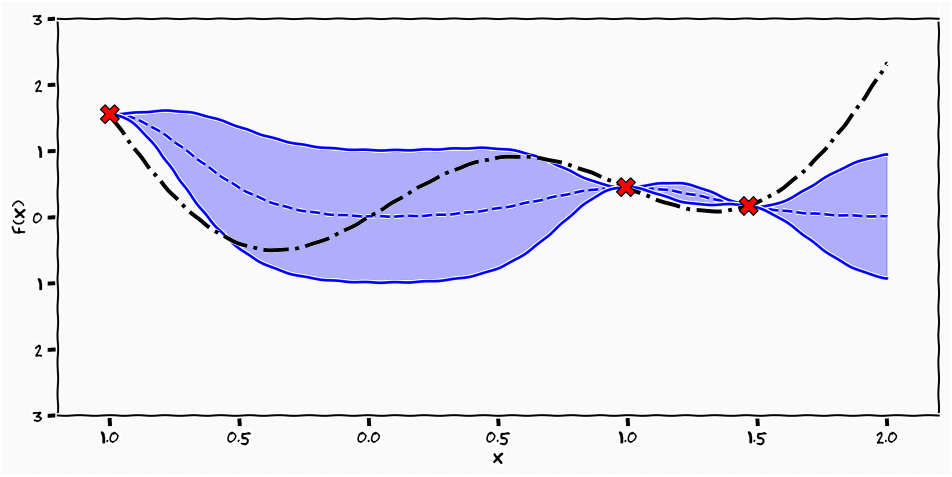

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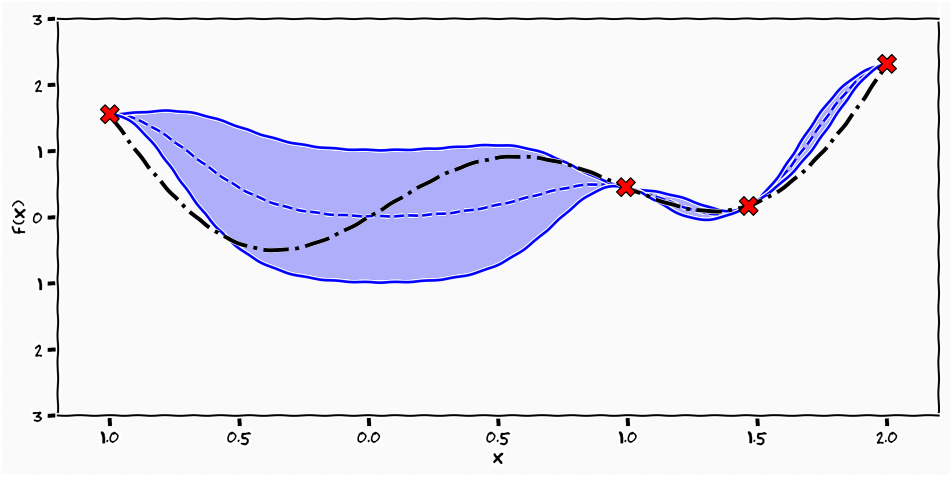

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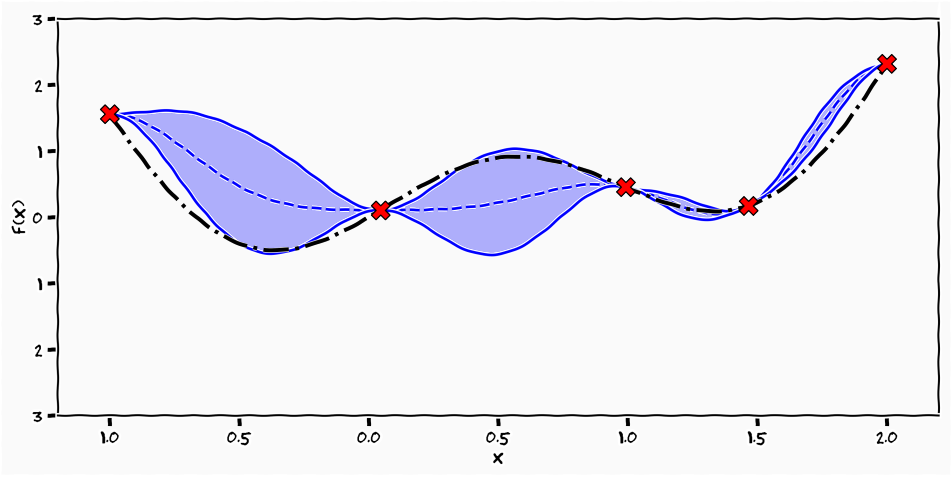

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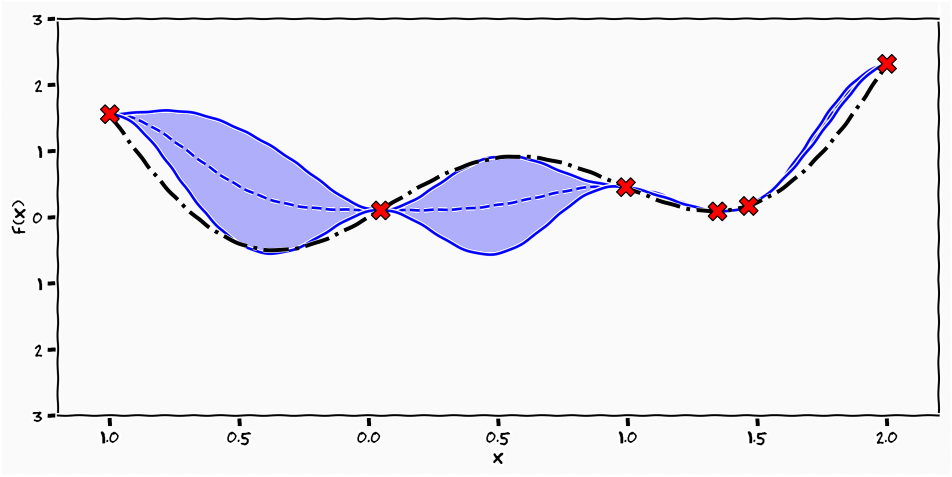

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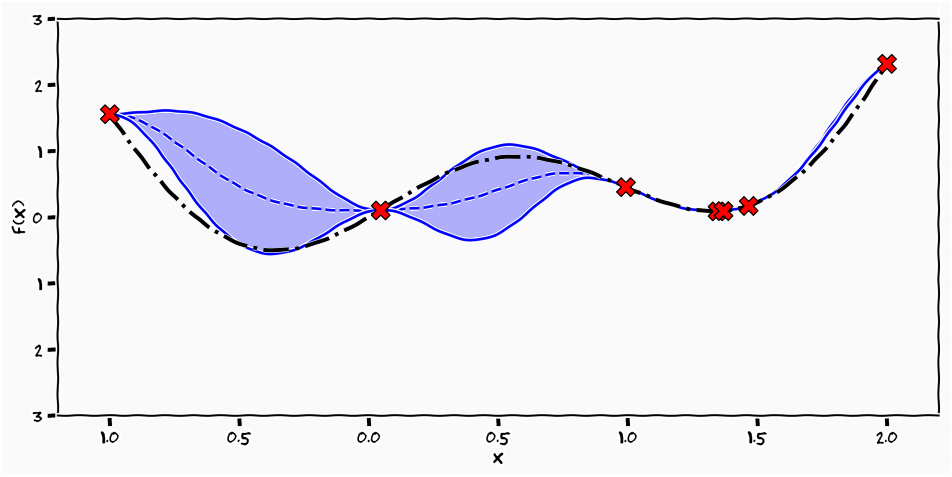

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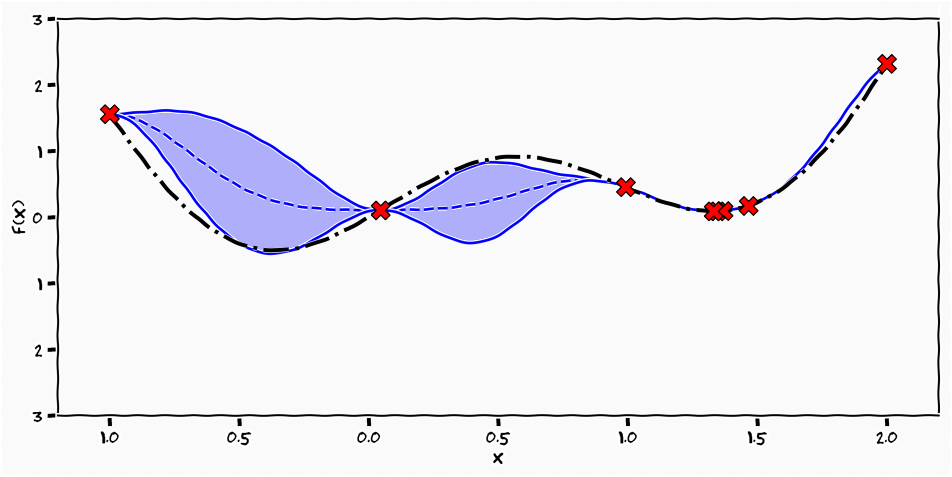

