University of BRISTOL

Machine Learning

Bayesian Optimisation

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http://www.carlhenrik.com

Introduction

Help Sessions

- Thursday 19/10 18-20 MVB 1.11
- Friday 20/10 17-19 MVB 1.11
- Potentially Thursday 26/10 17-19 (will confirm next week)

GitHub

`git pull`

Recap

Marginal Likelihood

$$p(\mathbf{Y}|\mathbf{X}, \theta) = \int p(\mathbf{Y}|\mathbf{f}) p(\mathbf{f}|\mathbf{X}, \theta) \mathrm{d}f$$

- We are not interested in f directly
- Marginalise out f
- Gaussian likelihood and Gaussian prior $\rightarrow$ Gaussian marginal

Marginalisation

- Deterministic world

$$\mathbb{E}[y] = \int y p(y) \mathrm{d}y$$

Marginalisation

- Deterministic world

$$\mathbb{E}[y] = \int y p(y) \mathrm{d}y$$

- Stochastic world

$$\mathbb{E}[p(y)] = \int p(y|x) p(x) \mathrm{d}x$$

Learning

$$\hat{\theta} = \text{argmax}_\theta p(\mathbf{Y}|\mathbf{X}, \theta) = \text{argmax}_\theta \int p(\mathbf{Y}|\mathbf{f}) p(\mathbf{f}|\mathbf{X}, \theta) \mathrm{d}\mathbf{f}$$

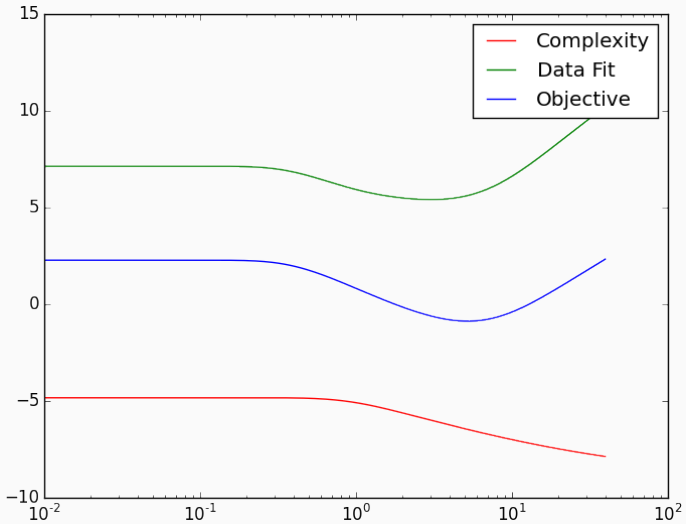
- Type-II Maximum likelihood [1] 3.5.0
- minimise logarithm of marginal likelihood

Learning

$$\text{argmax}_{\boldsymbol{\theta}} p(\mathbf{Y}|\mathbf{X}, \boldsymbol{\theta}) = \text{argmin}_{\boldsymbol{\theta}} - \log\left(p(\mathbf{Y}|\mathbf{X}, \boldsymbol{\theta})\right) = \text{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$$

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{2}\mathbf{y}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{y} + \frac{1}{2}\log|\mathbf{K}| + \frac{N}{2}\log(2\pi)$$

Learning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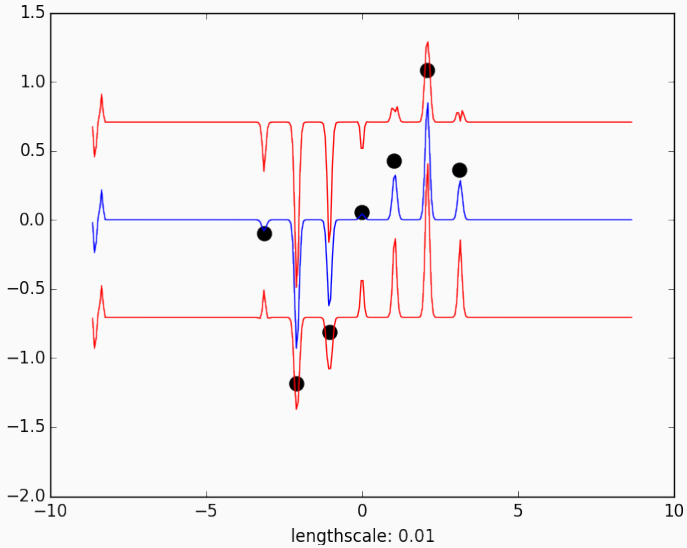
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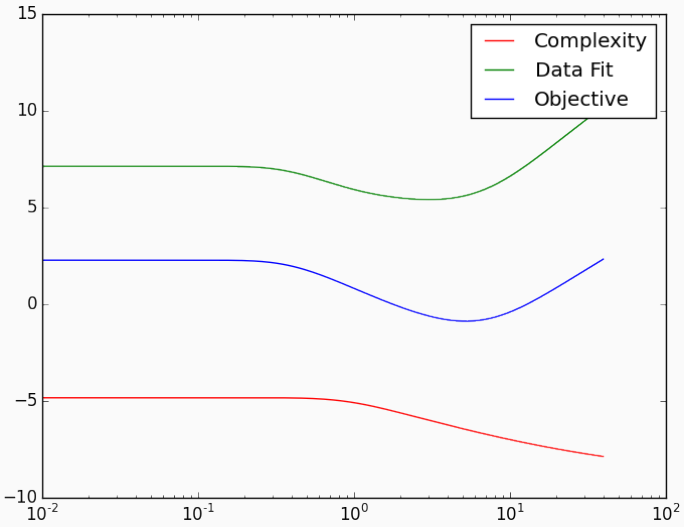
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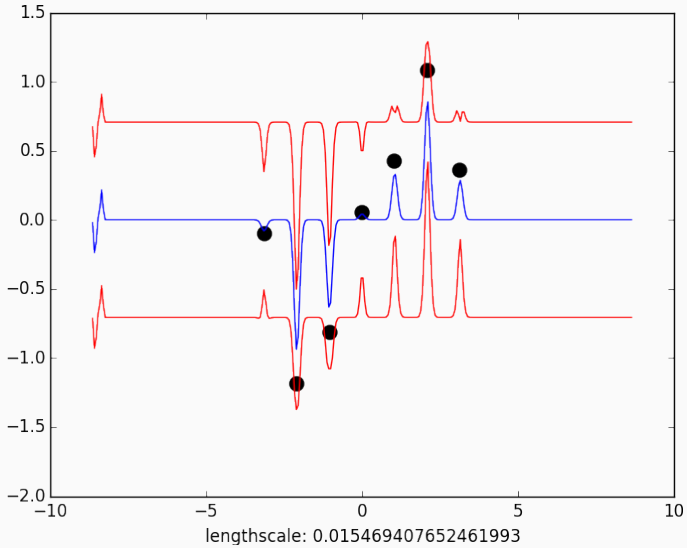
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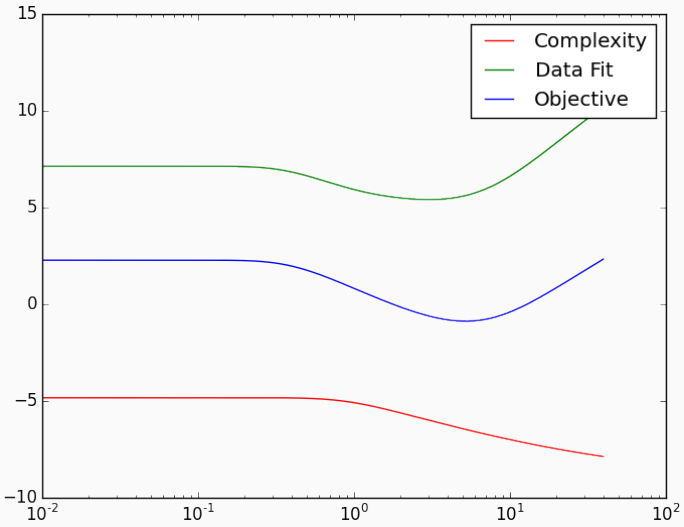
Learning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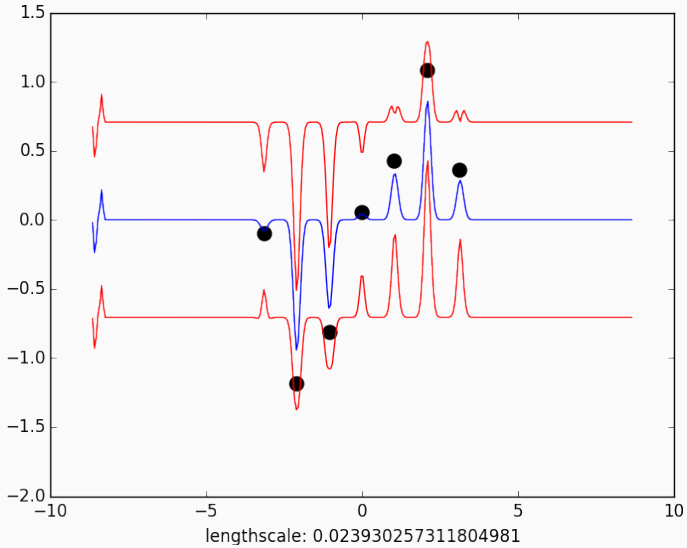
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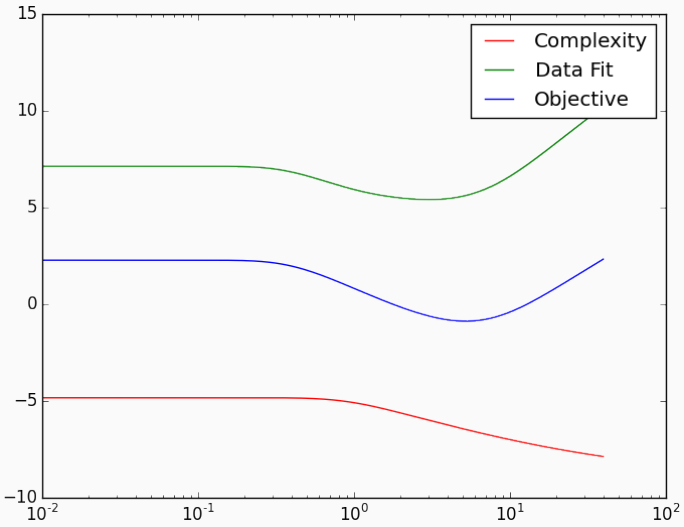
Learning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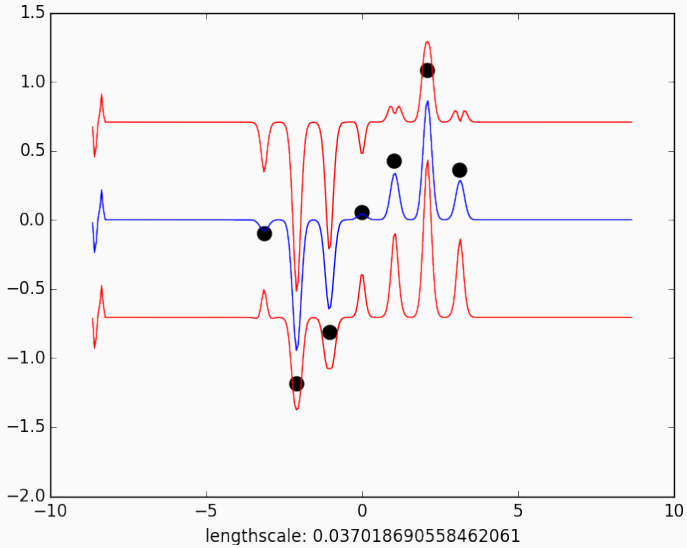
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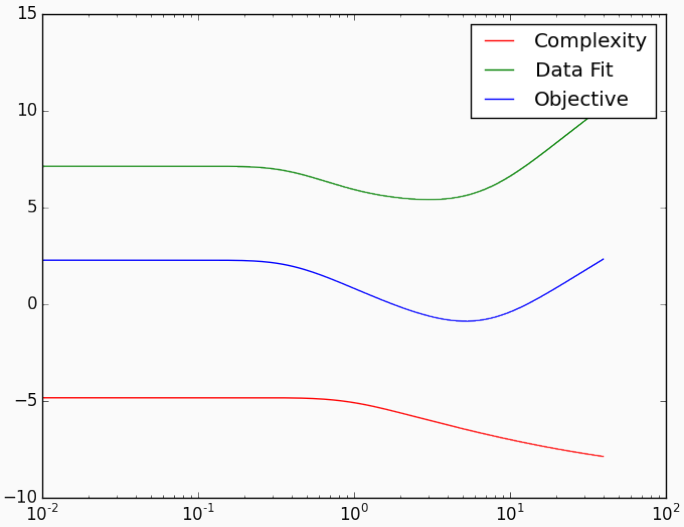
Learning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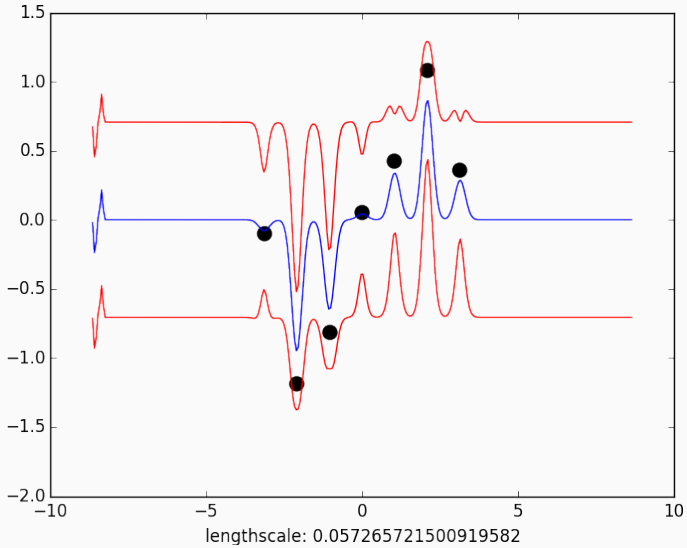
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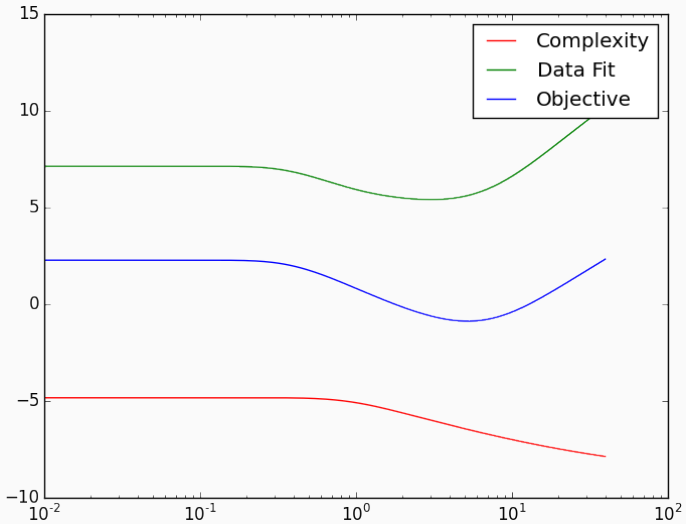
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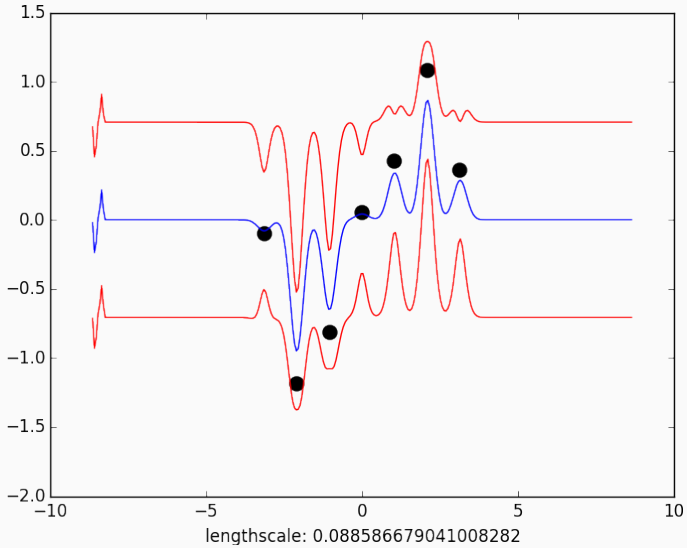
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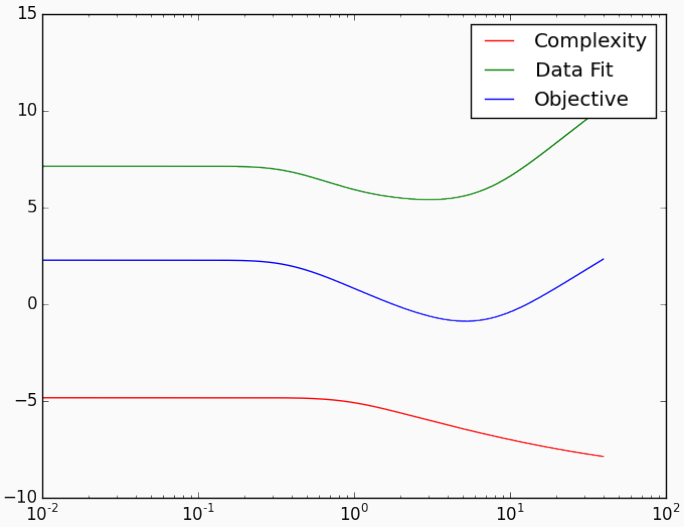
Learning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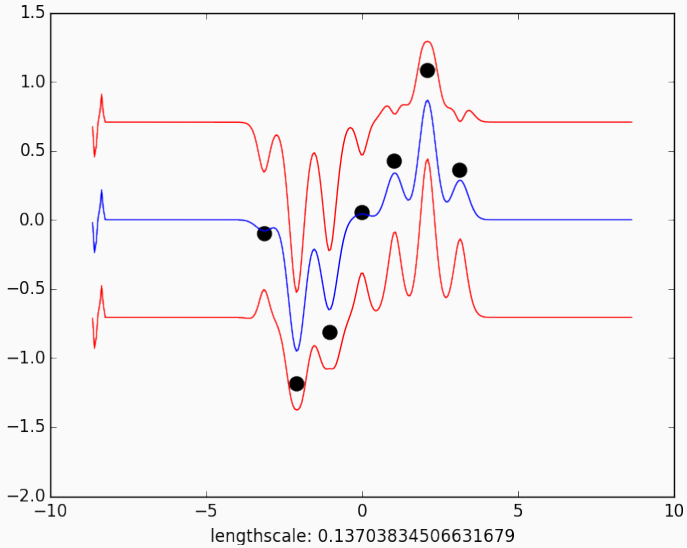
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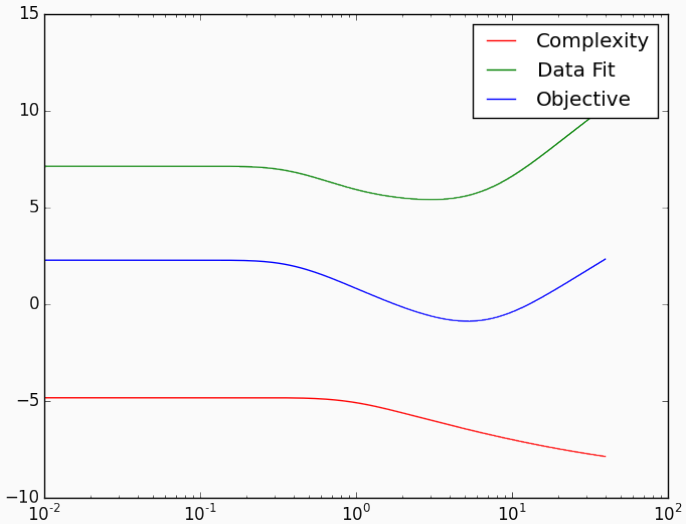
Learning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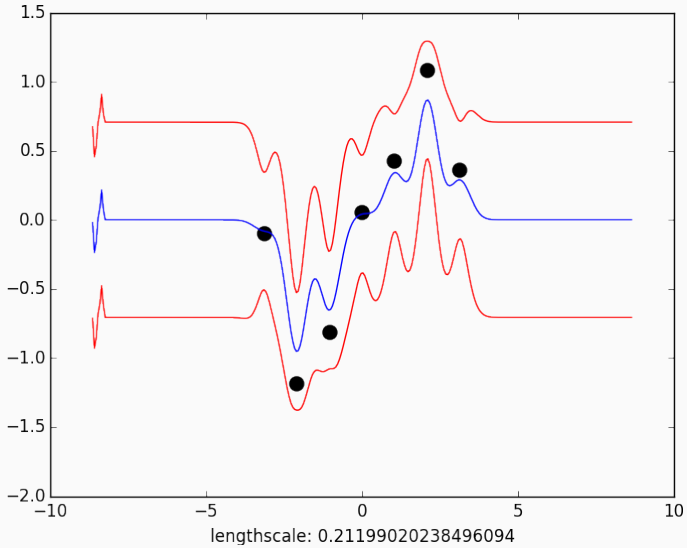
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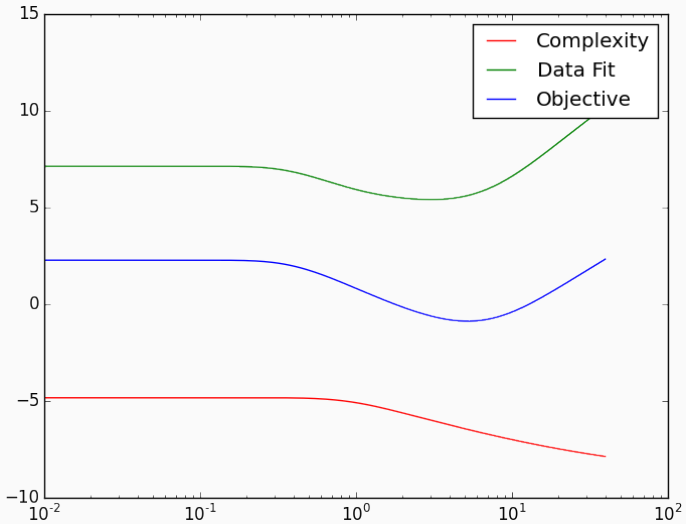
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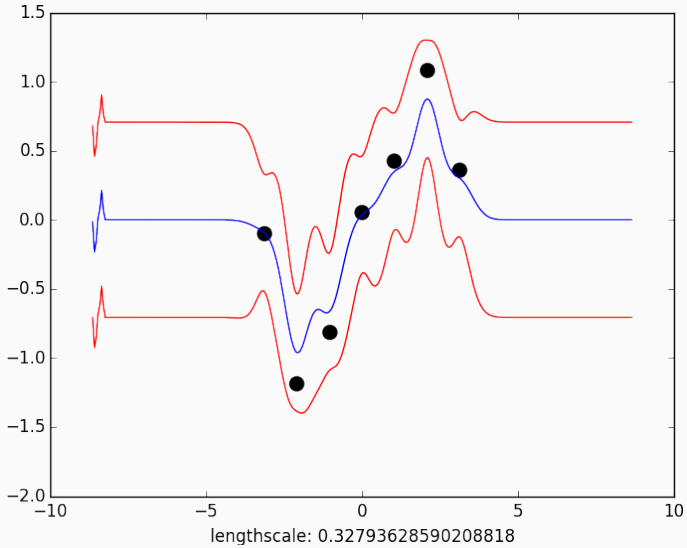
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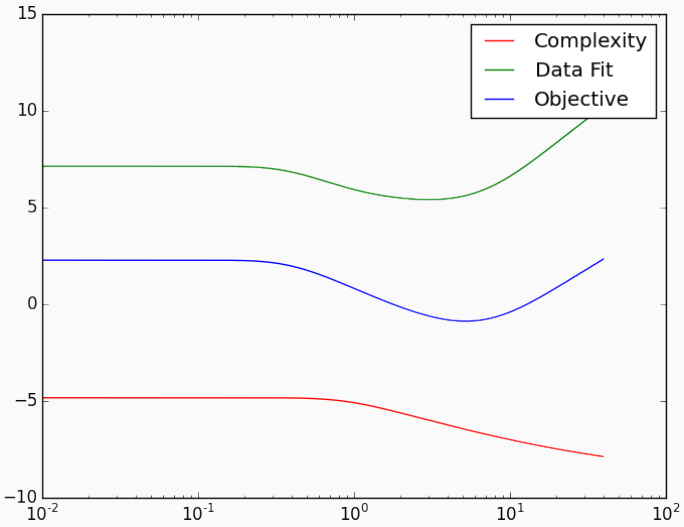
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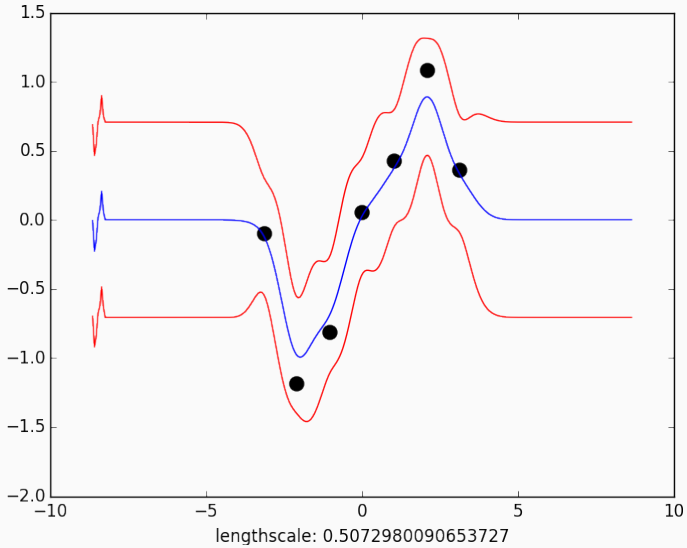
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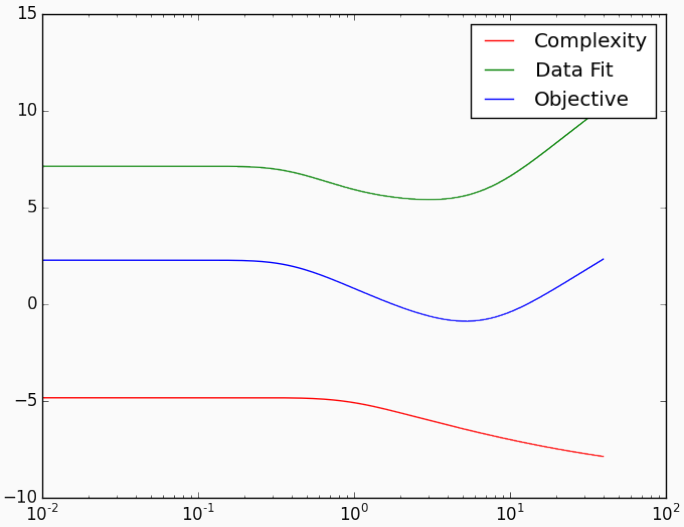
Learning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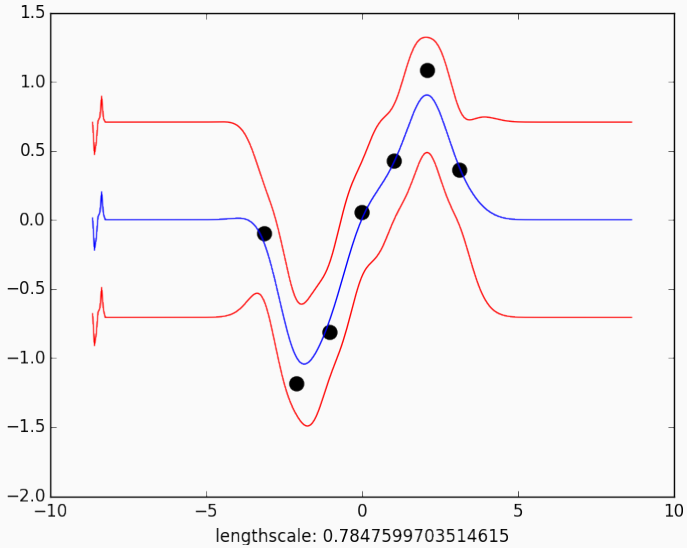
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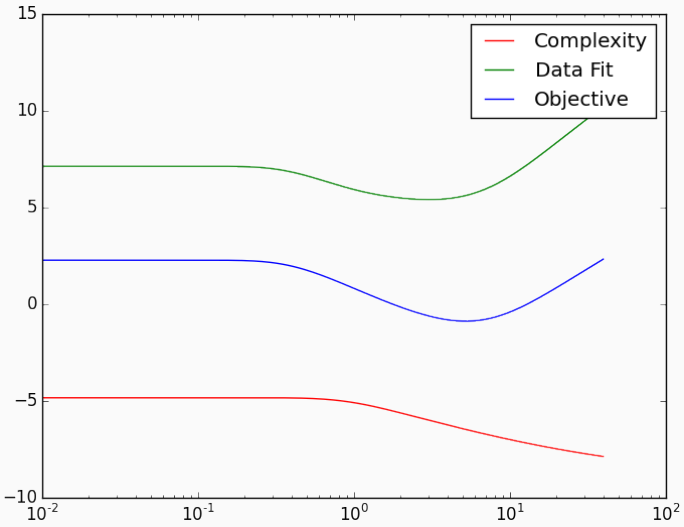
Learning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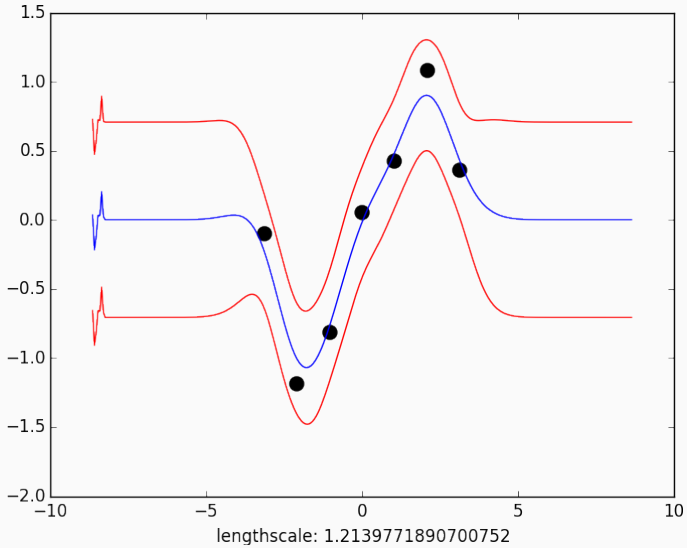
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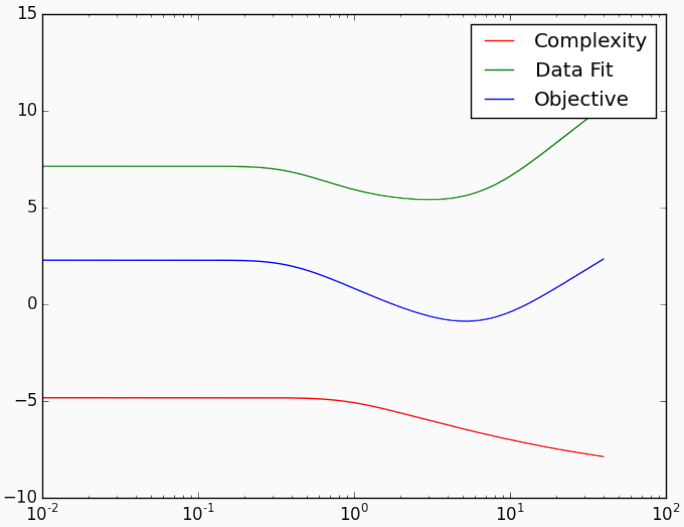
Learning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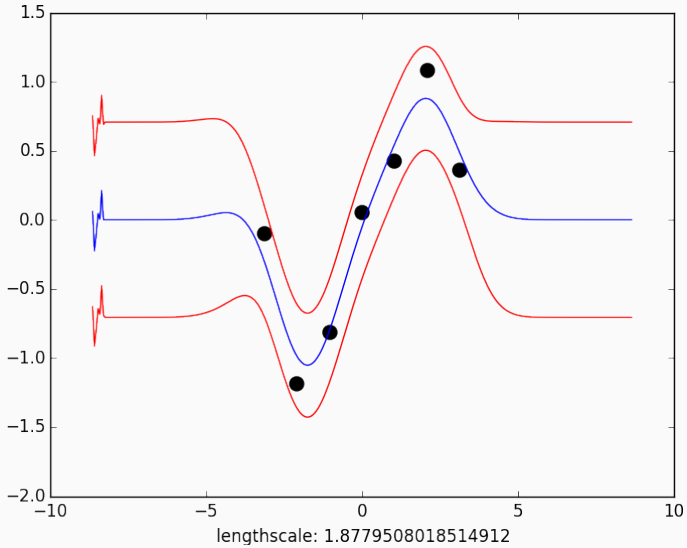
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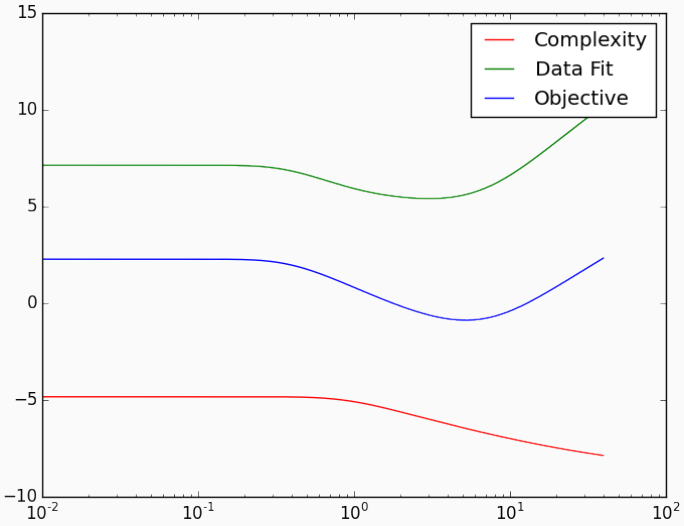
Learning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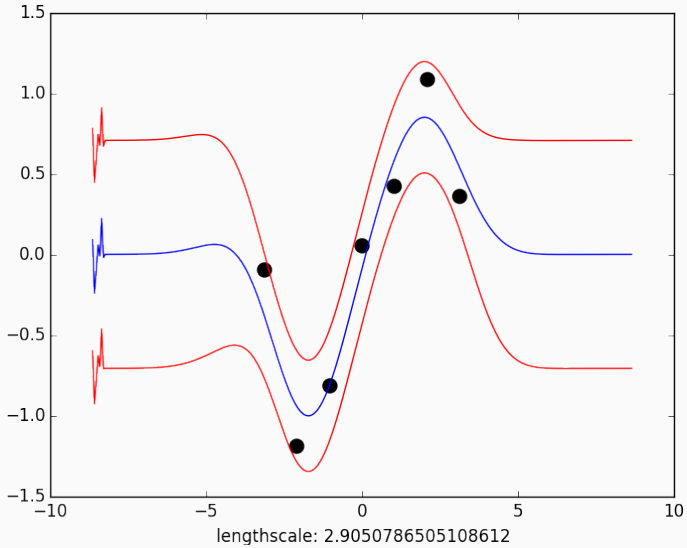
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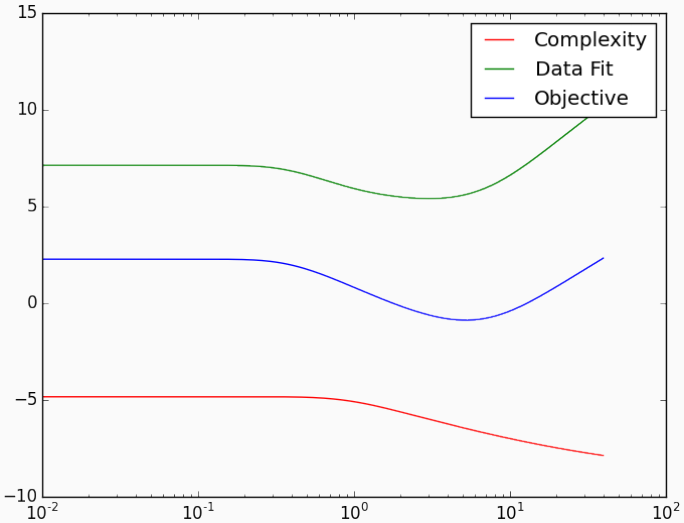
Learning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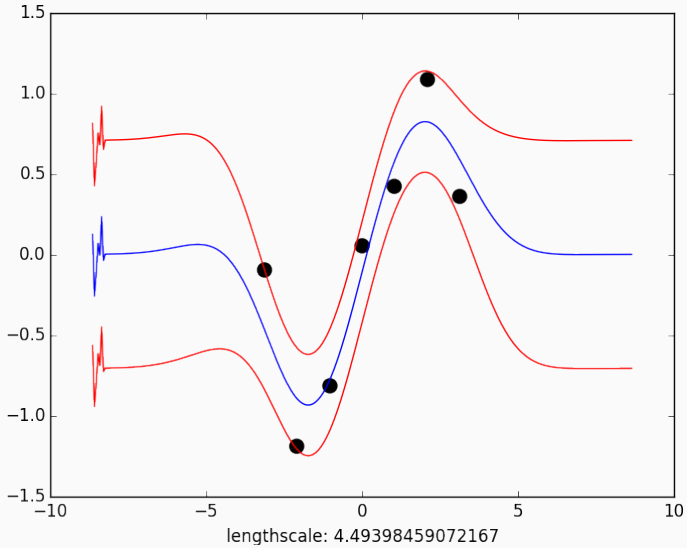
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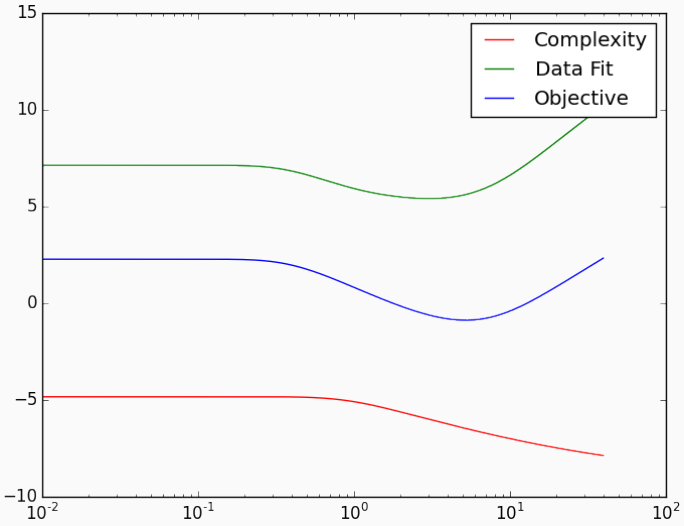
Learning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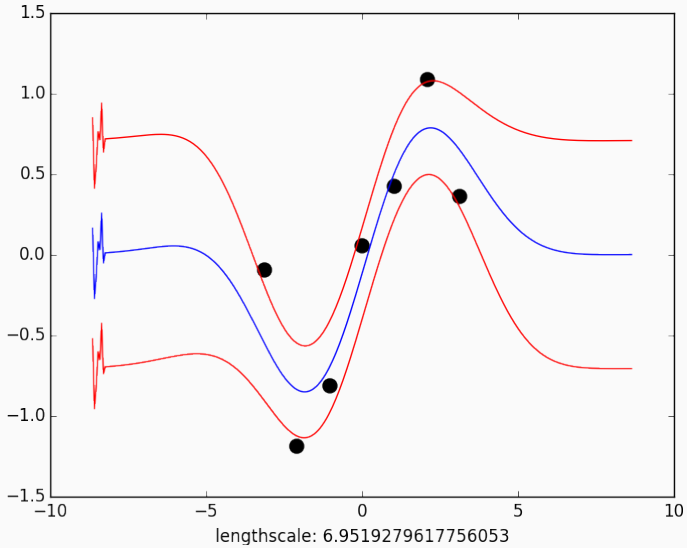
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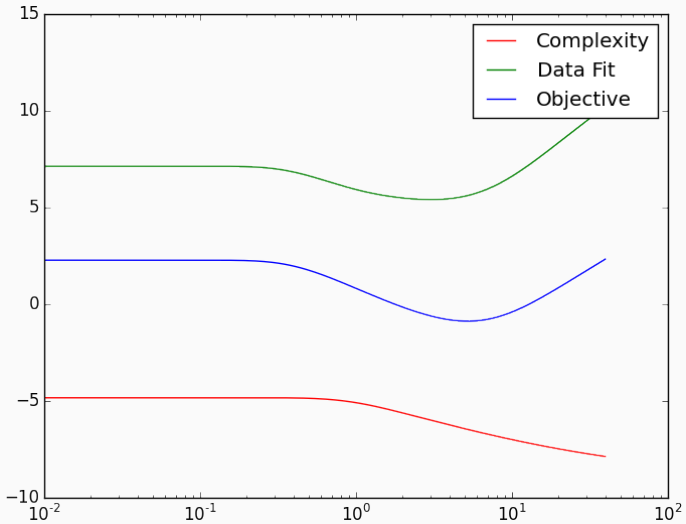
Learning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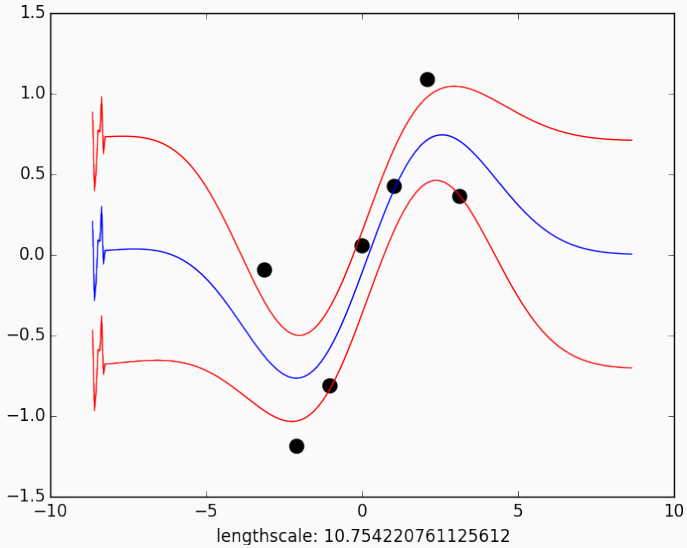
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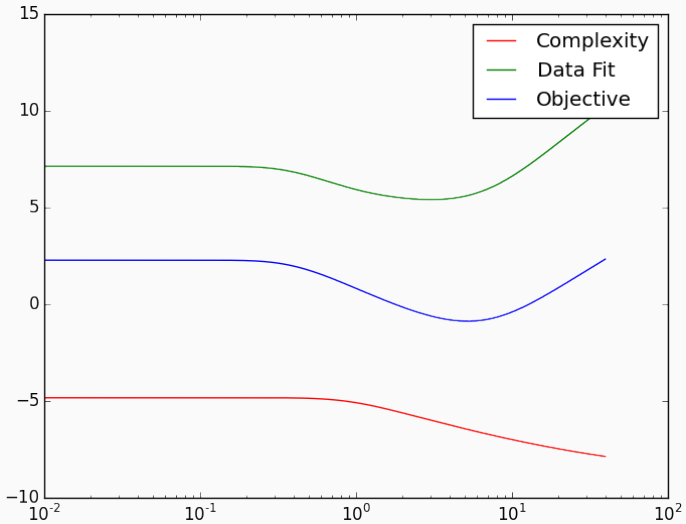
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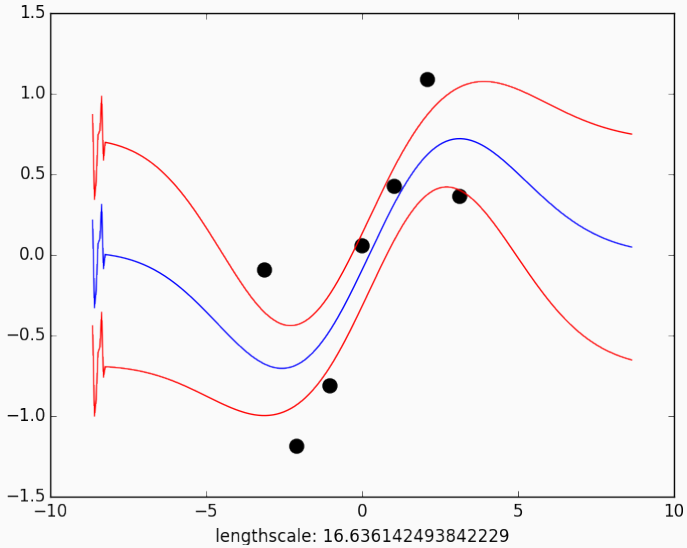
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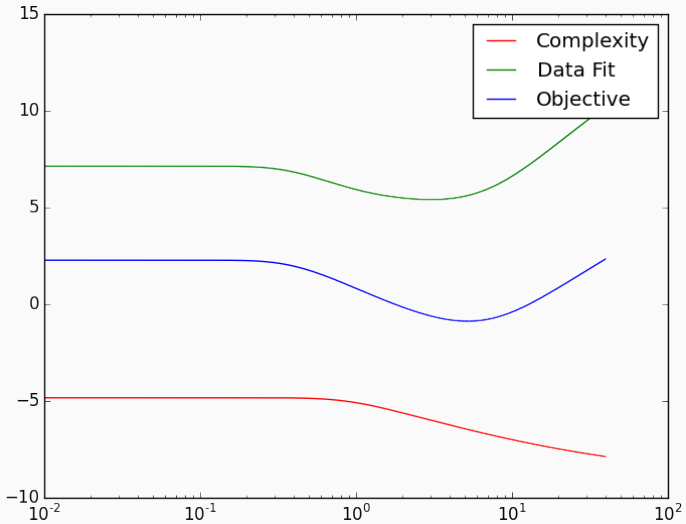
Learning


