Lecture 24
How to Optimize Expensive Functions

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Objectives

- Quantify the value of the information extracted from an experiment/simulation.
- Optimize an expensive black-box function under a limited budget.

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The problem

- Problem:

$$\mathbf{x}^{*} = \mathrm{argmax}_{\mathbf{x}} f(\mathbf{x})$$

- when the objective is:
  - very expensive to evaluate
  - you don't have gradients
  - dimensionality < 30 parameters

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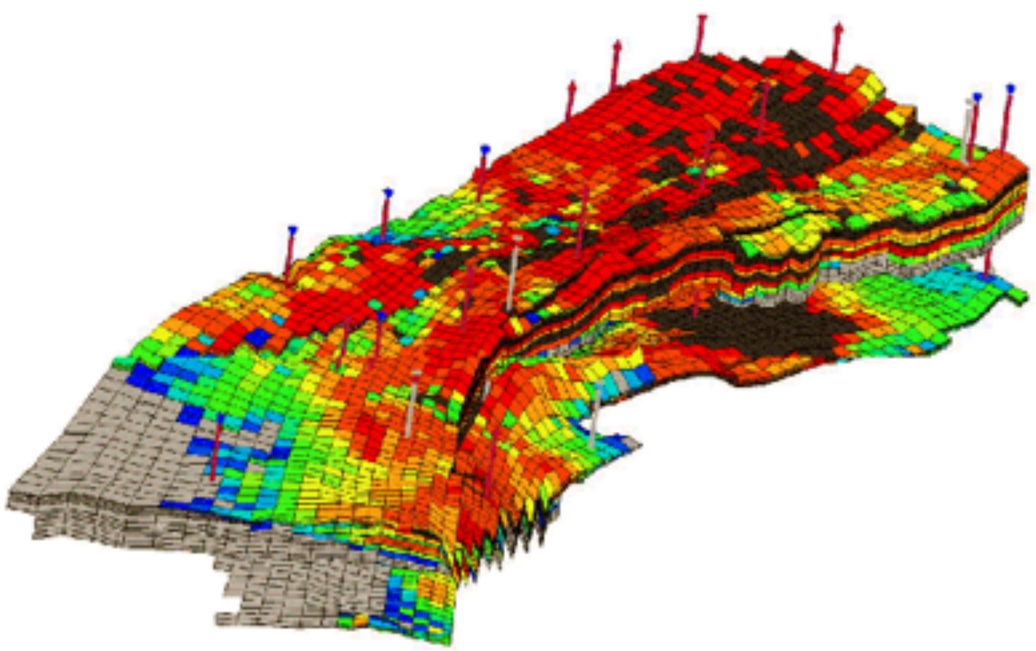
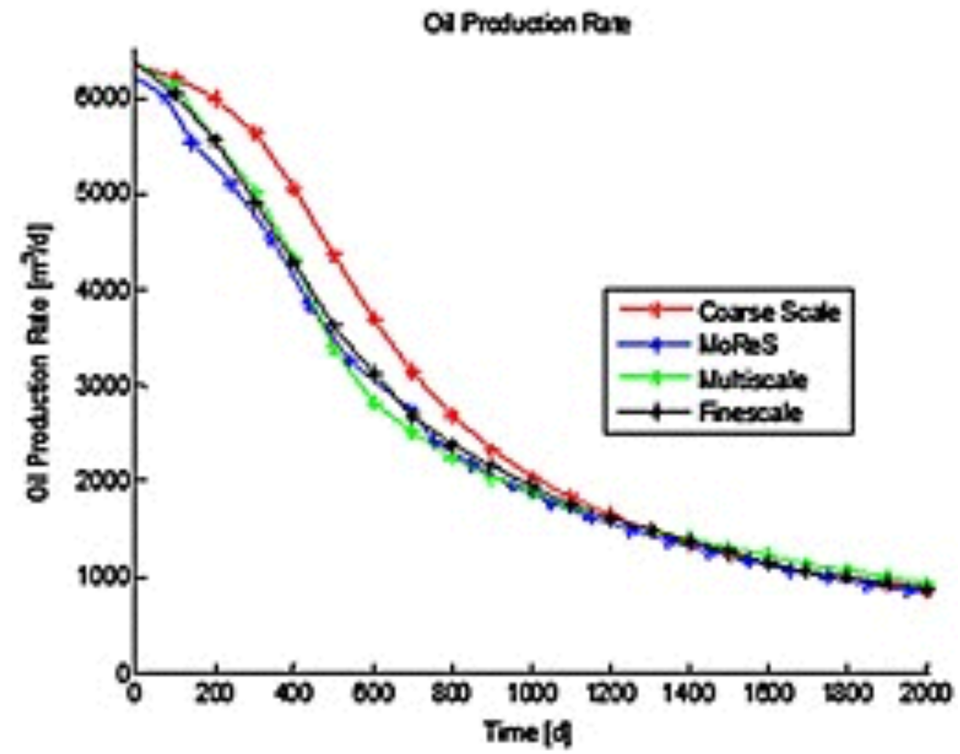
Example 1: Oil-well placement problem



Simulation



x = well locations

f(**x**) = expected net present cost of investment

Pandita, Bilionis, and Panchal, 2016
http://arxiv.org/abs/1604.01147

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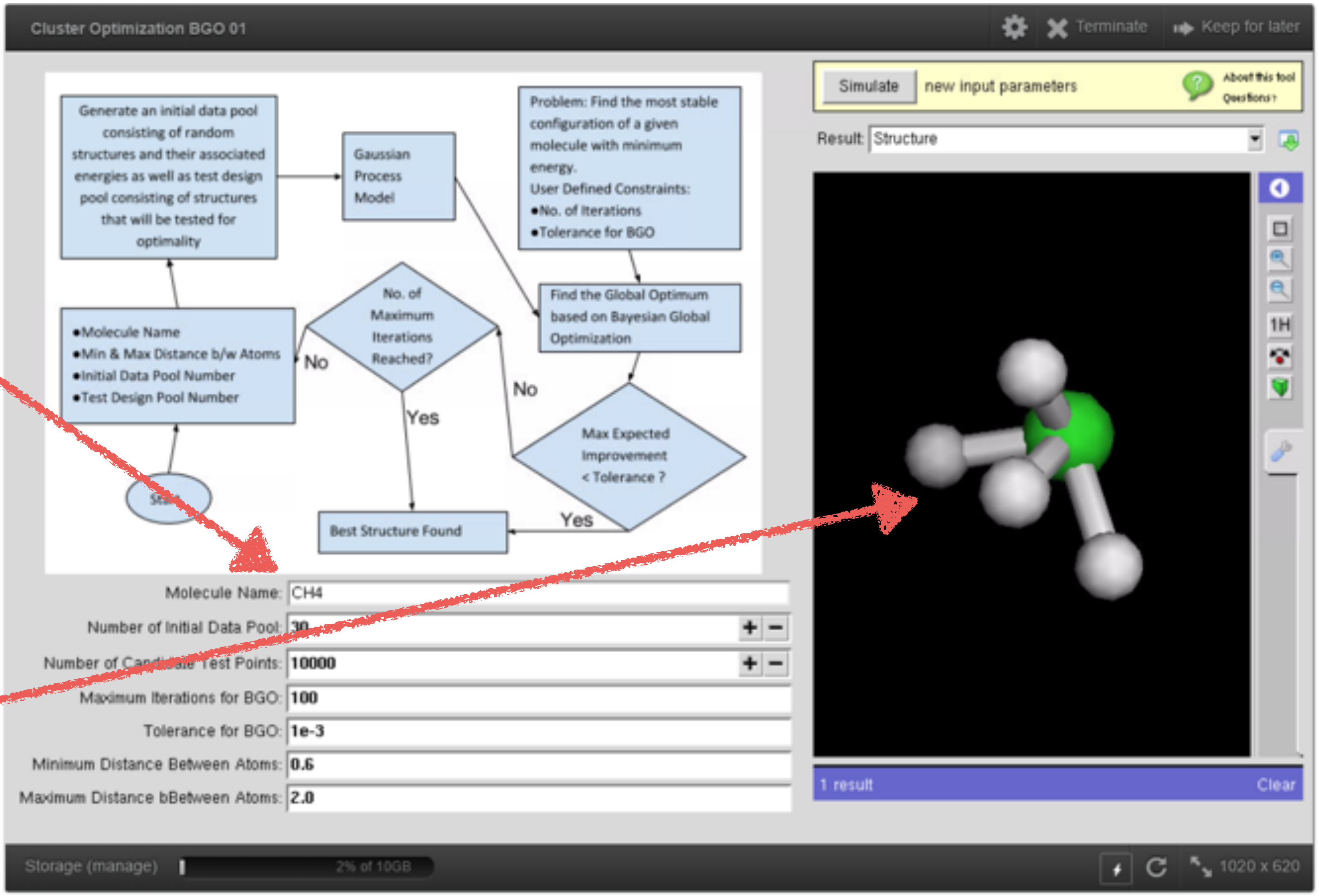
Example 2: Find stable structures

Surf student project

Chemical formula

Geometry (**x**) with minimum energy (y)



https://nanohub.org/tools/clusterbgopro

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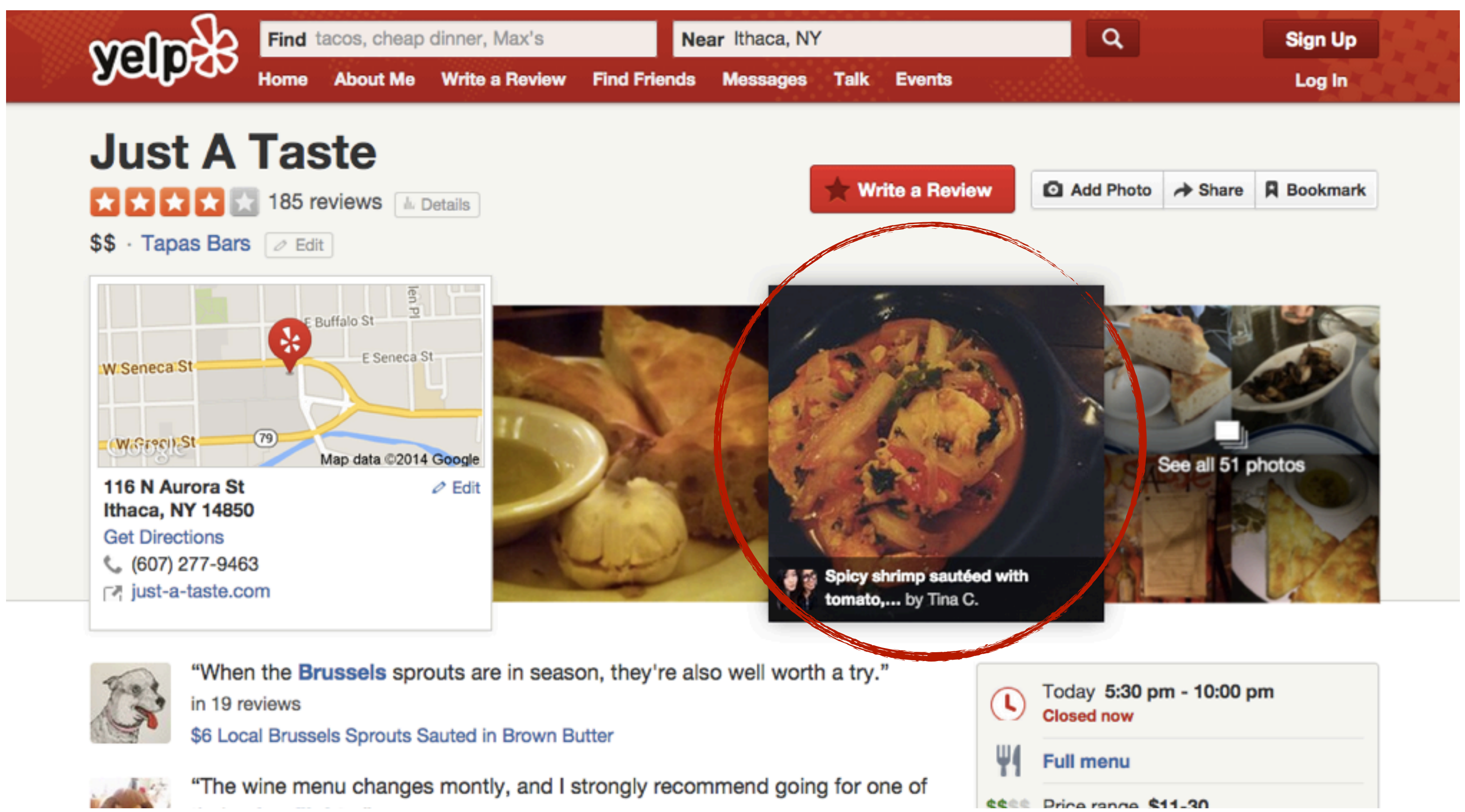
Example 3: Web site optimization

x = web design → measurement → -y = Number of views, seconds per view, etc.