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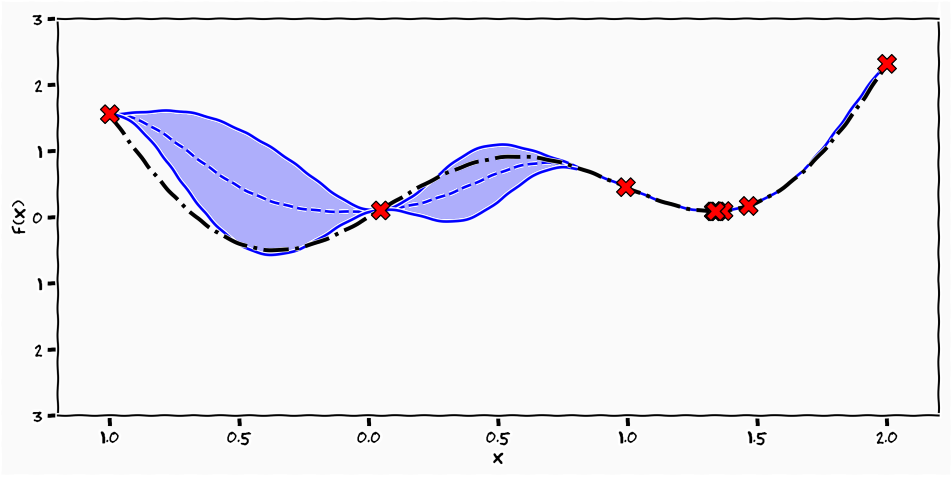


STRONGARM
CAMERONS
TIMOTHY TAYLOR'S
LANDLORD
FURNACE
NICK STAFFORD'S
West Coast
Mosaic IPA
4.0% ABV


Coca-Cola


Coca-Cola


WYE VALLEY
BITTER
Superior Quality
WYE VALLEY
BREWERY
WYE VALLEY
BREWERY


Coca-Cola


WYE VALLEY
BITTER
Superior Quality
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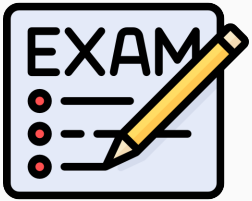
BREWERY


ALASKA
DISTILLERY
HANDCRAFTED
SMOKED SALMON
FLAVORED VODKA
PERFECT ANY BLOODY MARY
(80 PROOF)

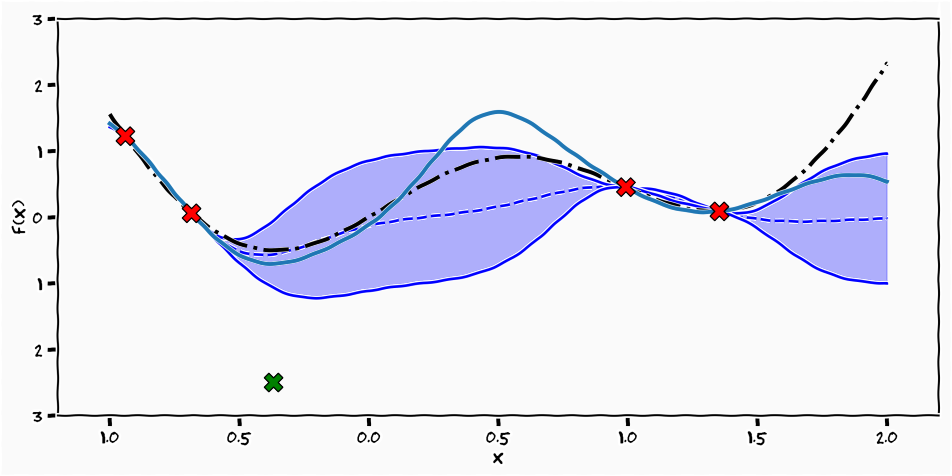
Exploration and Explotation



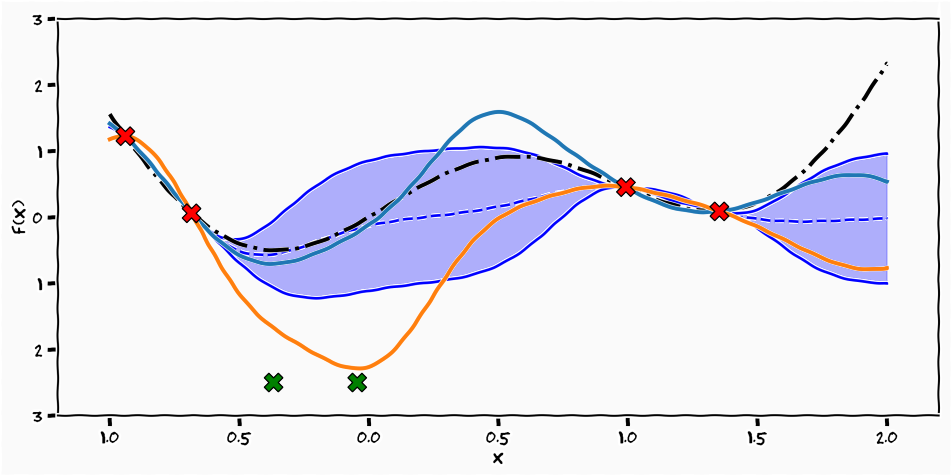
Exploitation use the knowledge that we currently have

Exploration try to gain new knowledge by trying new things

Surrogate Uncertainty



Surrogate Uncertainty



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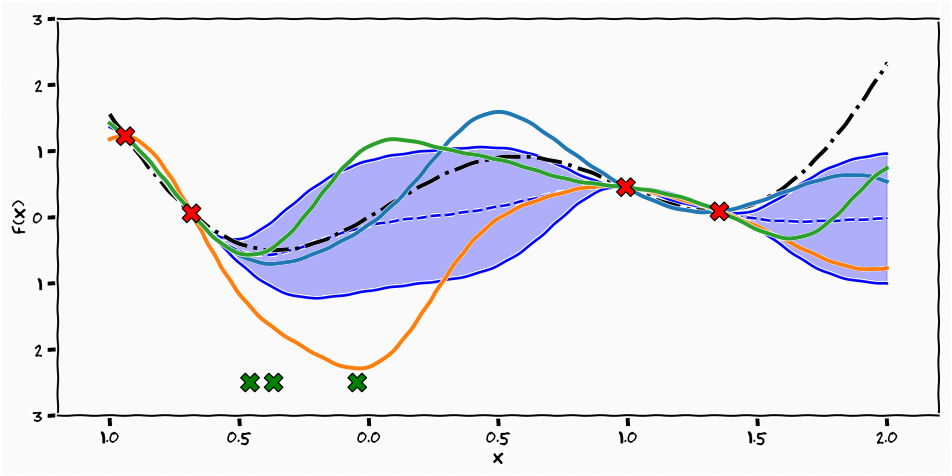

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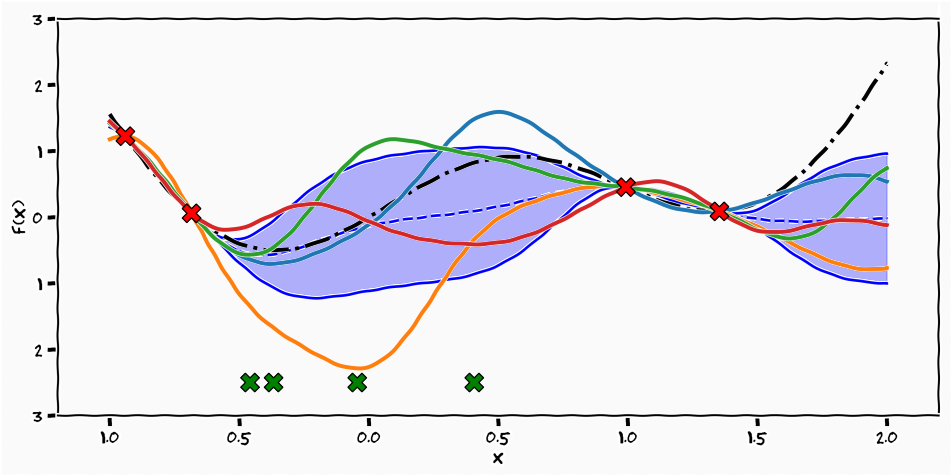

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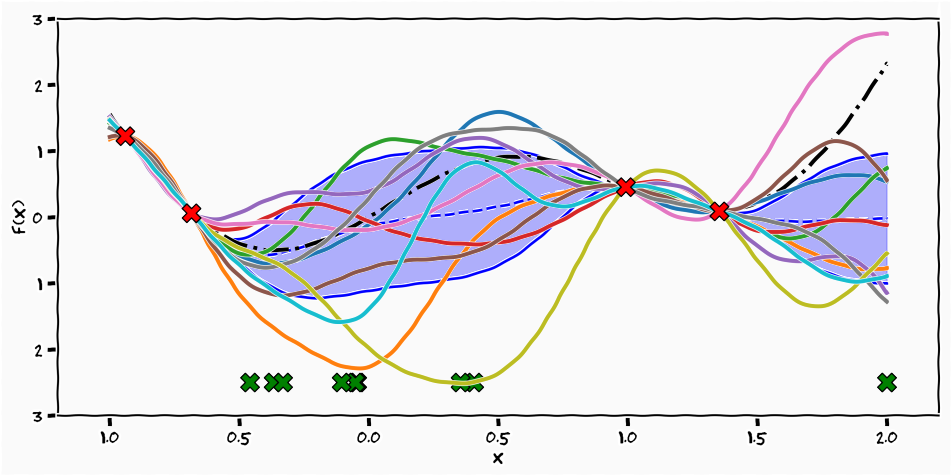