Complexity
Data Fit
Objective
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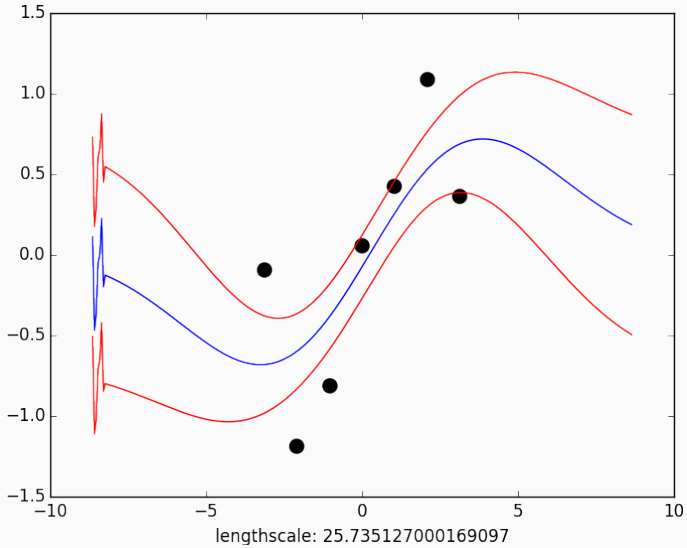
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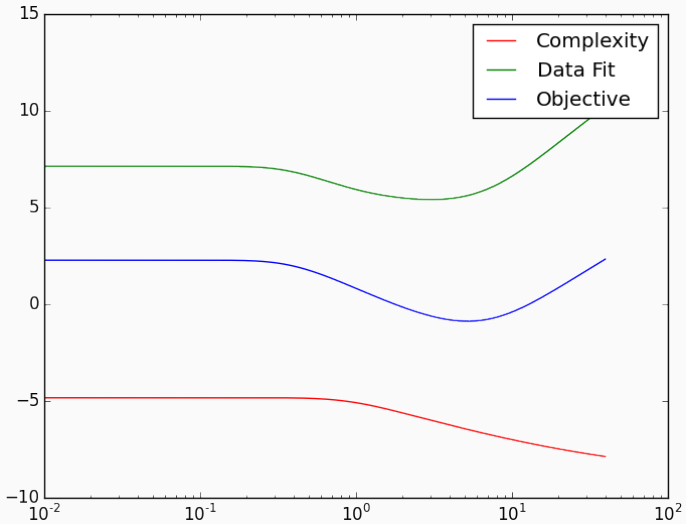
Learning


