Lecture 23: Bayesian global optimization

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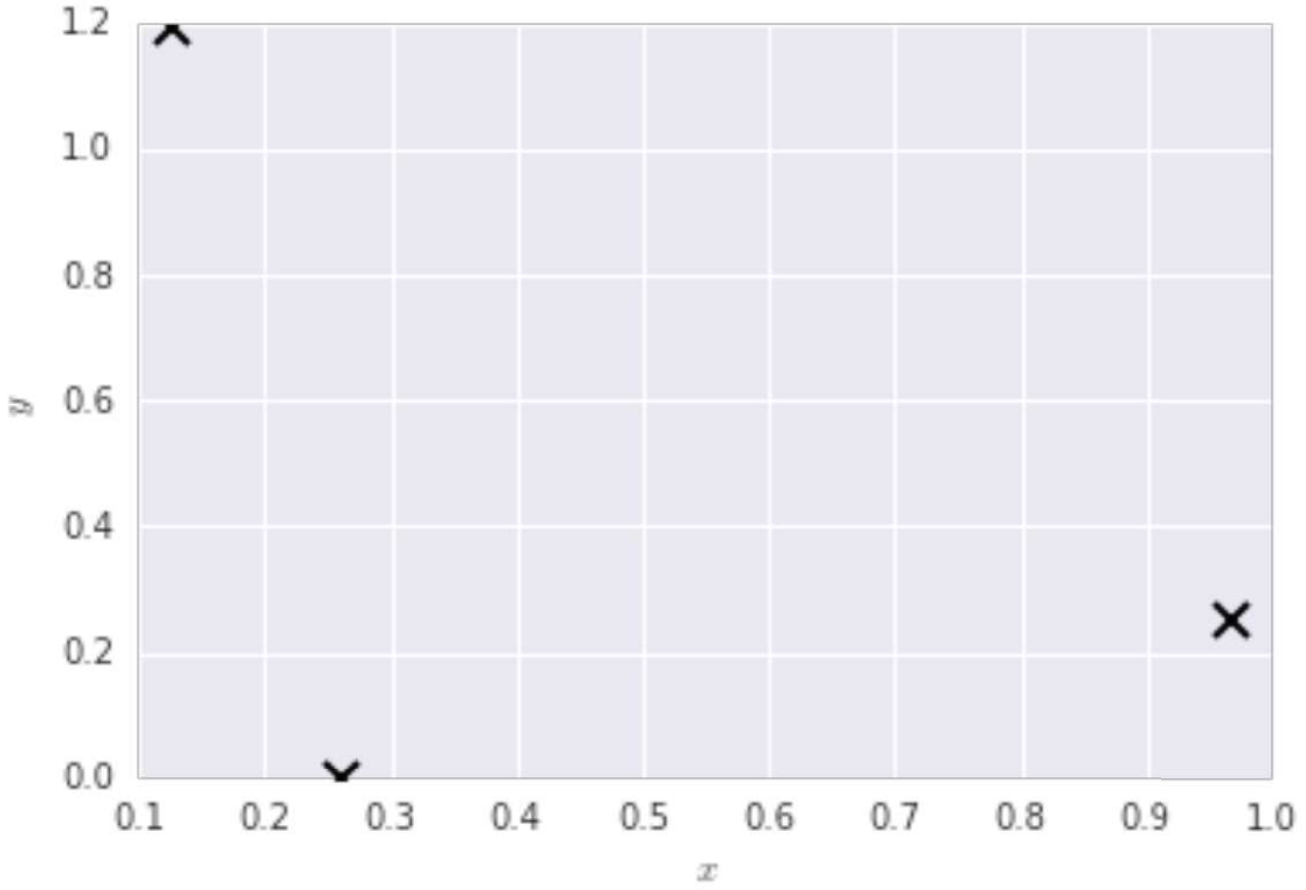