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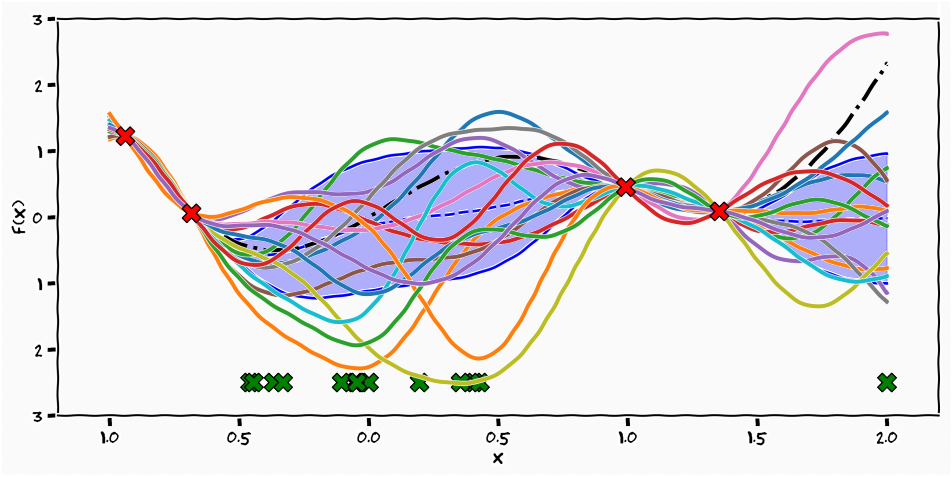
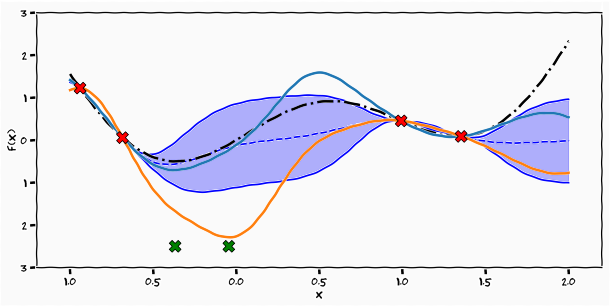


Acquisition Function

$$x_{n+1} = \underset{x \in \mathcal{X}}{\operatorname{argmax}}\, \alpha(x; \{x_i, y_i\}_{i=1}^{n}, \mathcal{M}_n)$$

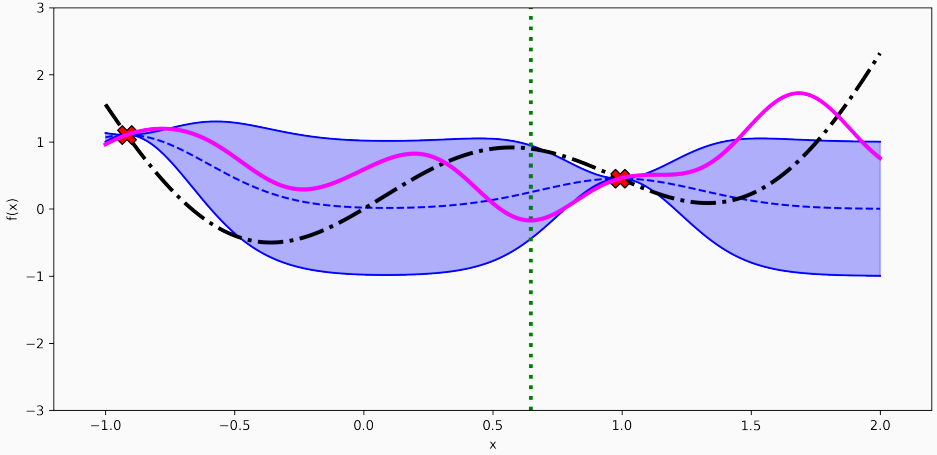
- Formulate a sequential decision problem
- This will work well if $\alpha(x)$
  - is cheap to compute
  - balances *exploration* and *exploitation*

Thompson Sampling [Thompson, 1933]



$$-\alpha(x; \{x_i, y_i\}_{i=1}^n, \mathcal{M}_n) \sim p(f \mid \{x_i, y_i\}_{i=1}^n)$$

Thompson Sampling



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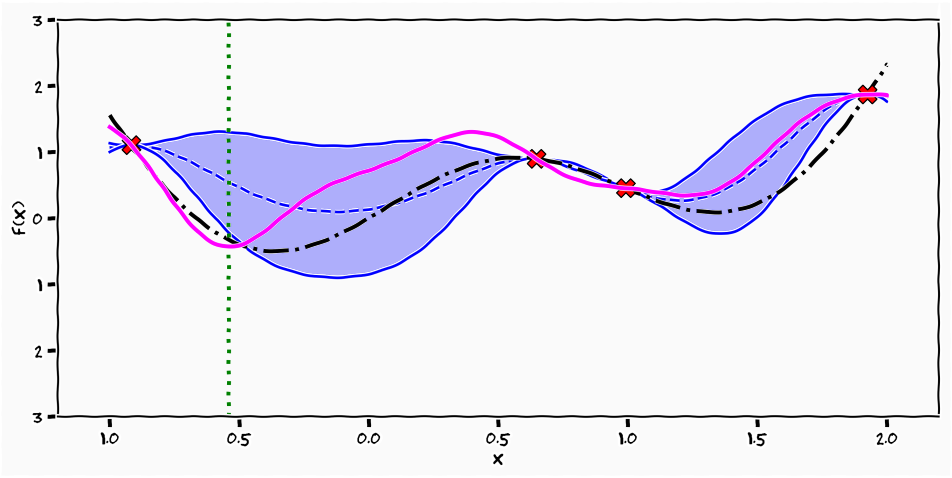

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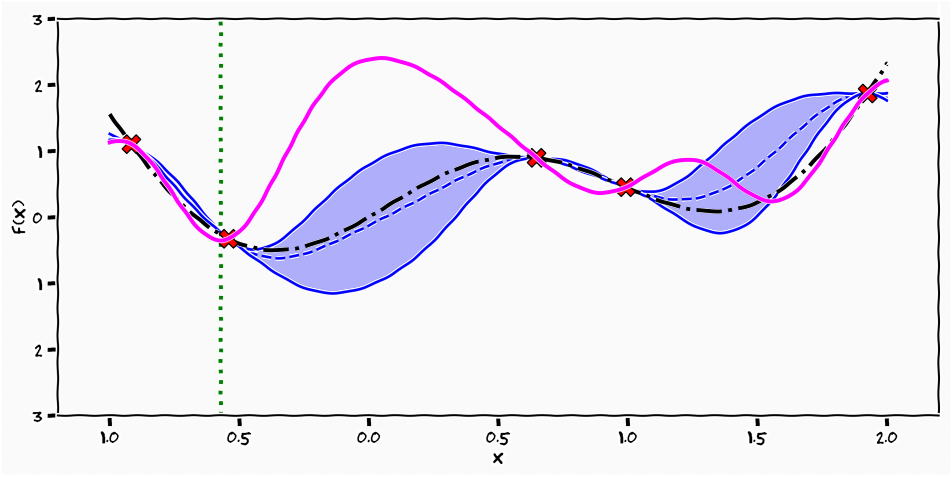

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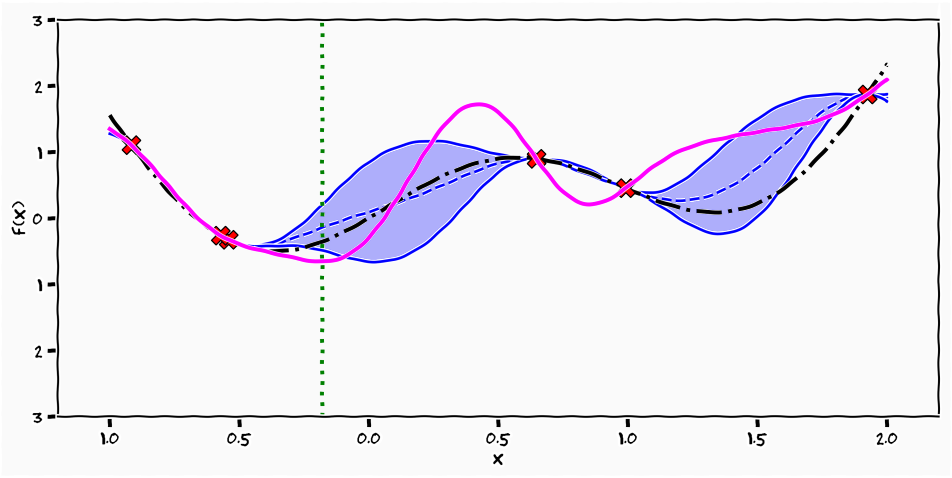

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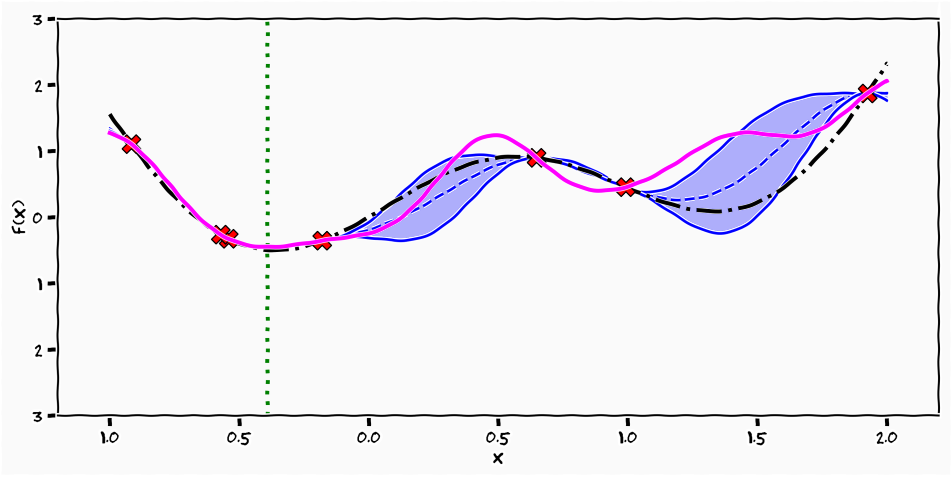

