



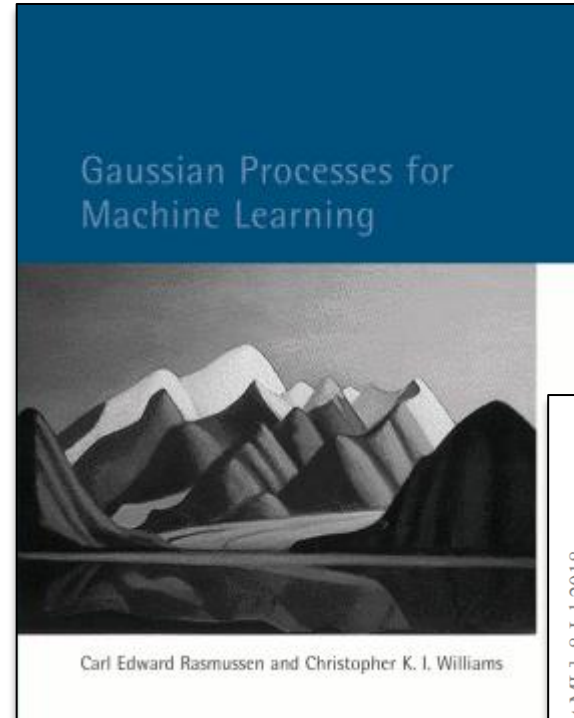
# Gaussian Processes and Bayesian Optimization

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# Outline

- Motivation for GPs
- Bayesian Statistics
  - Bayes Theorem
  - Bayesians vs. Frequentists
- Gaussian Processes
  - Derivation
  - Kernels
- Bayesian Optimization
  - Algorithm
  - Acquisition Functions



Rasmussen and Williams (2006)  
Gaussian Processes for Machine Learning.  
MIT Press.

<https://gaussianprocess.org/gpml/>

## A Tutorial on Bayesian Optimization

Peter I. Frazier

July 10, 2018

### Abstract

Bayesian optimization is an approach to optimizing objective functions that take a long time (minutes or hours) to evaluate. It is best-suited for optimization over continuous domains of less than 20 dimensions, and tolerates stochastic noise in function evaluations. It builds a surrogate for the objective and quantifies the uncertainty in that surrogate using a Bayesian machine learning technique, Gaussian process regression, and then uses an acquisition function defined from this surrogate to decide where to sample. In this tutorial, we describe how Bayesian optimization works, including Gaussian process regression and three common acquisition functions: expected improvement, entropy search, and knowledge gradient. We then discuss more advanced techniques, including running multiple function evaluations in parallel, multi-fidelity and multi-information source optimization, expensive-to-evaluate constraints, random environmental conditions, multi-task Bayesian optimization, and the inclusion of derivative information. We conclude with a discussion of Bayesian optimization software and future research directions in the field. Within our tutorial material we provide a generalization of expected improvement to noisy evaluations, beyond the noise-free setting where it is more commonly applied. This generalization is justified by a formal decision-theoretic argument, standing in contrast to previous ad hoc modifications.

## 1 Introduction

Bayesian optimization (BayesOpt) is a class of machine-learning-based optimization methods focused on solving the problem

$$\max_{x \in A} f(x), \quad (1)$$

where the feasible set and objective function typically have the following properties:

