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Gaussian Processes and Bayesian Optimization: An Introduction

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AI for atoms: How to machine learn STEM
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Gaussian Process Regression

- Splines, polynomials, other functional fits
  - Problem: Uncertainty depends on the model. Also, which model is the correct model?
- Bayesian approach:
  - Use Gaussian Processes
- A Gaussian process is a non-parametric Bayesian approach to regression, that finds a distribution over functions f(x) that are consistent with the observed data
  - The similarity between points is defined by a covariance matrix
  - The covariance is determined by a kernel function

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Gaussian Process Regression

- Why bother with multivariate normal distributions? Two reasons:
  - (1) Easy to marginalize: when you have many, if you want to limit yourself to some subset, it is simple to integrate out the variables you don't want
  - (2) Easy to condition: Can write analytical solutions for conditioning. The conditioned distribution is also normal.

Multivariate Gaussian Distribution

$$y \sim N(\mu, \Sigma)$$ Mean vector, covariance matrix

Generalizes to a Gaussian Process

$$f \sim GP(m(x), \mathrm{k}(\mathrm{x}, \mathrm{x}'))$$ Mean function, covariance function

Covariance Function returns the Covariance Matrix

$$\Sigma \sim k(x, x' | \Phi)$$ Pass function values, return Cov. Mat.

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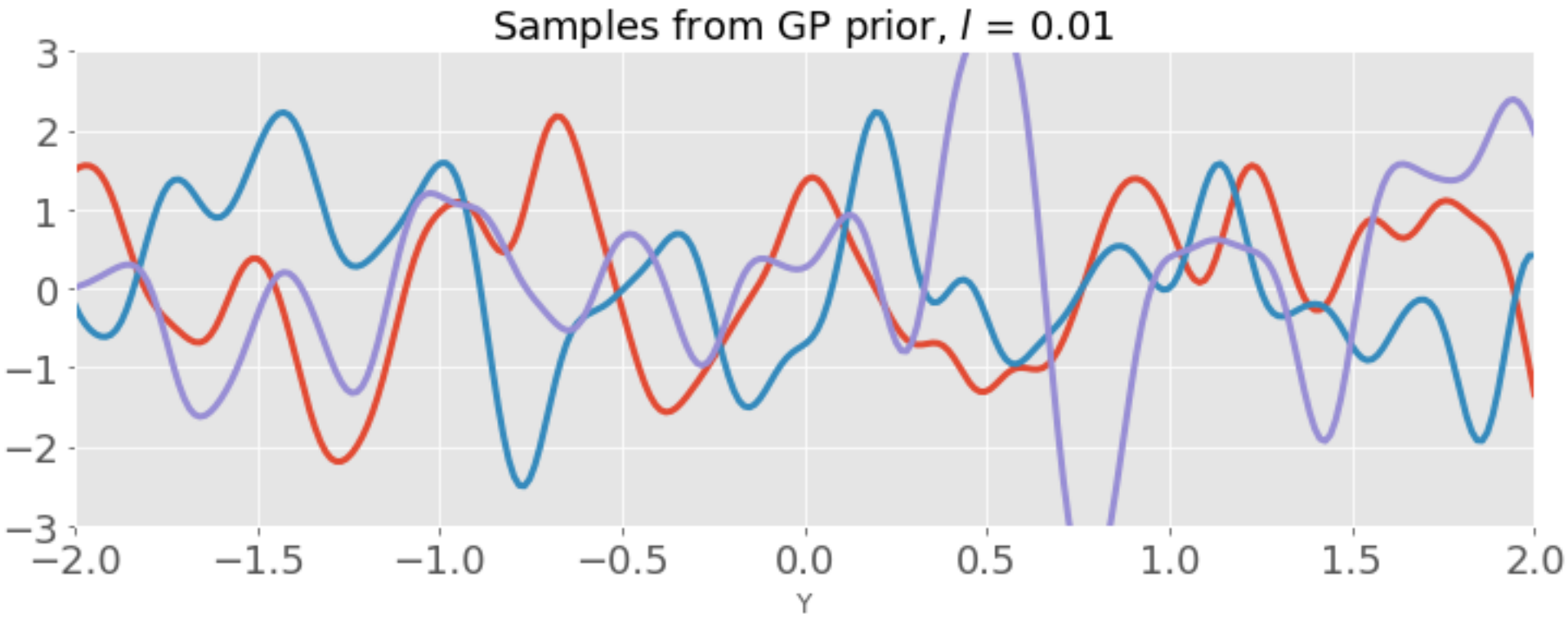
Gaussian Process Regression