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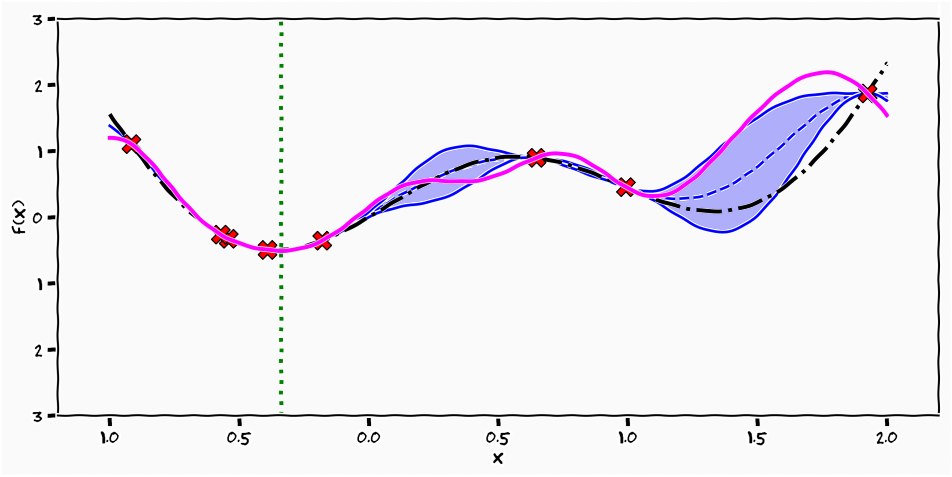

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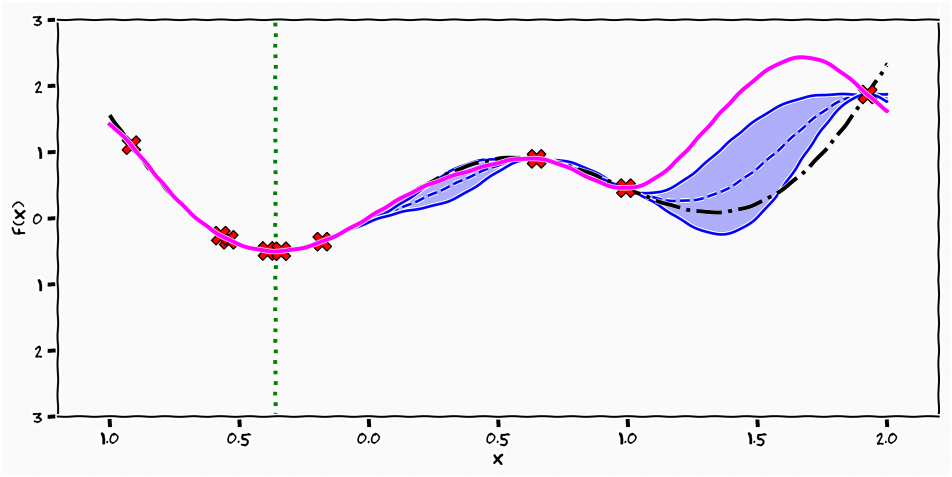
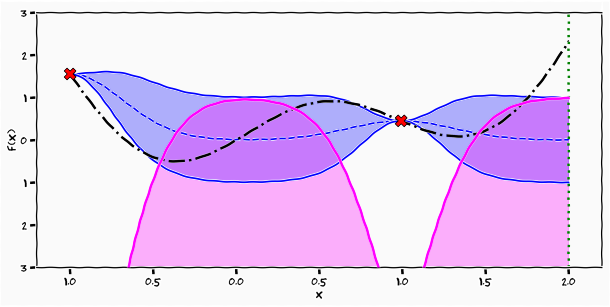


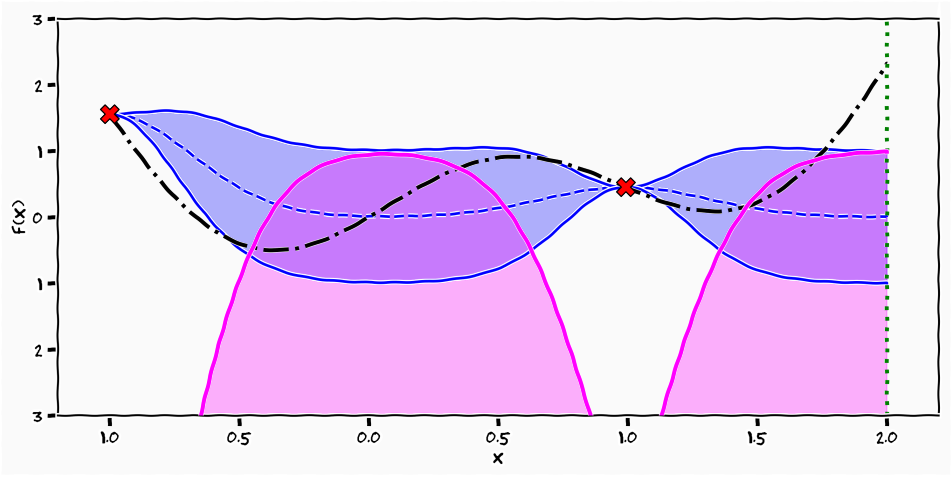
Upper Confidence Bound [Cox et al., 1997]



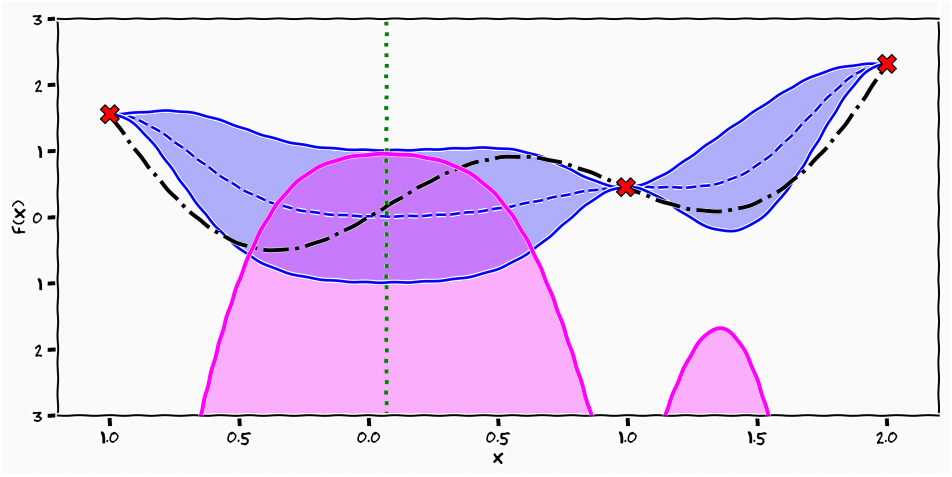
- Acquisition Function

$$\alpha(x; \{x_i, y_i\}_{i=1}^n, \mathcal{M}_n) = -\mu(x; \{x_i, y_i\}_{i=1}^n) + \beta\sigma(x; \{x_i, y_i\}_{i=1}^n)$$

Upper Confidence Bound



Upper Confidence Bound



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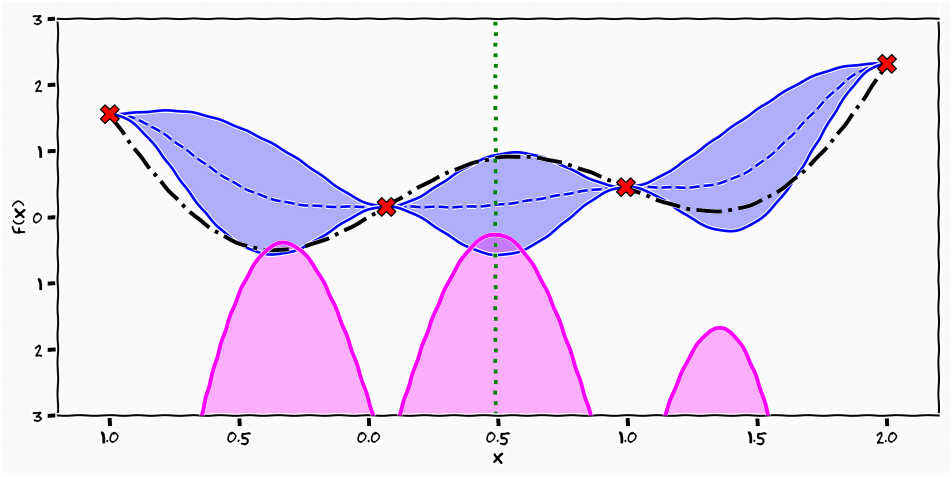
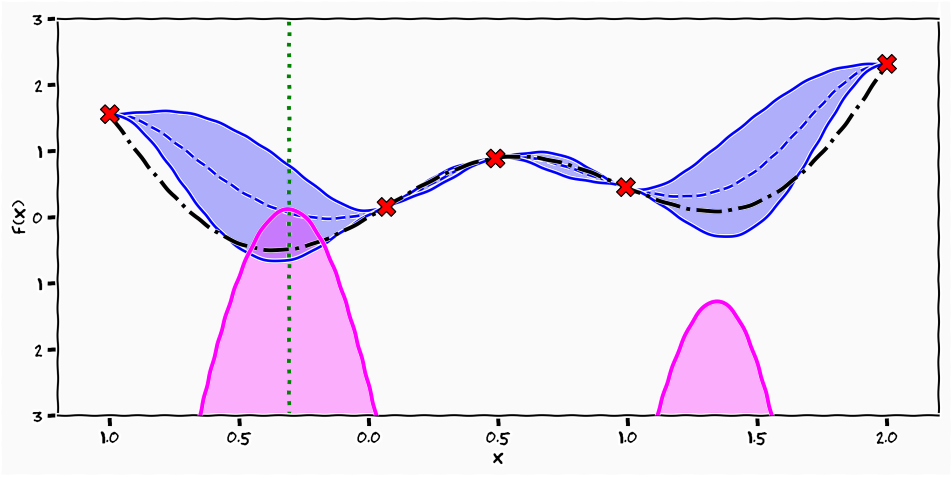
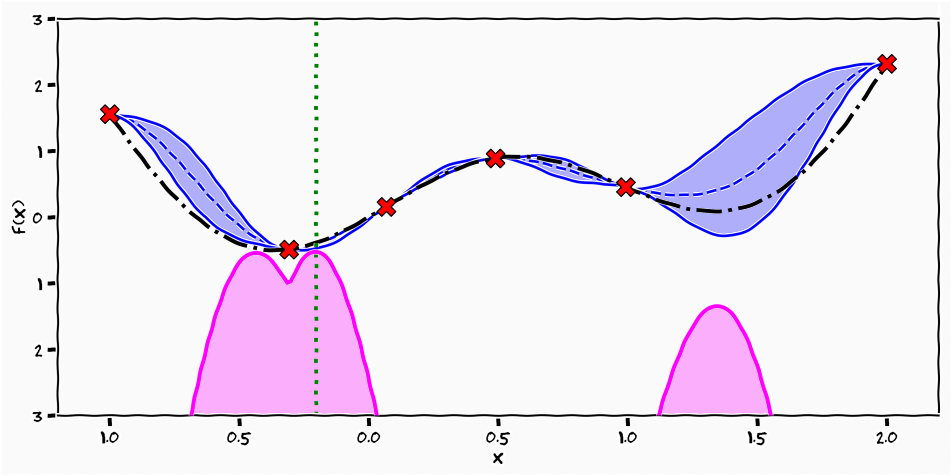