Complexity
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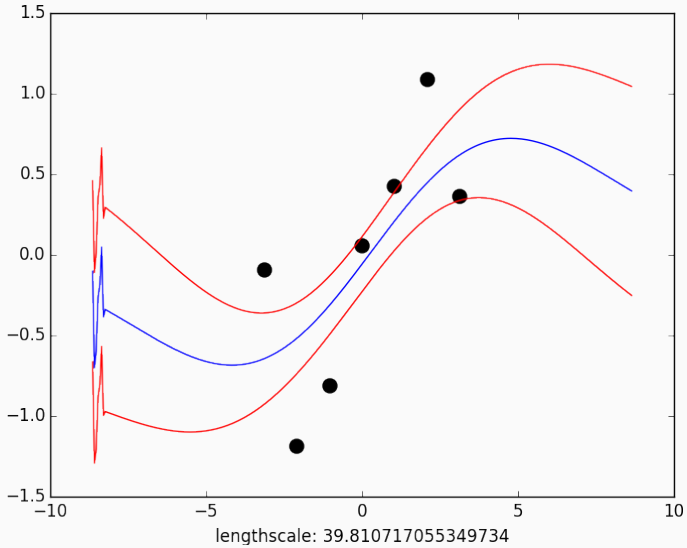
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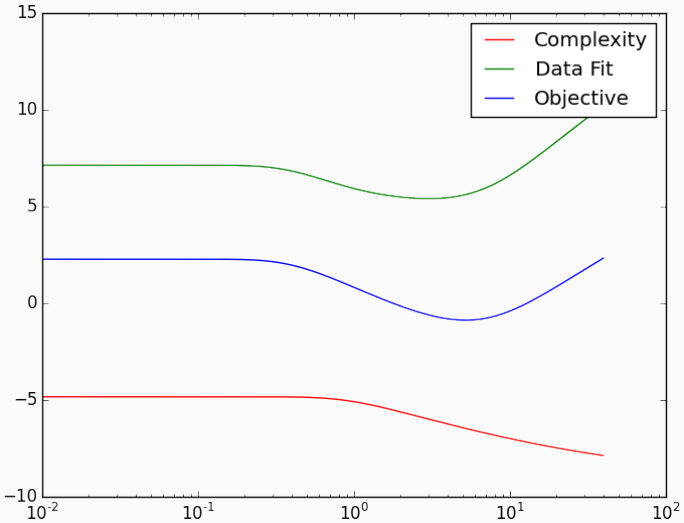
Learning


Complexity
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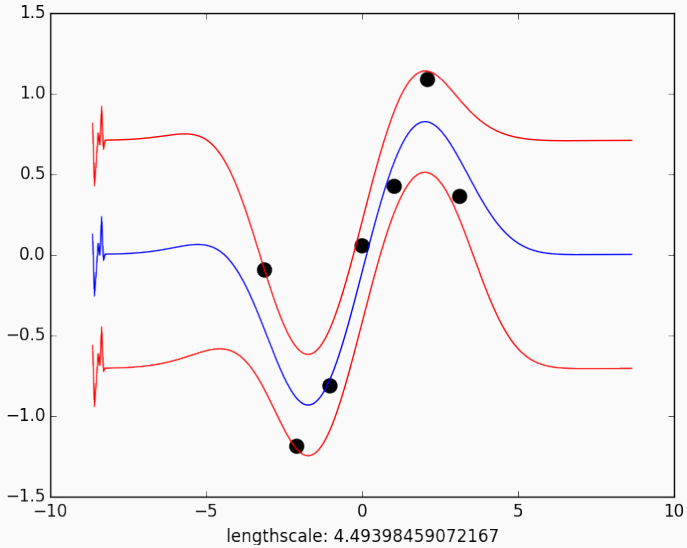
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lengthscale: 4.49398459072167

Linear Latent Variable Models [1] 12.2

- Linear Regression

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

Linear Latent Variable Models [1] 12.2

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- Linear Unsupervised Learning

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

Linear Latent Variable Models [1] 12.2

- Linear Regression

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

- Linear Unsupervised Learning

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

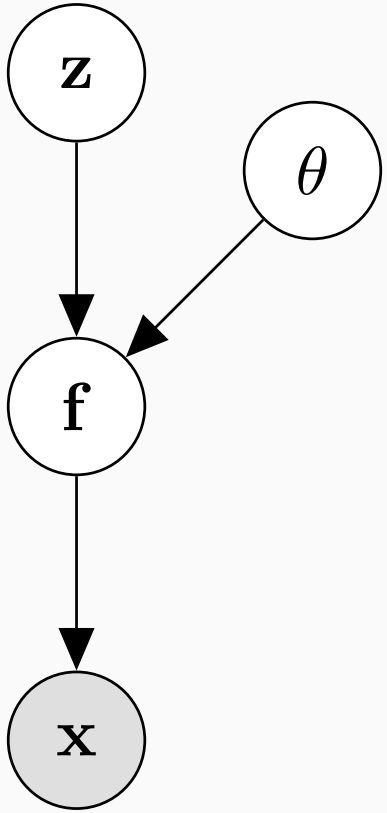
- Actually formulating the posterior over both $\mathbf{W}$ and $\mathbf{z}$ is intractable

Type II Maximum Likelihood

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

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

Non-linear Latent variable model



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

Demo

Font Demo

Bayesian Optimisation

Next lectures

Today Bayesian Optimisation

Monday Dirichlet Processes

Tuesday Topic Models

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.

Uncertainty

- Deterministic world

$$x = 4$$

- Point estimate world

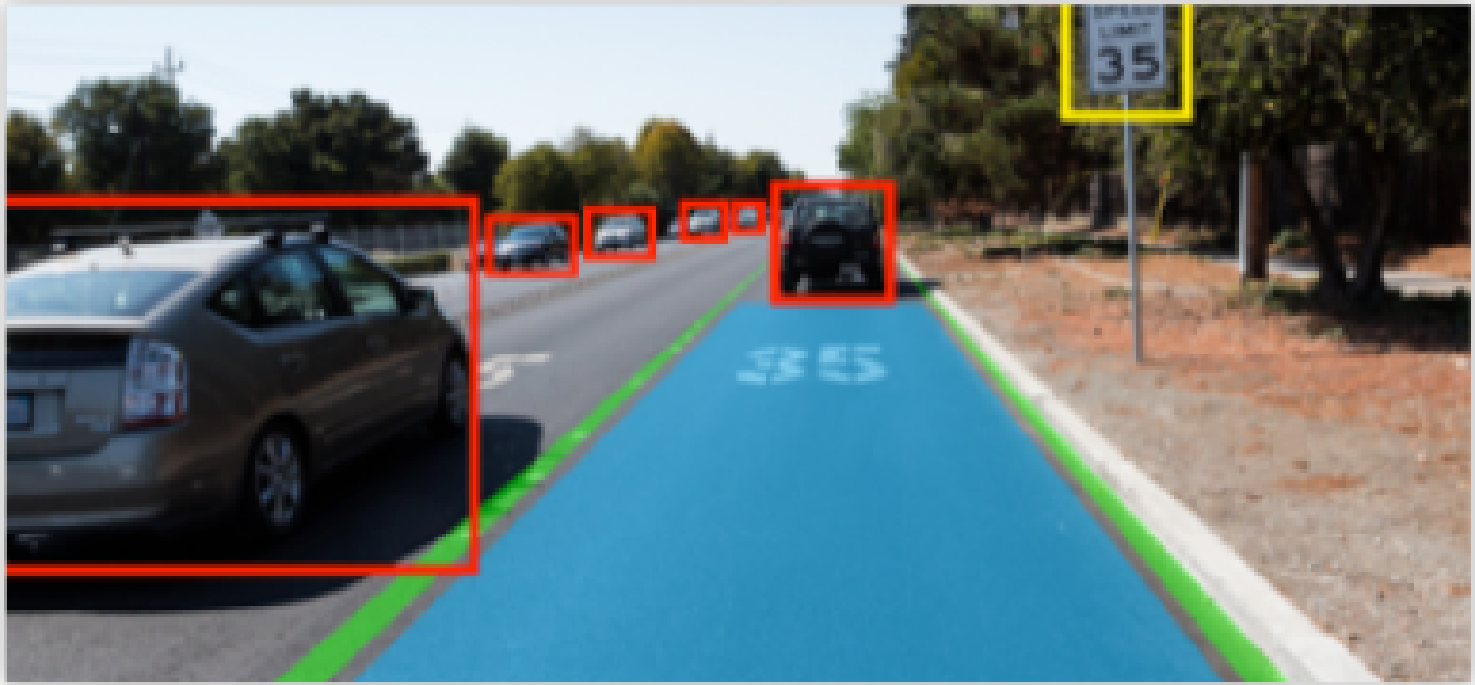
$$\text{argmax}_x p(x) = 4$$

- Stochastic world

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

Uncertainty

Uncertainty

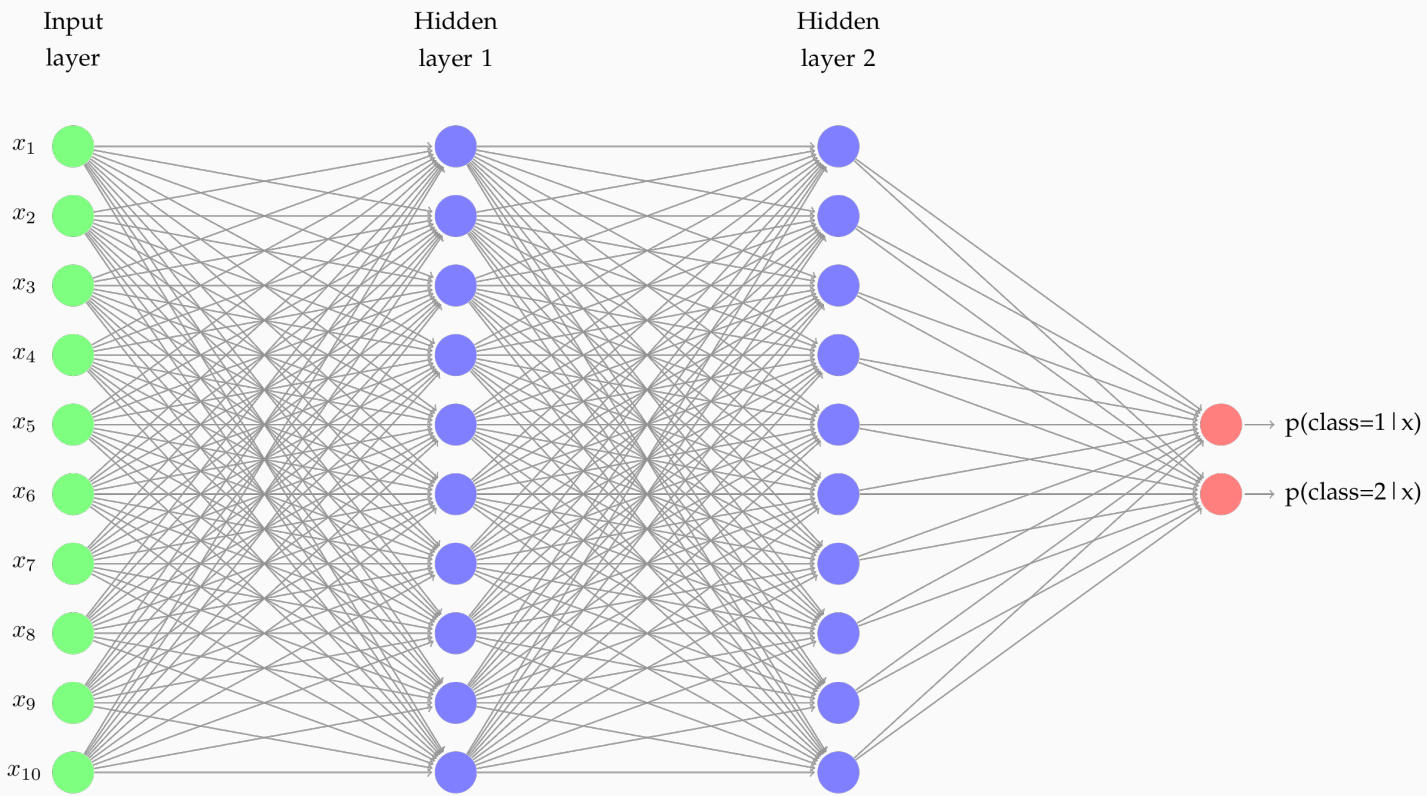


Real Doctors

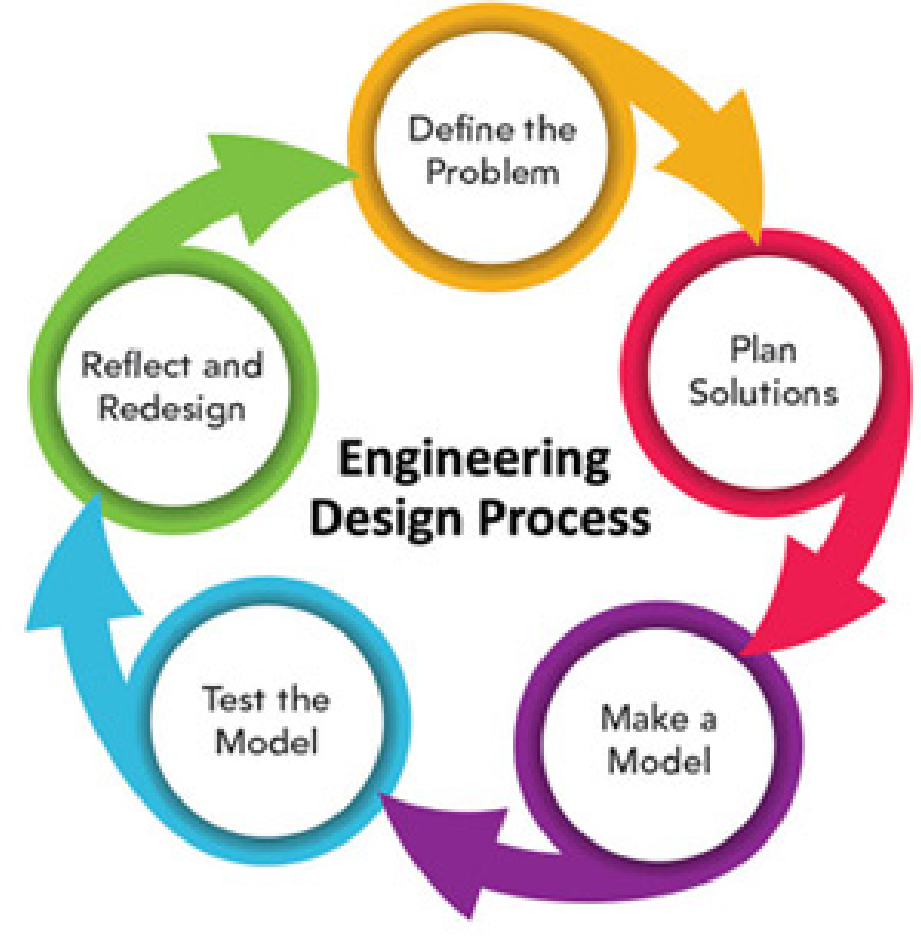
Real Doctors

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

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

- Much more common

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

Implicit understanding

Optimisation

- in most cases we have an objective function that we do not know

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- 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