- Covariance matrix determines what type of functions we will allow.

$$\mathrm{k}(\mathrm{x}, \mathrm{x}') = \exp\left(-\frac{1}{2l}(x - x')^2\right)$$



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Gaussian Process Regression

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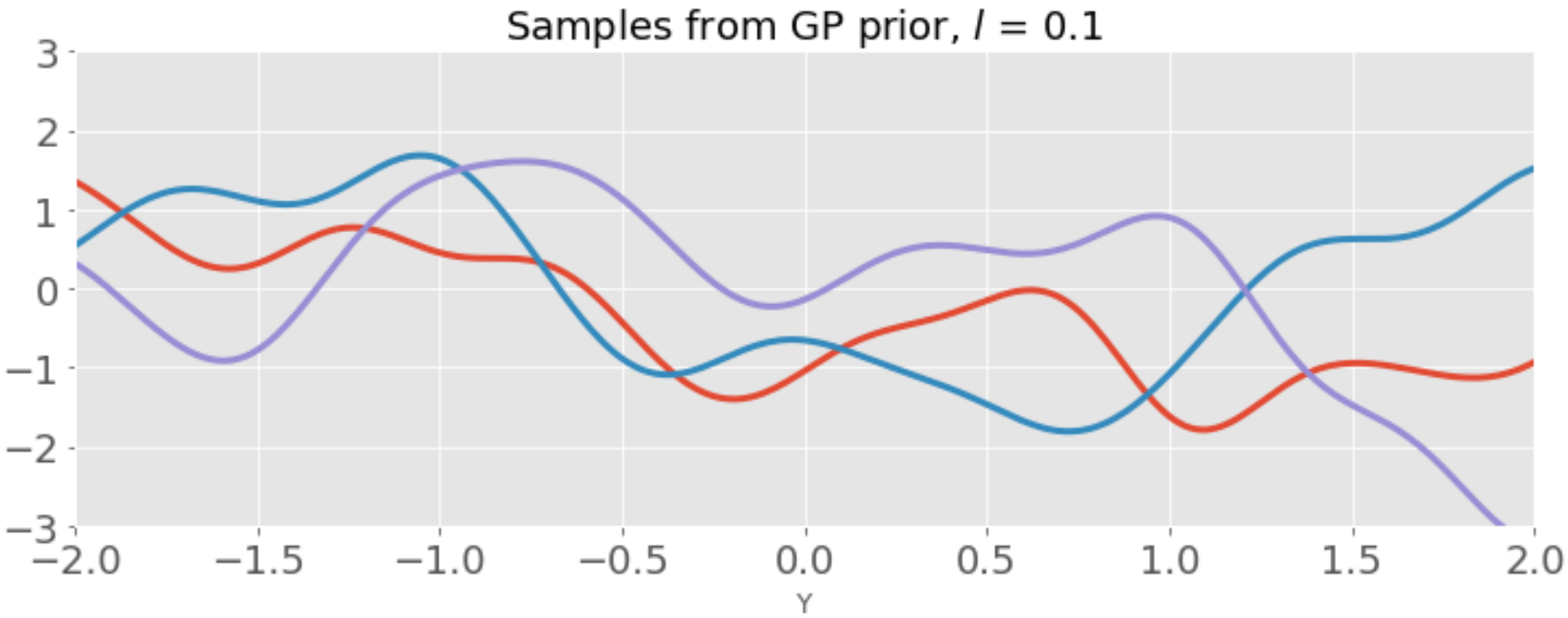