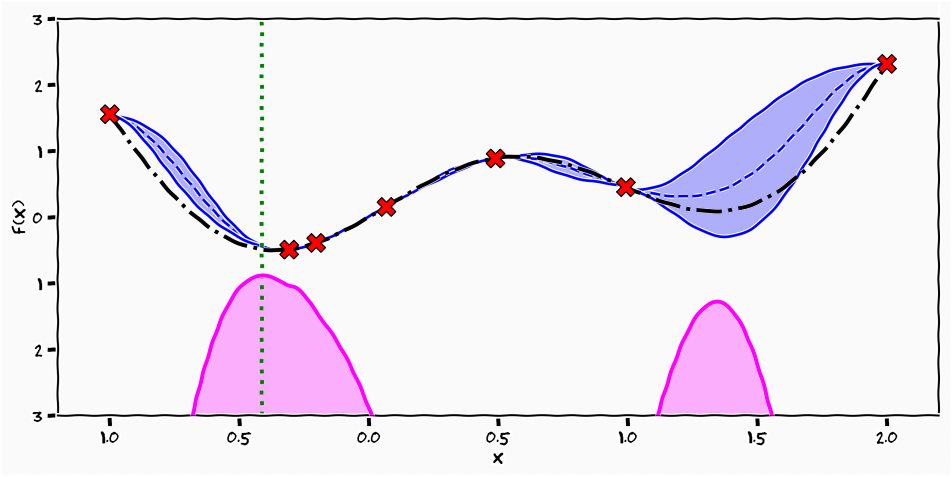
Upper Confidence Bound



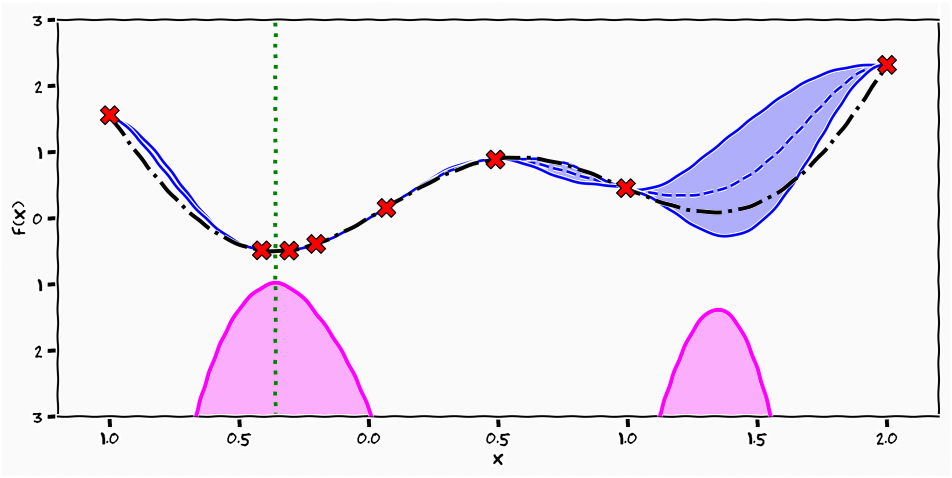
Upper Confidence Bound



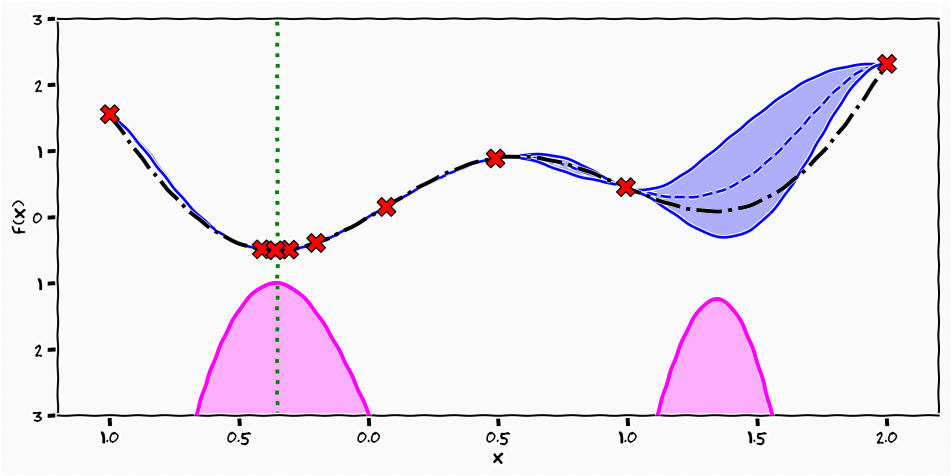
Upper Confidence Bound



Upper Confidence Bound



Upper Confidence Bound



Utility

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- Define a function that defines the utility of observing each location

$$u(x, f(x^{(*)}), \mathcal{M}_n)$$

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- Define a function that defines the utility of observing each location

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- Define the acquisition function as the expected utility

$$\begin{aligned}\alpha(x; \{x_i, y_i\}_{i=1}^n, \mathcal{M}_n) &= \mathbb{E}_{p(f)}[u(x)] \\ &= \int u(x, f(x^{(*)}), \mathcal{M}_n) p(f \mid \{x_i, y_i\}_{i=1}^n) \mathrm{d}f\end{aligned}$$

Probability of Improvement [Kushner, 1963]

- Utility Function

$$u(x) = \begin{cases} 0 & f(x) > f(x^{(*)}) \\ 1 & f(x) \leq f(x^{(*)}) \end{cases}$$

Probability of Improvement [Kushner, 1963]

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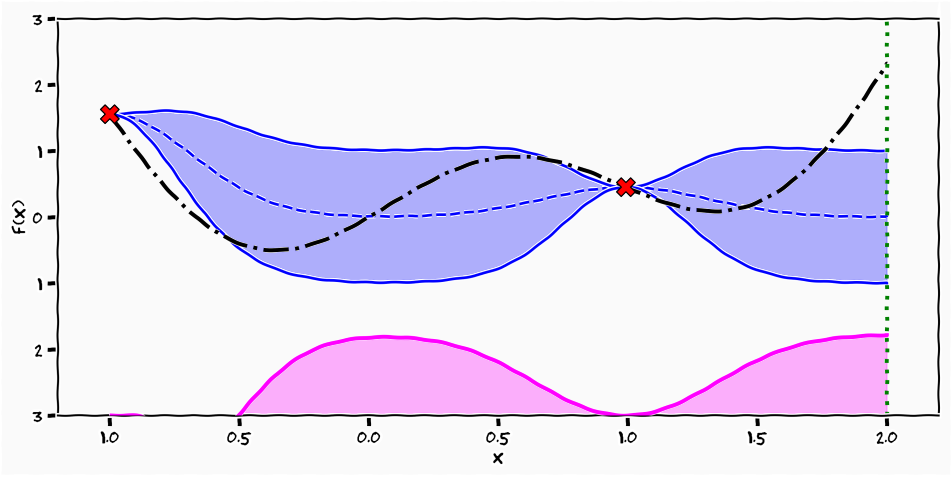
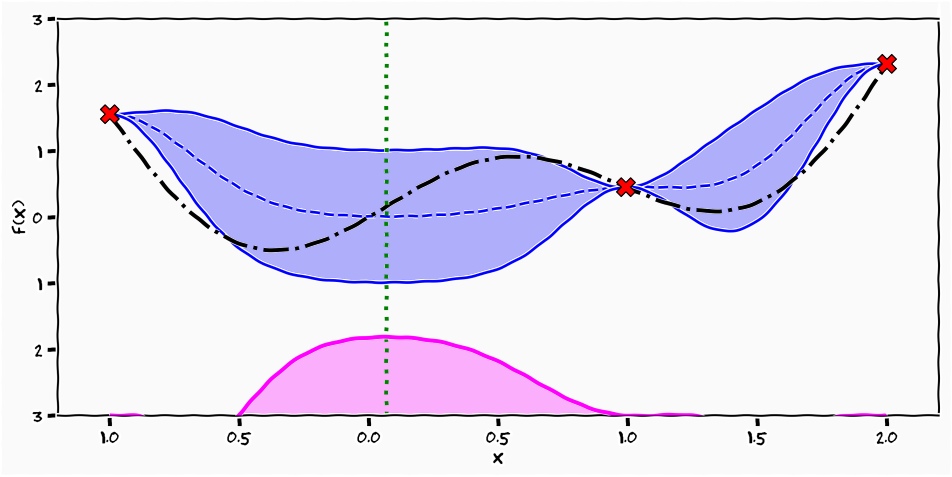
- Acquisition Function

$$\begin{aligned} \alpha(x; \{x_i, y_i\}_{i=1}^n, f(x^{(*)}), \mathcal{M}_n) &= \mathbb{E}[u(x)] = p(f(x) \leq f(x^{(*)})) \\ &= \int_{-\infty}^{f(x^{(*)})} \mathcal{N}\left(f \mid \mu(x), K(x,x)\right) \mathrm{d}f \\ &= \Phi\left(f(x^{(*)}) \mid \mu(x), K(x,x)\right) \end{aligned}$$