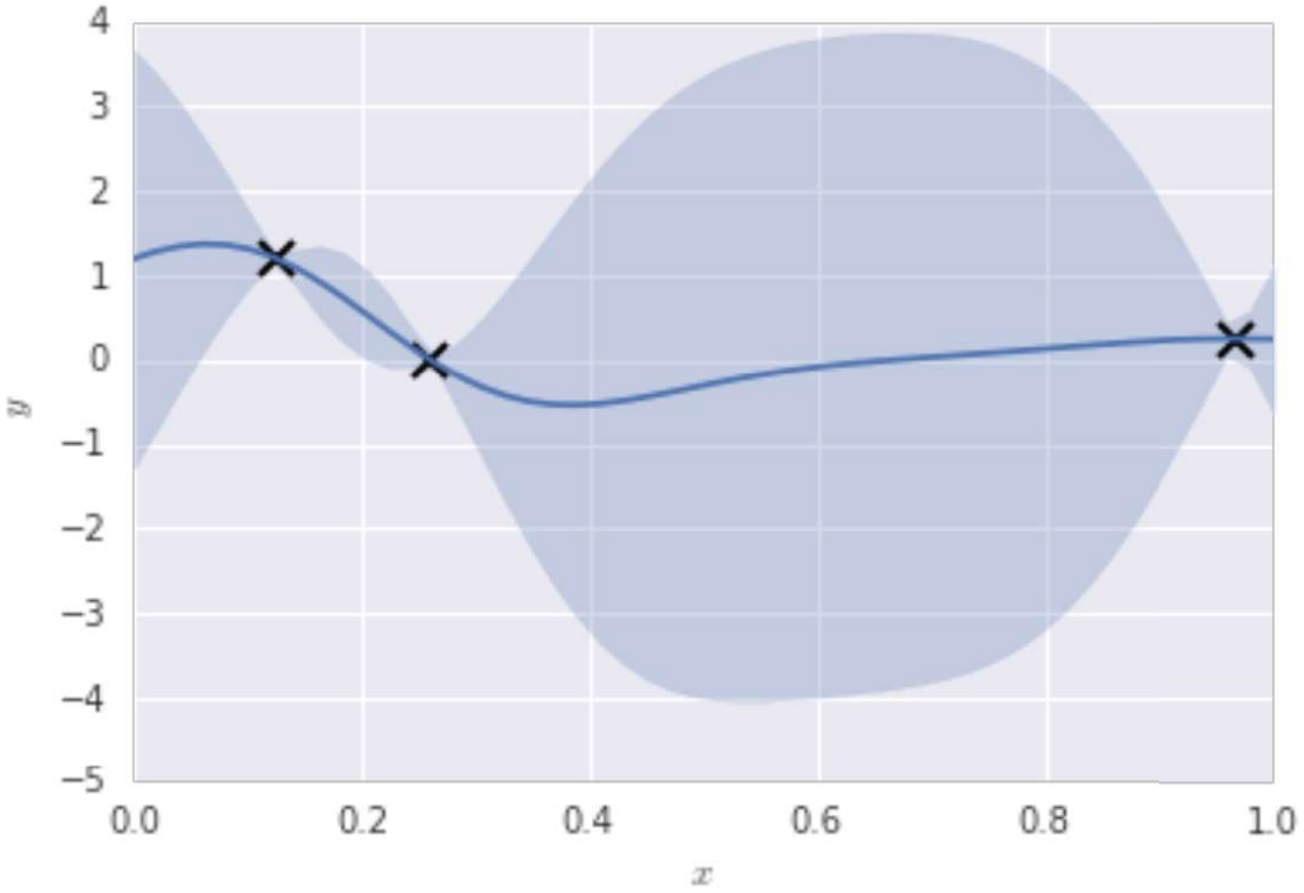
Overview of the Bayesian global optimization algorithm