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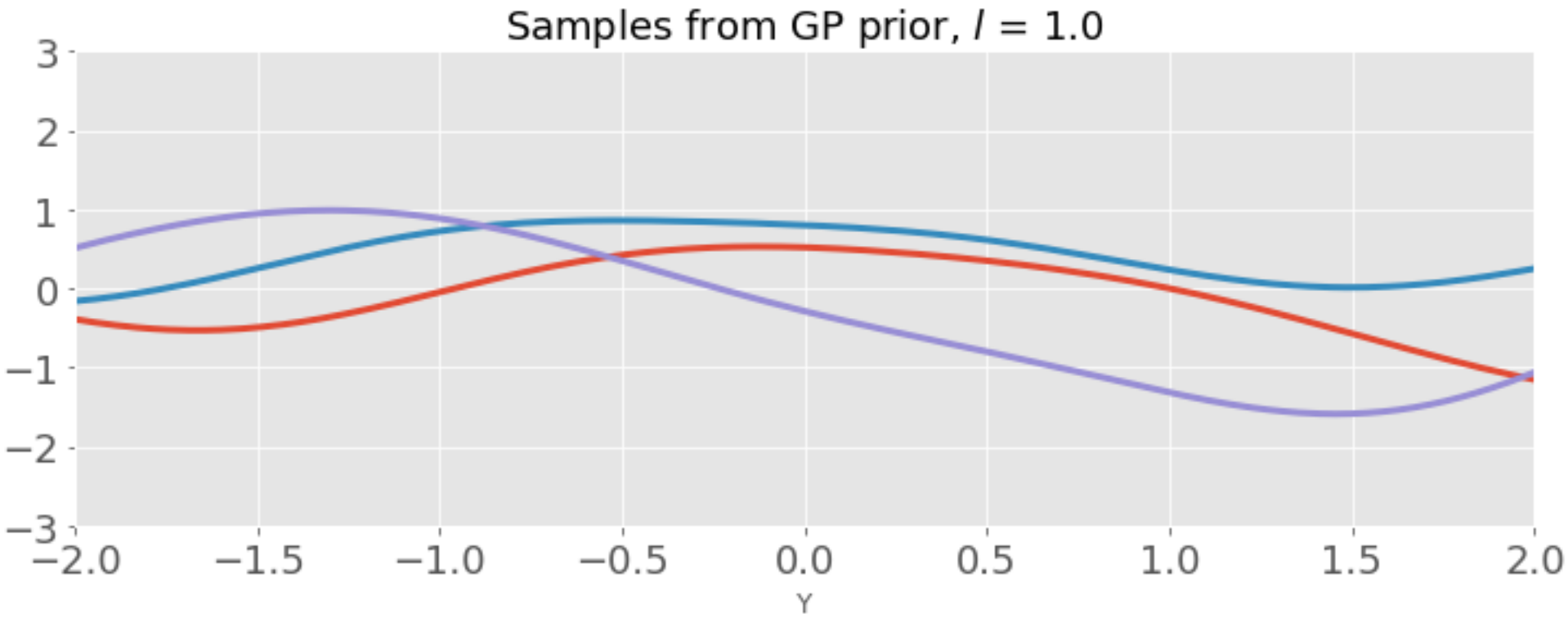
Gaussian Process Regression

- Covariance matrix (kernel) determines what type of functions we will allow.

$$\mathrm{k}(\mathrm{x}, \mathrm{x}') = \exp\left(-\frac{1}{2l}(x - x')^2\right)$$



L controls the lengthscale – sort of how far points should be to make them independent of each other.

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Gaussian Process Regression

- Consider a (gaussian) joint probability distribution with two variables, as follows

Similarity of x_1 values to x_2 values

Variance in x_1

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \right)$$

Variance in x_2

Nonzero entries off-diagonal indicate the correlations

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Gaussian Process Regression

- Generalize this to the function space
- When we observe the data, we now have to calculate the posterior over the functions. This posterior is a joint distribution over function values observed and those not observed.

Function values training points

Similarity to observed points

Similarity of training values to test values

$$\begin{pmatrix} f \\ f_* \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu_1 \\ \mu_* \end{pmatrix}, \begin{pmatrix} K & K_* \\ K_*^T & K_{**} \end{pmatrix} \right)$$

Function values test points

Similarity of test values to each other

Read Rasmussen and Williams for all the math
http://www.gaussianprocess.org/gpml/