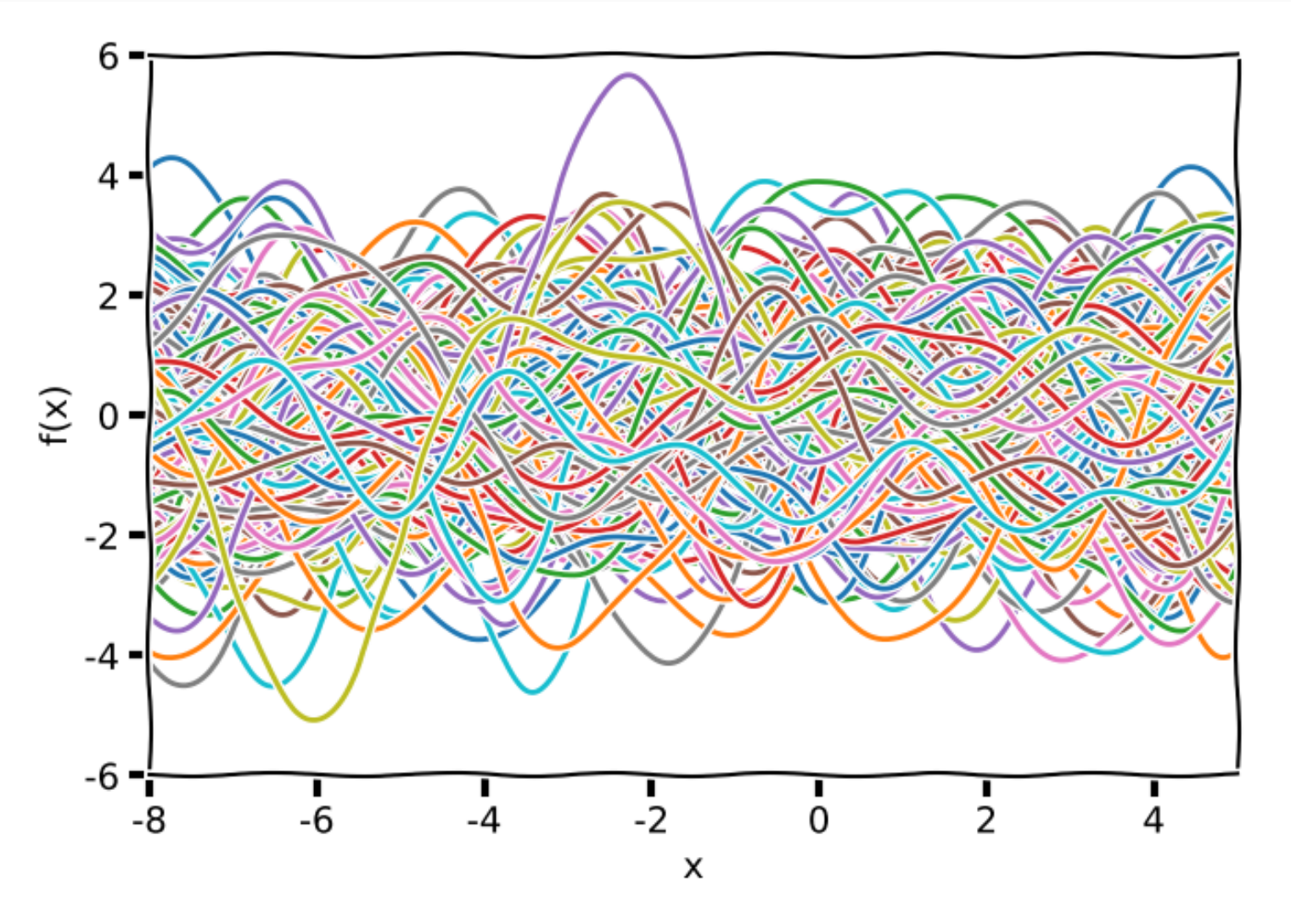
Strategies

- Implicit knowledge
- Grid search

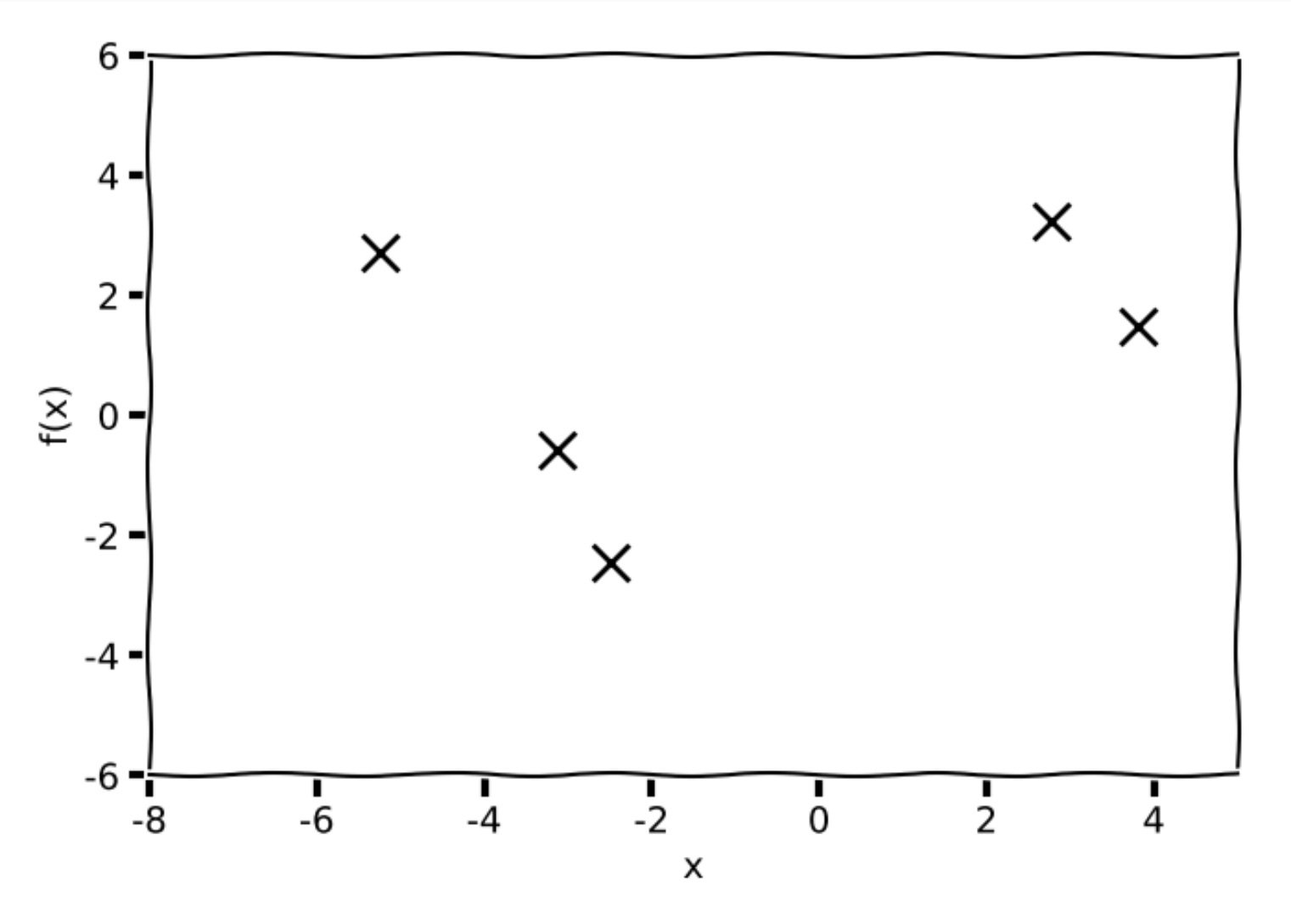
  $$f(x_M) - f(x'_M) \leq \epsilon$$

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

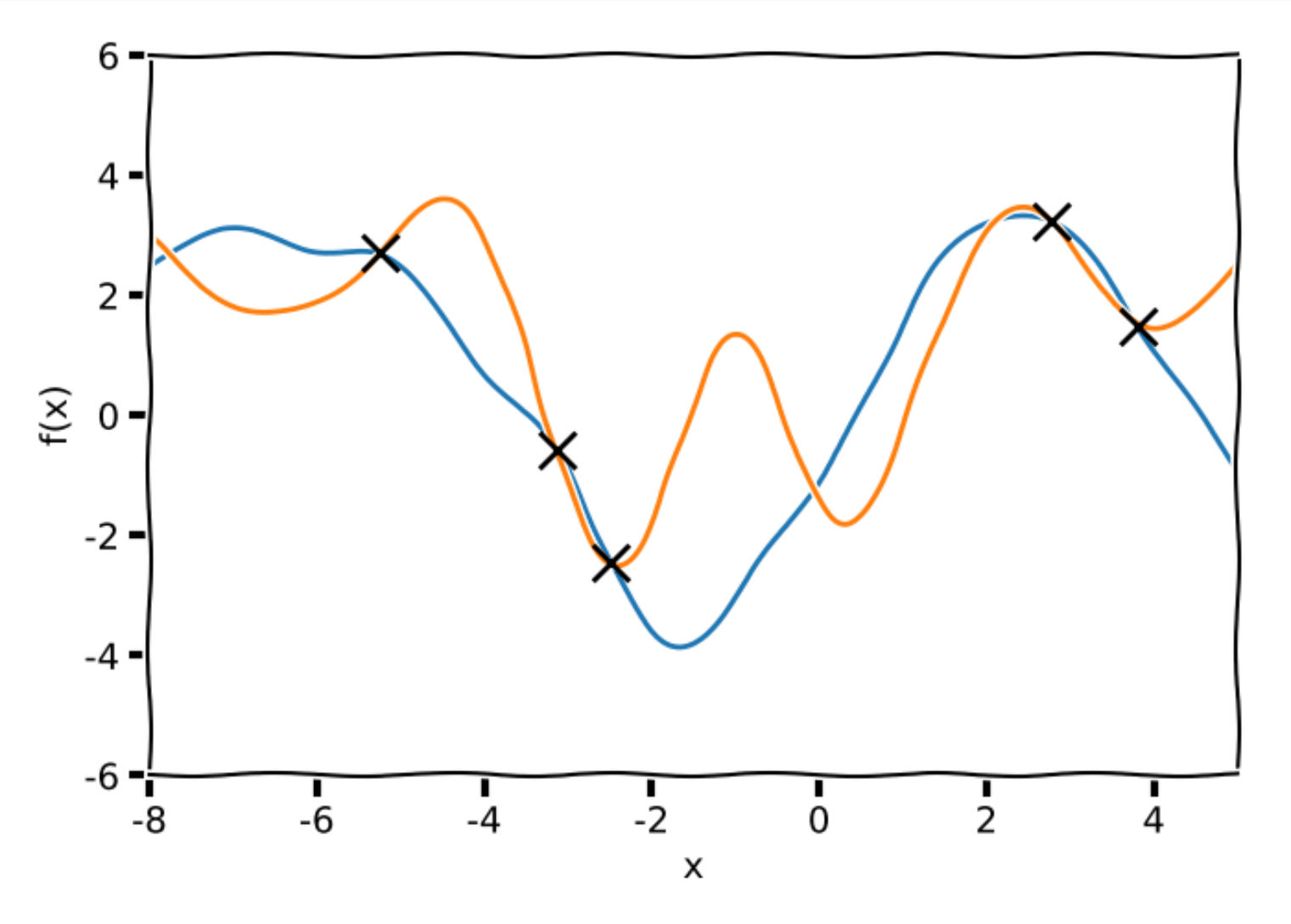
BO in practice



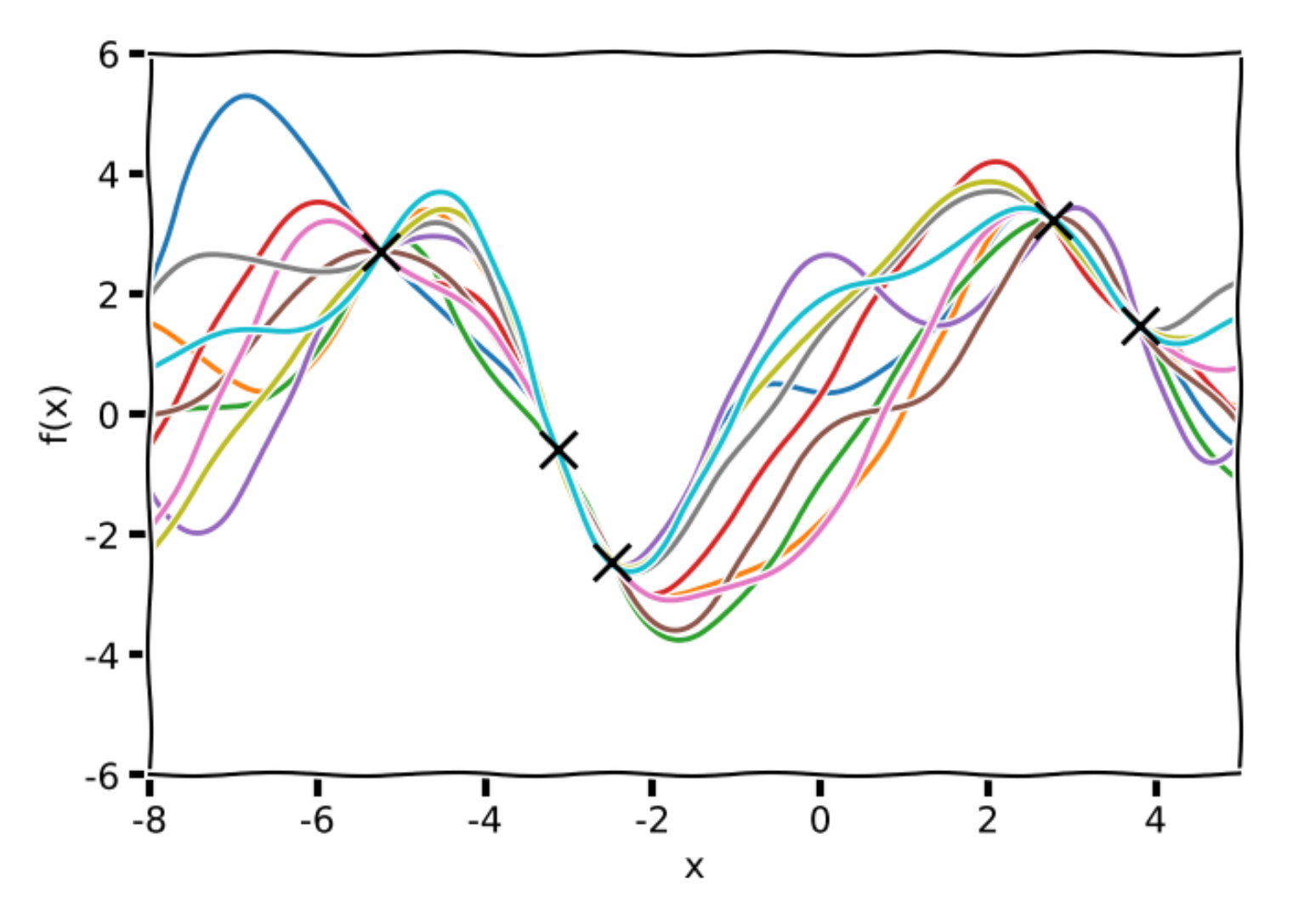
BO in practice



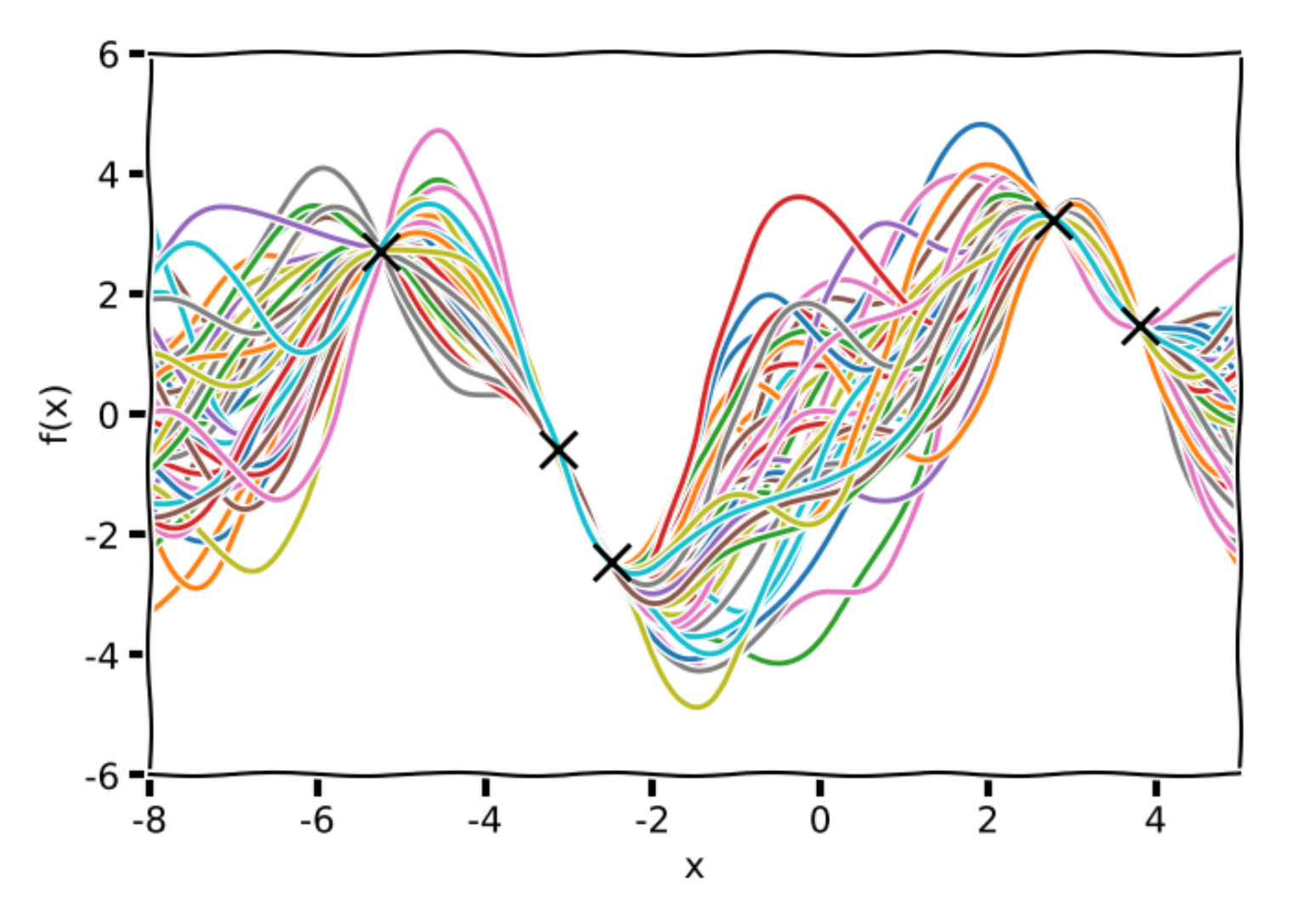
BO in practice



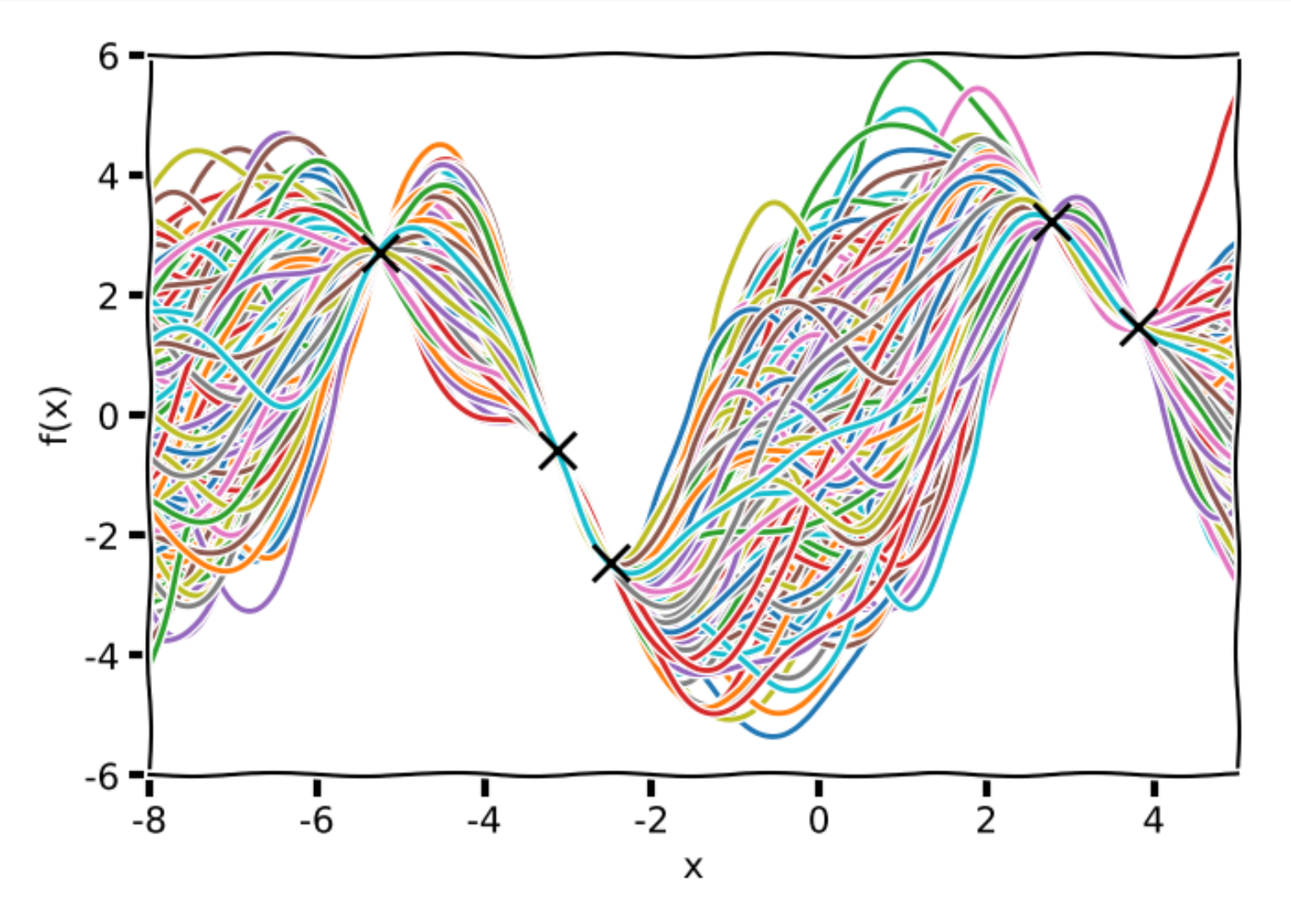
BO in practice



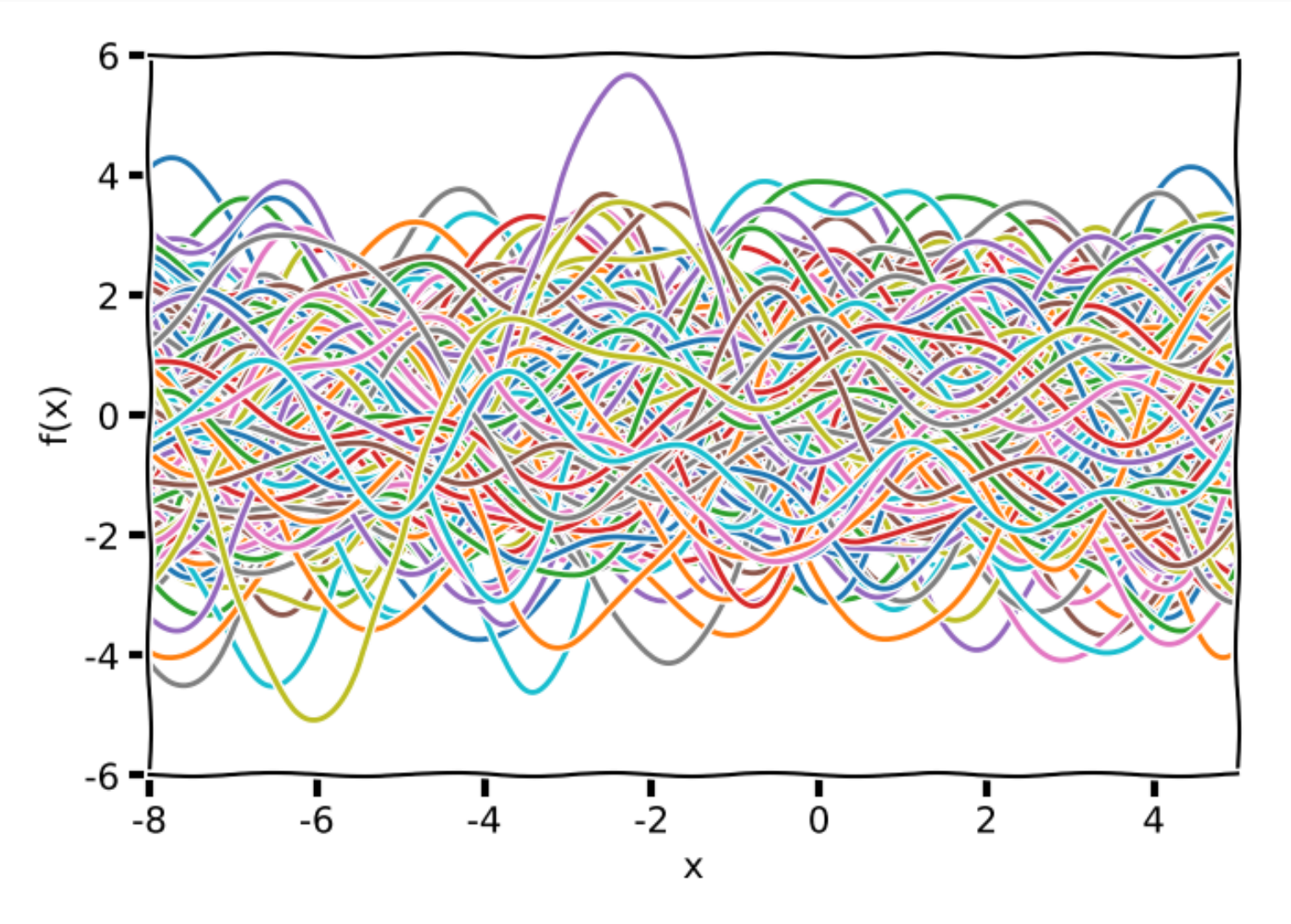
BO in practice



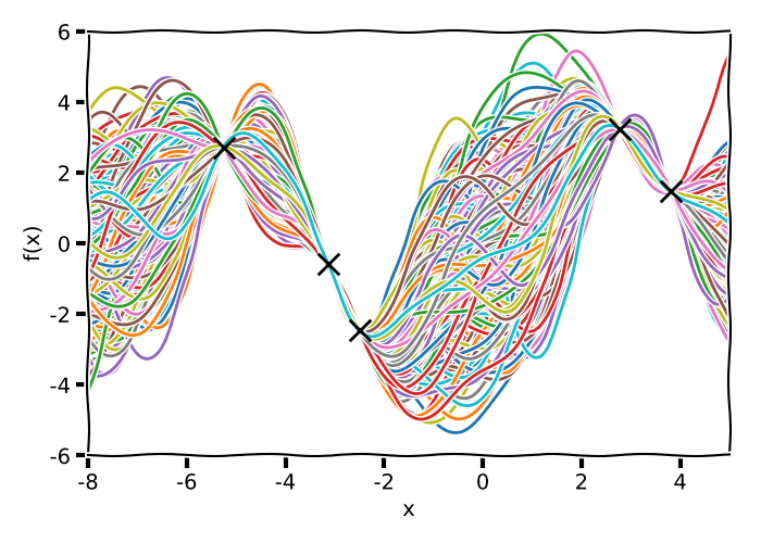
BO in practice

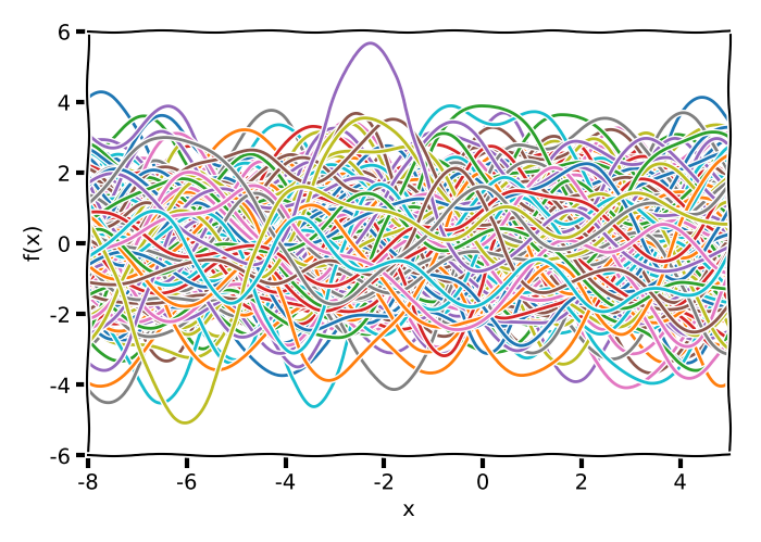


BO in practice



What did we actually do





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

Bayesian Optimisation