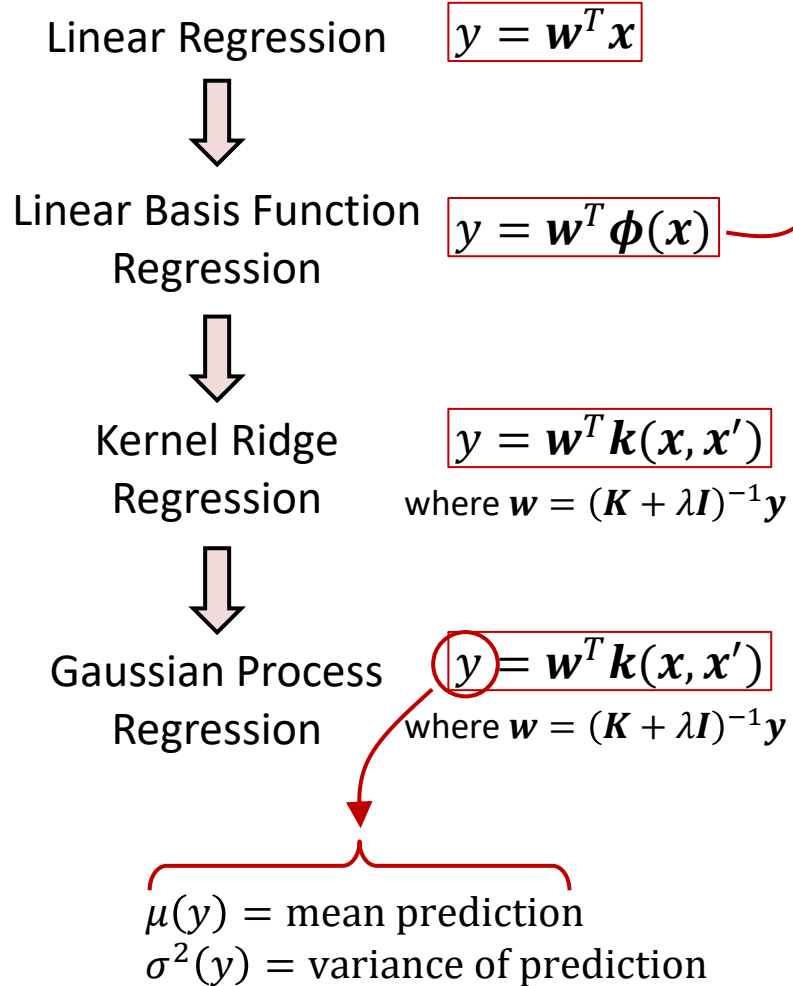
- The input  $x$  is in  $\mathbb{R}^d$  for a value of  $d$  that is not too large. Typically  $d \leq 20$  in most successful applications of BayesOpt.
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- The objective function  $f$  is continuous. This will typically be required to model  $f$  using Gaussian process regression.
- $f$  is “expensive to evaluate” in the sense that the number of evaluations that may be performed is limited, typically to a few hundred. This limitation typically arises because each evaluation takes a substantial amount of time (typically hours), but may also occur because each evaluation bears

Frazier (2018). A Tutorial on Bayesian Optimization  
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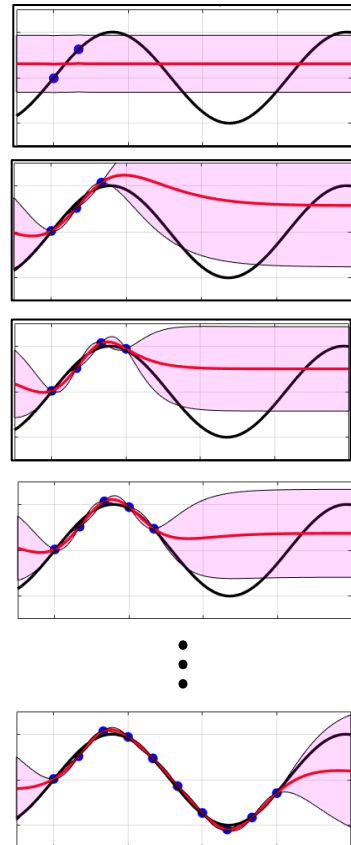
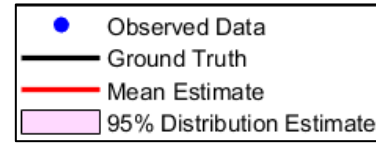
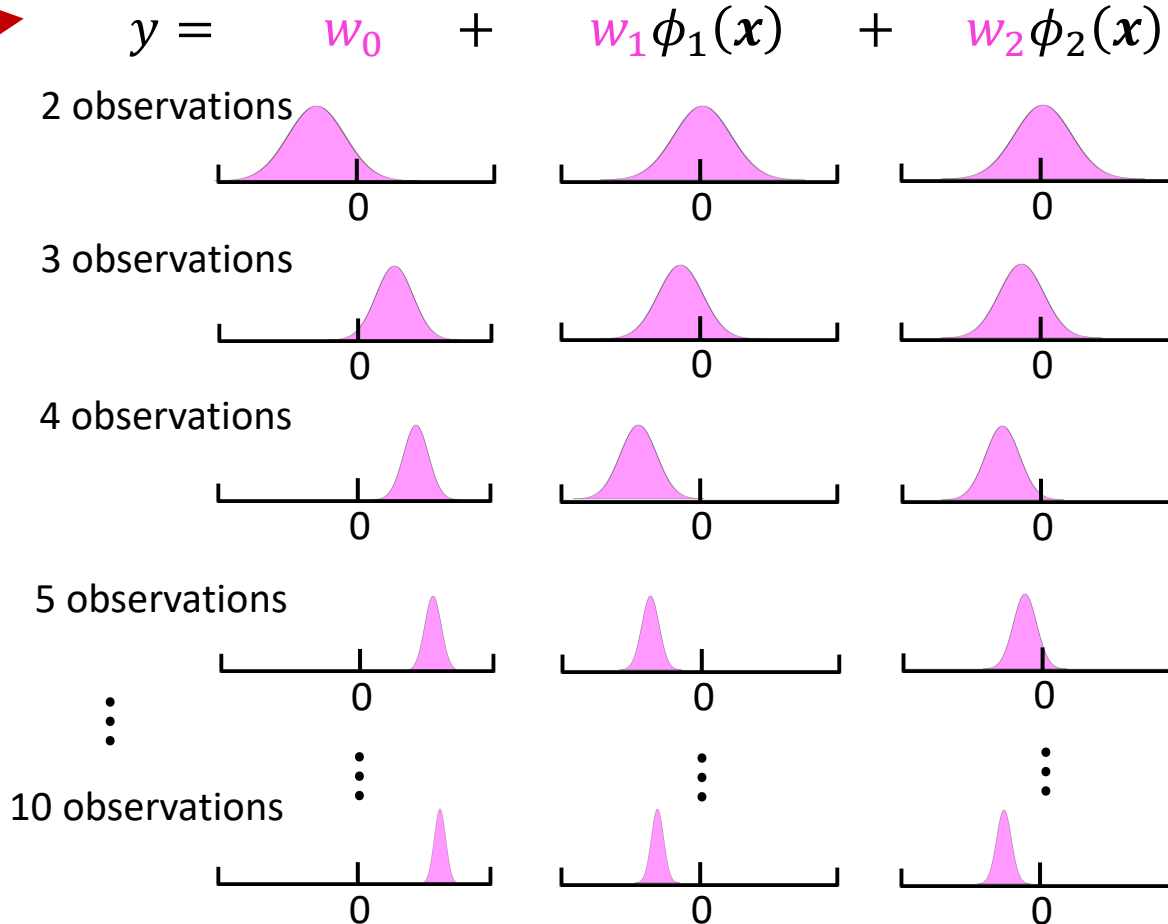
arXiv:1807.02811v1 [stat.ML] 8 Jul 2018