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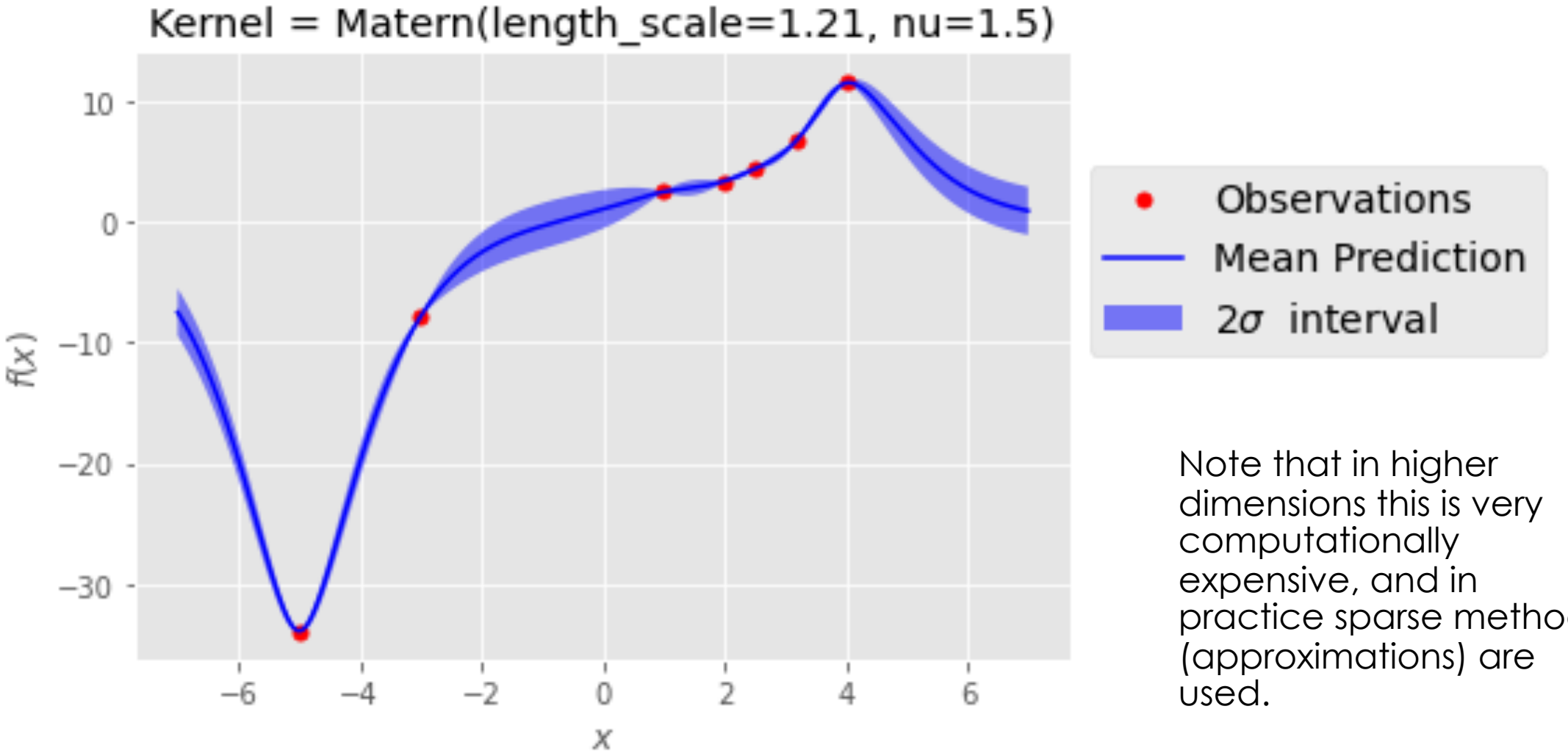
Gaussian Process Regression



Note that in higher dimensions this is very computationally expensive, and in practice sparse methods (approximations) are used.

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Gaussian Process Regression

Open (01_Gaussian_Processes.ipynb)