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http://yelp.github.io/MOE

Example 4: Training a robot to walk

https://www.youtube.com/watch?v=ualnbKfkc3Q

https://www.youtube.com/watch?v=GiqNQdzc5TI

Other examples

- Model calibration (if posed as an optimization problem).
- Maximize efficiency in solar cells.
- Drug development.
- …

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Startup idea

https://sigopt.com/

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Free options

- https://github.com/PredictiveScienceLab/py-bgo (features stochastic and multi-objective optimization)

- https://github.com/SheffieldML/GPyOpt (features parallel optimization)

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pip install GPyOpt

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Idea

1. We have some observed data (designs **x** - vs - objectives **y**).

2. We fit a **statistical regression model** to the data.

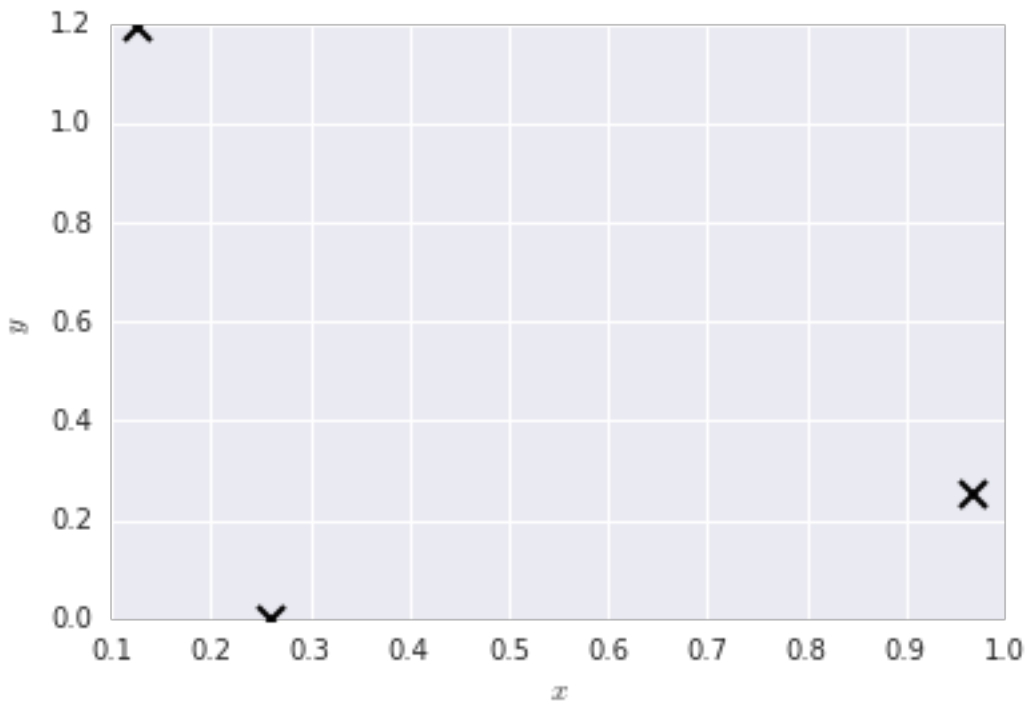
3. For each candidate design, compute the **value of information (VoI)**.

4. We find the design with the **maximum VoI**.

5. We compute the objective for this design.

Repeat until:
- budget is exhausted;
- VoI low.

We have some data



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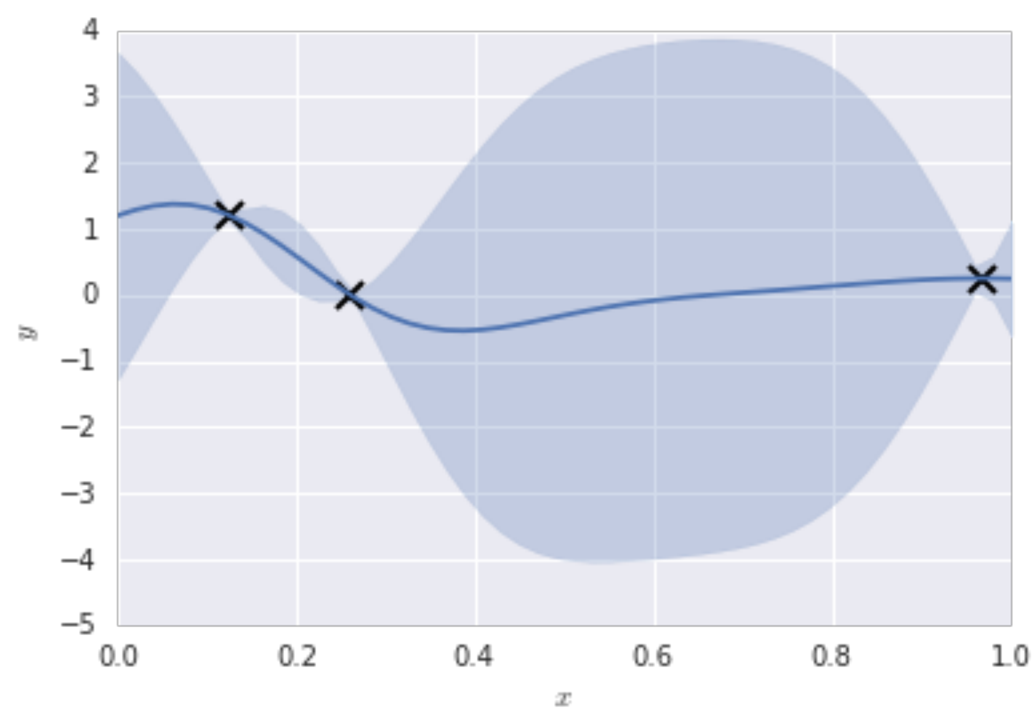
We fit a statistical model



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$$p(y \mid \mathbf{x}) \approx \mathcal{N}\left(y \mid m(\mathbf{x}), \sigma^2(\mathbf{x})\right)$$

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Gaussian process regression

- Assume that we have observed:

$$\mathbf{X} = \{x_1, \ldots, x_N\},$$
$$\mathbf{f} = \{f(x_1), \ldots, f(x_N)\}$$

- and that we want to make predictions at an arbitrary set of *test* inputs:

$$\mathbf{X}^* = \{x_1^*, \ldots, x_{N^*}^*\}$$
$$\mathbf{f}^* = \{f(x_1^*), \ldots, f(x_{N^*}^*)\}$$

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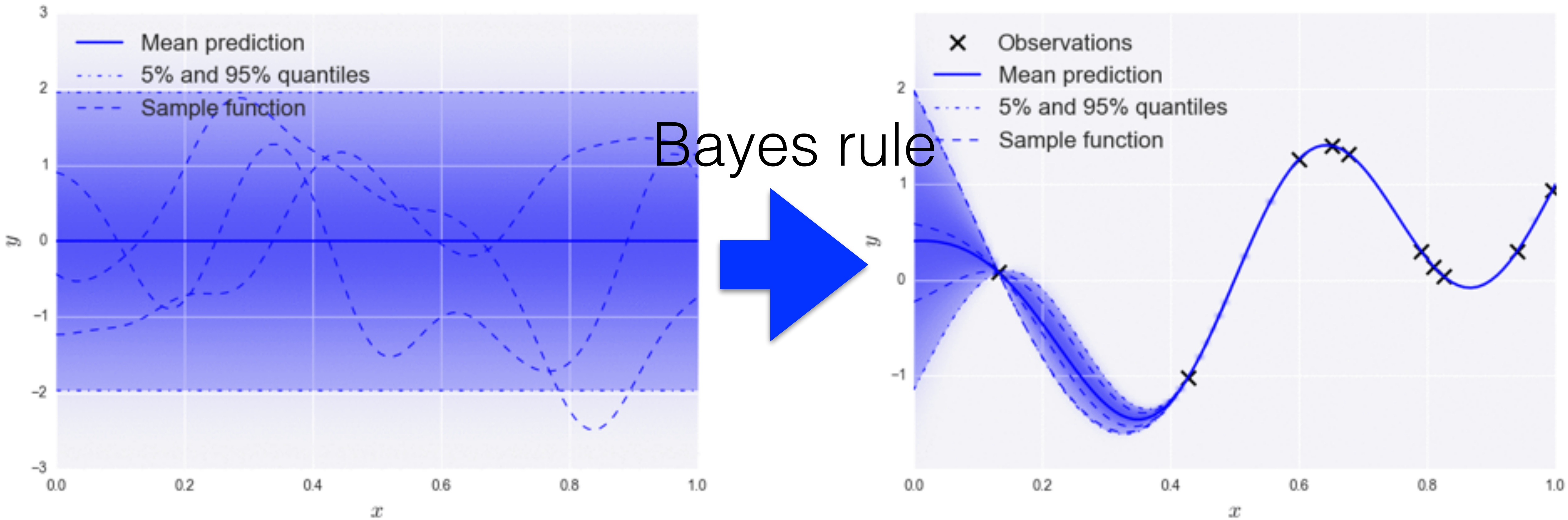
Gaussian process regression



Prior GP

Posterior GP

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The point predictive distribution

- Posterior GP:

$$f(\cdot) \mid \mathbf{X}, \mathbf{f} \sim \mathrm{GP}\left(f(\cdot) \mid \tilde{m}(\cdot), \tilde{k}(\cdot,\cdot)\right),$$

- Looking at just one point, we get the *point predictive distribution:*

$$y \mid \mathbf{x}, \mathbf{X}, \mathbf{f} \sim \mathcal{N}\left(y \mid \tilde{m}(\mathbf{x}), \tilde{\sigma}^2(\mathbf{x})\right),$$

$$\tilde{\sigma}^2(\mathbf{x}) = \tilde{k}(\mathbf{x}, \mathbf{x}).$$

- You may use the mean as a surrogate.