We have some data



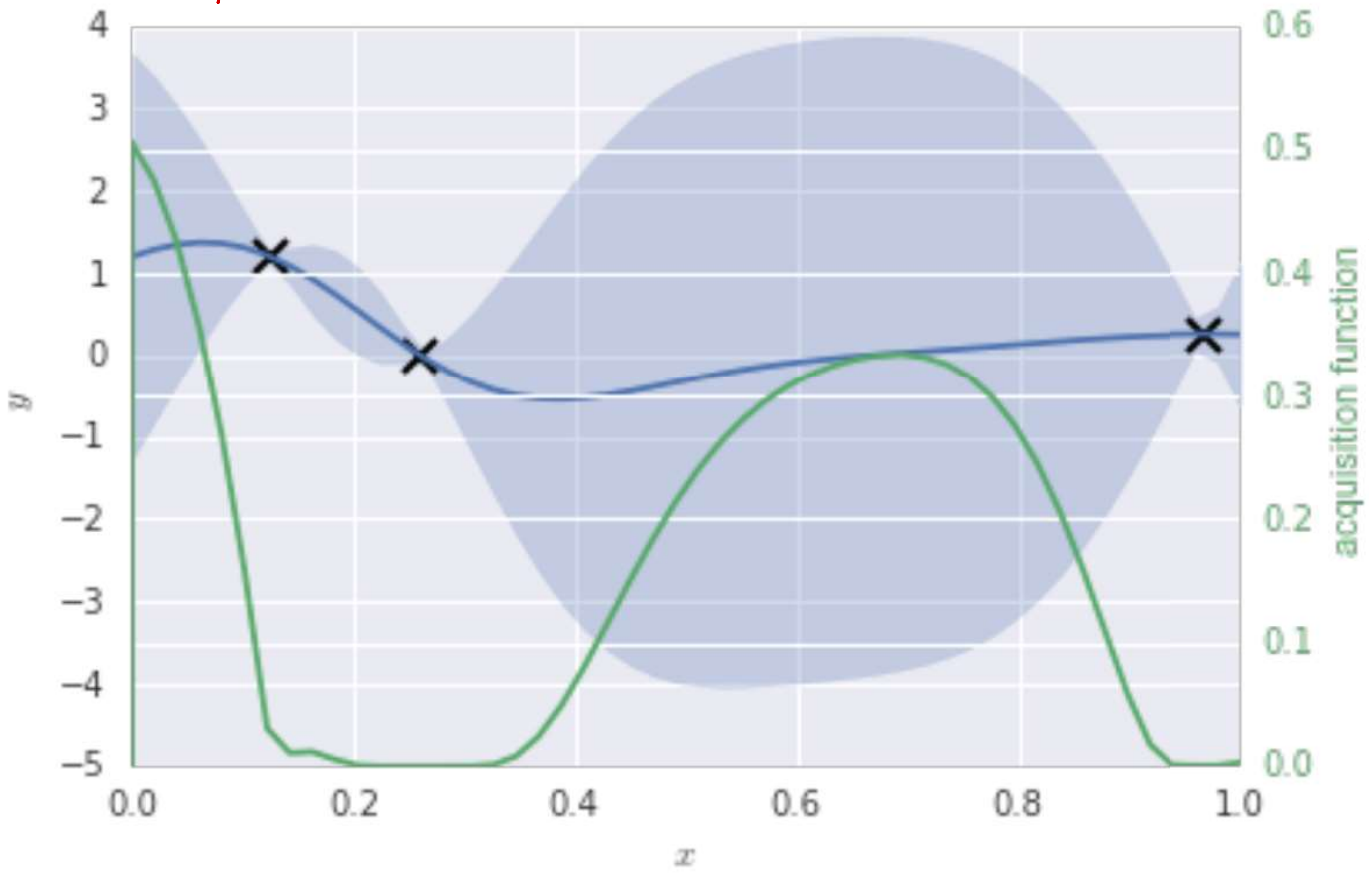
We fit a statistical model

↳ in this case: Gaussian Process Regression
w/ zero measurement noise