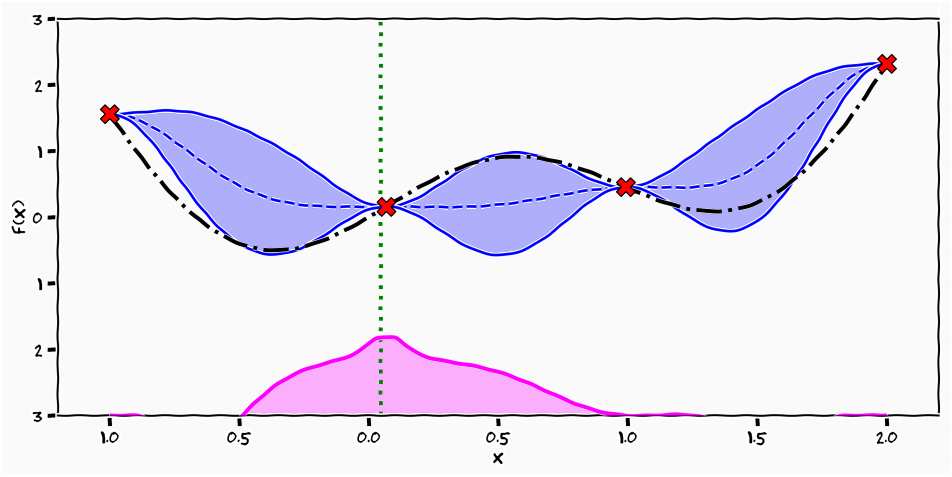
Probability of Improvement



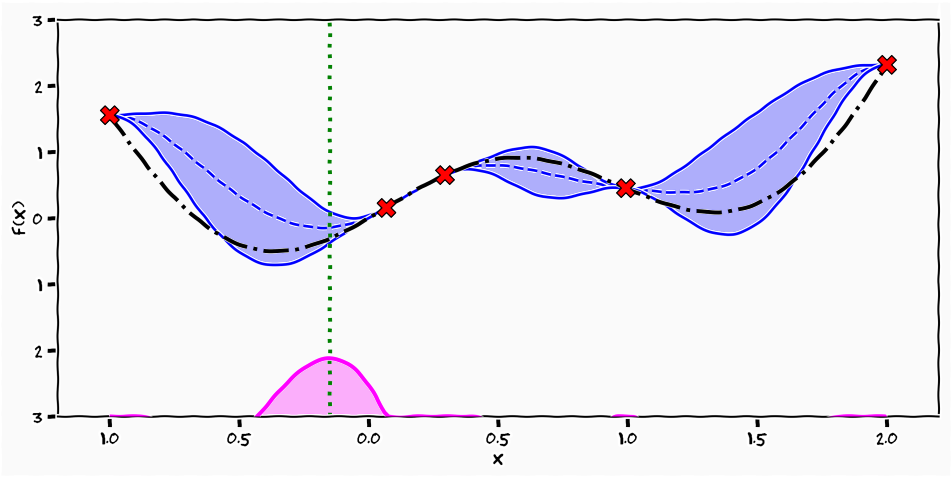
Probability of Improvement



Probability of Improvement



Probability of Improvement



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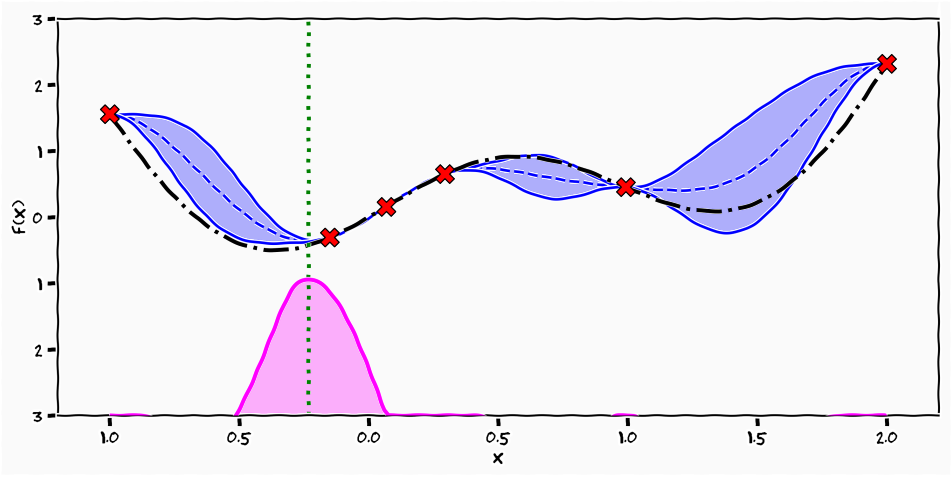
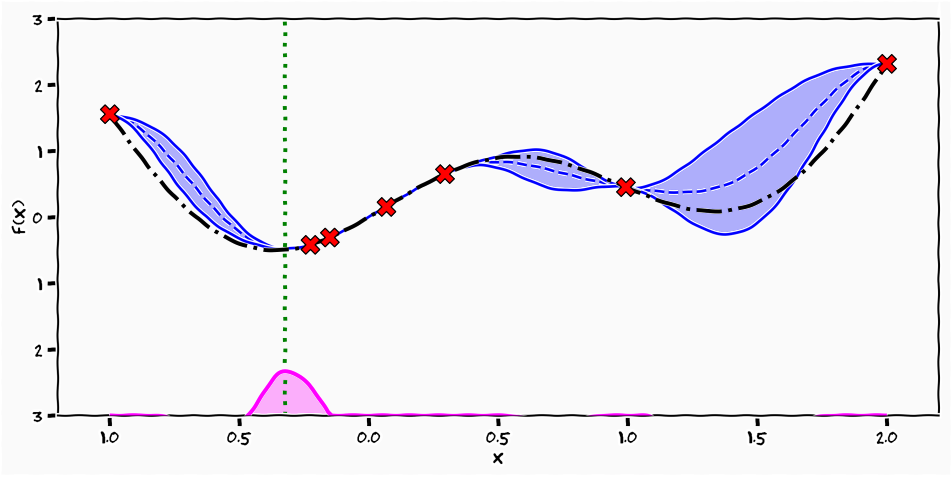


Probability of Improvement



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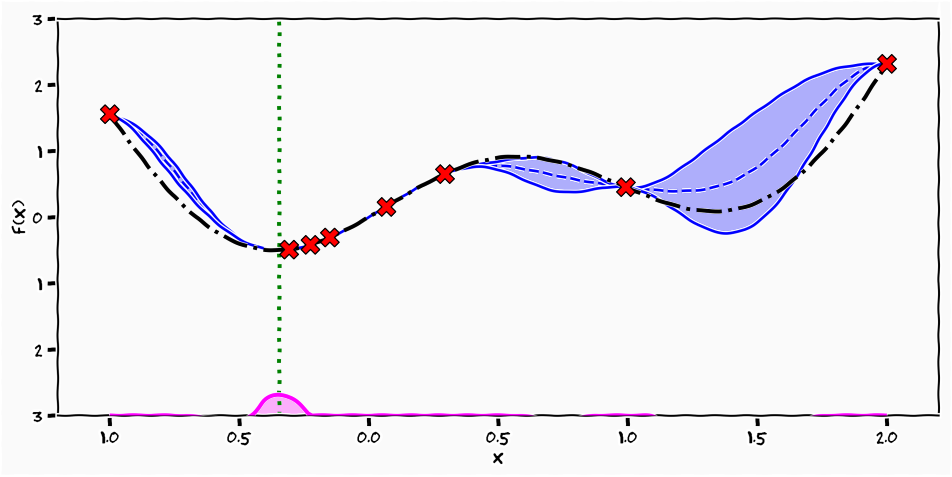

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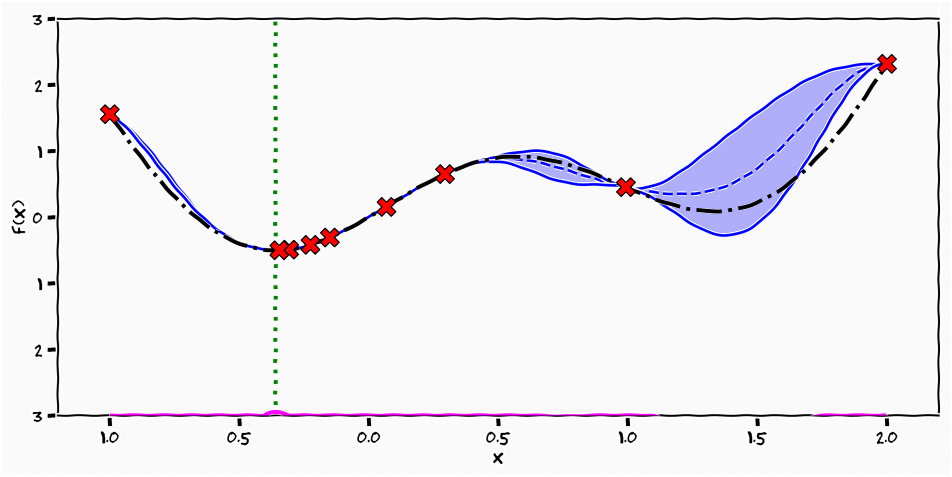