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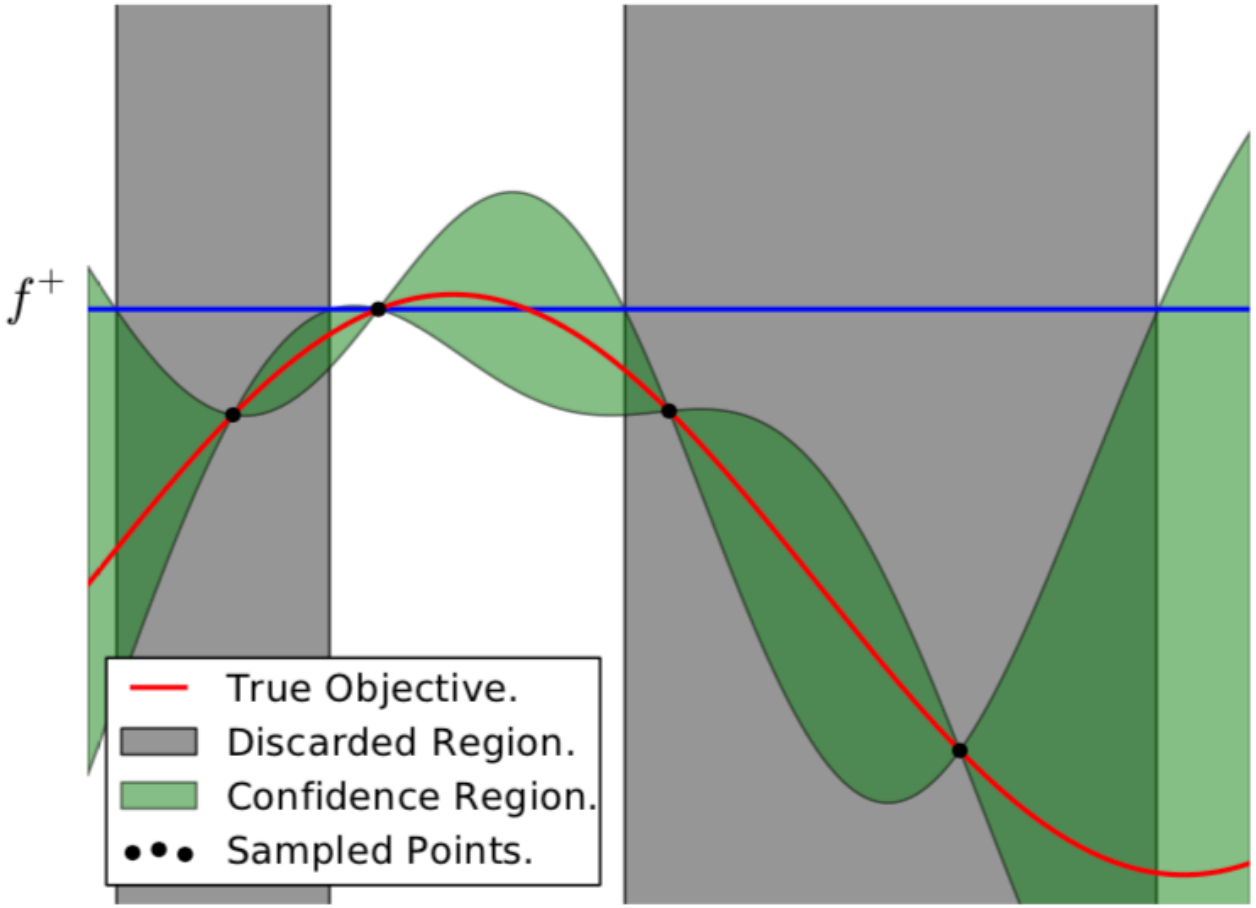
Bayesian Optimization



N. de Freitas et al., Taking the Human Out of the Loop: A Review of Bayesian Optimization , *Proceedings of the IEEE* **104**, 148 (2015)

- We have some measurements in space X, and we want to maximize some property f(X).
- How can we decide what point to measure next to best maximize f?
- We need to balance the exploration of the space with exploitation of regions near we have already know