1. Choose a prior over the space of possible objective functions f

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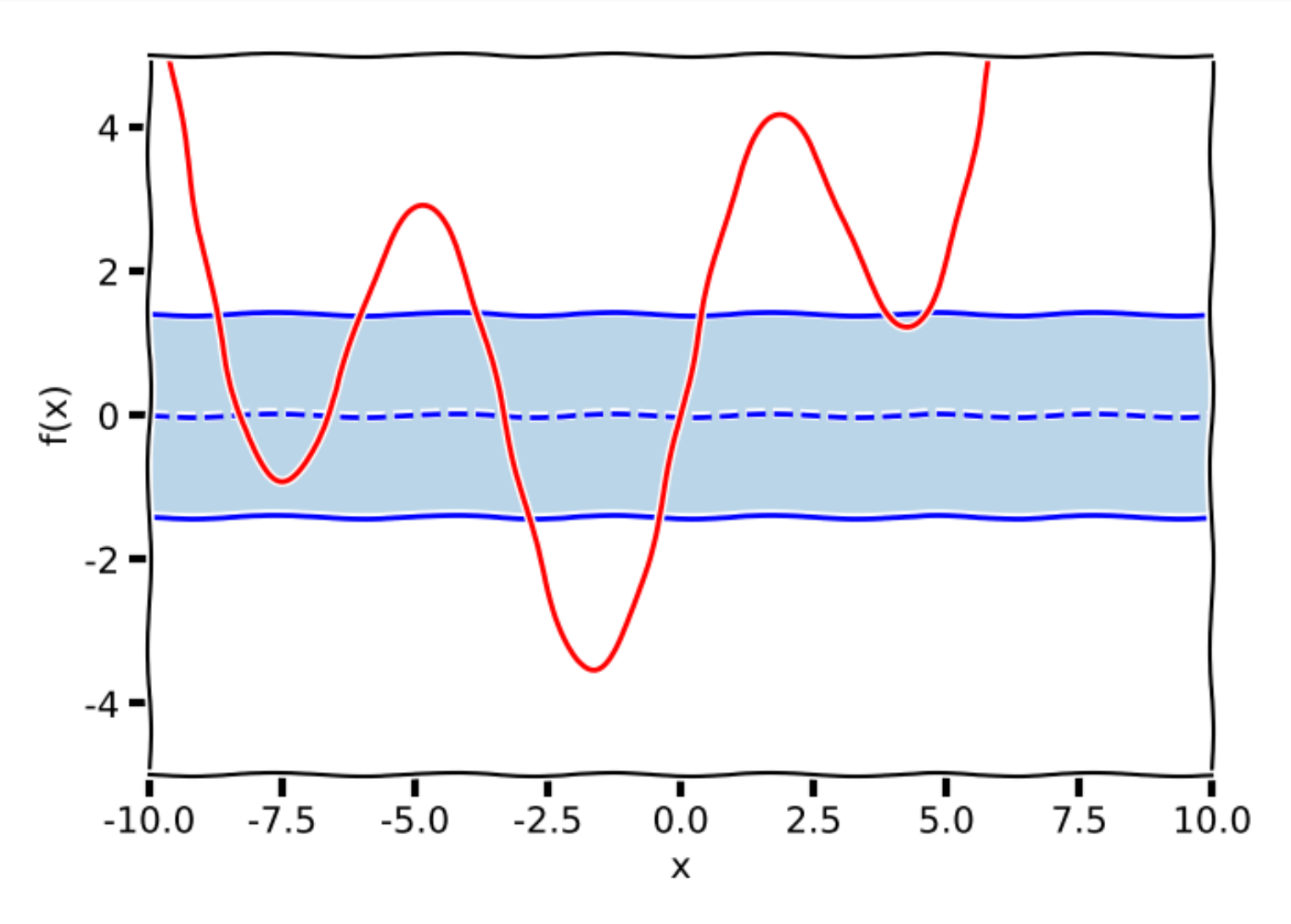
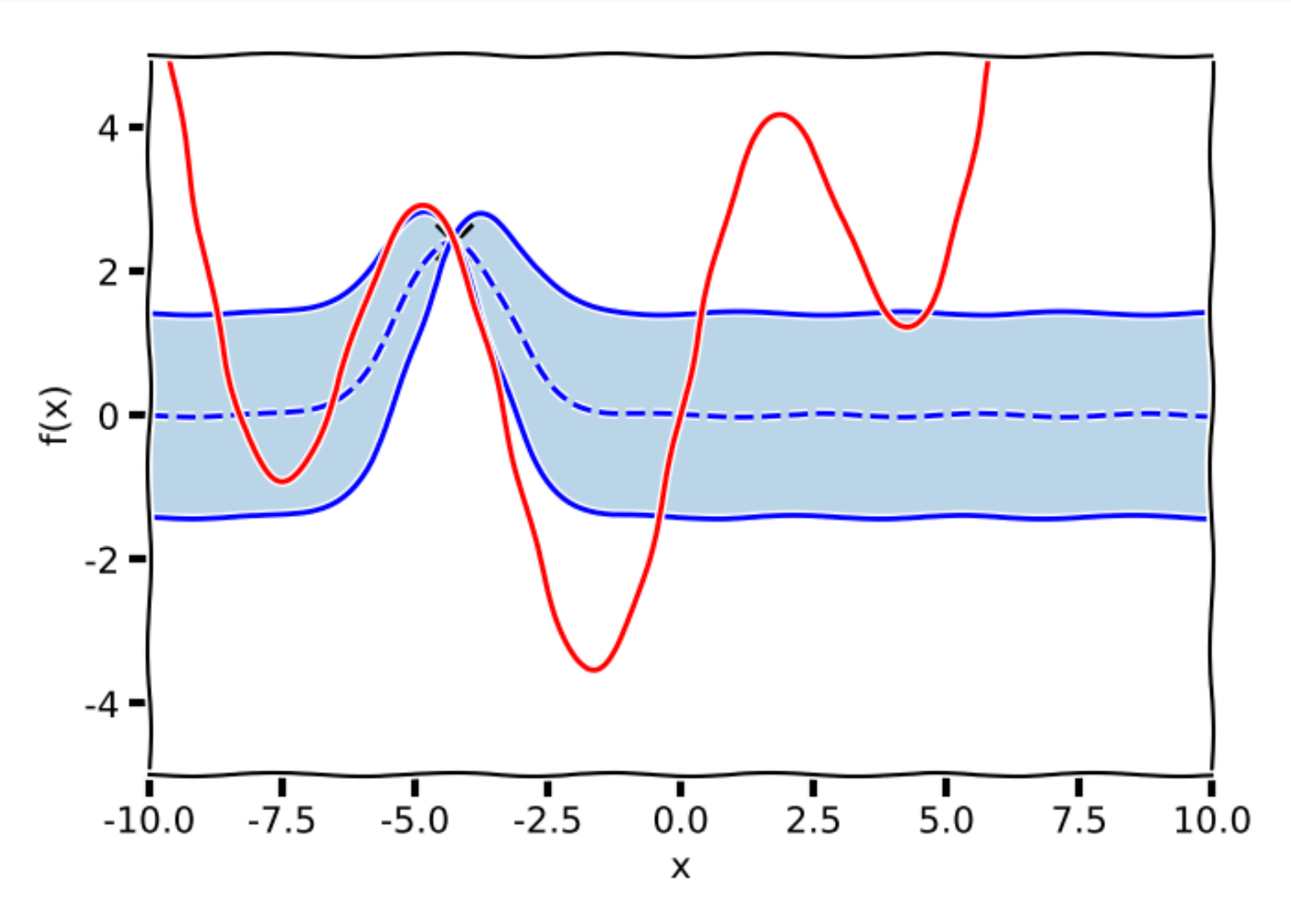
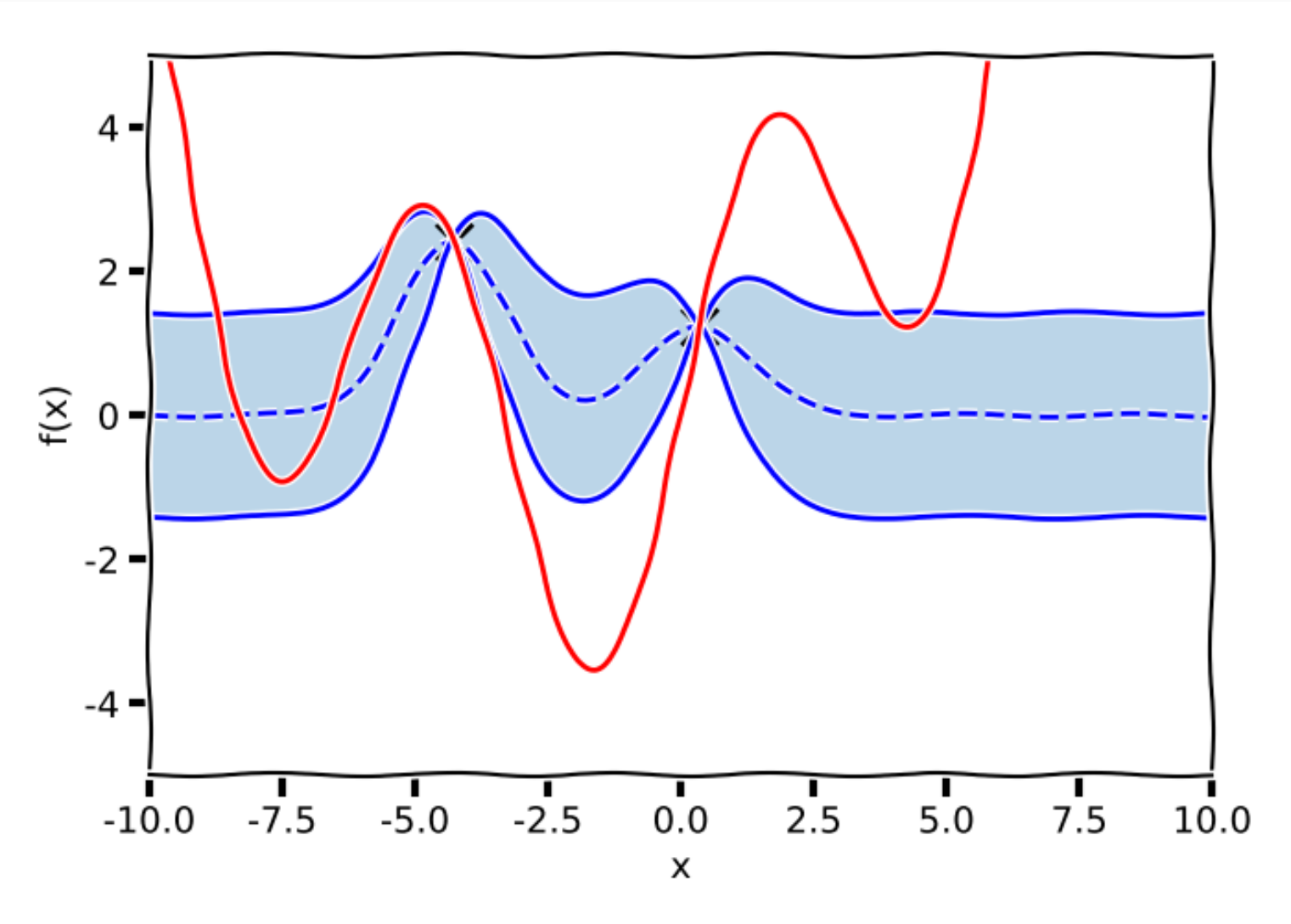
Gaussian Processes



Gaussian Processes



Gaussian Processes



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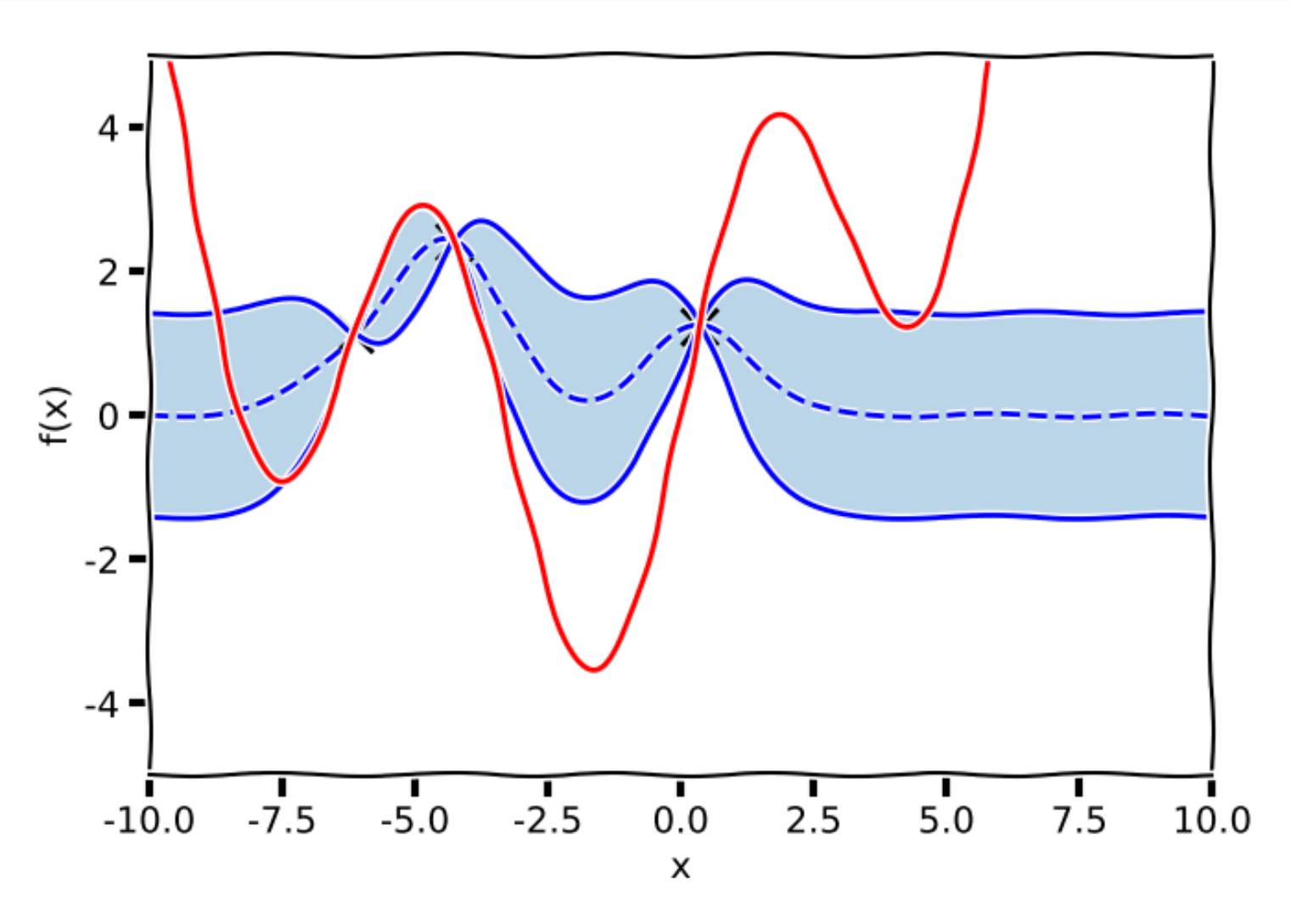

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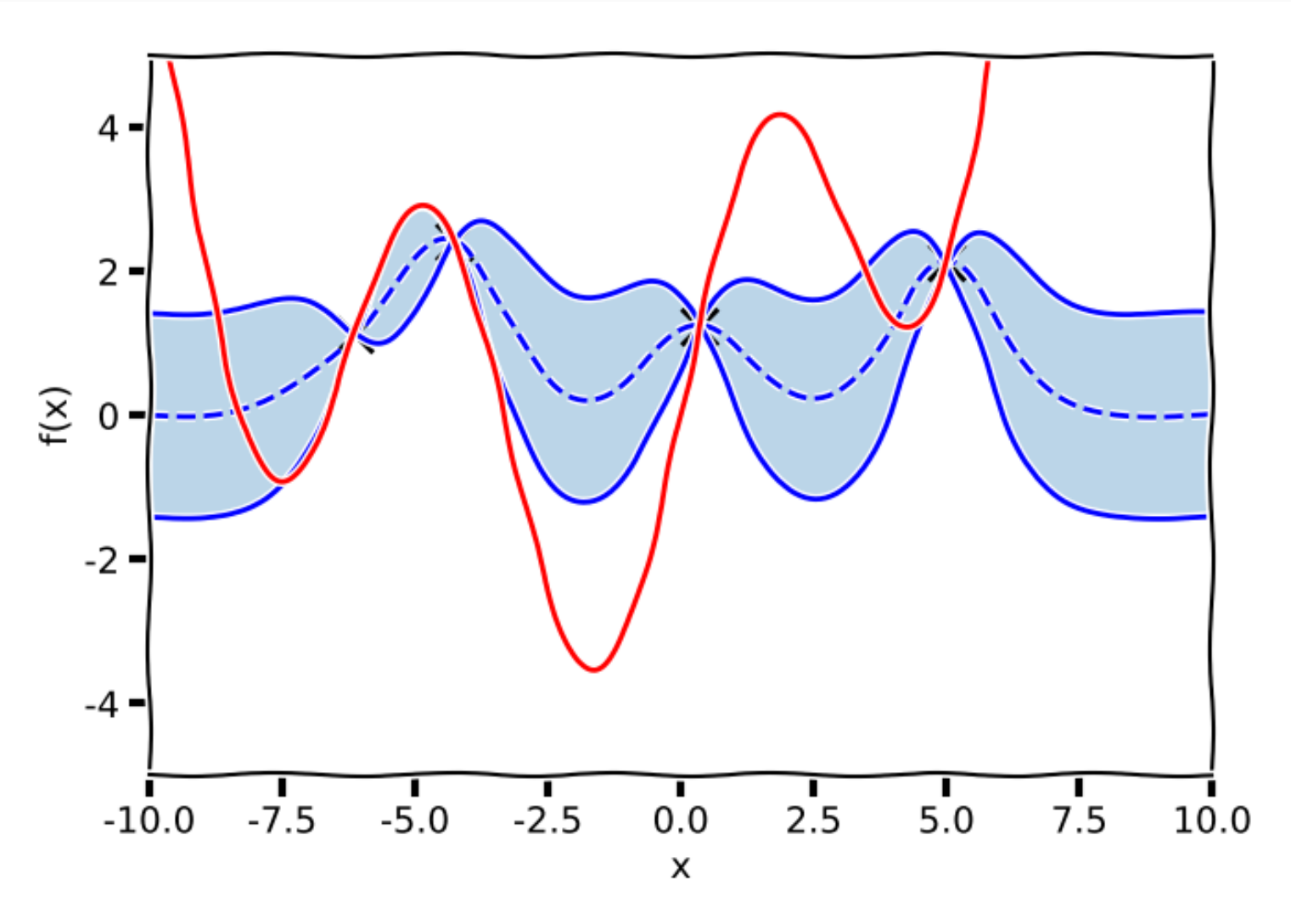

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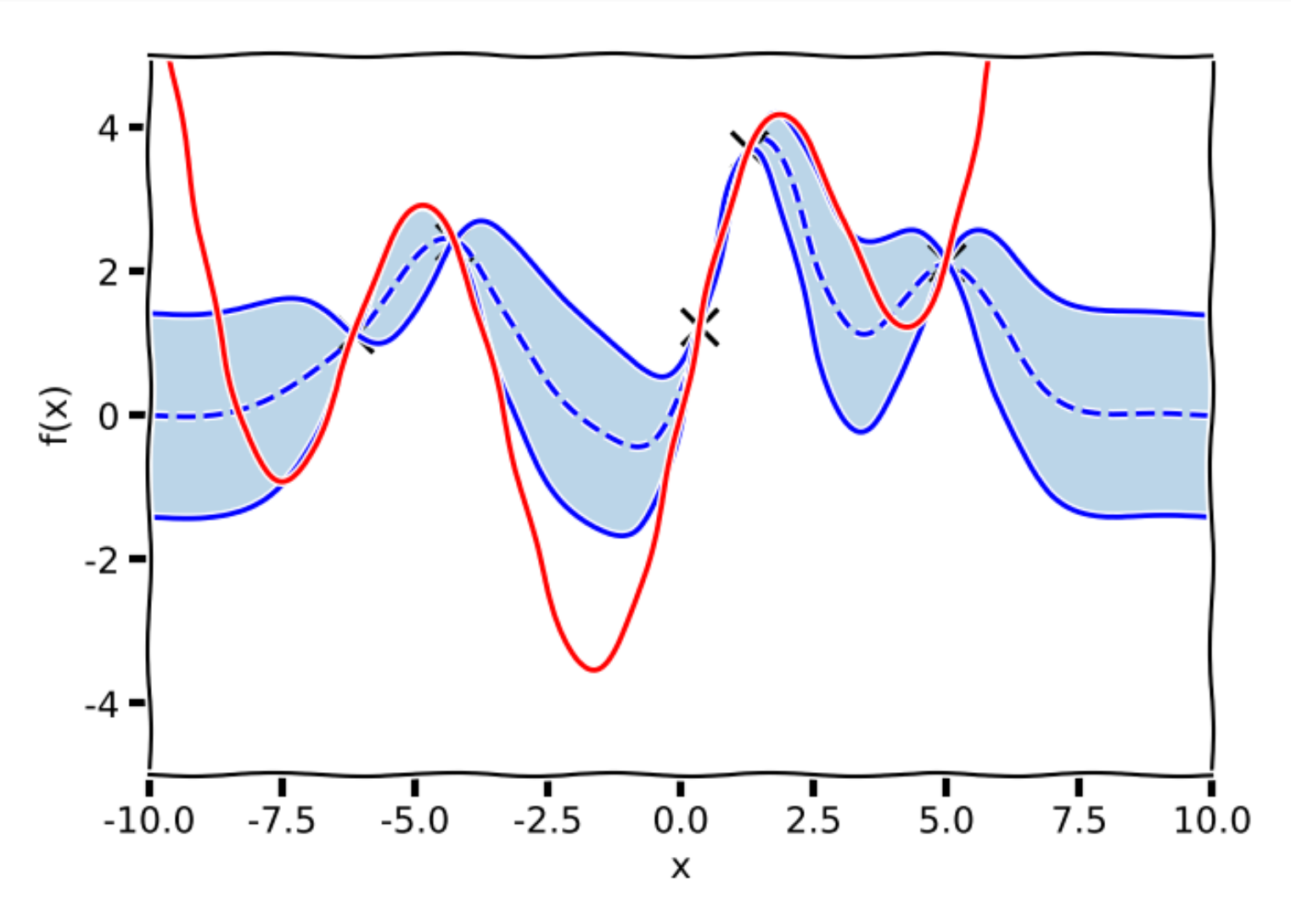

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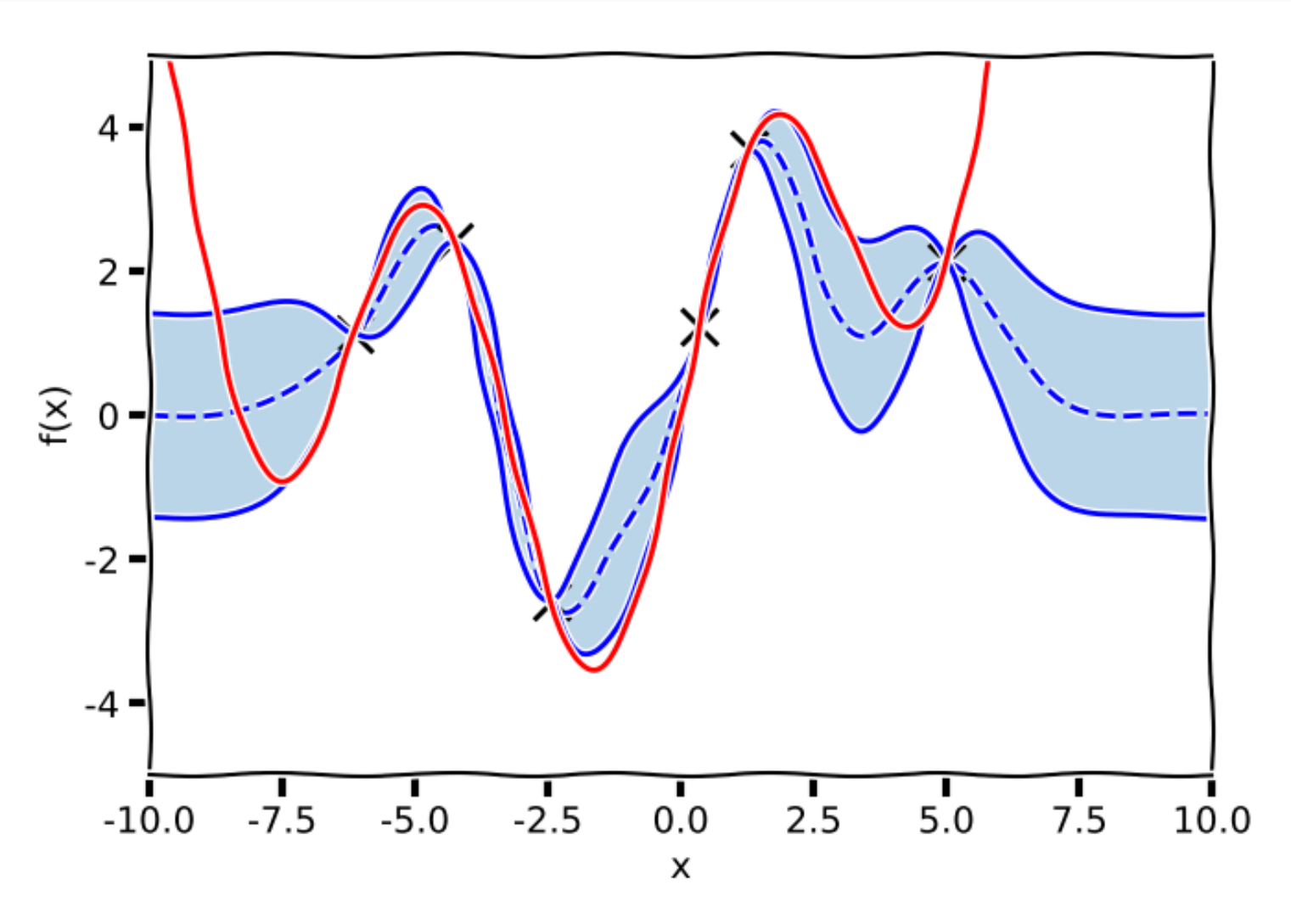

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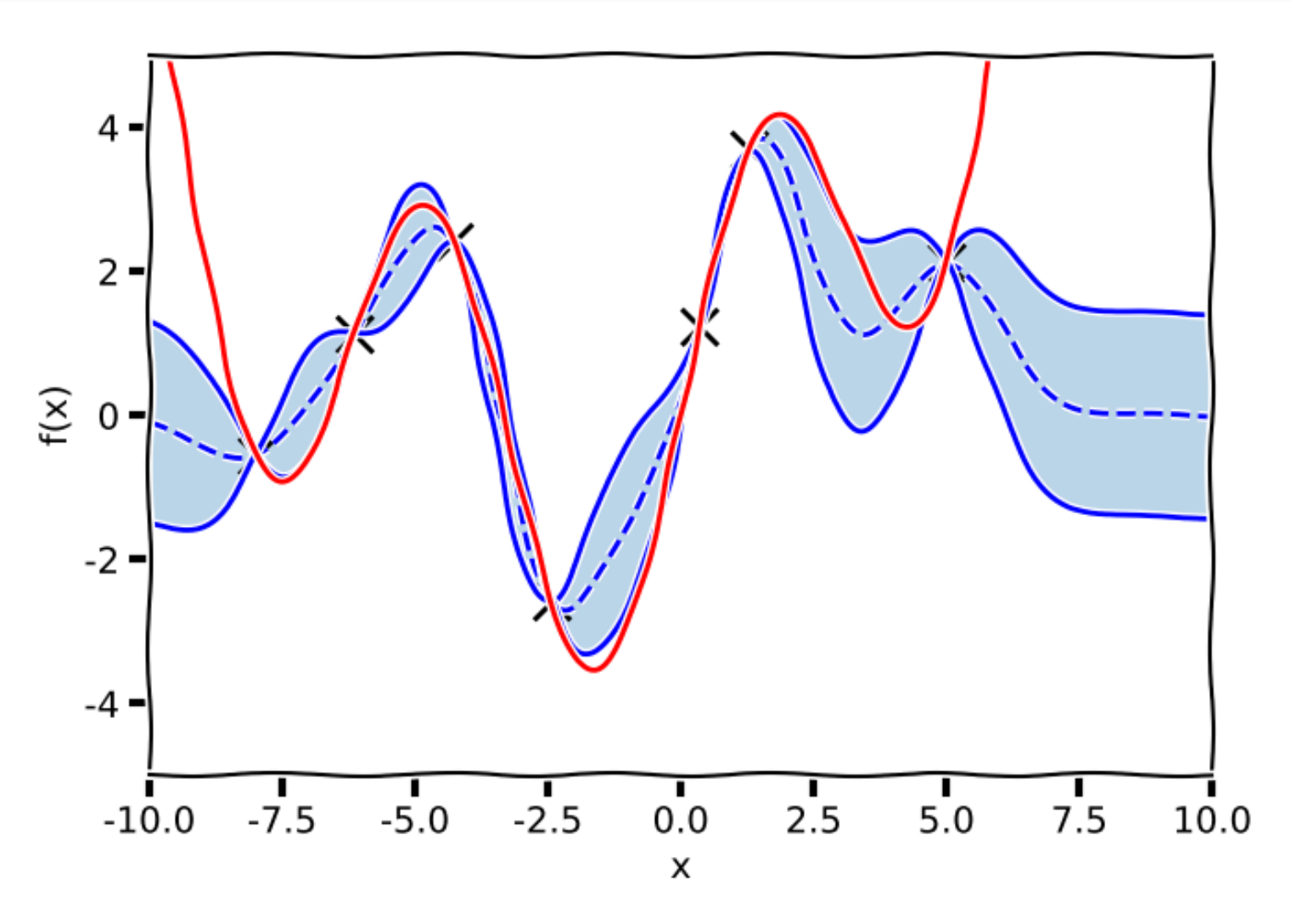