Expected Improvement Mockus et al., 1978

- Utility Function

$$u(x) = \max(0, f(x^{(*)}) - f(x))$$

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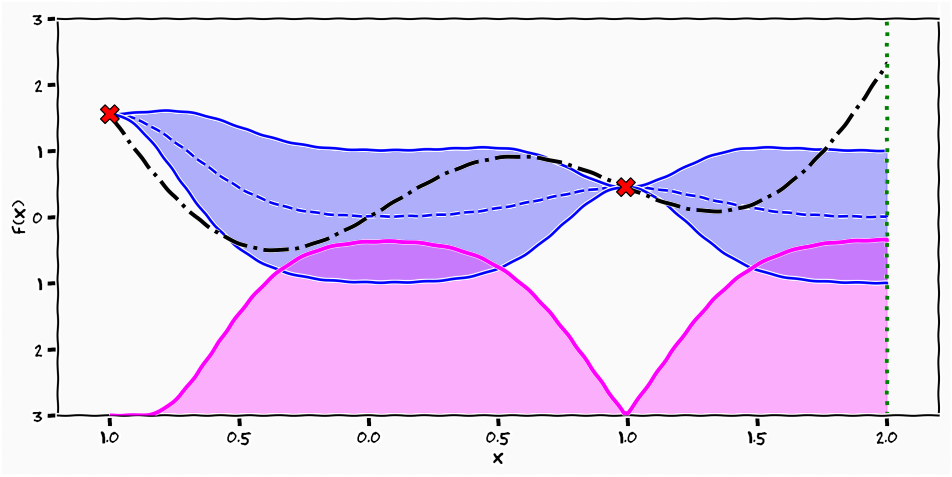
$$\begin{aligned}
\alpha(x; \{x_i, y_i\}_{i=1}^n, f(x^{(*)}), \mathcal{M}_n) &= \mathbb{E}[u(x)] \\
&= \int_{-\infty}^{f(x^{(*)})} (f(x^{(*)}) - f)\mathcal{N}\left(f \mid \mu(x), K(x,x)\right) \mathrm{d}f \\
&= (f(x^{(*)}) - \mu(x))\Phi\left(f(x^{(*)}) \mid \mu(x), K(x,x)\right) \\
&+ K(x,x)\mathcal{N}\left(f(x^{(*)}) \mid \mu(x), K(x,x)\right)
\end{aligned}$$

Expected Improvement



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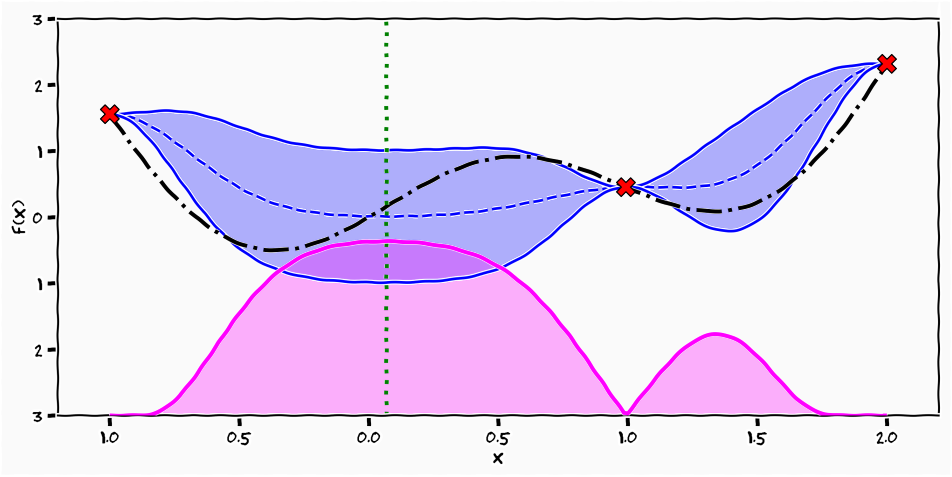
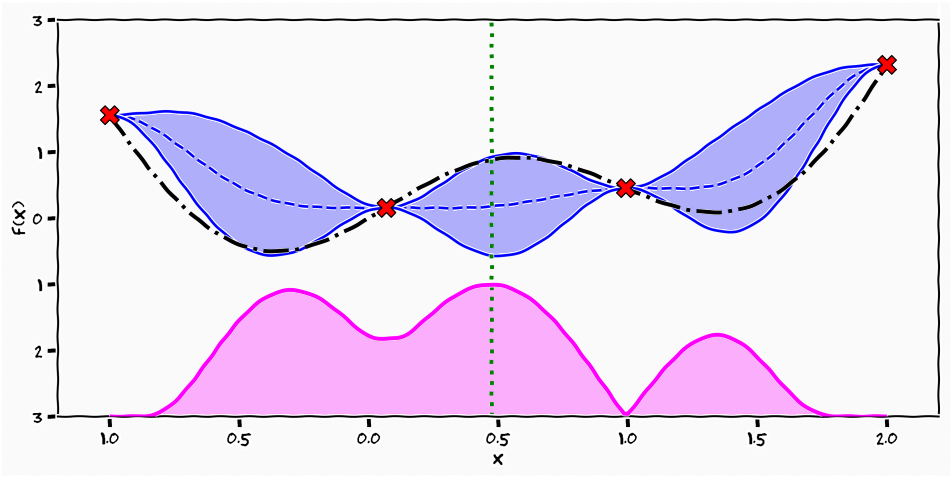


Expected Improvement



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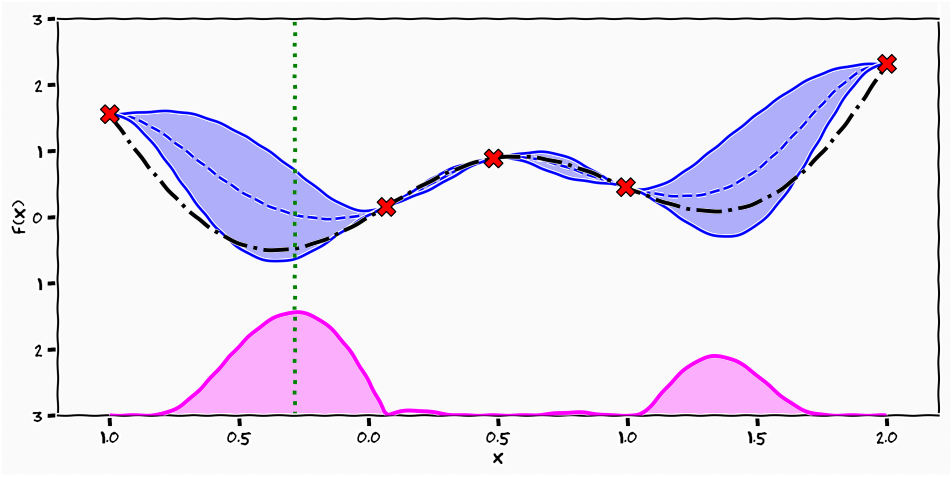
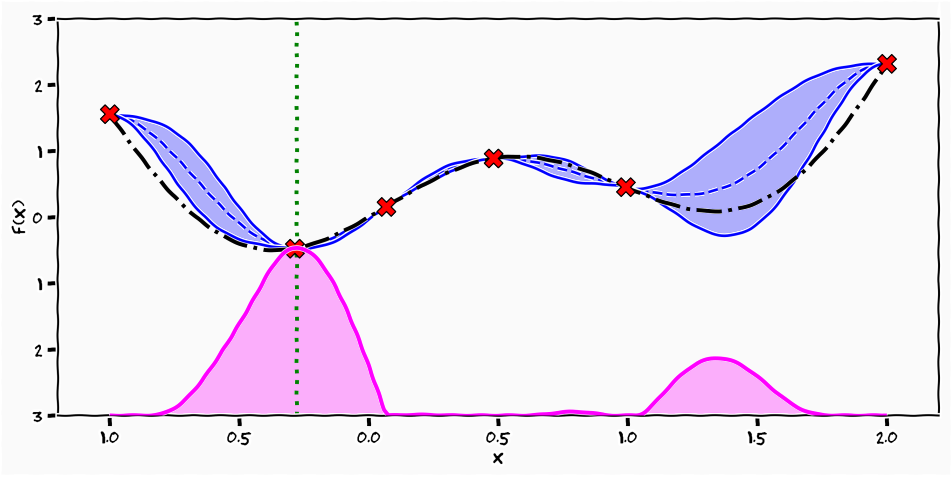
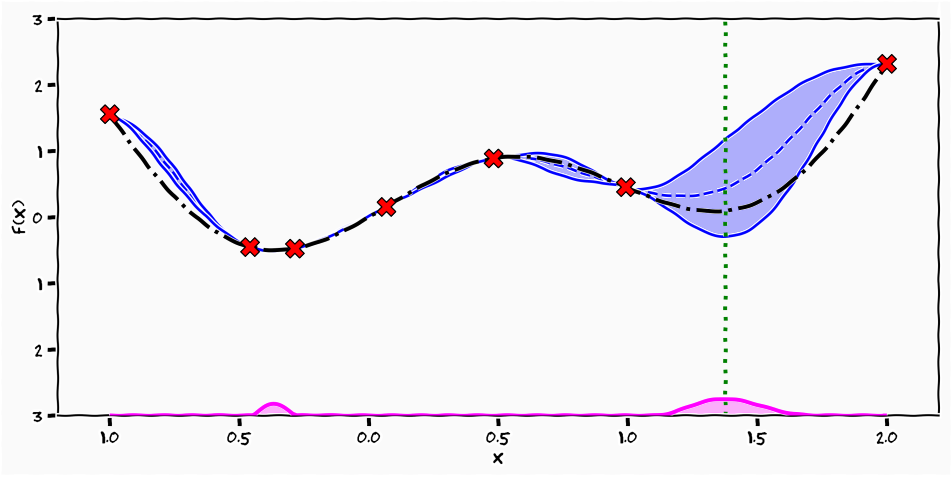