Quantify the value of information via an acquisition function

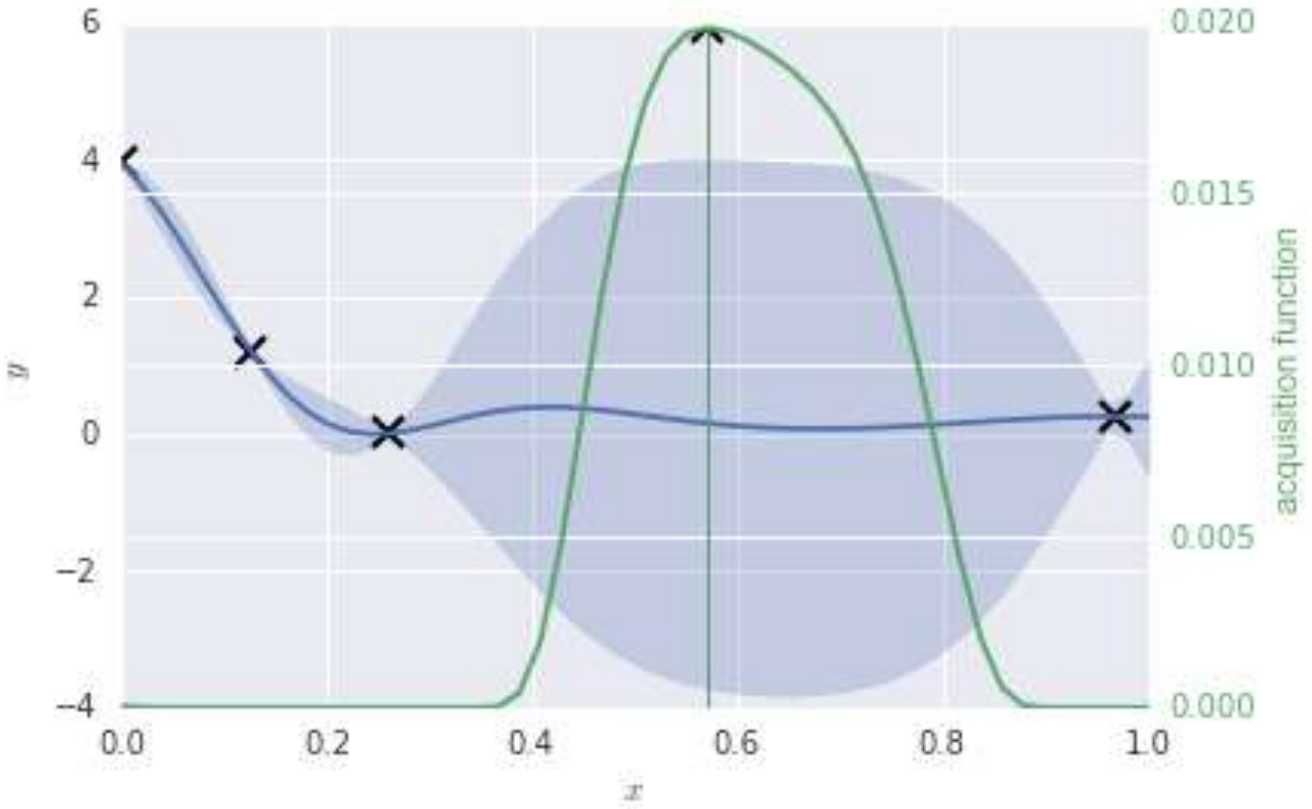
captures the value of making an observation at any input point