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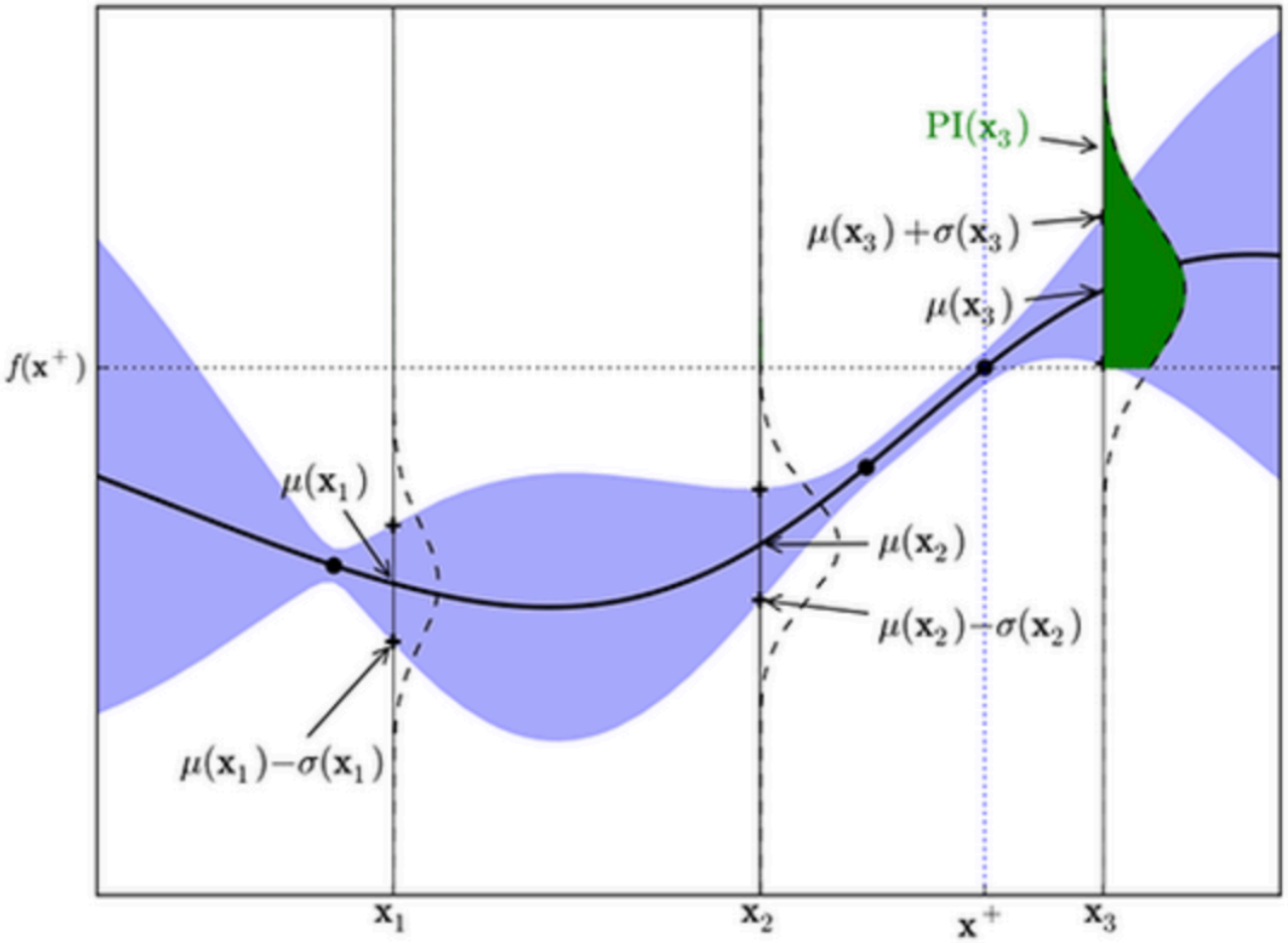
Acquisition Functions

Probability of Improvement Acquisition Function



1. **Confidence bound:** simplest possible - just take the upper confidence bound from the prediction
2. **Probability of Improvement:** Integral from current functional maximum to upper limit of distribution as test point
3. **Expected Improvement:** Instead of probability of improvement, we want to maximize the expected increase in the function value
4. **There are (always) more…**