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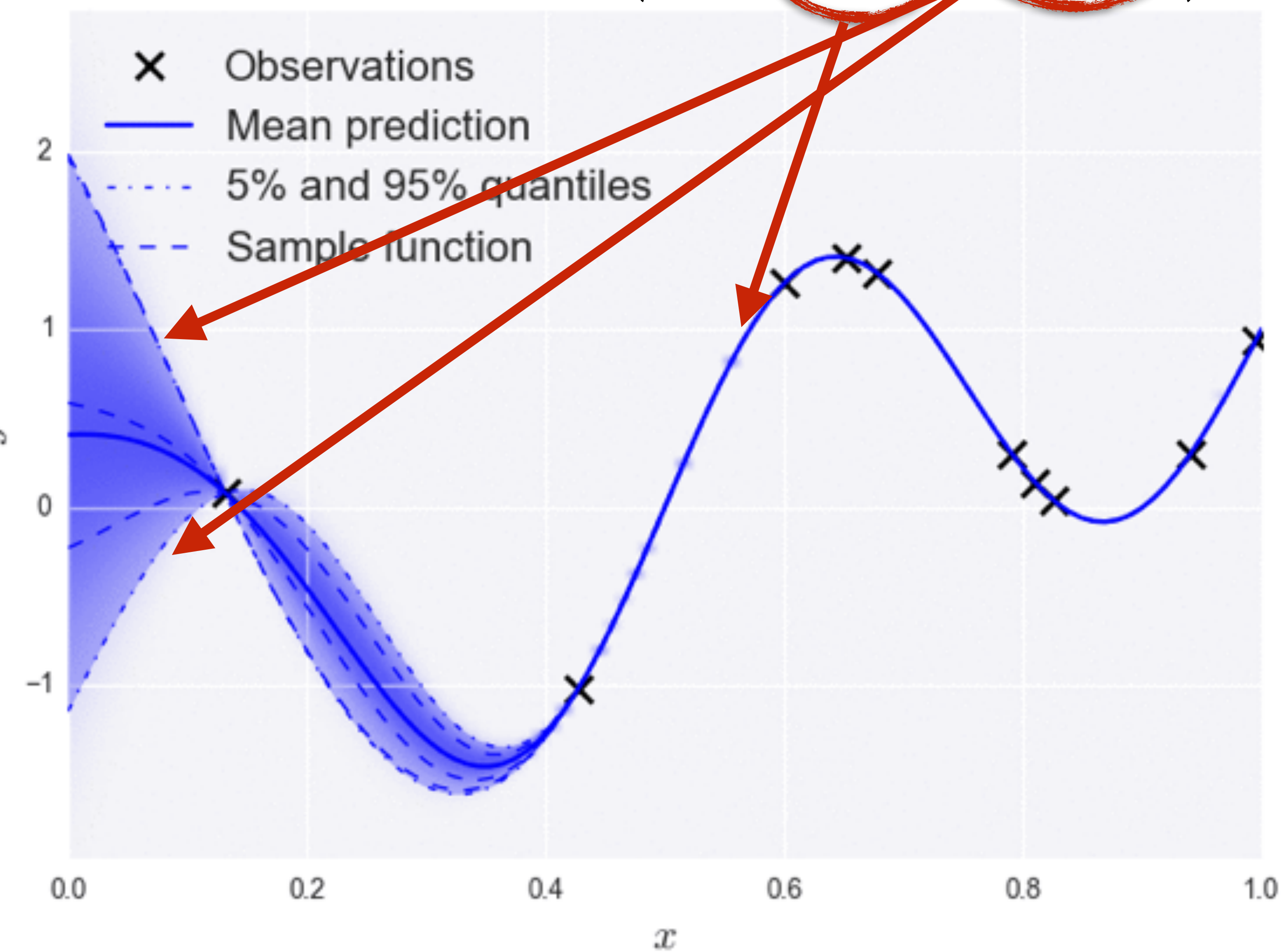
Gaussian process regression

$$y \mid \mathbf{x}, \mathbf{X}, \mathbf{f} \sim \mathcal{N}\left(y \mid \tilde{m}(\mathbf{x}), \tilde{\sigma}^2(\mathbf{x})\right),$$

$$f(\mathbf{x}) = \tilde{m}(\mathbf{x}) \pm 2\tilde{\sigma}(\mathbf{x})$$



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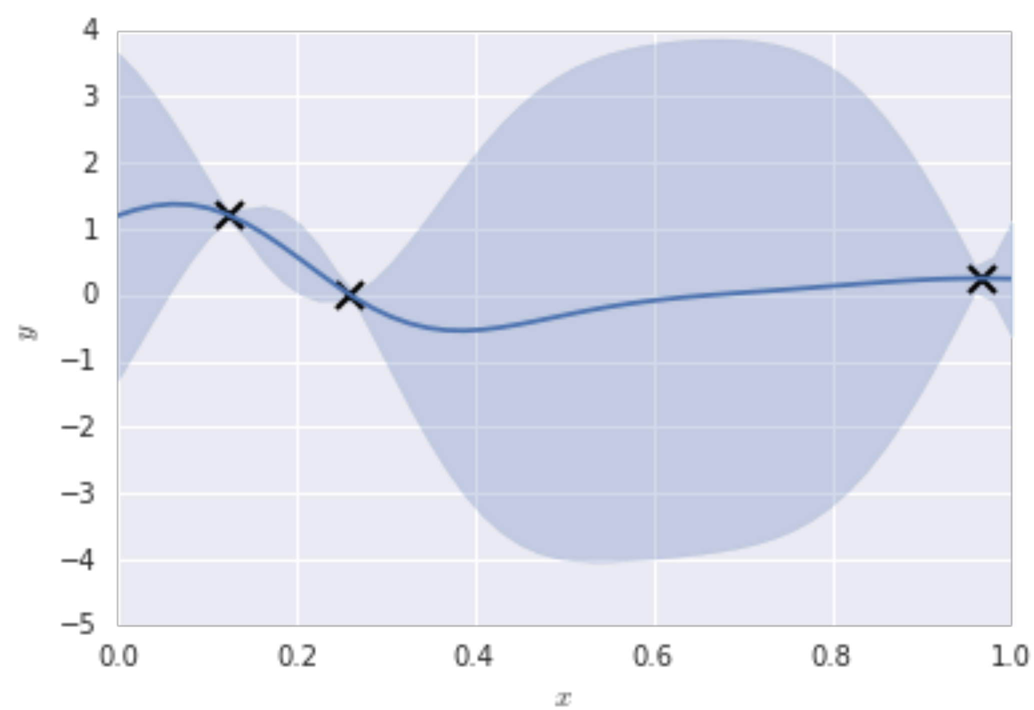
We fit a statistical model



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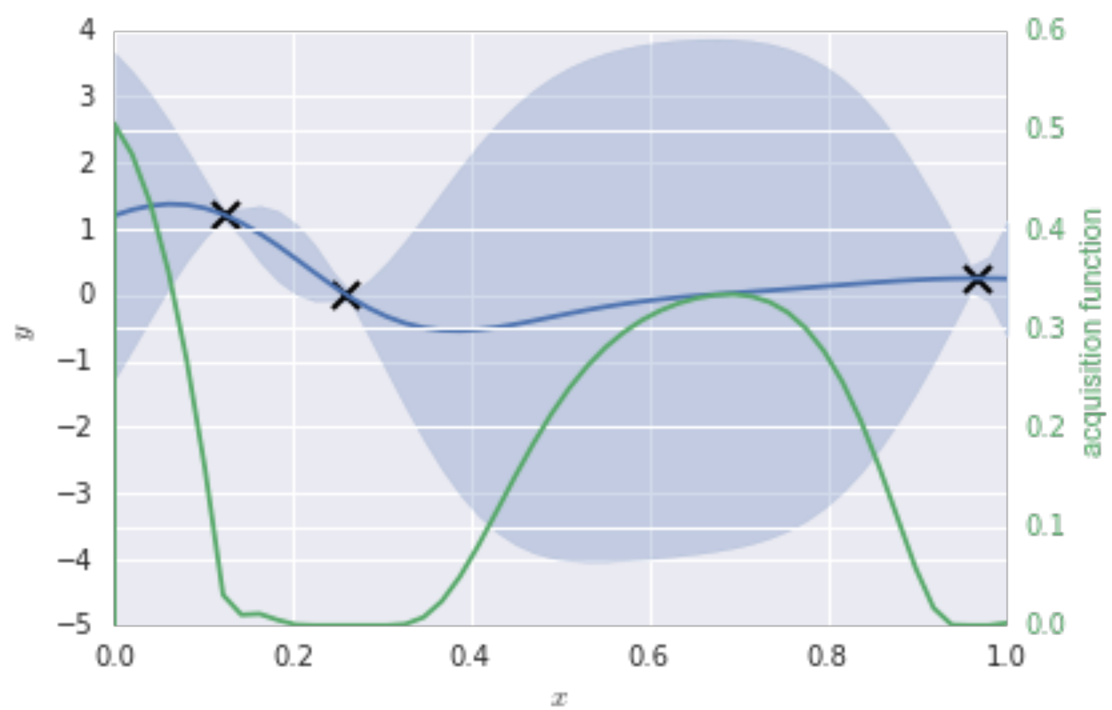
Quantify the value of information via an acquisition function



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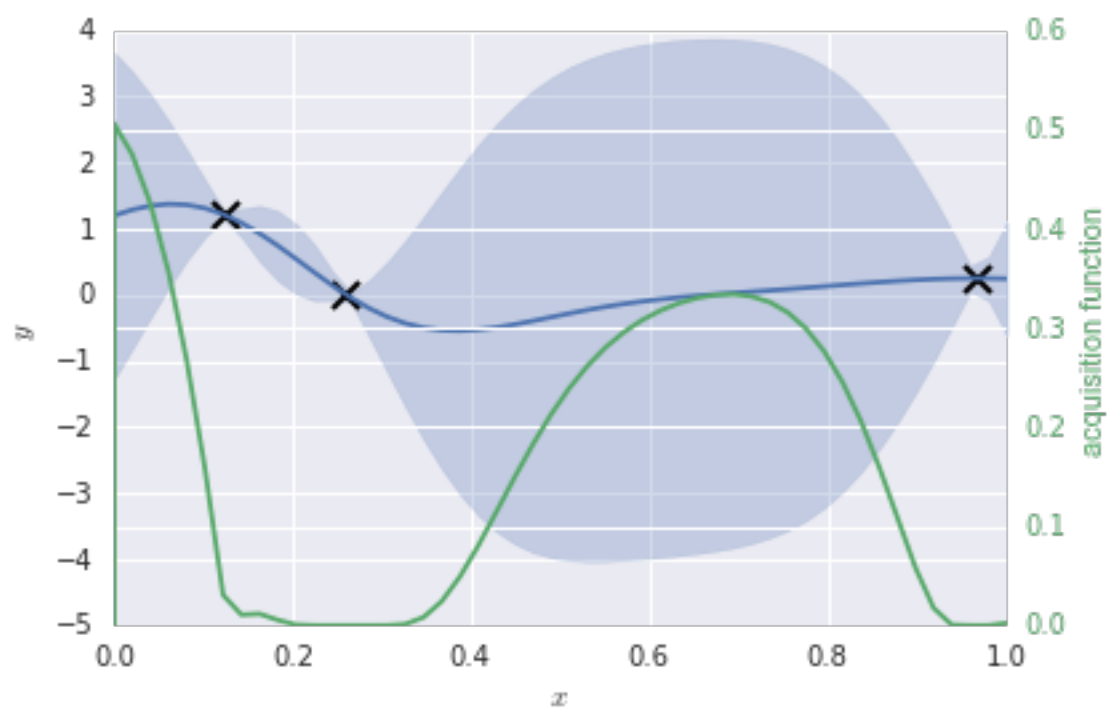

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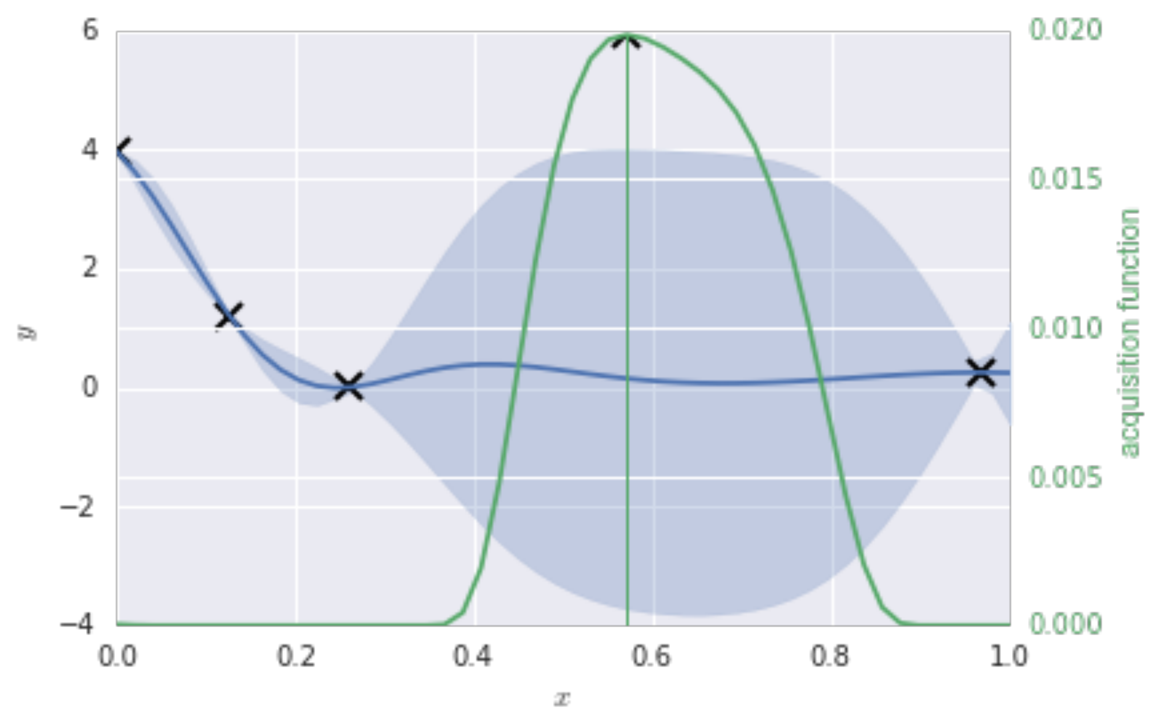
Repeat (Iteration 2)