the larger this is, the larger the value of making an observation

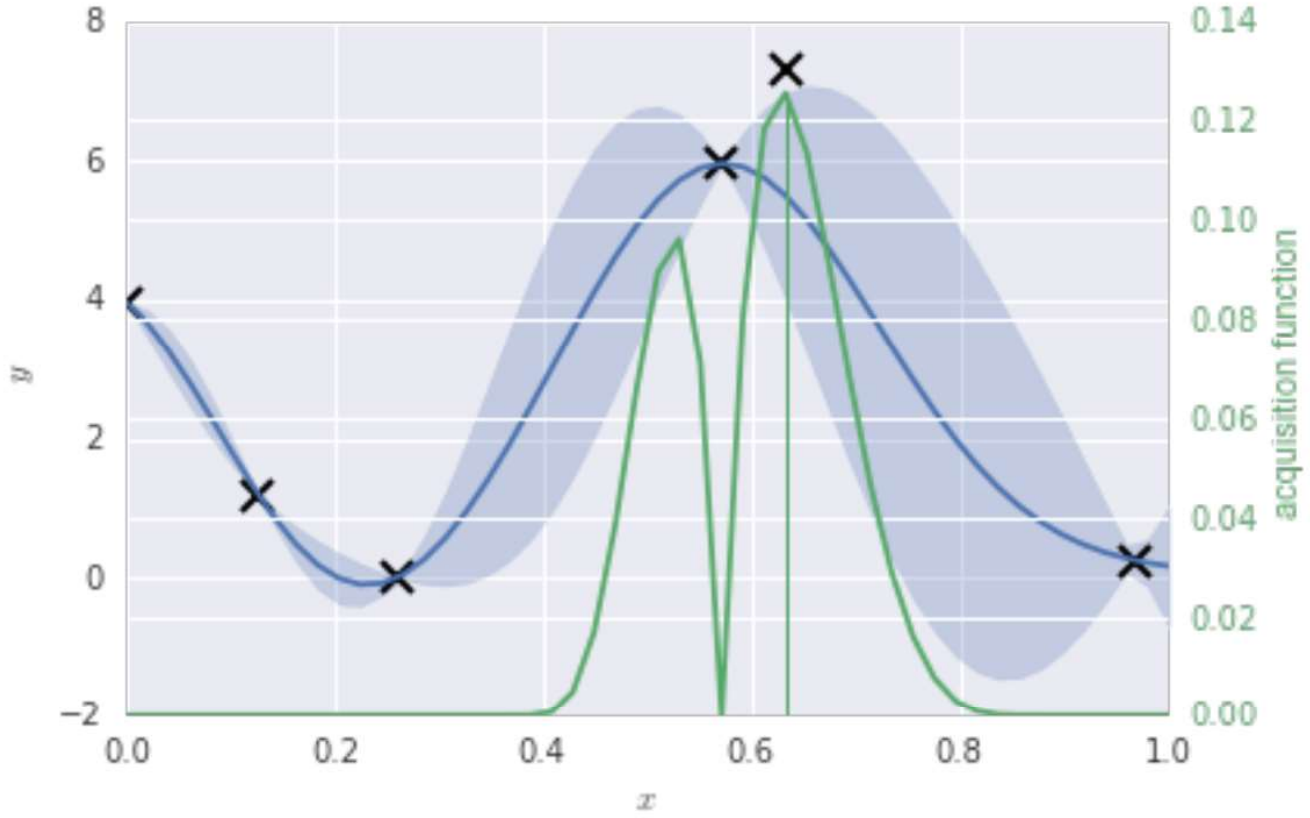
Repeat (Iteration 2)

↳ re-condition the model on this new observation
(re-train, new posterior)



Repeat (Iteration 3)

. . .