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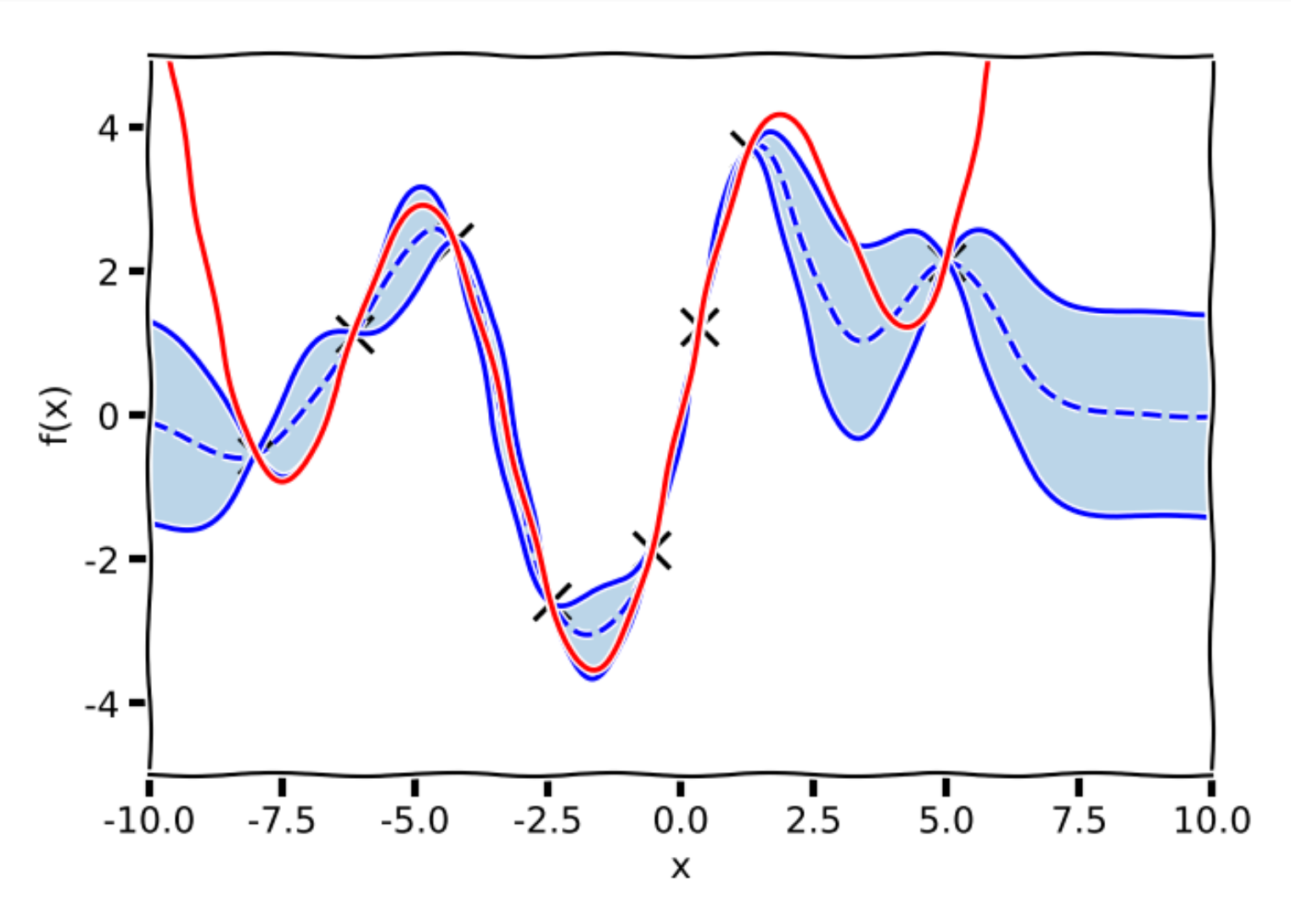

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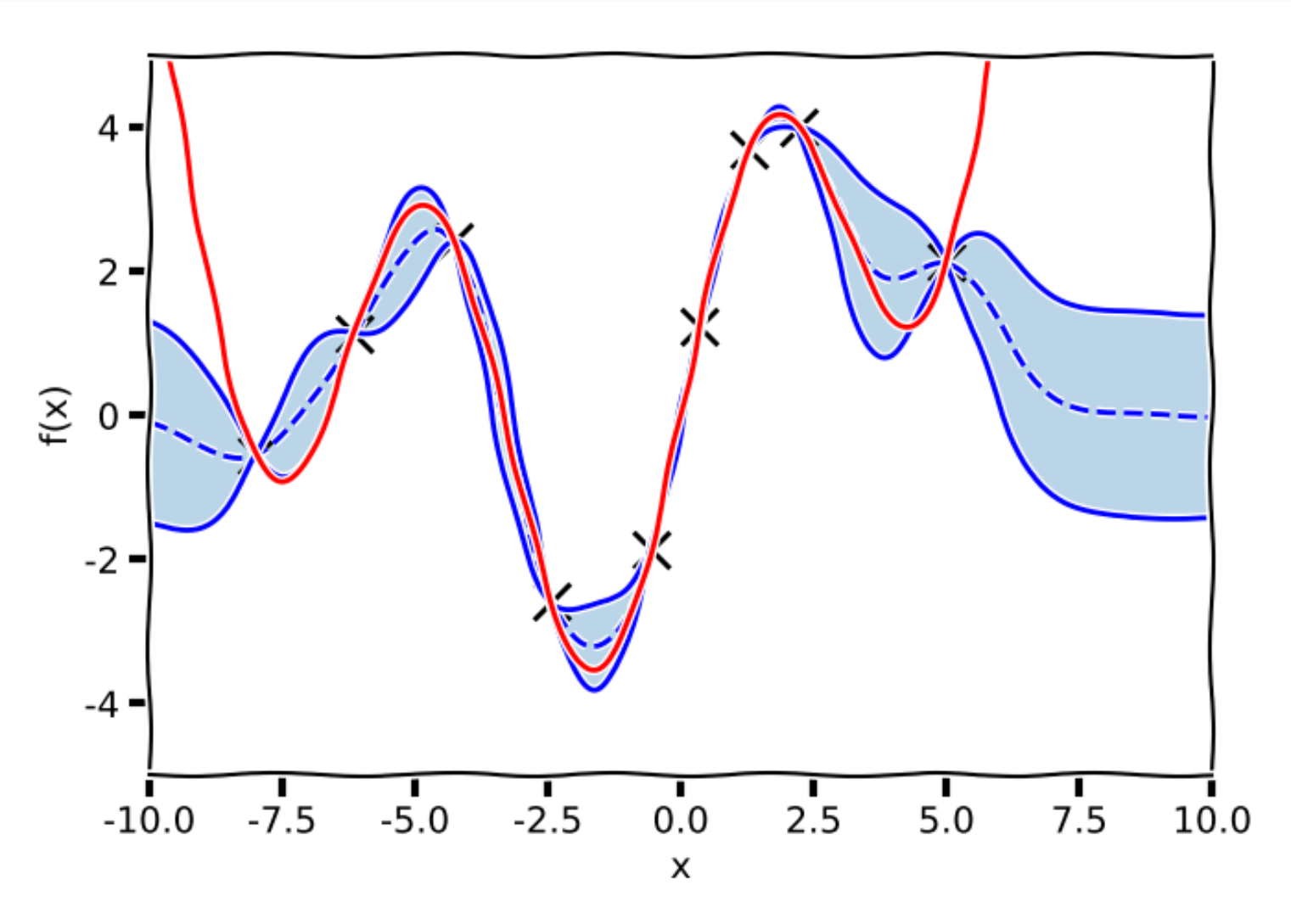

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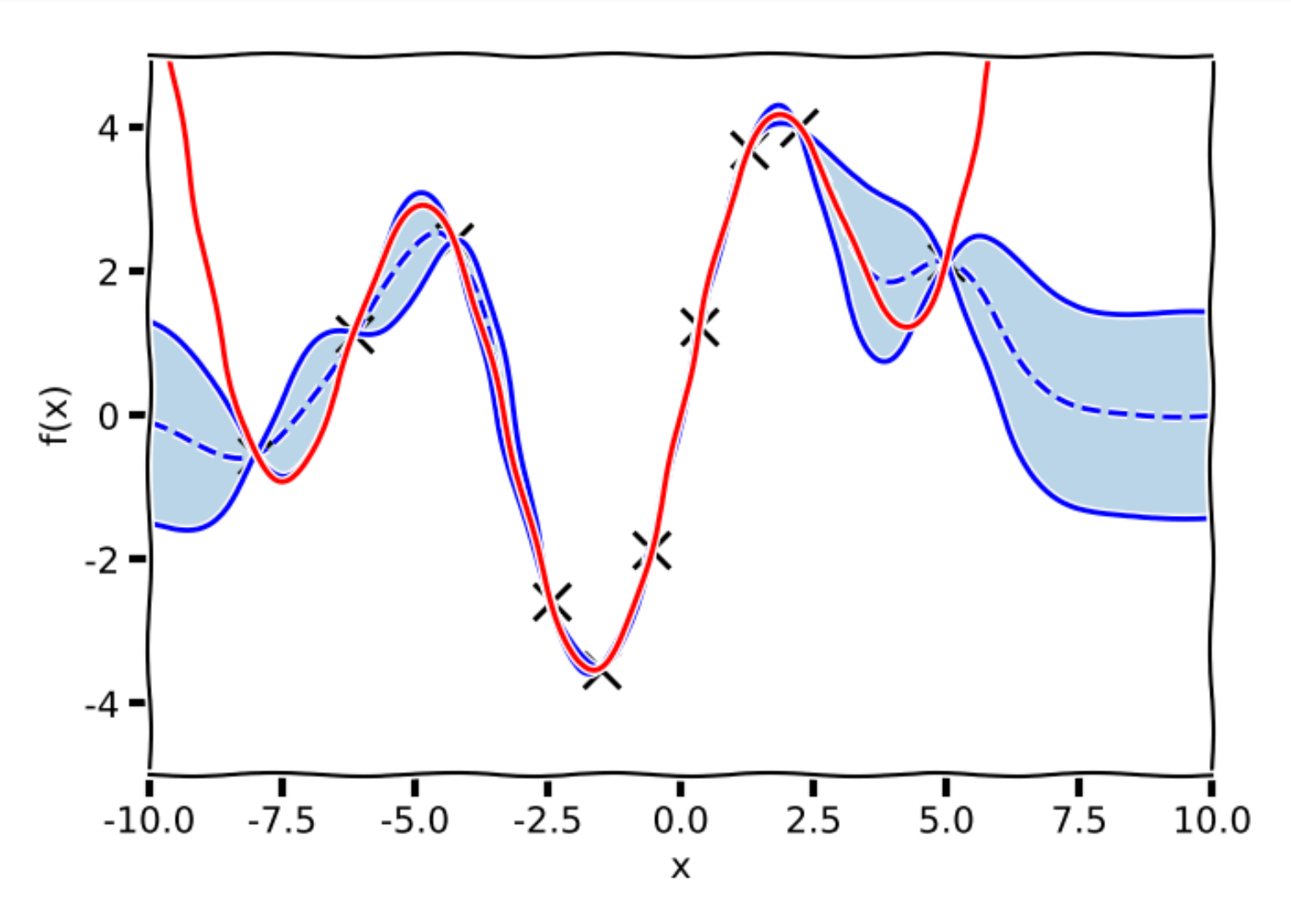

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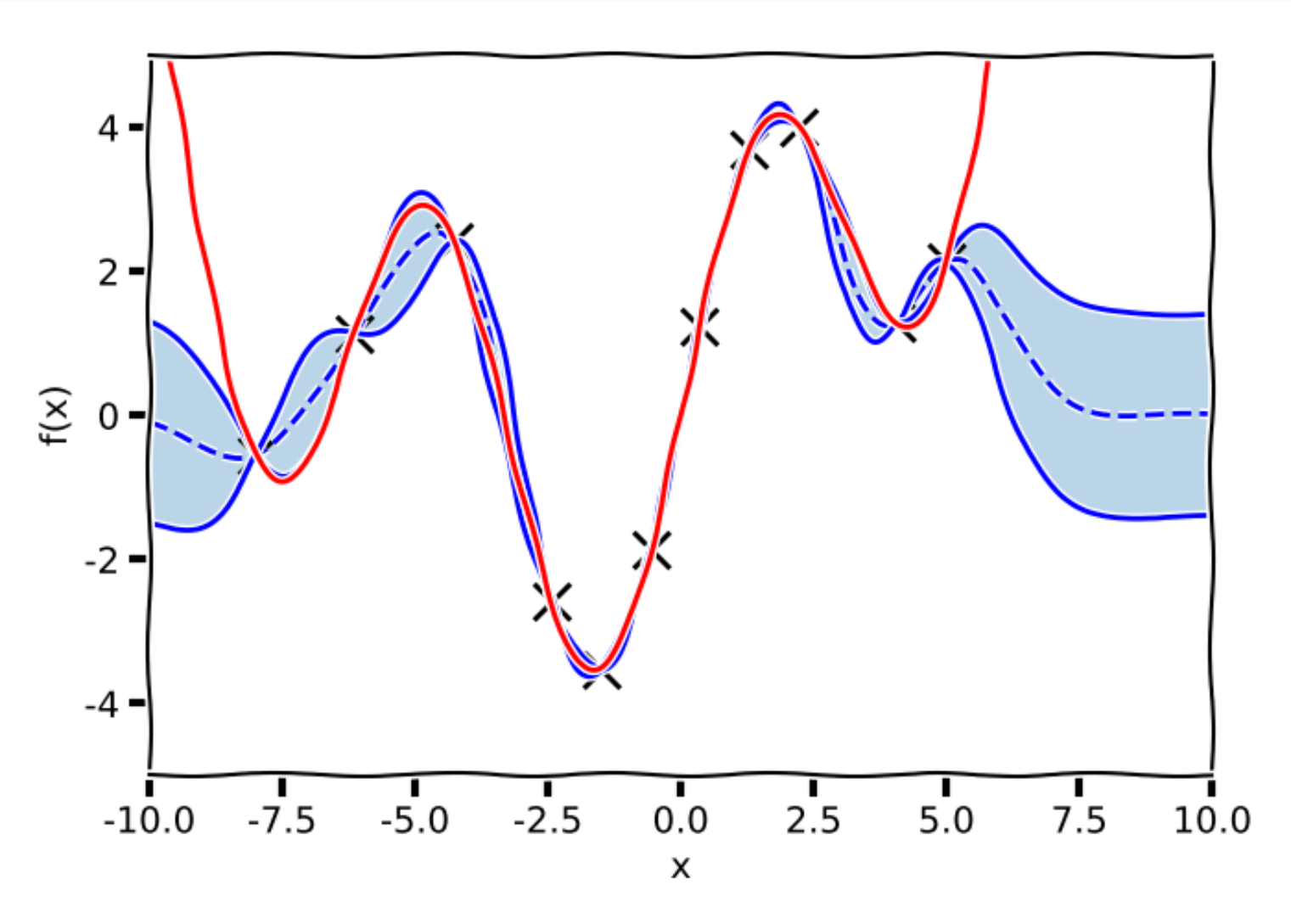

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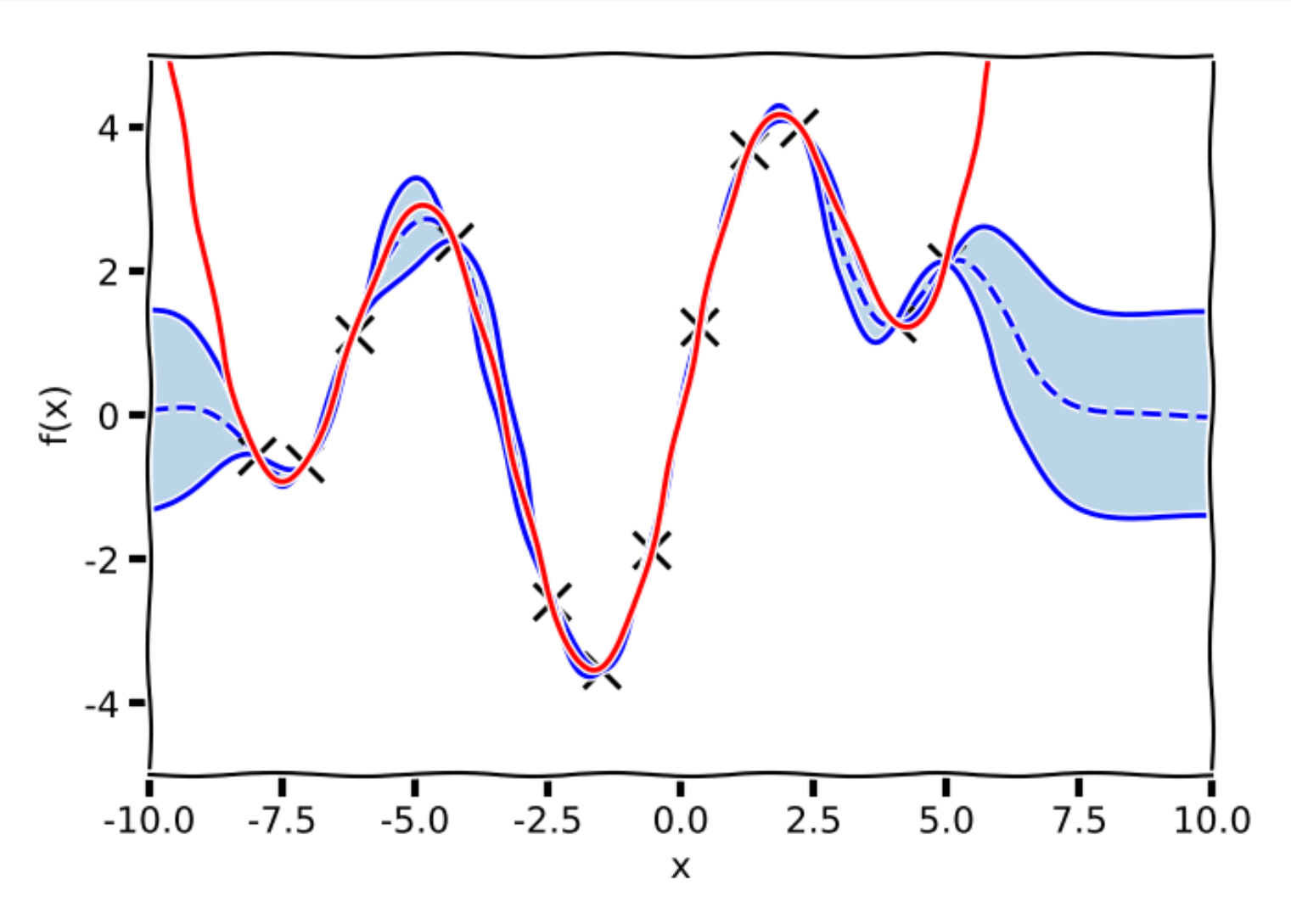

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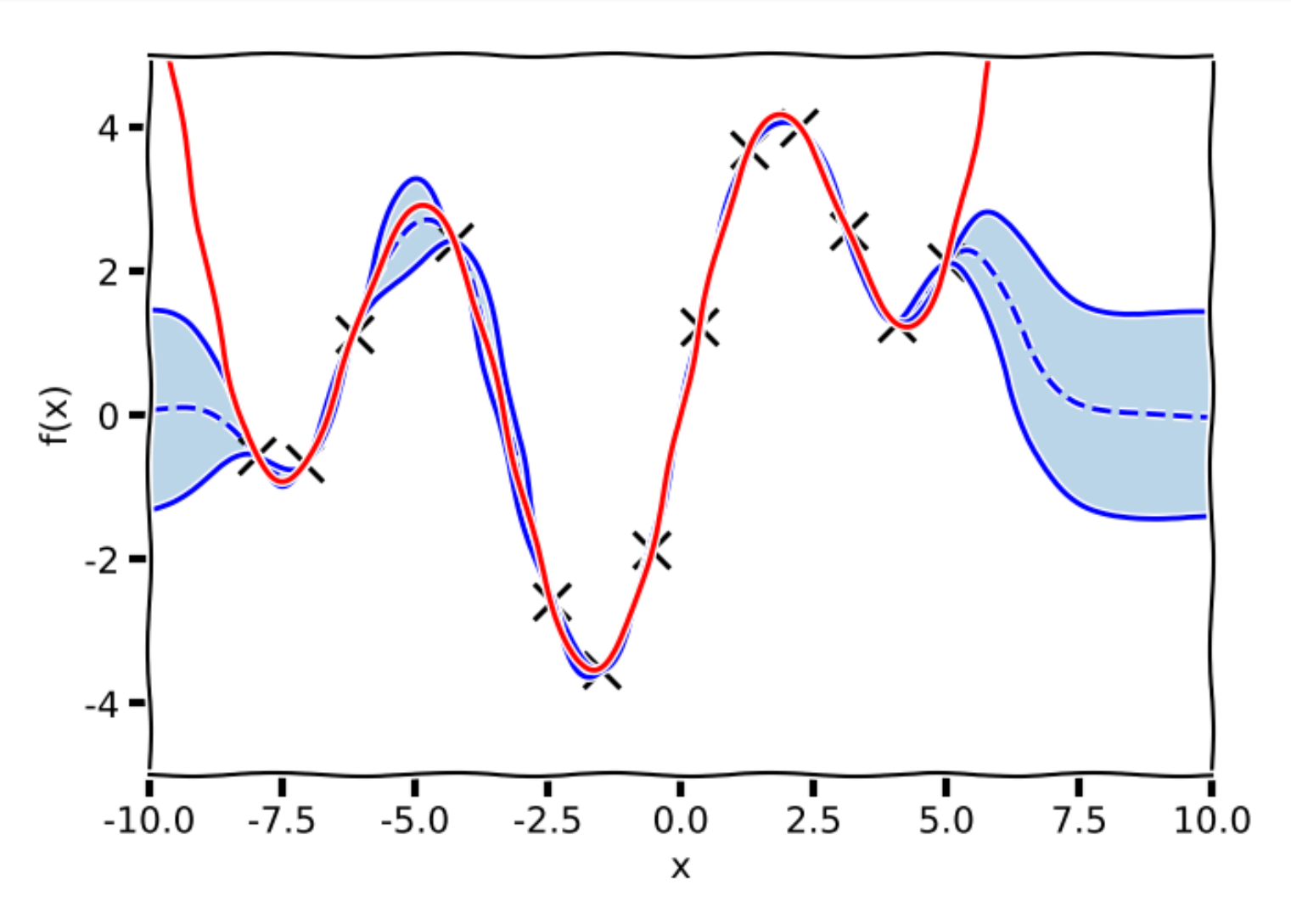