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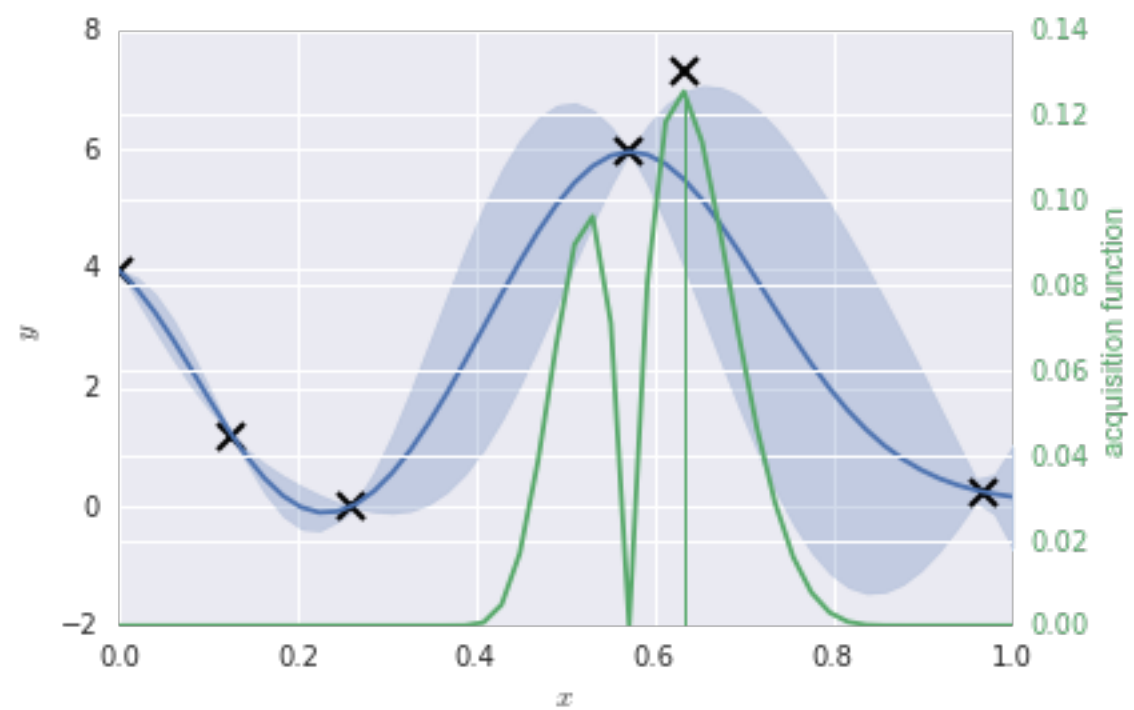

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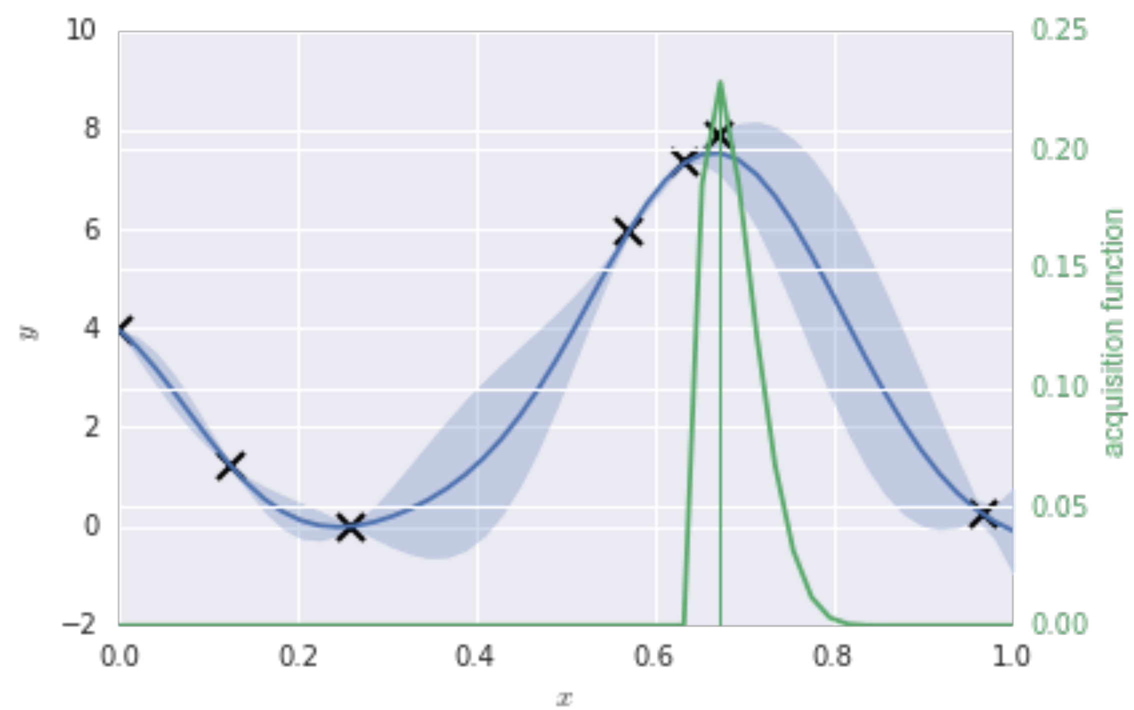

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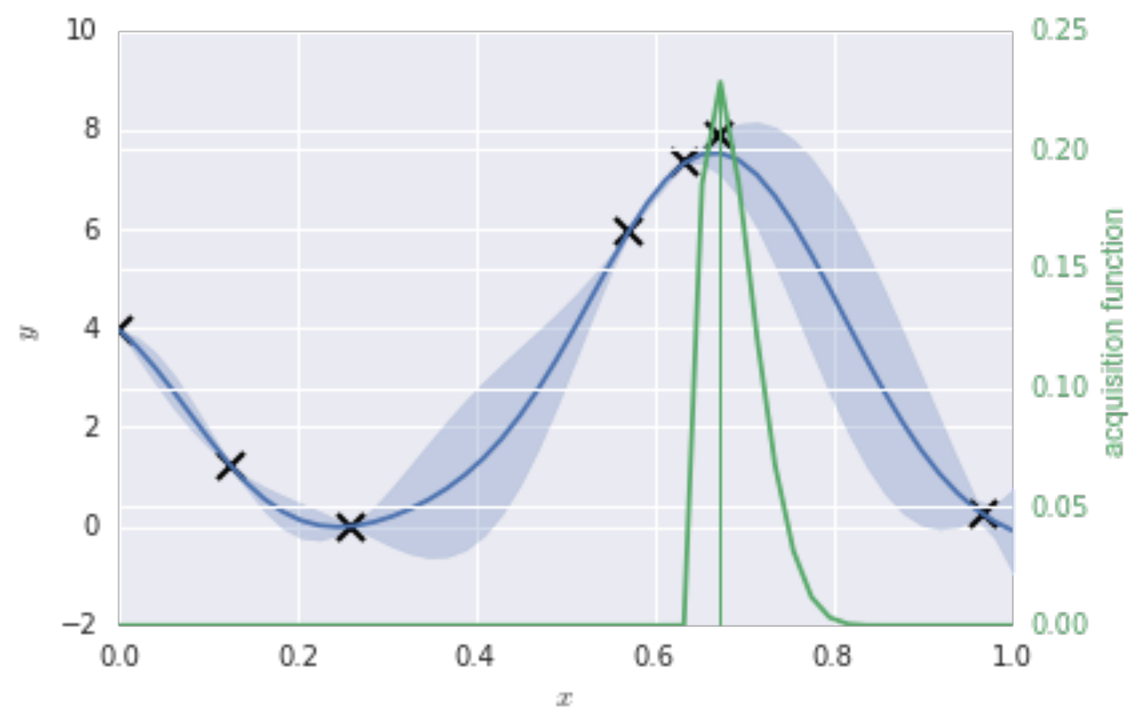
Repeat (Iteration 4)



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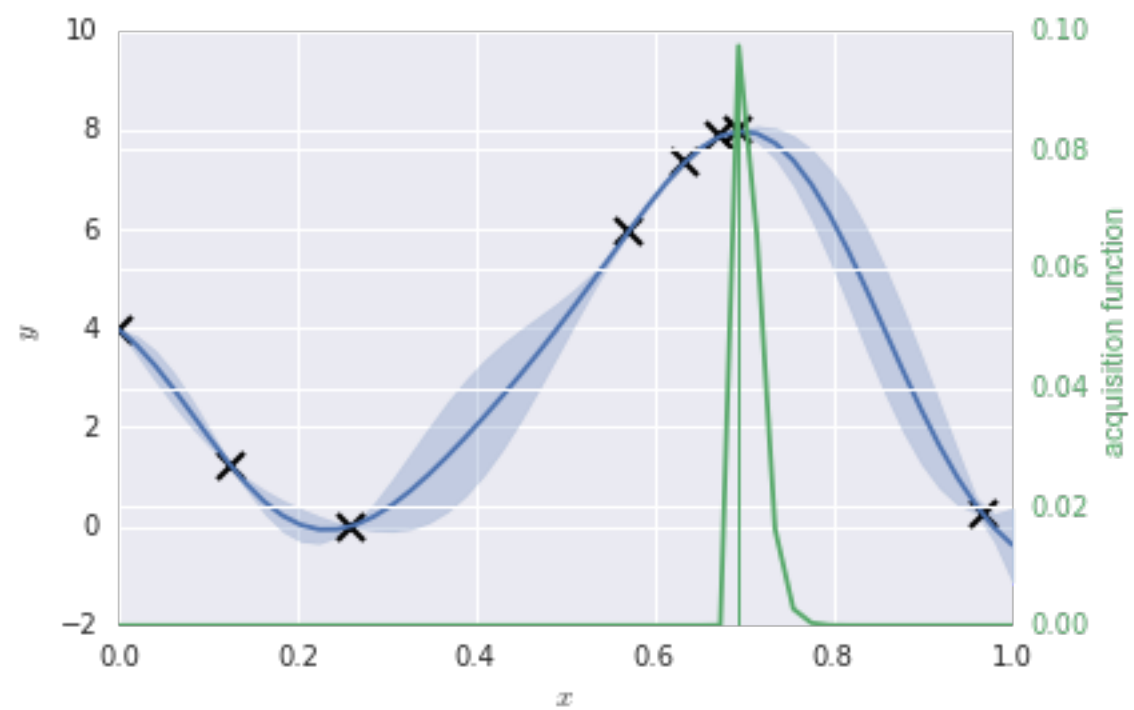
Repeat (Iteration 5)



$a(\mathbf{x})$

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$$\mathbf{x}_{n+1} = \operatorname{argmax}_{\mathbf{x}} a(\mathbf{x})$$

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The problem

- Problem:

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- when the objective is:
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Dynamic vs Myopic Information Acquisition

- Optimal information acquisition policies…
- => Dynamic programming/control theory.
- Too hard mathematical/computational problems.
- What if, we just pick one piece of information at a time?
- Myopic (one-step-look-ahead) policies.