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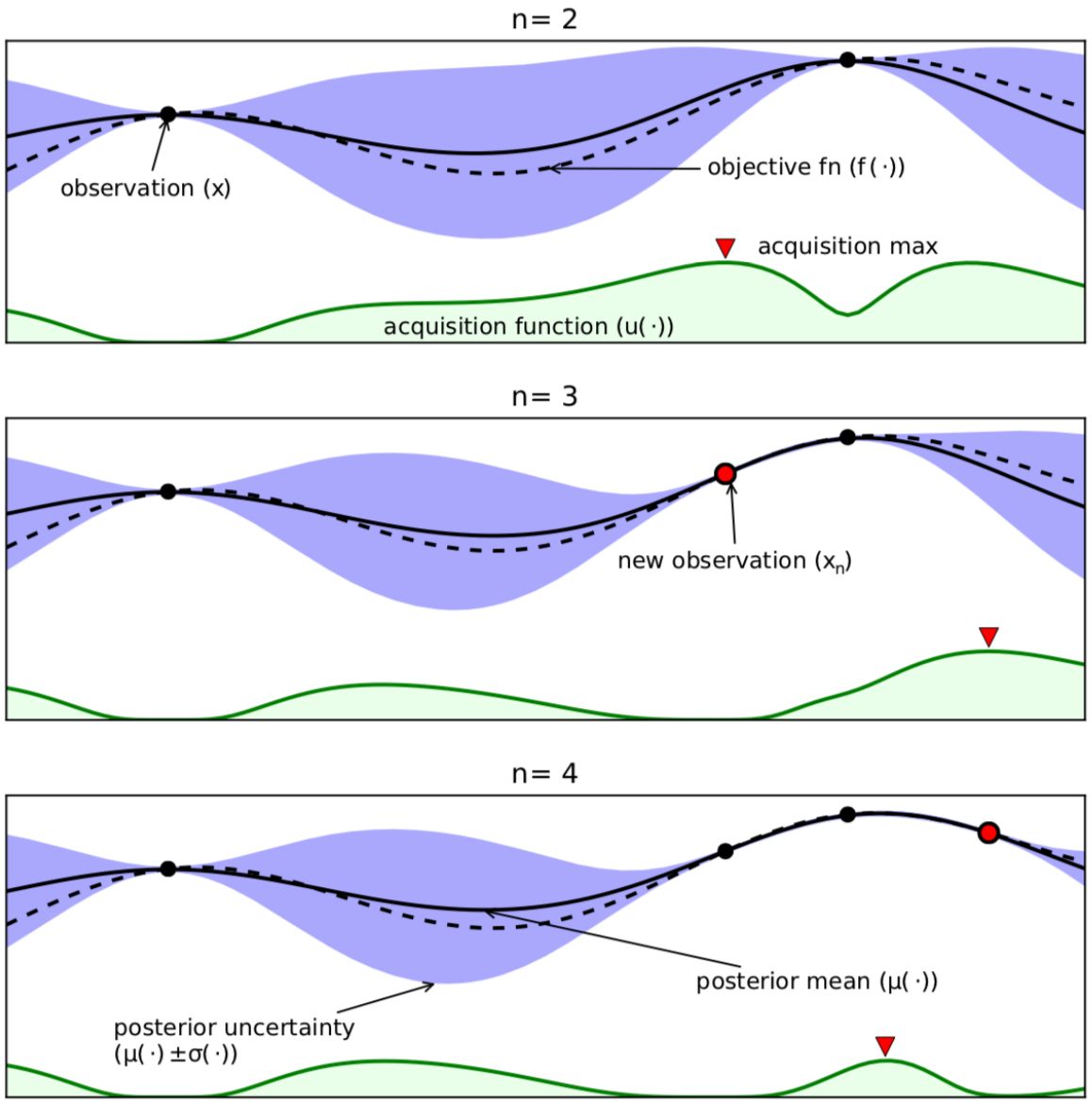
"Active Learning"



- Shown here are three iterations of Bayesian optimization
- We can do this for dictating how to collect new observations in our experiment