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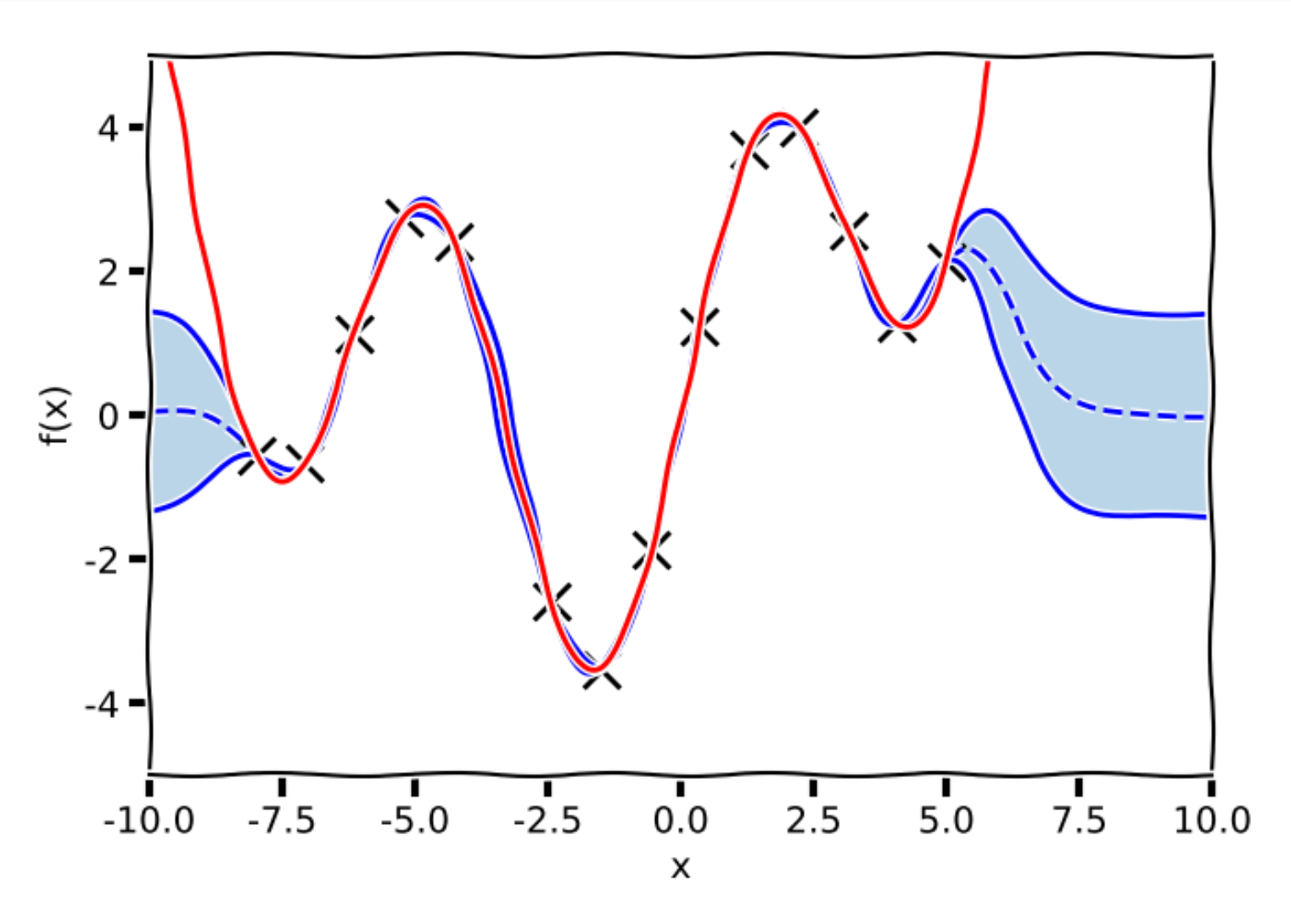
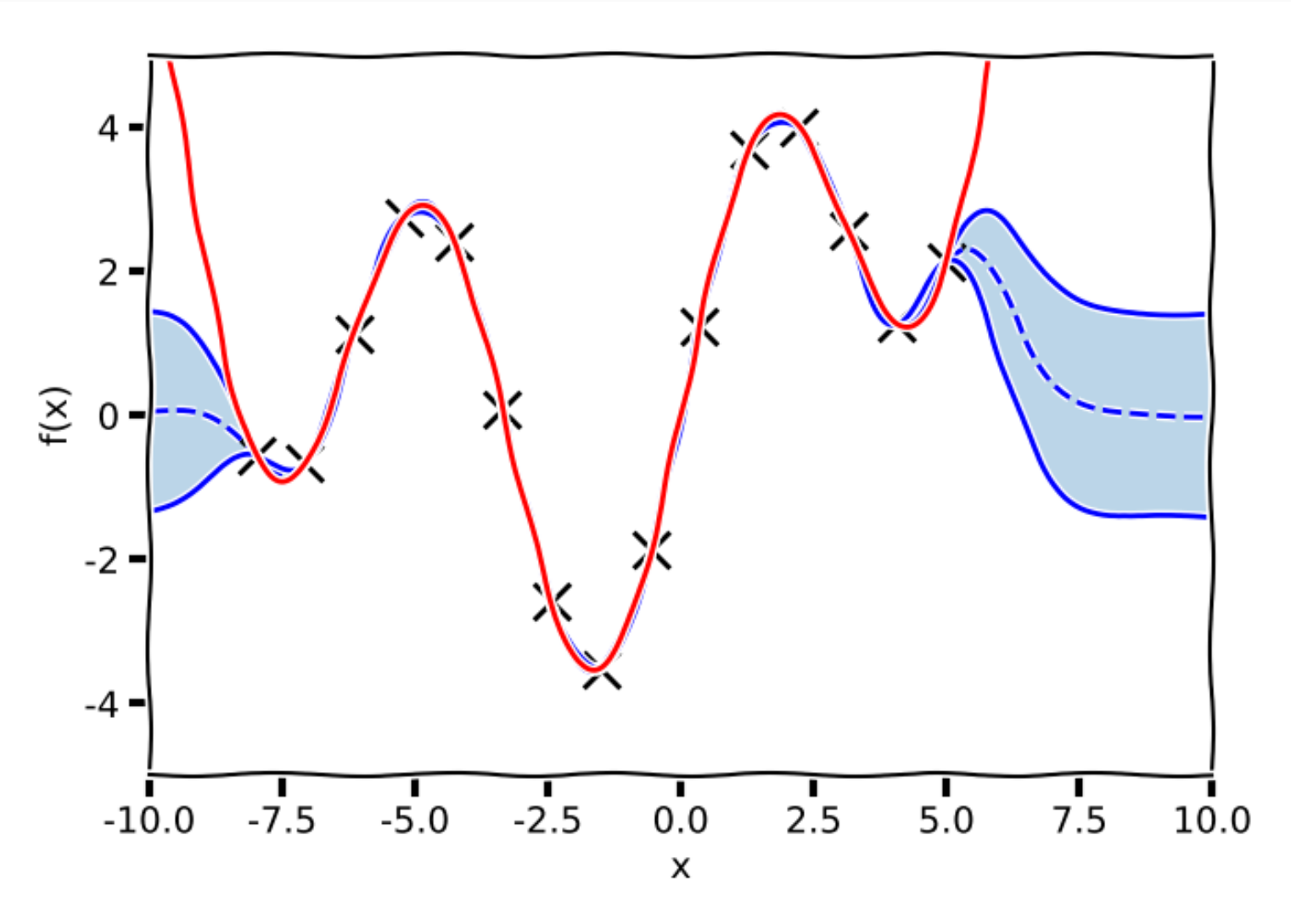


Gaussian Processes



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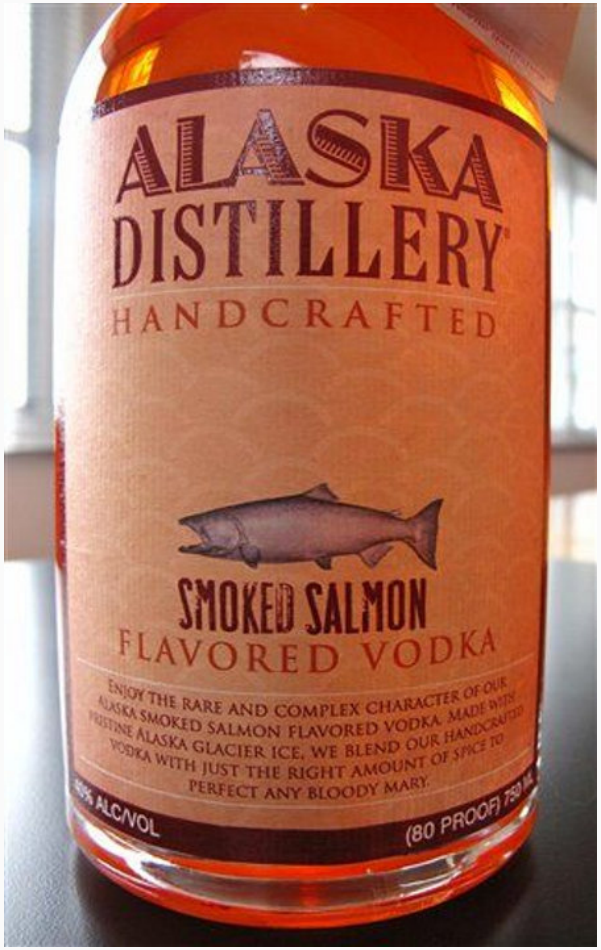
Exploration vs Exploitation

Exploration vs Exploitation

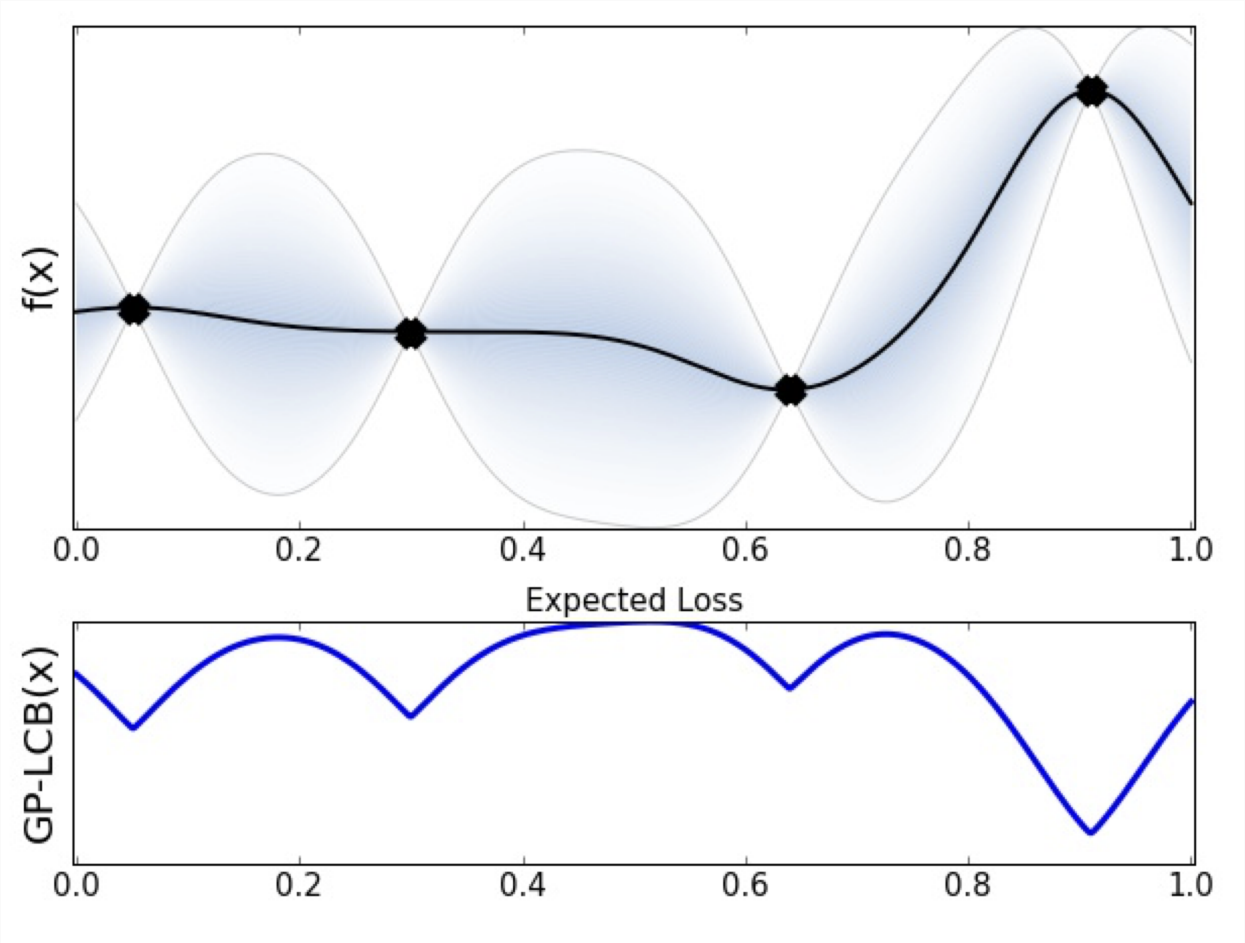
Balance is the key



Aquisition function

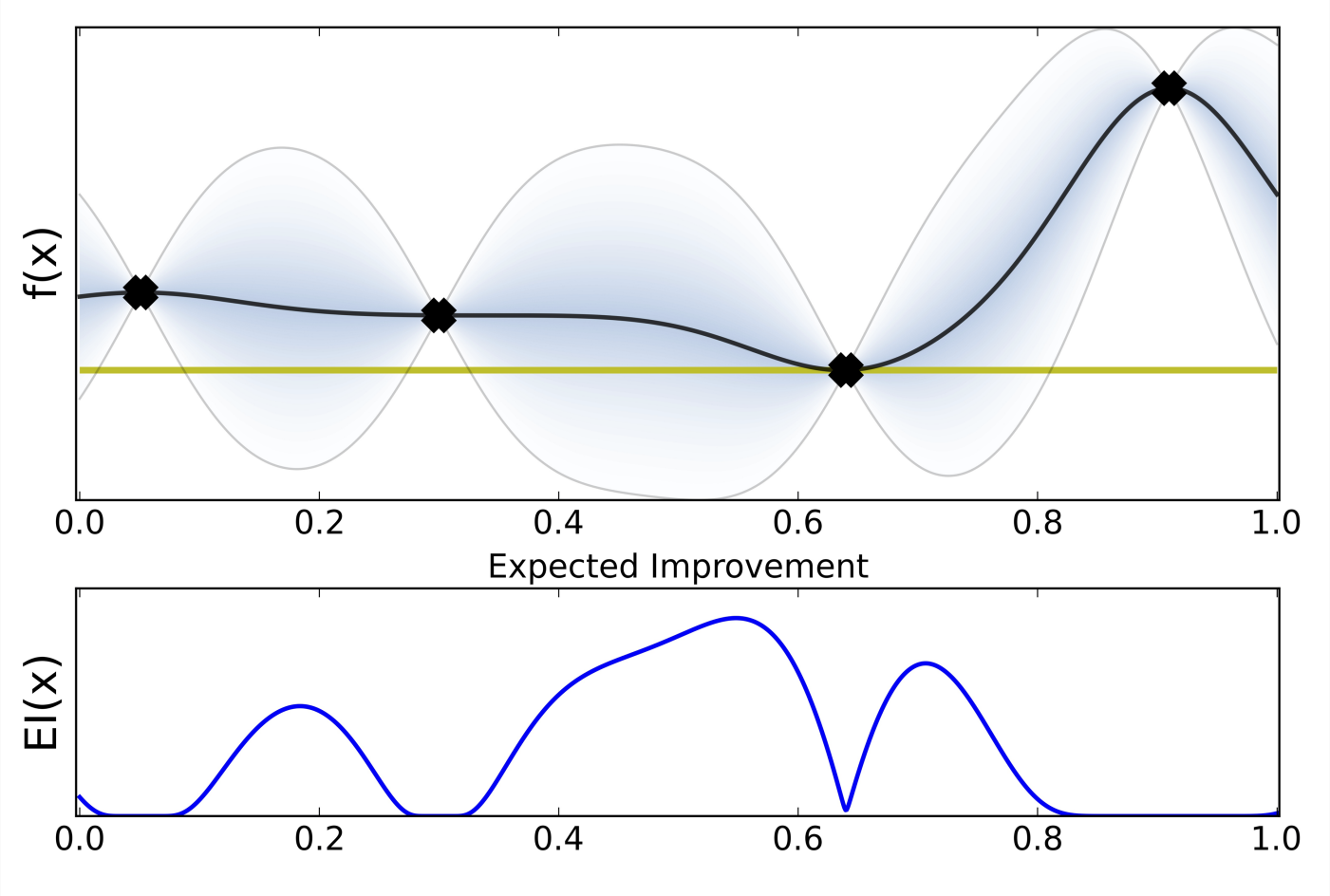
- how should we explore the space?
- humans do active search?
    - studying for exam
-

Confidence



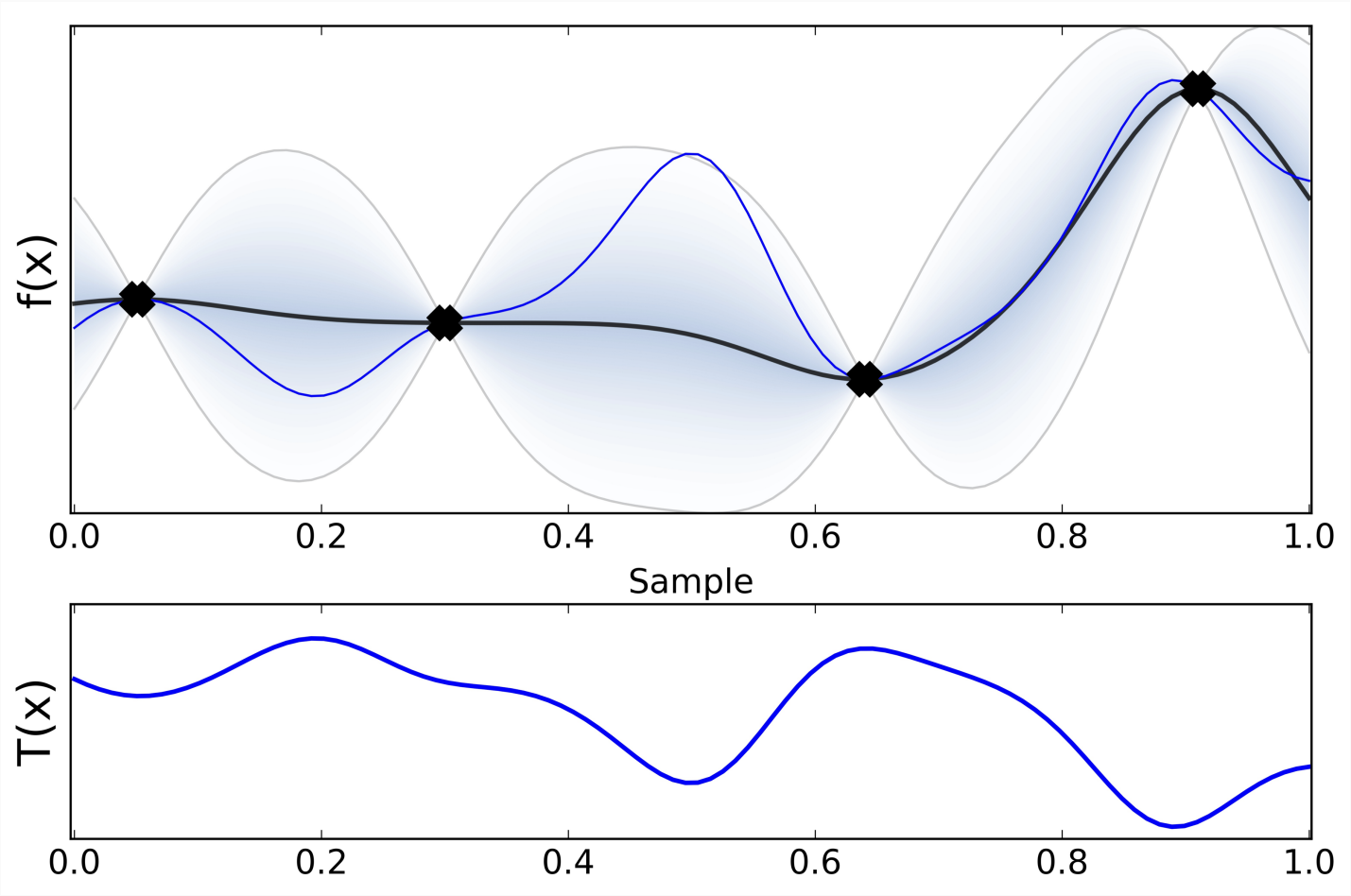
$$\alpha(\mathbf{x}; \theta, \mathcal{D}) = -\mu(\mathbf{x}; \theta, \mathcal{D}) + \beta_t \sigma(\mathbf{x}; \theta, \mathcal{D})$$

Expected Improvement



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

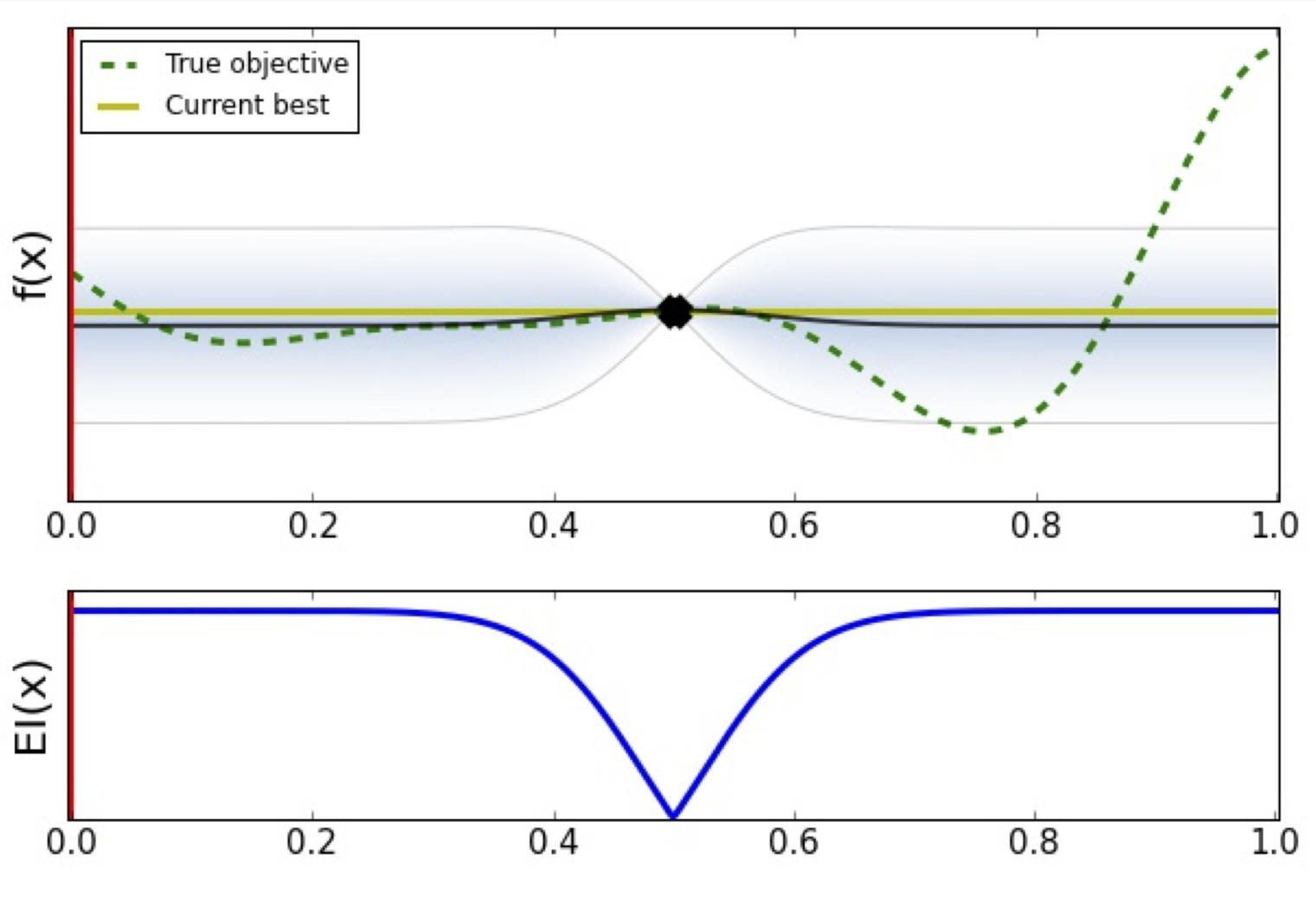
Thomson Sampling



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

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

Bayesian Optimisation [1]