The value of information

- The value of information (VoI) depends on what you want to do.
- Can be quantified objectively if:
  - you have assigned probabilities over all possibilities.
  - you can quantify your profit/loss if any of the possibilities happen.

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The value of information

VoI of **x** = how much expected gain if I measure at **x**

= expected profit if I measure at **x**
- current best alternative

= expected income if I measure at **x**
- cost of measuring **x**
- current best alternative

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Acquisition function

- Most of the times, we don’t have the details to find the VoI.
- We use heuristic approximations to VoI such as:
    - the probability of improvement
    - the expected improvement
    - the knowledge gradient
    - the expected information gain
    - …

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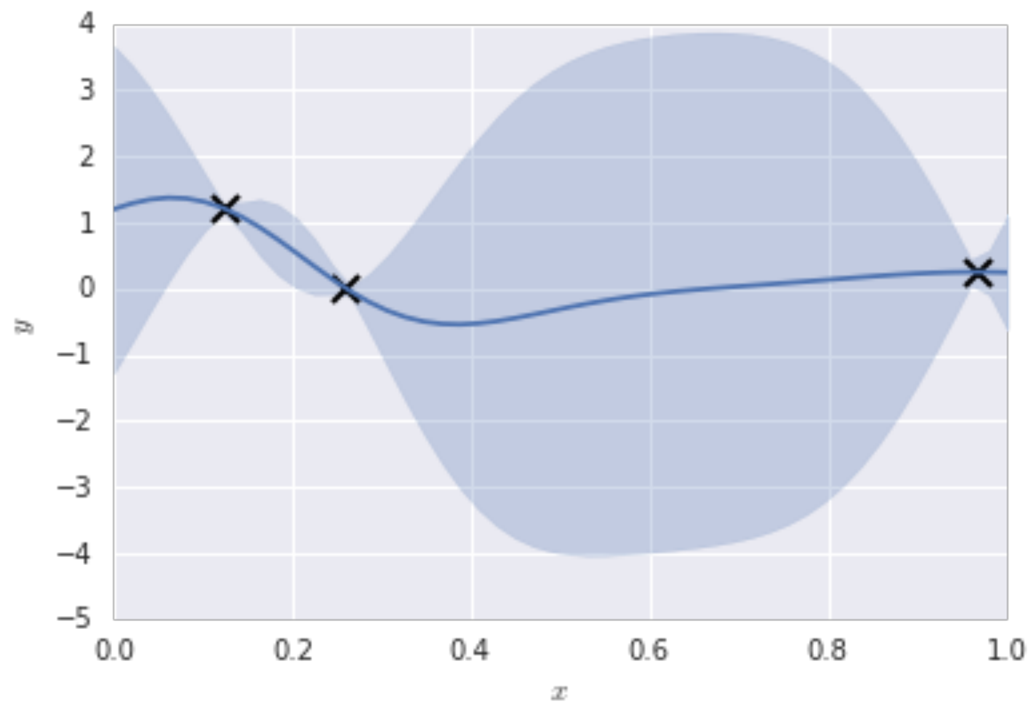
Maximum Mean



Add the point with the maximum expected mean:

$$a(\mathbf{x}) = m(\mathbf{x})$$

Tries to exploit what we know.

It does not converge.

How can we add some elements of exploration?

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$$
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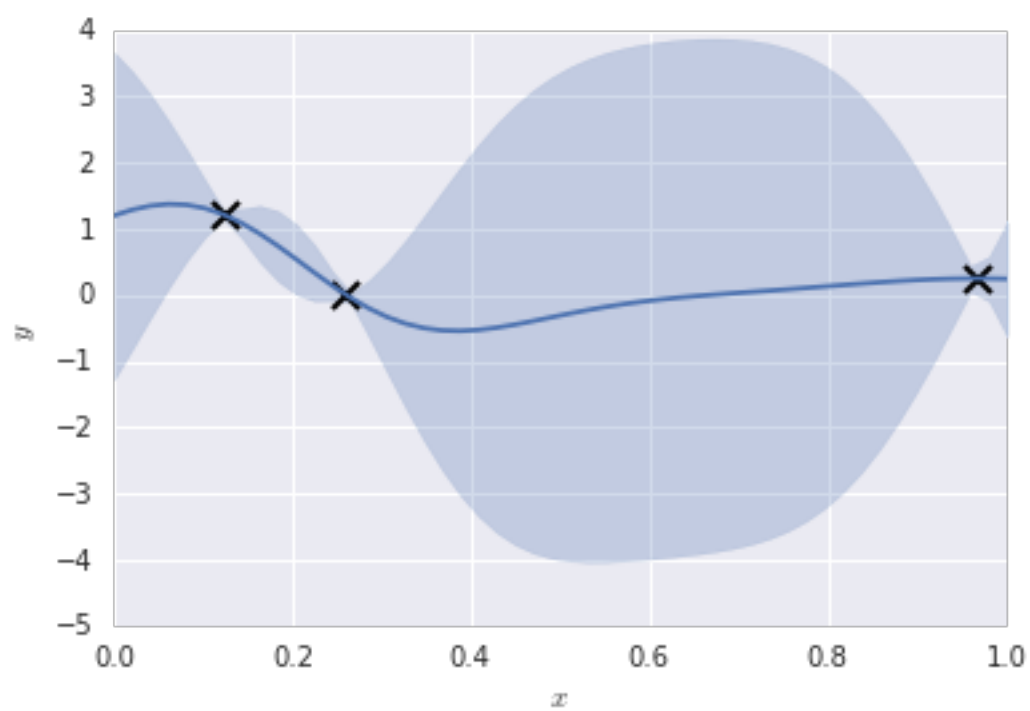
Maximum Upper Interval



Use the variance to explore:

$$a(\mathbf{x}) = m(\mathbf{x}) + \psi\sigma(\mathbf{x})$$

Adds upper quantile.

Provable convergence to the global maximum!

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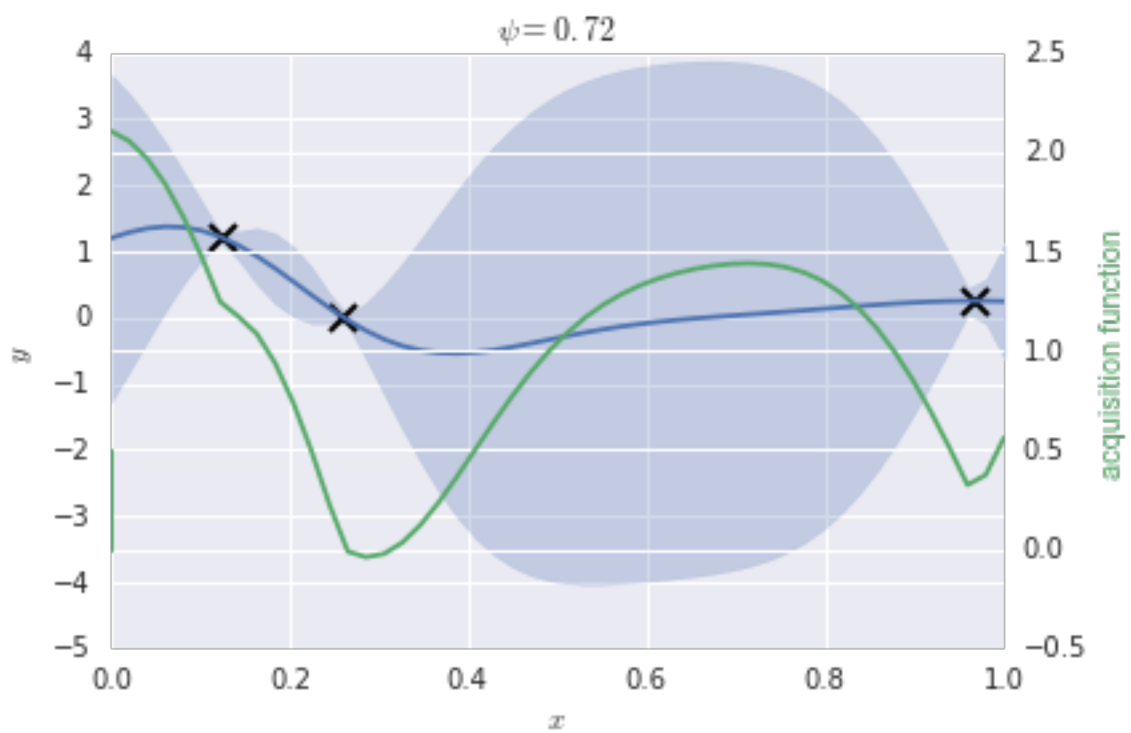
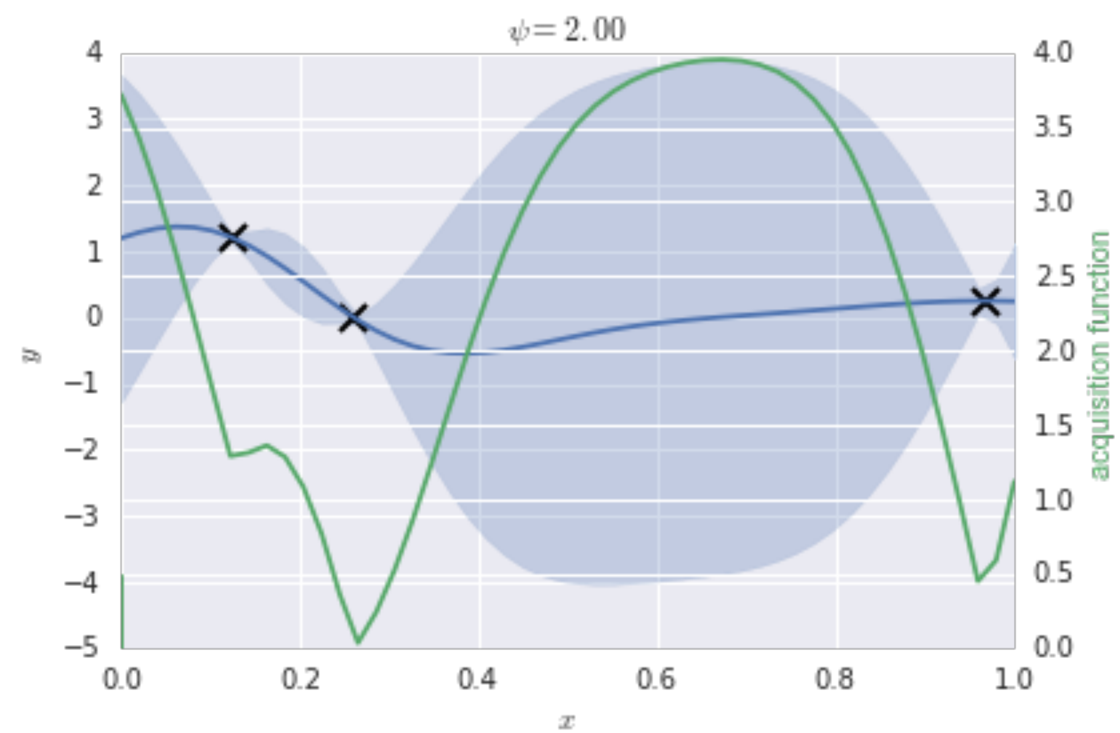
Maximum Upper Interval