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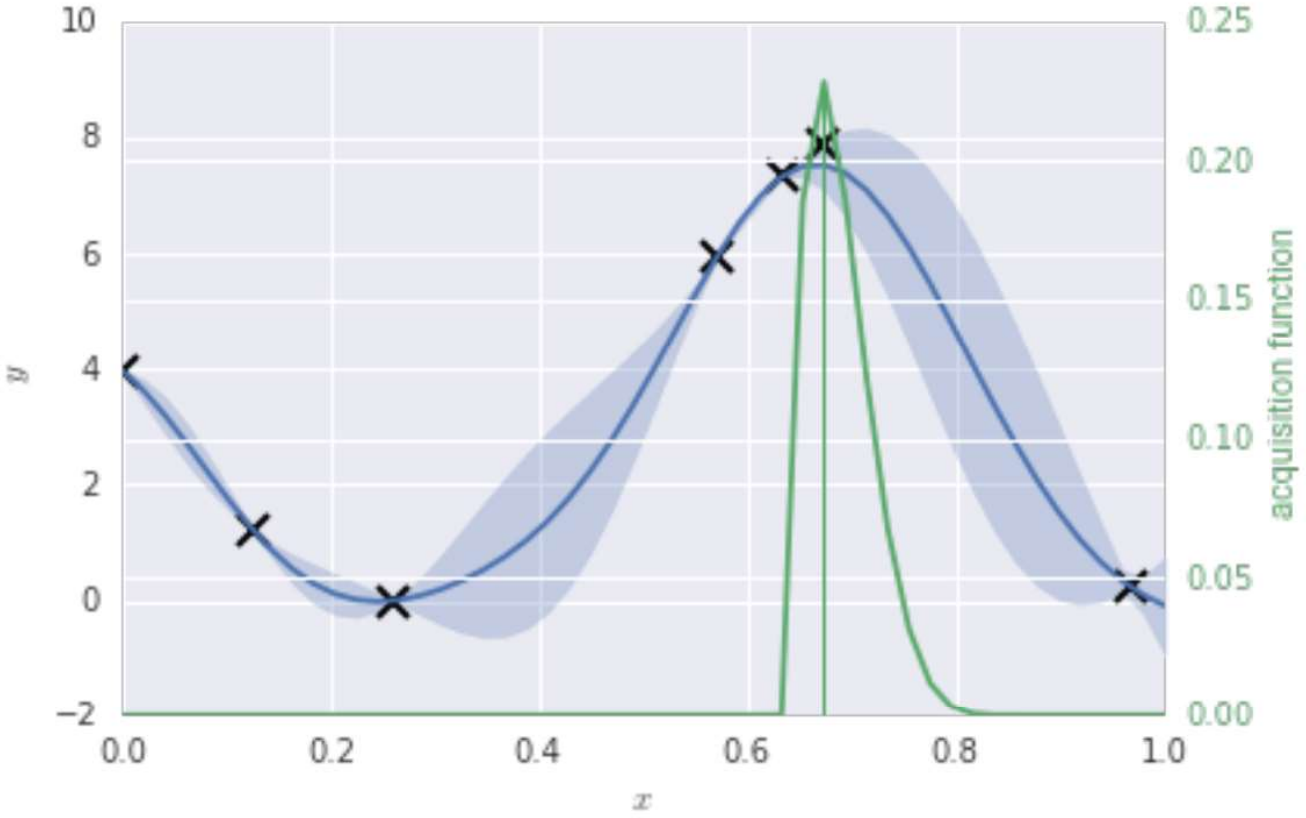
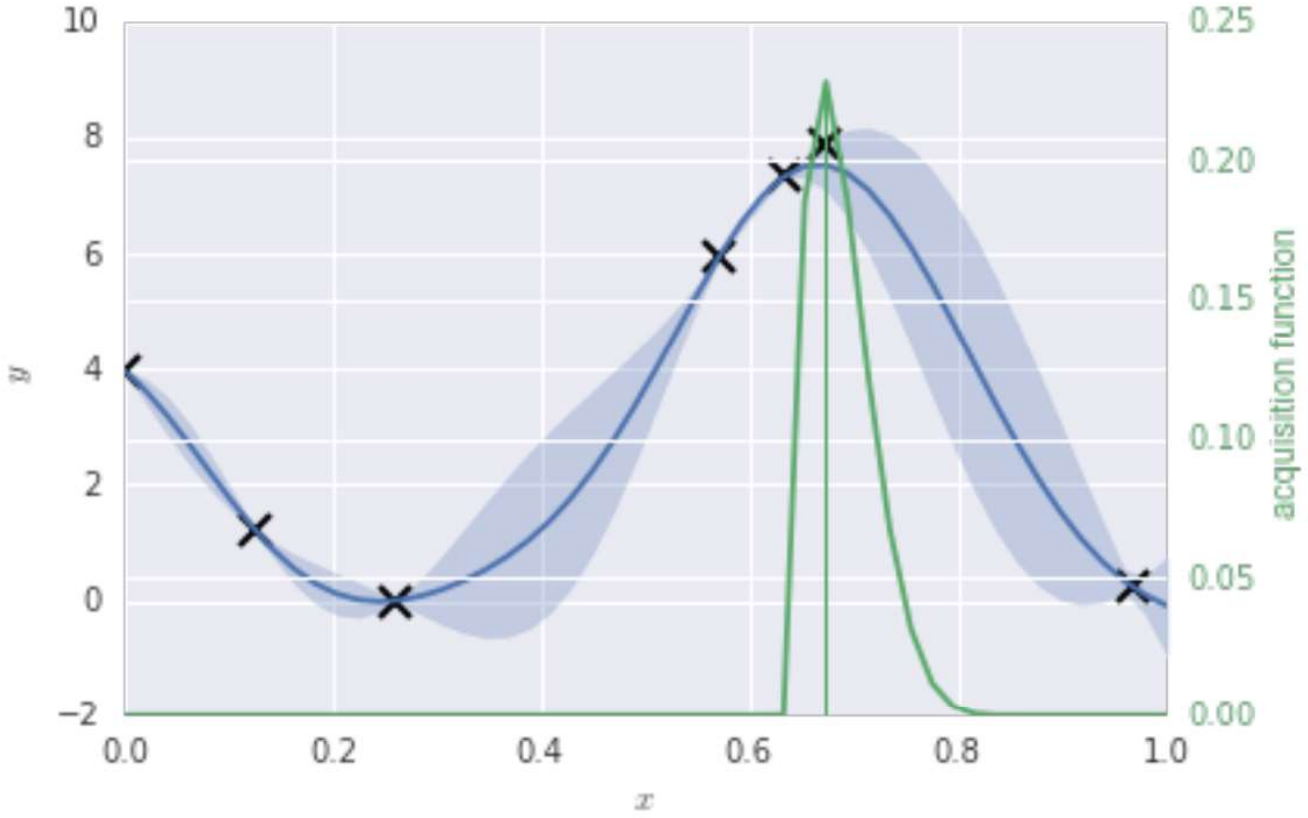
Repeat (Iteration 4)