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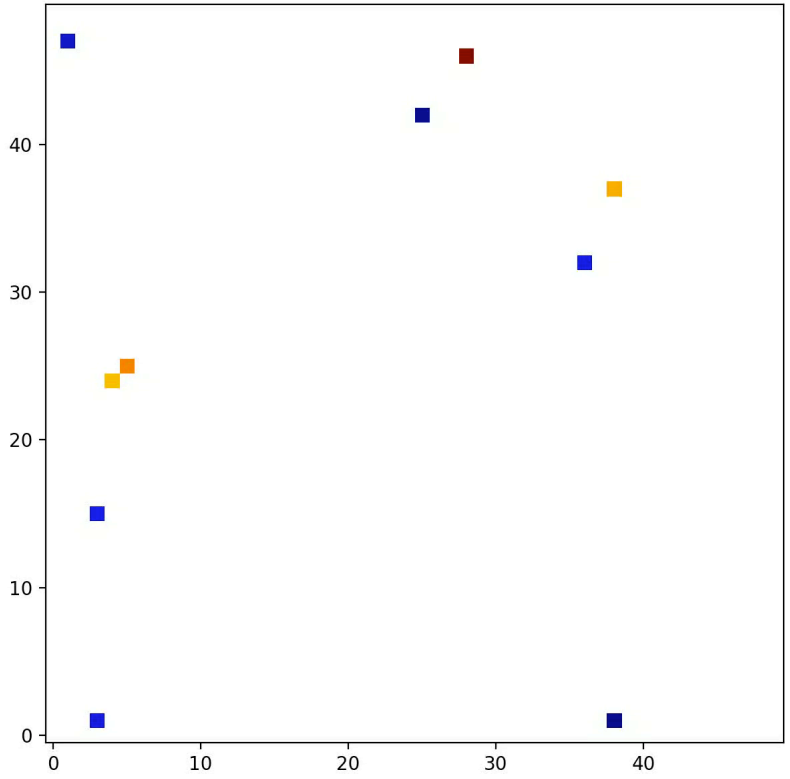
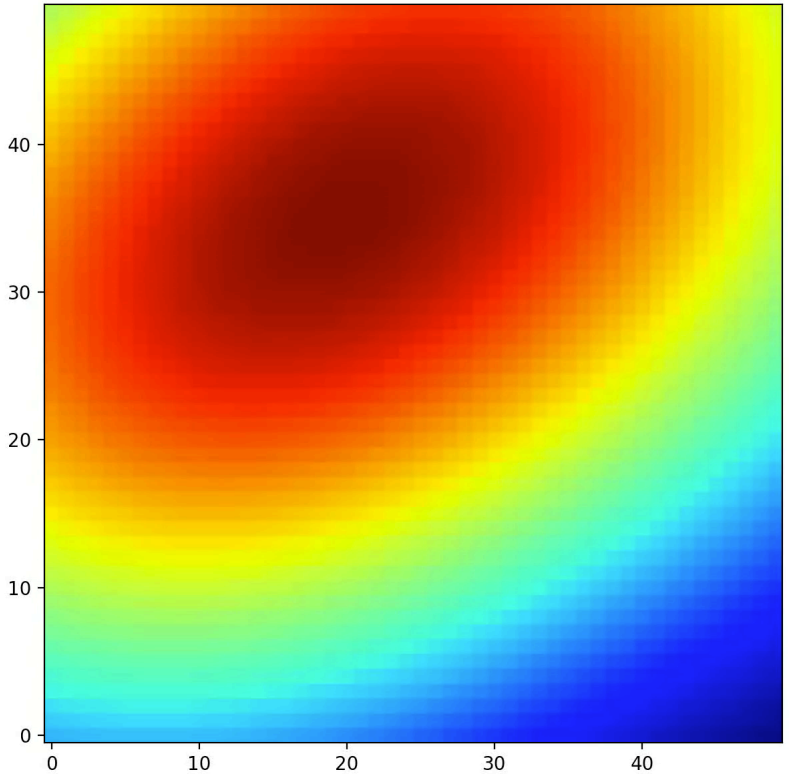
Example: Hysteresis Loops Area Maximization

Batch size = 10. 2.35s/pixel, and each iteration took ~6s on dgx. 410 points in total (40 GP iterations). 1200s in total. Total time for all pixels: 5875s (20% the time)

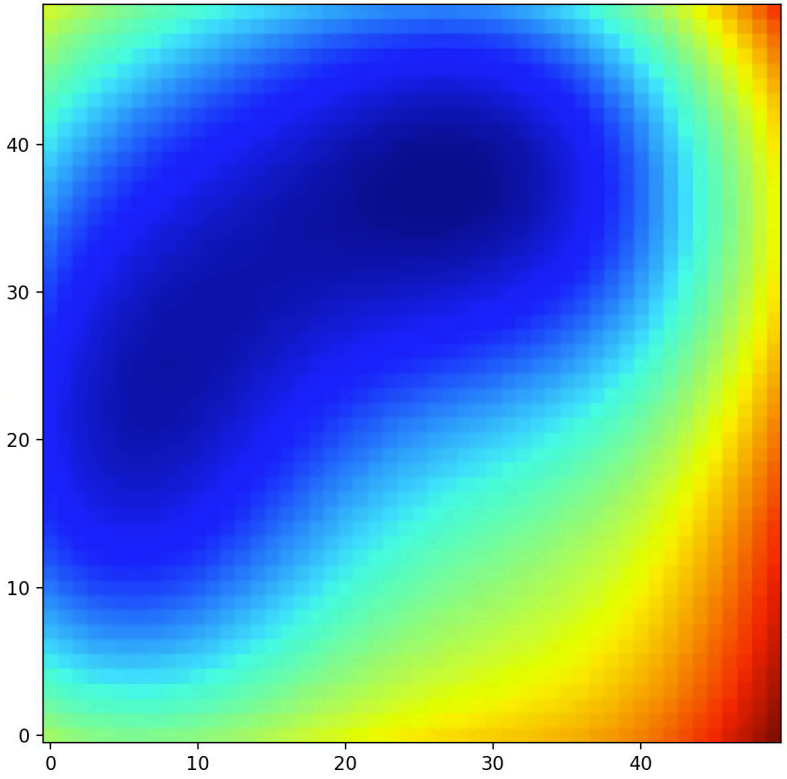
Measured Loop Areas



GP Prediction



GP Uncertainty



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