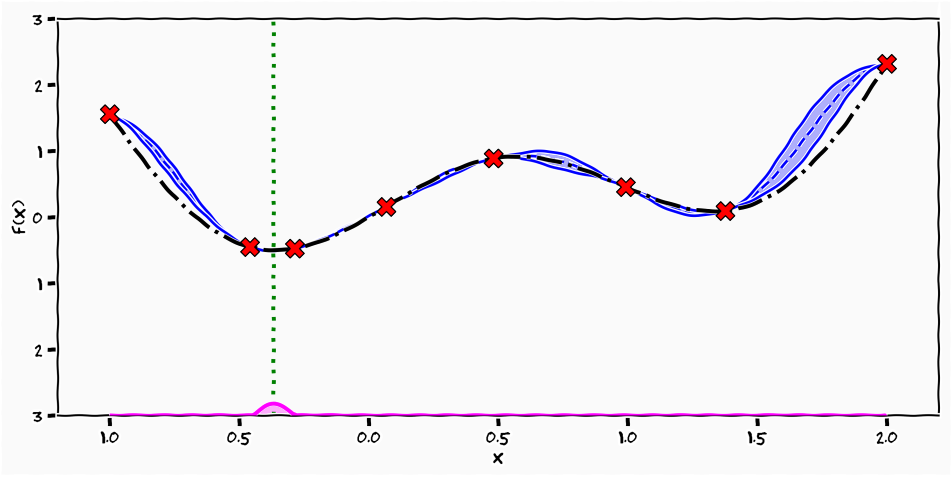
Expected Improvement



Expected Improvement



Expected Improvement



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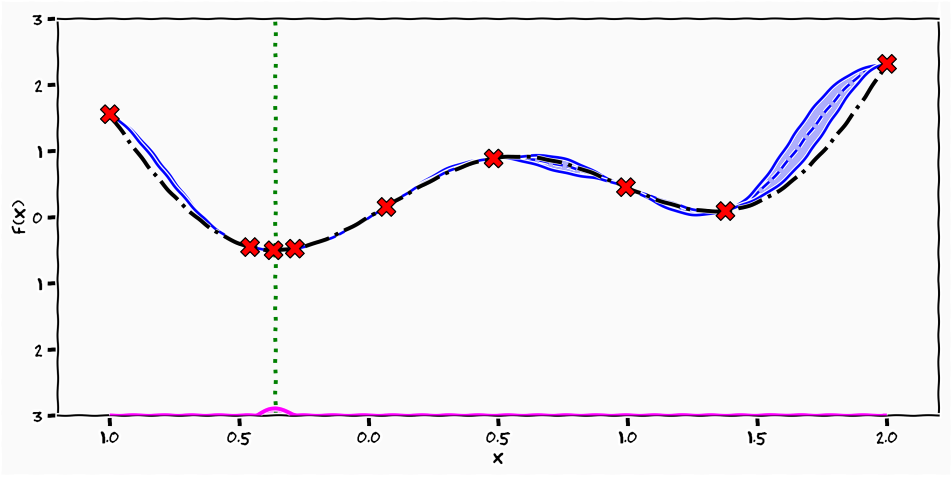

Task 1 encode your knowledge about the function in the GP prior

[1] till they open the door to the exam.

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Task 2 randomly sample some data

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Task 4 evaluate and maximise the acquisition function

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Task 5 add new data to model and re-estimate hyperparameters

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Loop 4-5 till budget is gone[1]

[1] till they open the door to the exam.

Learning Hyper-parameters

$$\{\hat{\beta}, \hat{\ell}, \hat{\sigma}\} = \underset{\beta,\ell,\sigma}{\operatorname{argmax}} \quad \log \quad \int p(y \mid f) p(f) \mathrm{d}f$$

- Update the hyper-parameters of the GP
- We can do this by gradient based optimisation
  - *or with a Bayes Opt loop!*

[2] *. . . .and here I was thinking that you guys had some principles in life*

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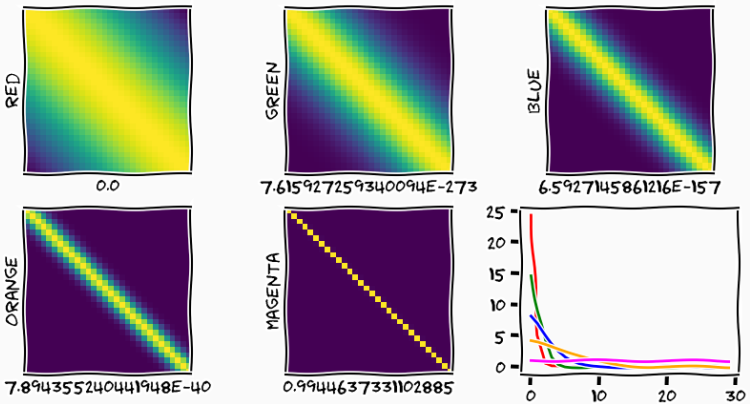
- Update the hyper-parameters of the GP
- We can do this by gradient based optimisation
  - *or with a Bayes Opt loop!*
- *Are we doing MLE*[2]?

[2] *. . . .and here I was thinking that you guys had some principles in life*

$$
\begin{aligned}
\{\hat{\beta}, \hat{\ell}, \hat{\sigma}\} &= \underset{\beta,\ell,\sigma}{\operatorname{argmax}} \quad \log \int p(y \mid f) p(f) \mathrm{d}f \\
&= \underset{\beta,\ell,\sigma}{\operatorname{argmin}} - \log \quad p(y) \\
&= \underset{\beta,\ell,\sigma}{\operatorname{argmin}} \frac{1}{2} \operatorname{trace}\left(\mathbf{Y}\mathbf{K}^{-1}\mathbf{Y}^{\mathrm{T}}\right) + \frac{1}{2} \log|K| + \frac{N}{2} \log(2\pi)
\end{aligned}
$$

- $Data - fit$ *how well does the observations fit the model*
- $"Complexity"$ *how "smooth" is the functions*

Determinant



N

How to implement

Summary

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- GPs are quite useful surrogates!

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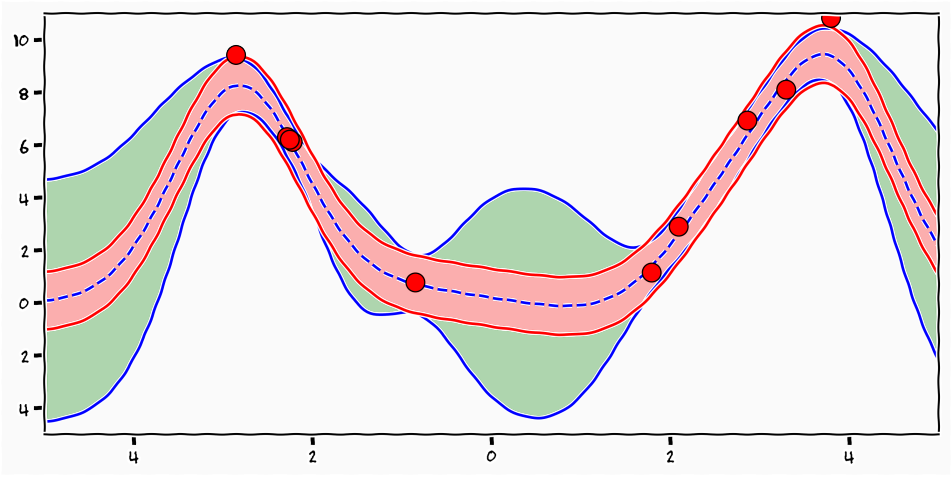
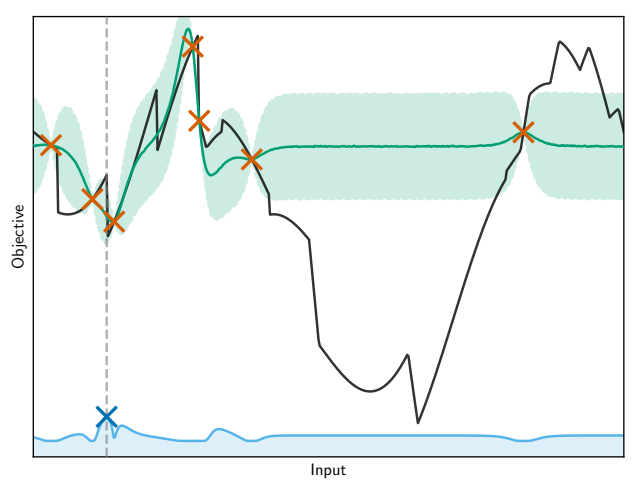
- GPs are quite useful surrogates!
- Degrees of beliefs are really useful
- The uncertainty allows us to design rich strategies for how to aquire data
- The factorisation of uncertainty allows us to describe search strategies in simple acquisition functions

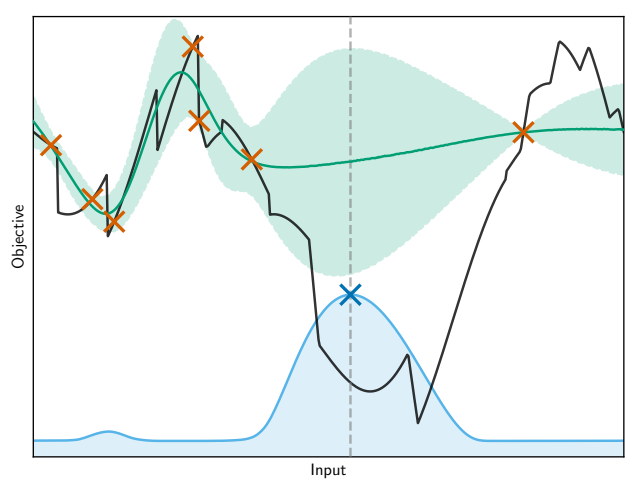
Uncertainty Quantification/Factorisation



Irrelevant structures Bodin et al., 2020



Relevant structures Bodin et al., 2020



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