Exploits more

Explores more

Too much exploration…

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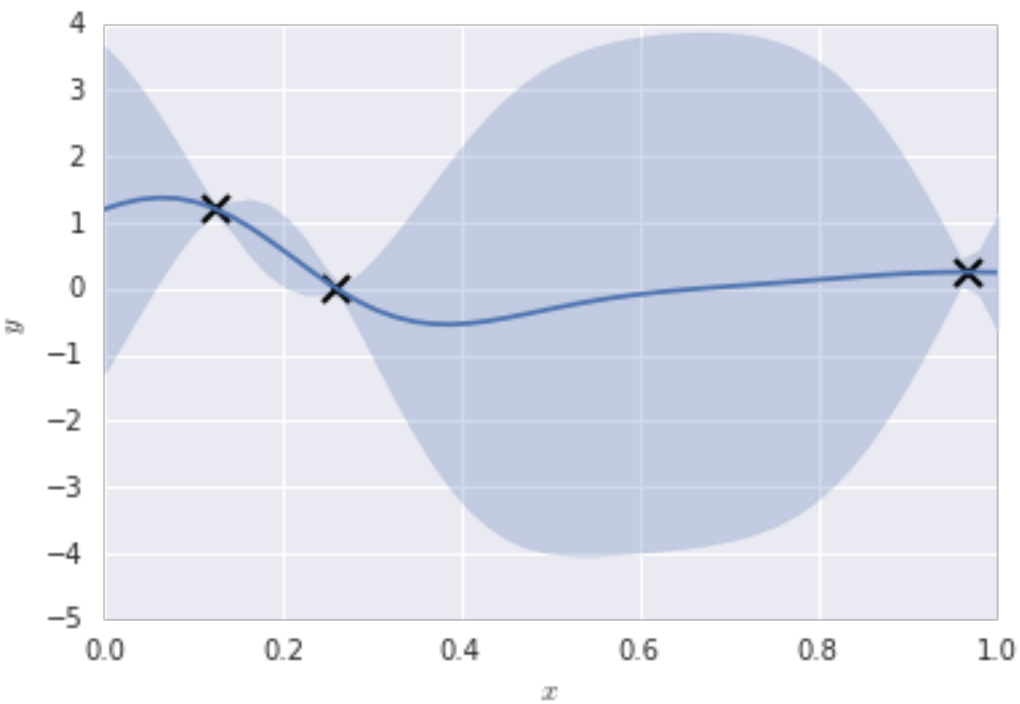
Probability of Improvement



Current best:

$$\tilde{y}_n = \max_{1\le i\le n} y_i$$

Hypothetical simulation at **x** yields y

The probability of improvement is:

$$\begin{aligned} a(\mathbf{x}) &= P[y > \tilde{y}_n + \psi \mid \mathbf{x}] \\ &= \int_{\tilde{y}_n+\psi}^{\infty} p(y \mid \mathbf{x}) dy \\ &= 1 - \Phi\left(\frac{\tilde{y}_n + \psi - m(\mathbf{x})}{\sigma(\mathbf{x})}\right) \end{aligned}$$

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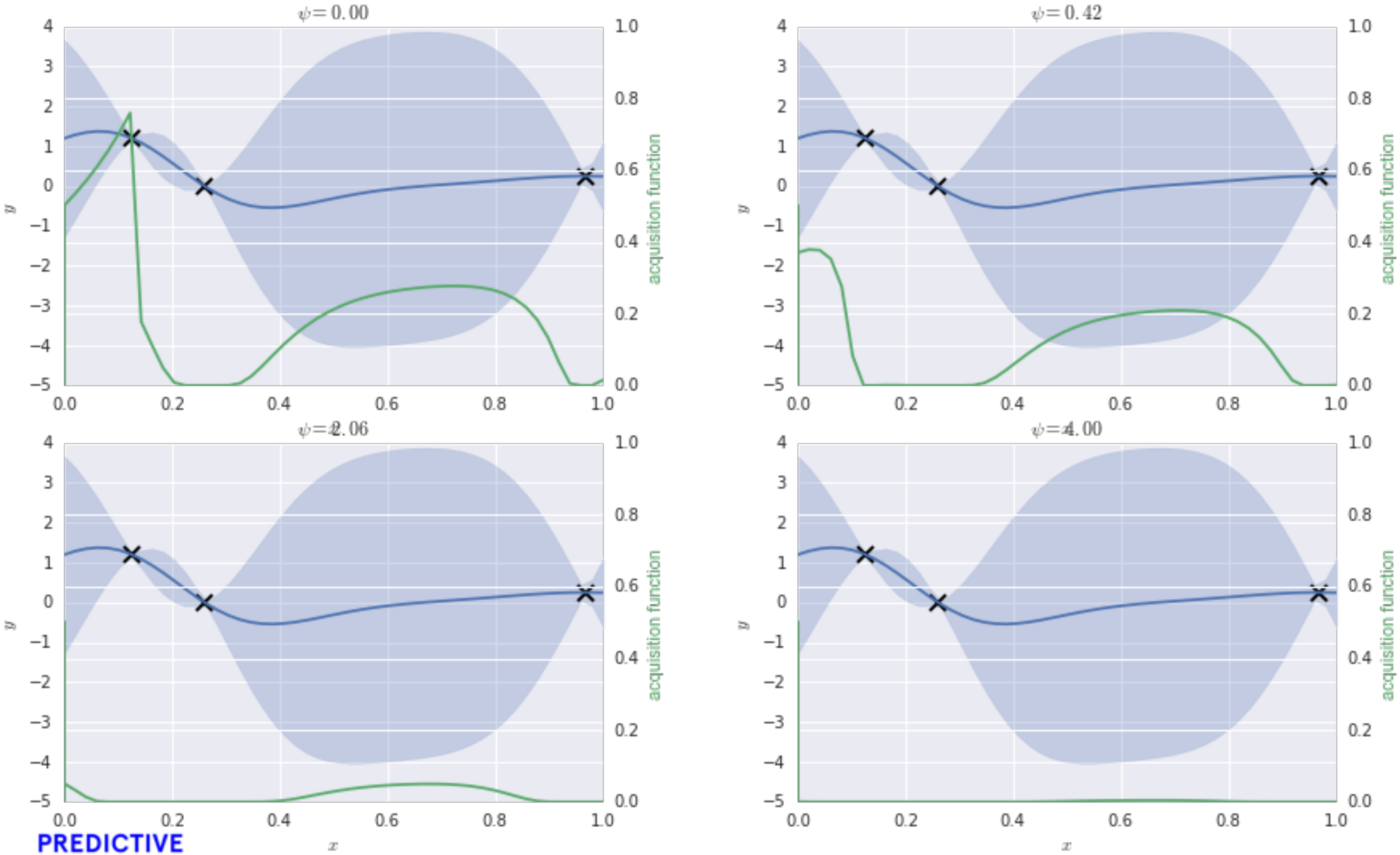
Probability of Improvement



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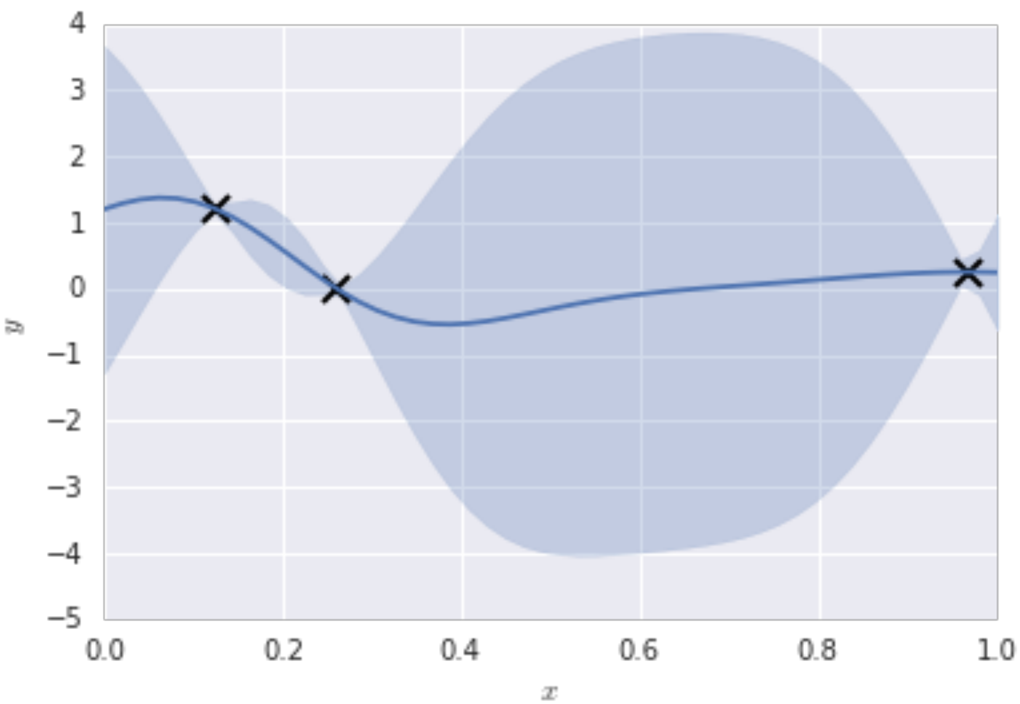
Probability of Improvement - Why not use it?

- Large value of psi -> exploration.
- Small value of psi -> exploitation.
- But how to you pick it?

Expected Improvement



Current best:

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Hypothetical simulation at **x** yields y

The improvement is:

$$a(\mathbf{x}, y) = \max\{0, y - \tilde{y}_n\}$$

Integrate over y:

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$$p(y\mid\mathbf{x}) \approx \mathcal{N}\left(y\mid m(\mathbf{x}), \sigma^2(\mathbf{x})\right)$$

$$a(\mathbf{x}) = \int_{-\infty}^{\infty} \max\{0, y - \tilde{y}_n\} p(y\mid\mathbf{x})dy$$
$$= (m(\mathbf{x}) - \tilde{y}_n)\Phi\left(\frac{m(\mathbf{x}) - \tilde{y}_n}{\sigma(\mathbf{x})}\right) + \sigma(\mathbf{x})\phi\left(\frac{m(\mathbf{x}) - \tilde{y}_n}{\sigma(\mathbf{x})}\right)$$