Exploitation vs. Exploration

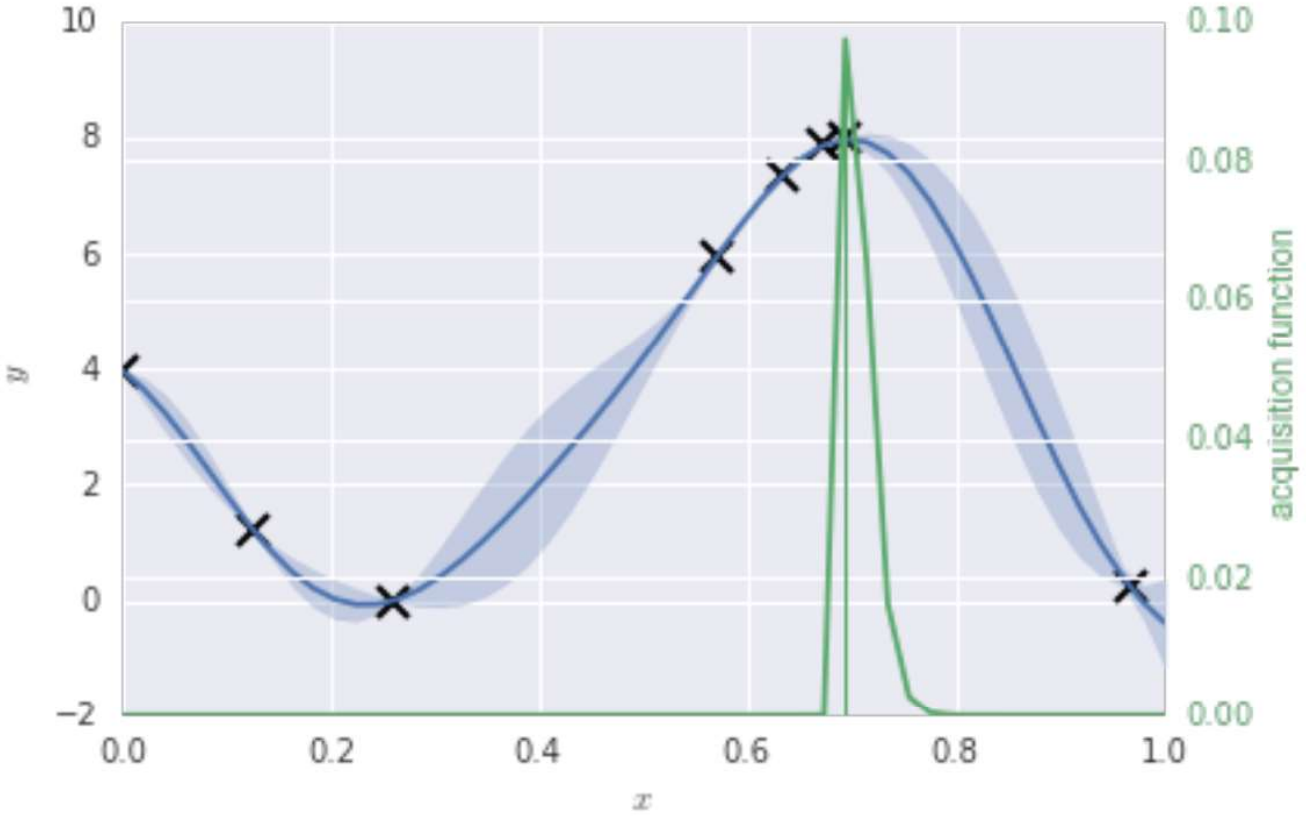


Repeat (Iteration 5)