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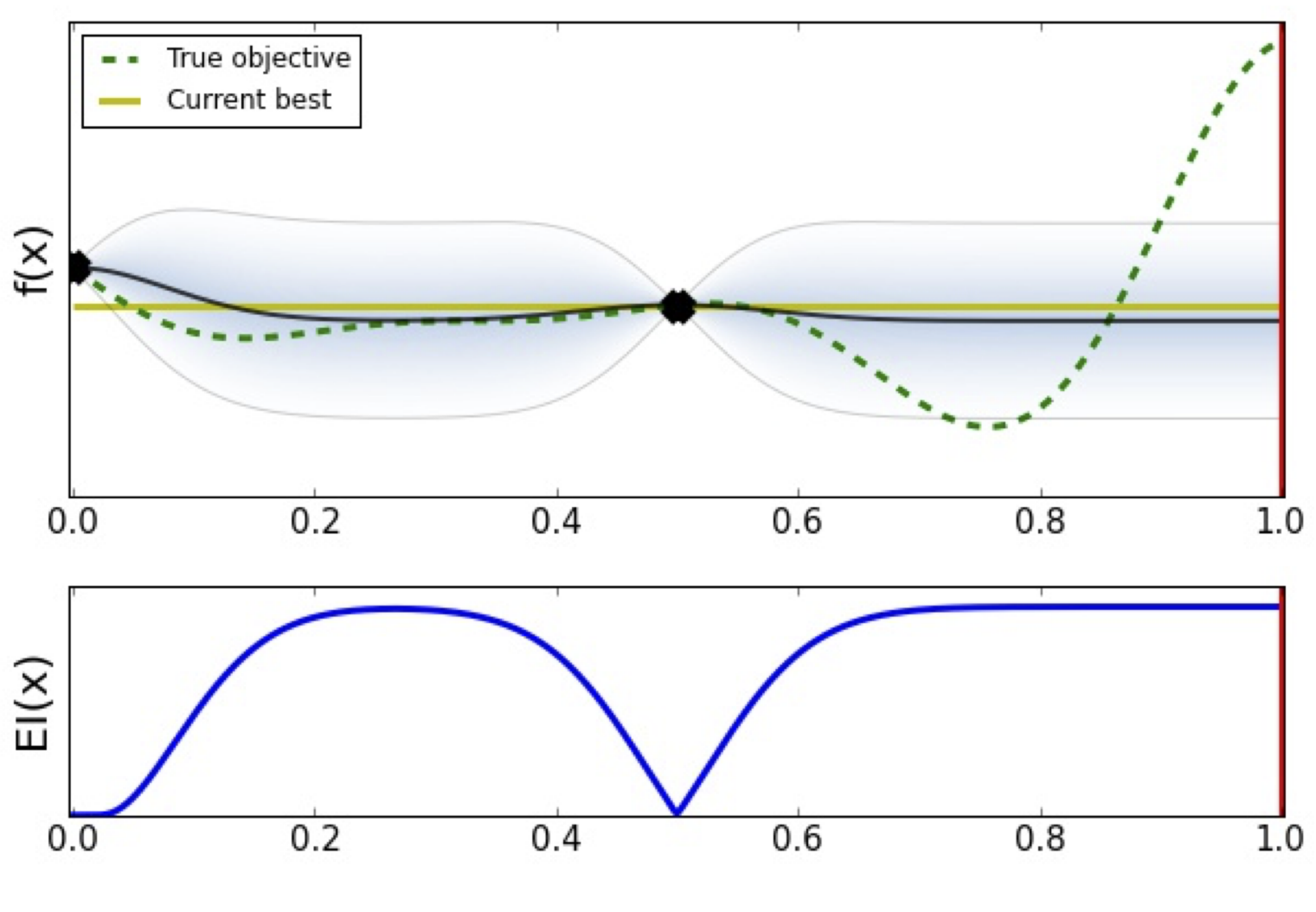

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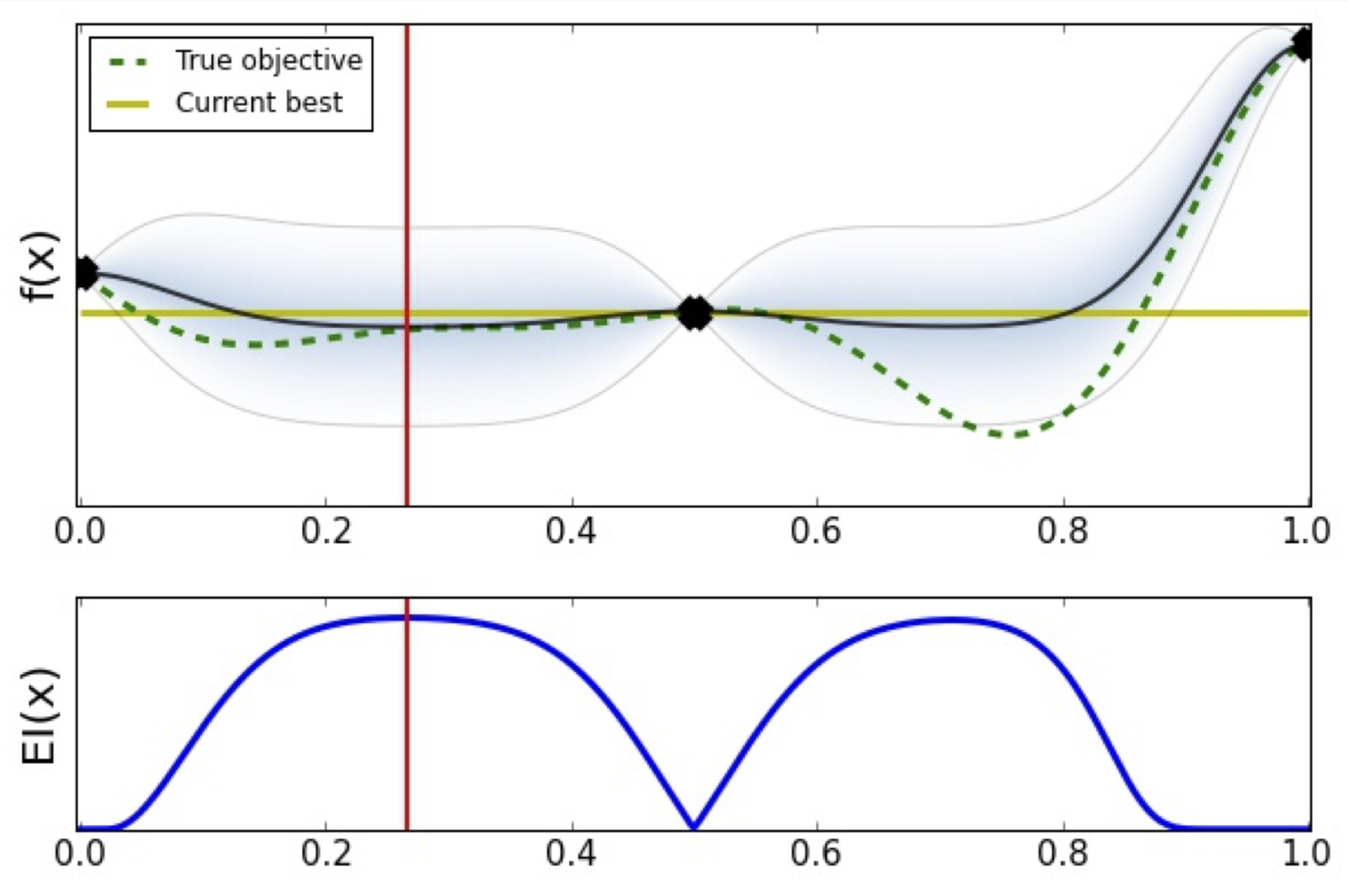

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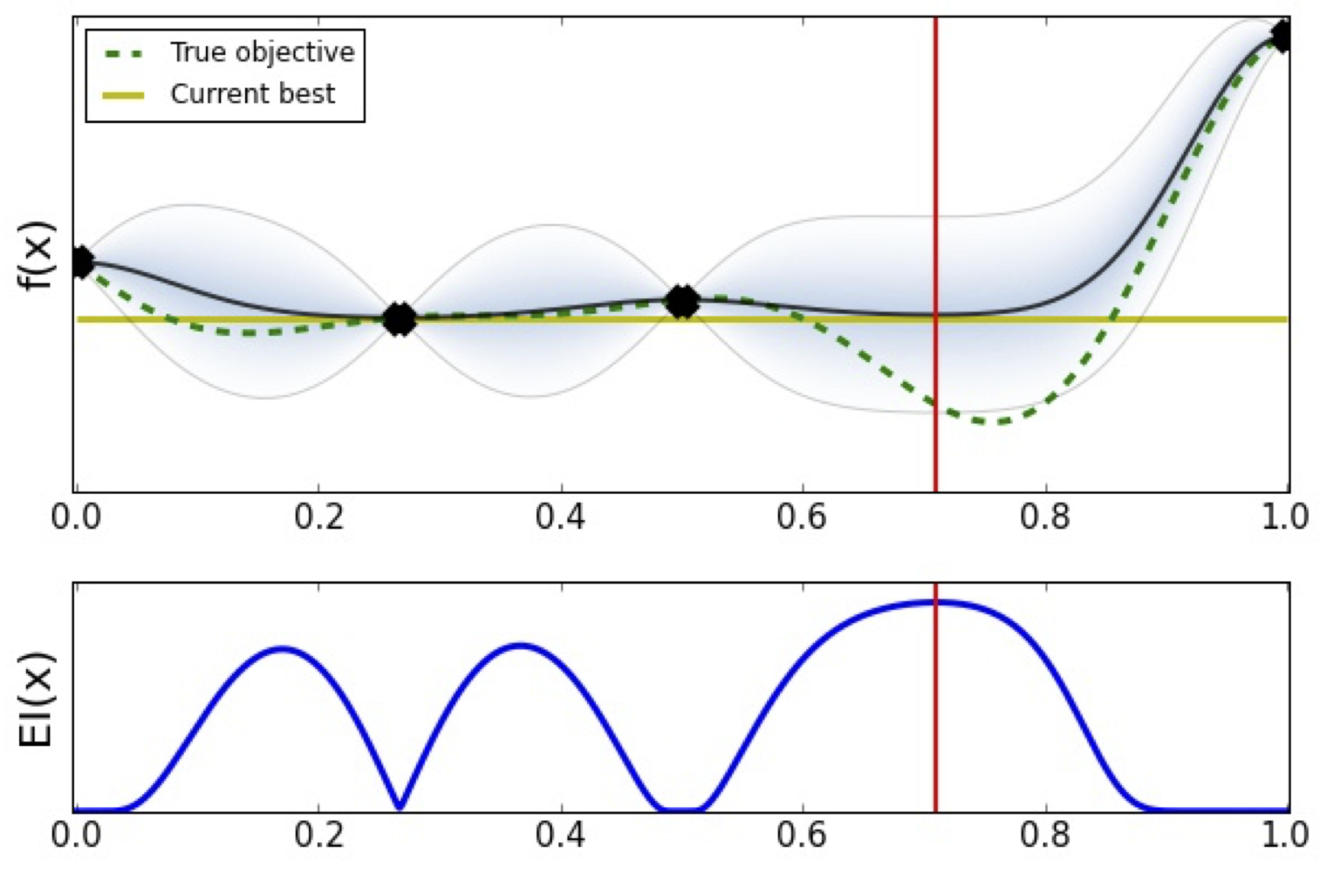

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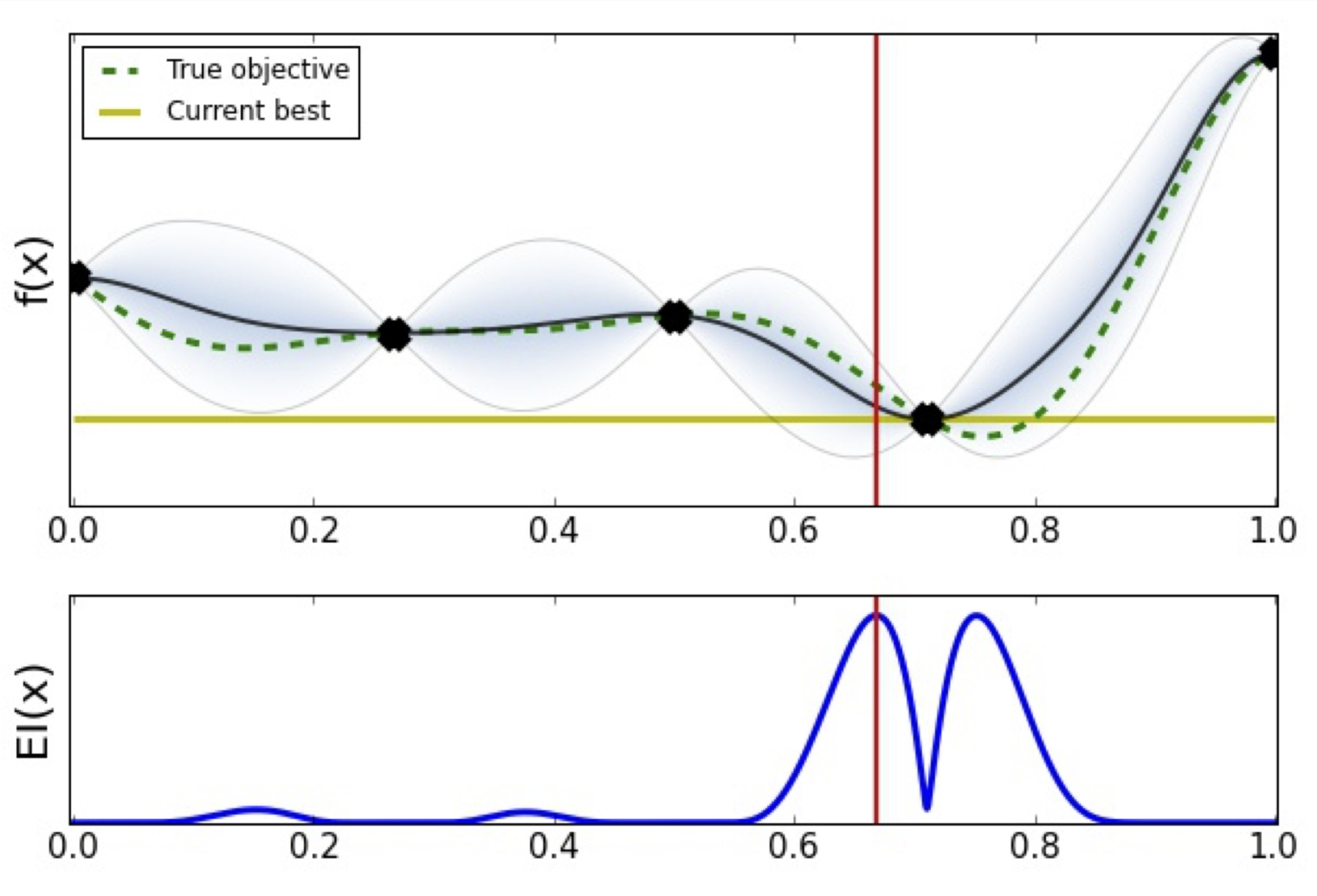

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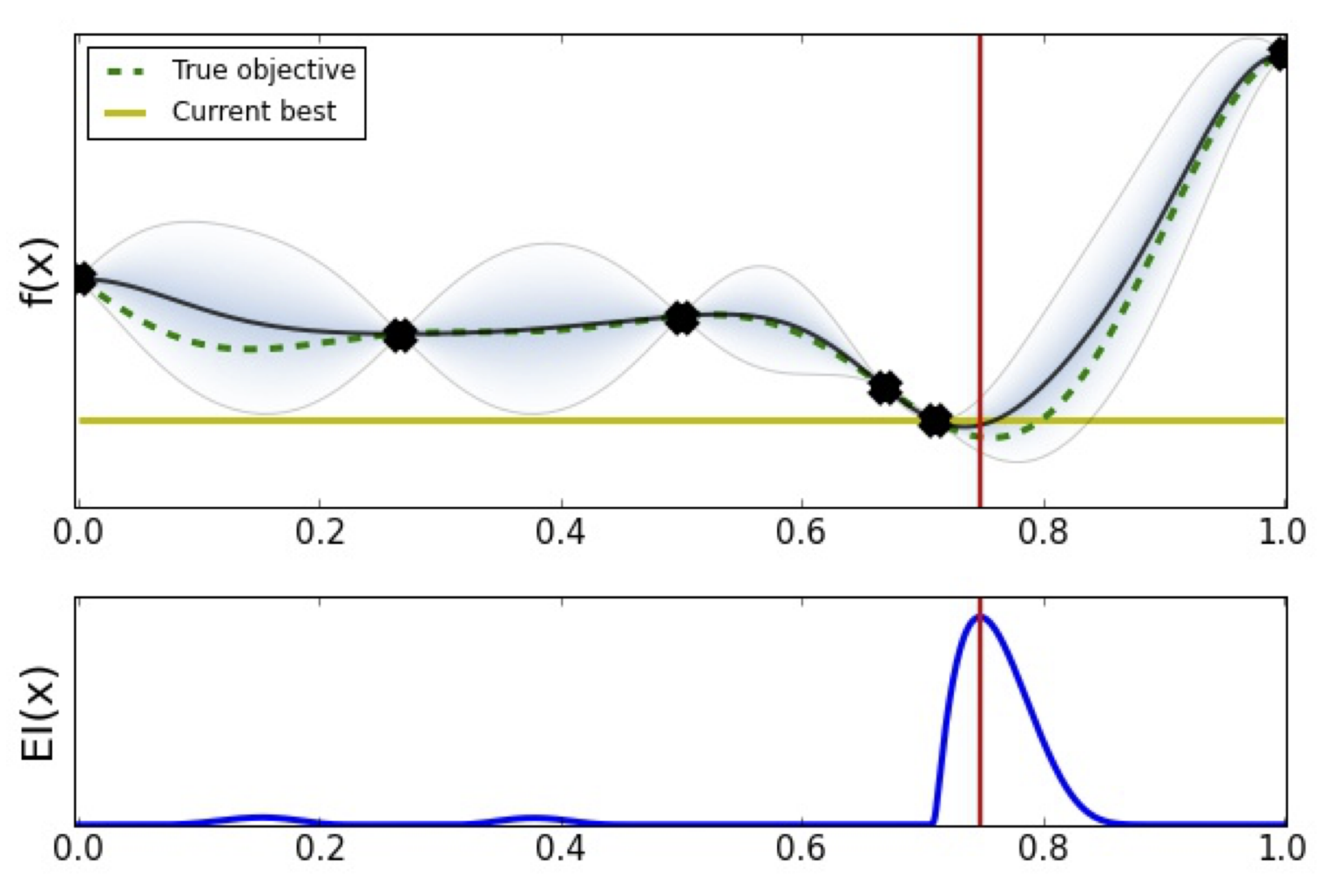

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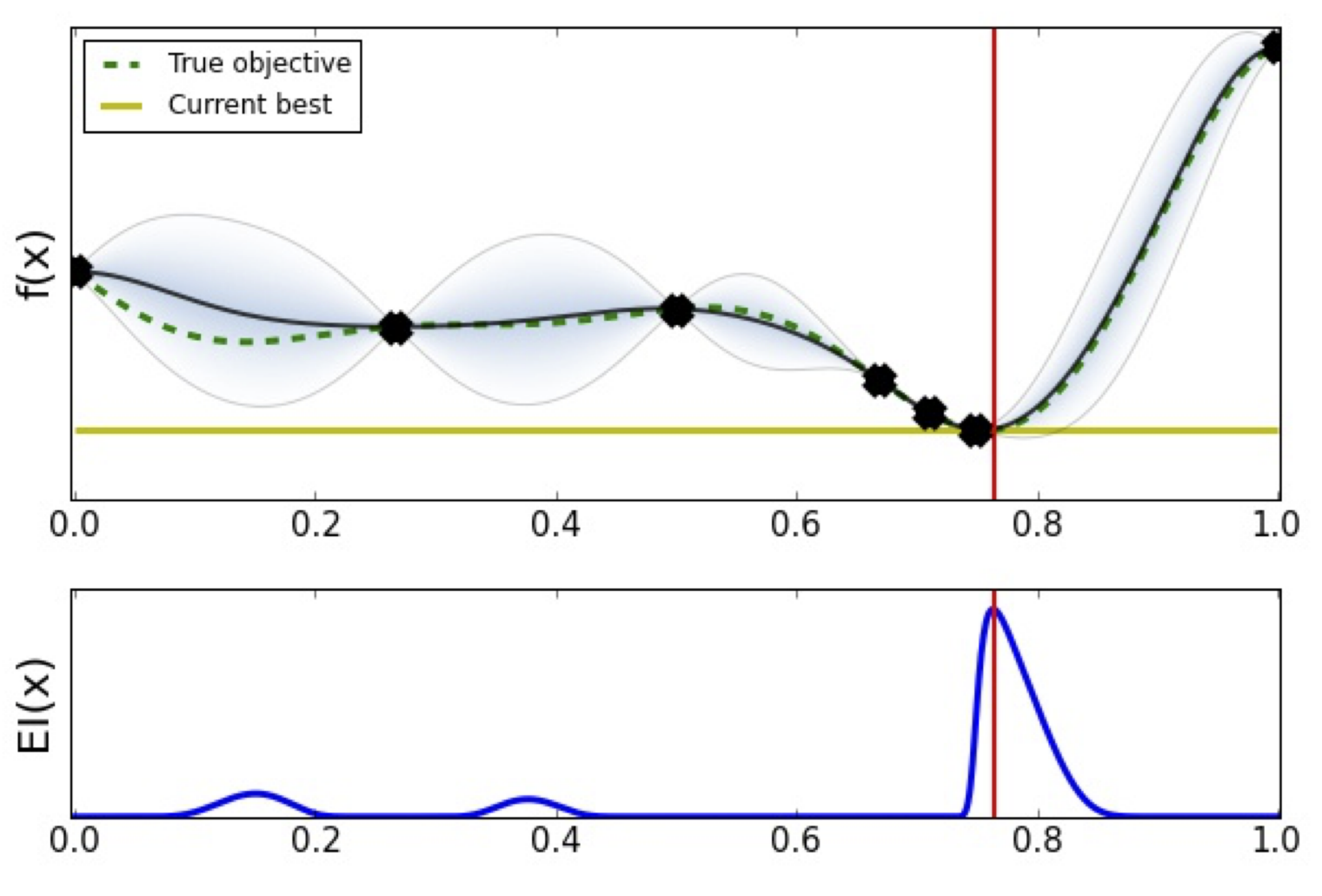

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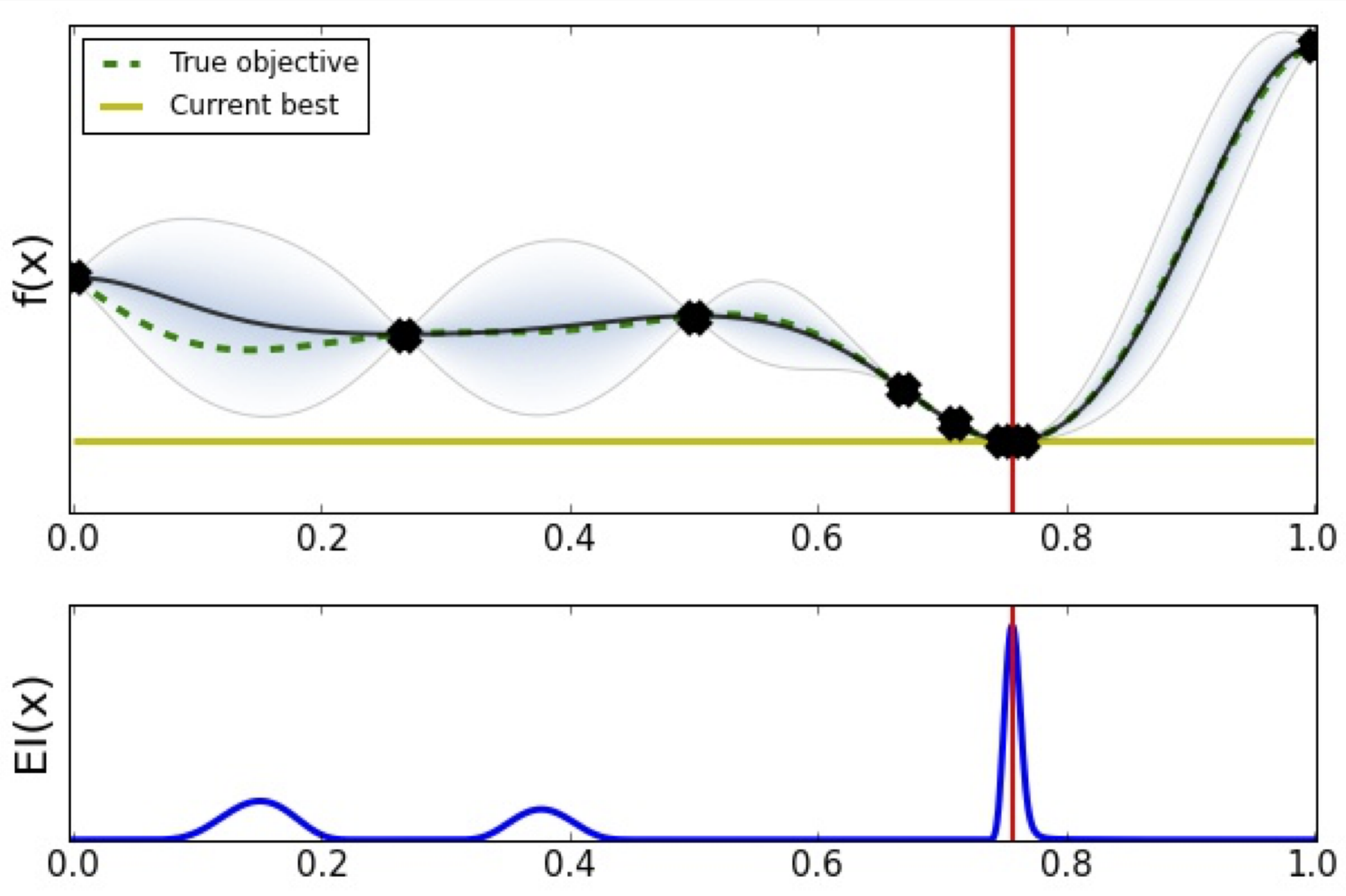

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Bayesian Optmisation

- 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

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- Constraints

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- Take home message: *uncertainty matters*

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References


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