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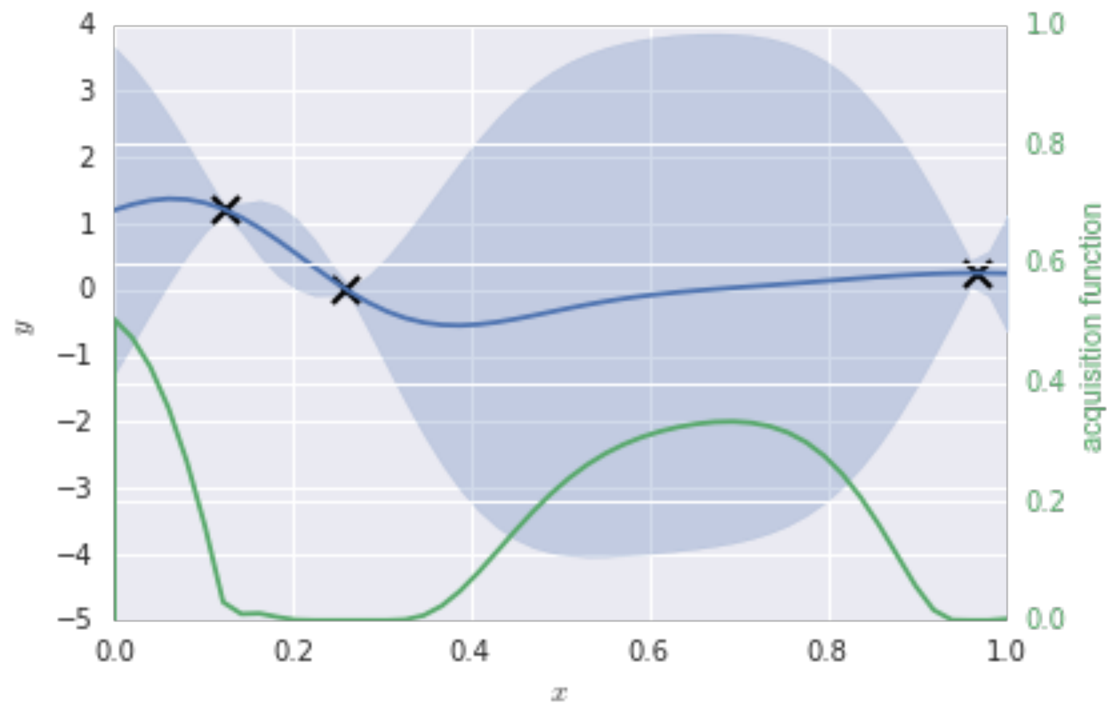
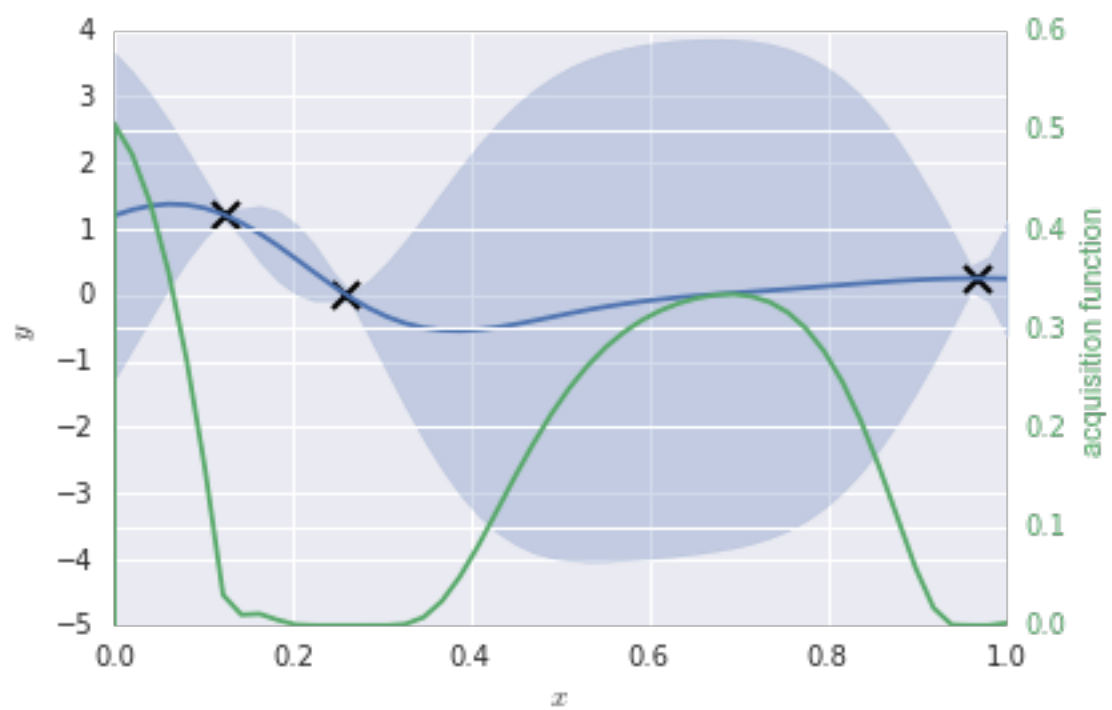
Expected Improvement



Automatic exploration vs exploitation…

Quantify the value of information via an acquisition function



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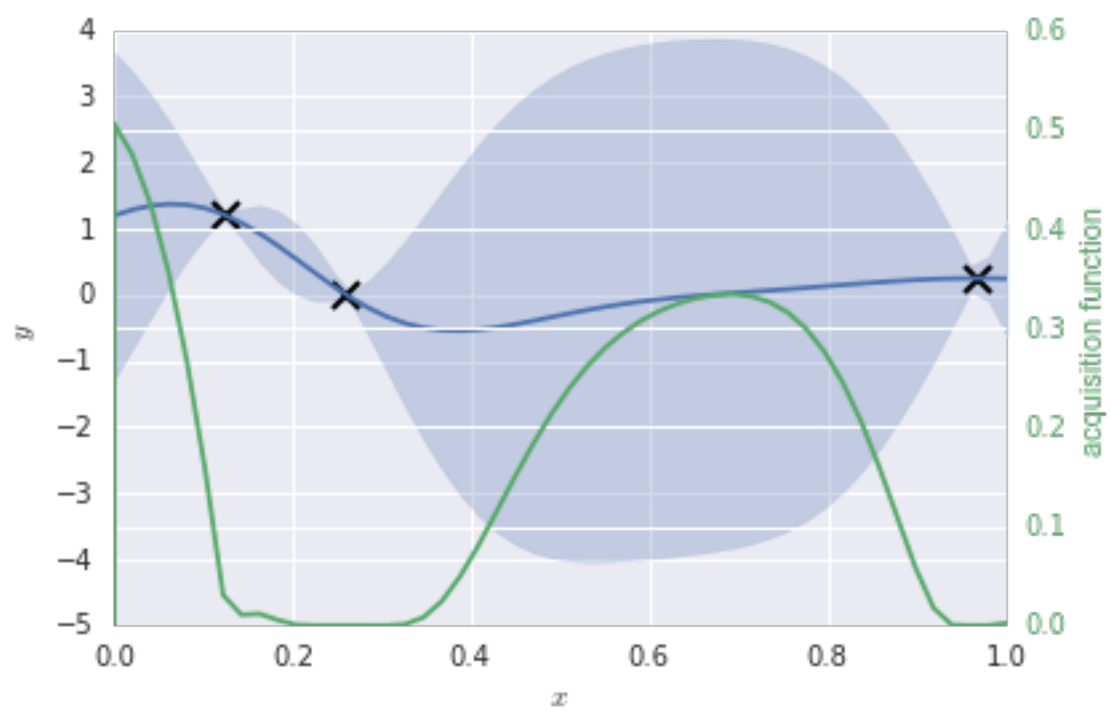

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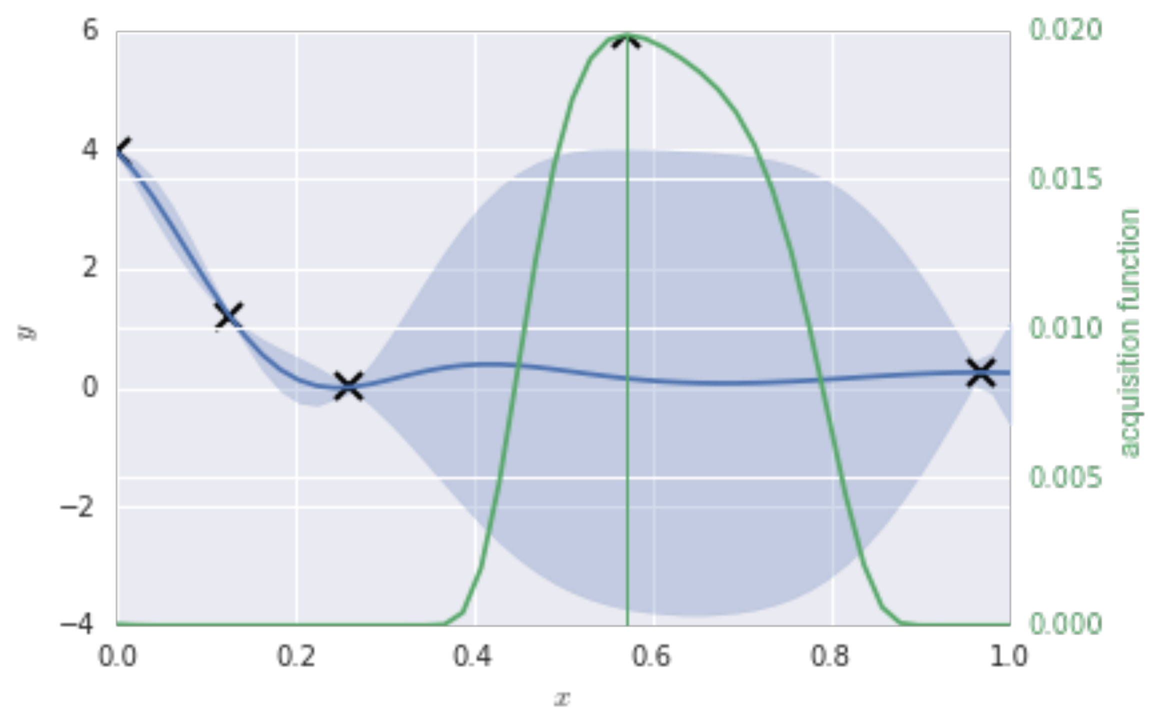
Repeat (Iteration 2)



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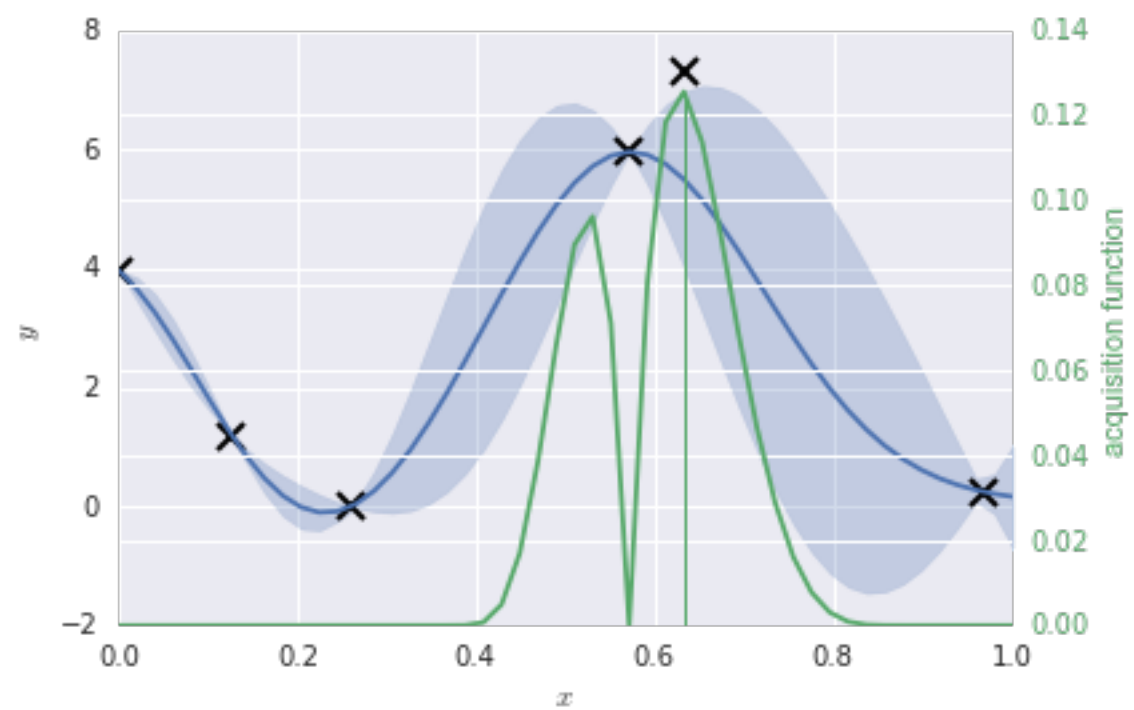