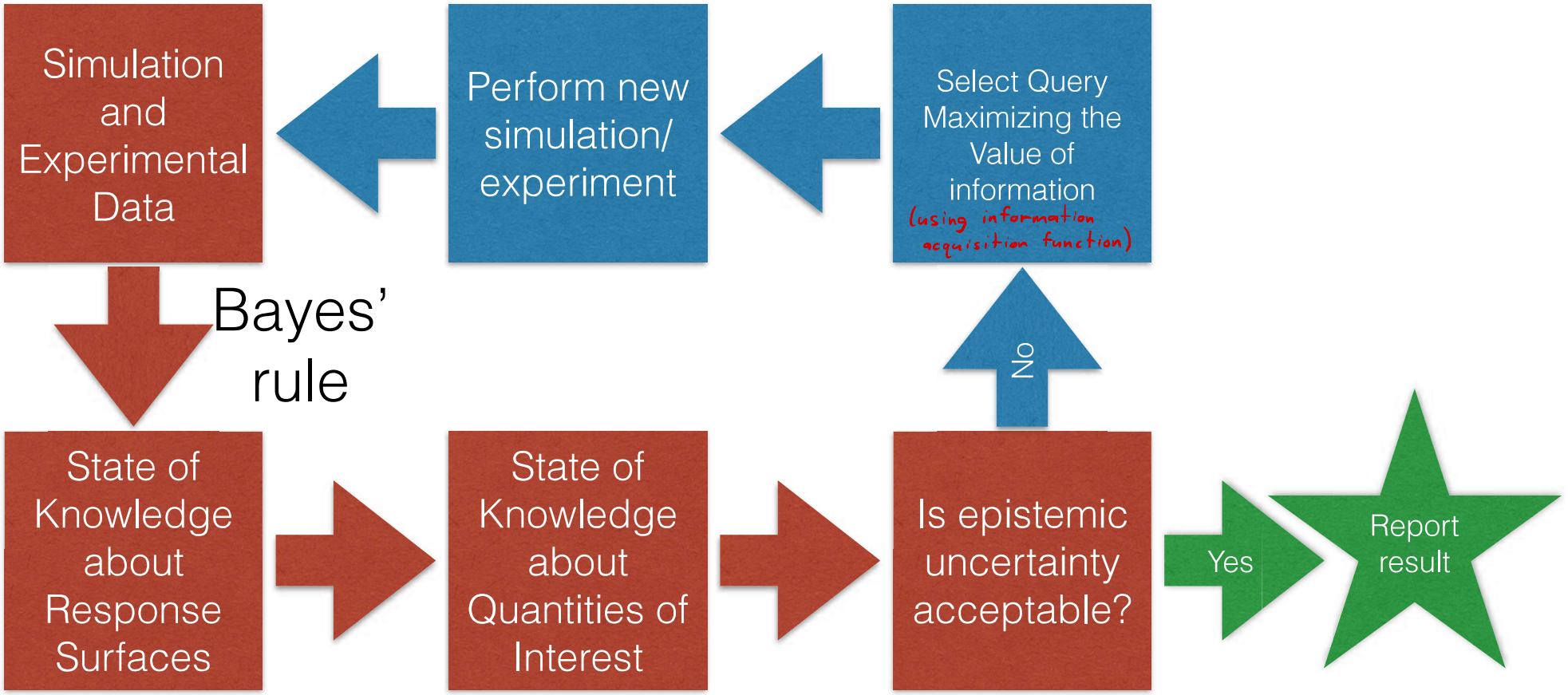
Repeat (Iteration 6)

values decrease as convergence is approached



Schematic Algorithm Framework

Bayesian global optimization



Example codes

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