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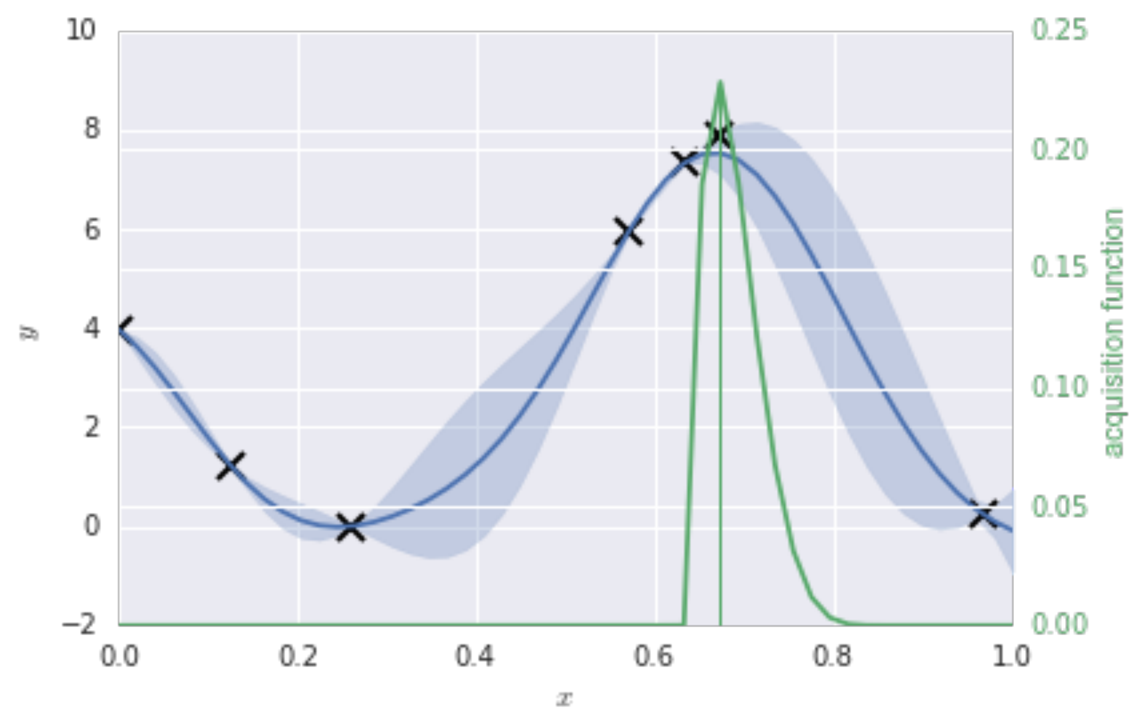

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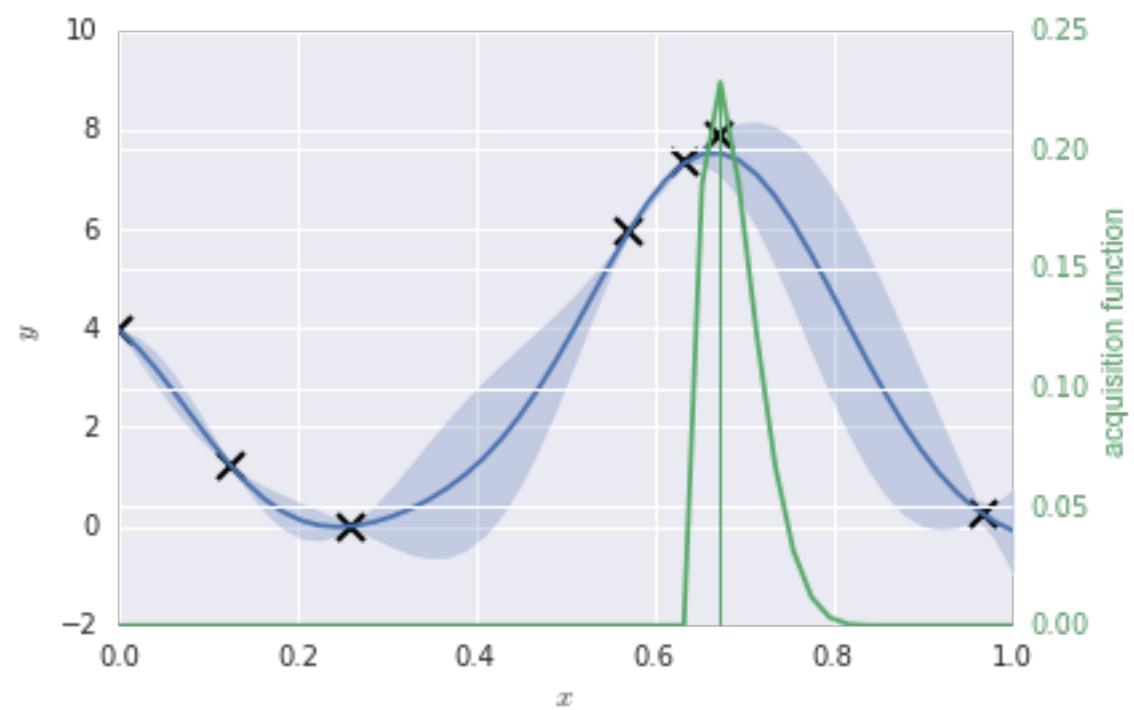

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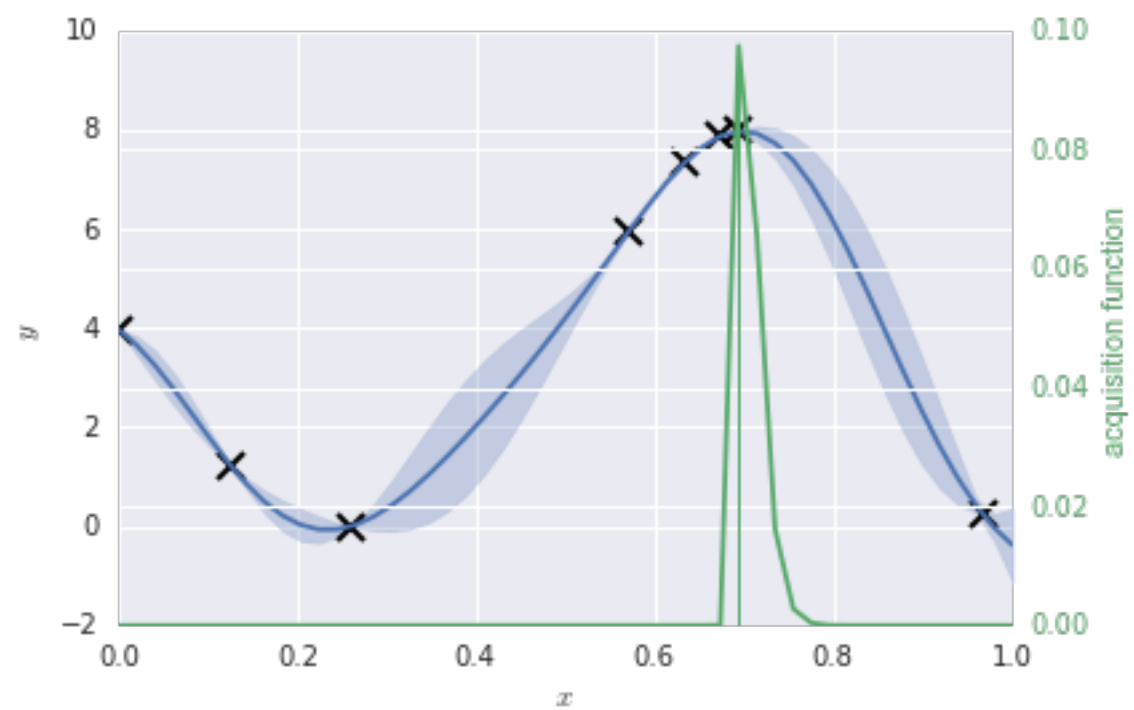
Repeat (Iteration 5)



$a(\mathbf{x})$

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$$
$$y_{1:n} = \{y_1, \ldots, y_n\}$$
$$p(y \mid \mathbf{x}) \approx \mathcal{N}\left(y \mid m(\mathbf{x}), \sigma^2(\mathbf{x})\right)$$
$$\mathbf{x}_{n+1} = \operatorname{argmax}_{\mathbf{x}} a(\mathbf{x})$$

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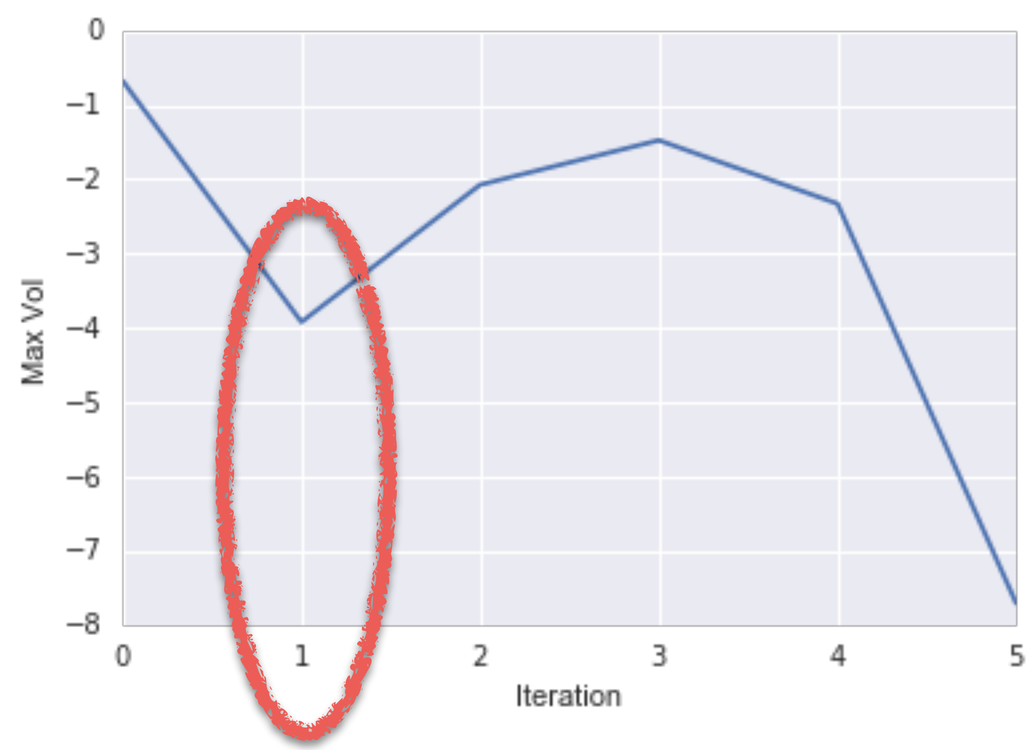
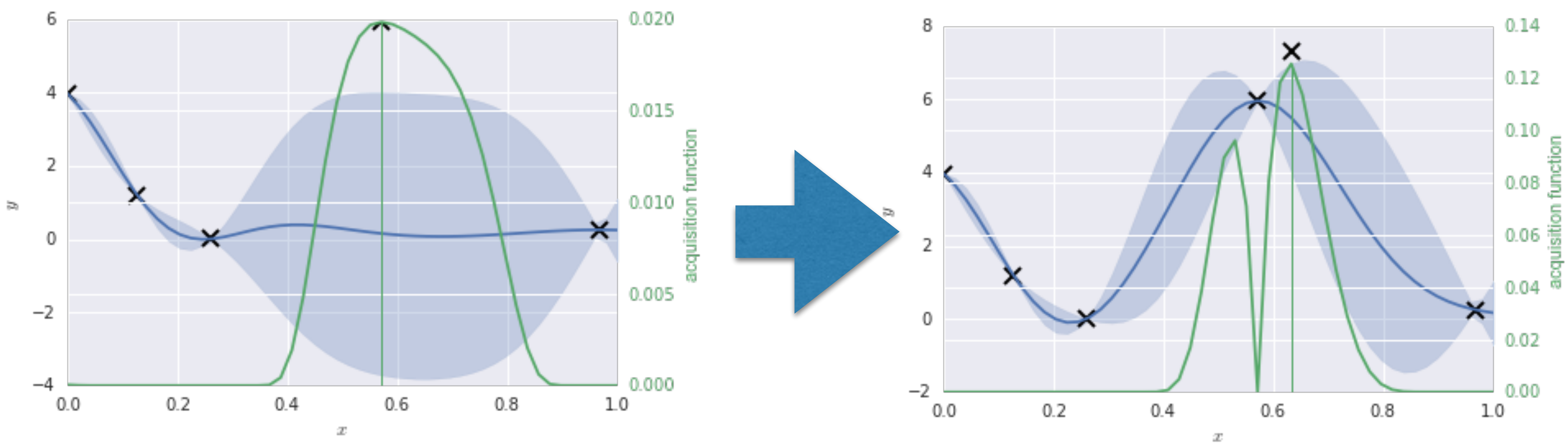
The S-curve Phenomenon of Information



Unexpected information

The S-curve Phenomenon of Information



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Advanced Topics for Next Time

- Enforcing optimization constraints.
- Information acquisition for multi-objective optimization.
- Information acquisition under uncertainty.
- Information acquisition from various heterogeneous sources.

Start the notebook of lecture 24