# Motivation for Gaussian Processes

Recall:

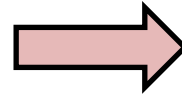
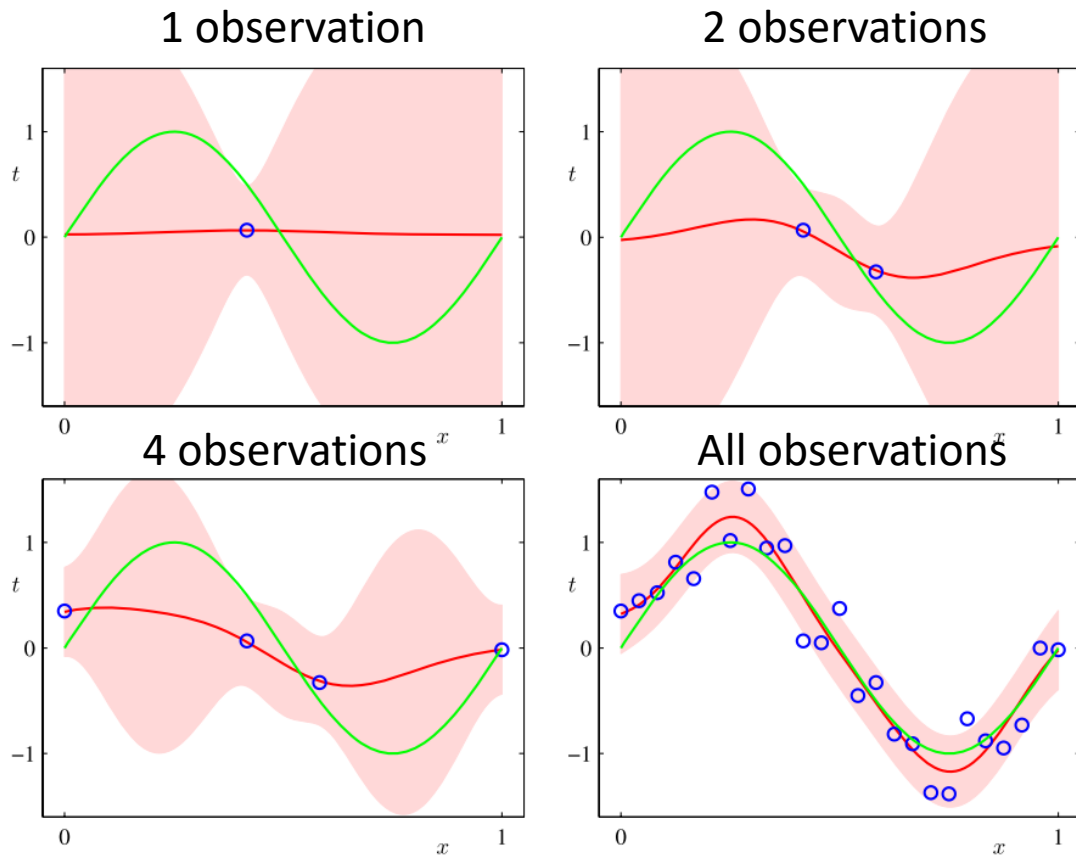
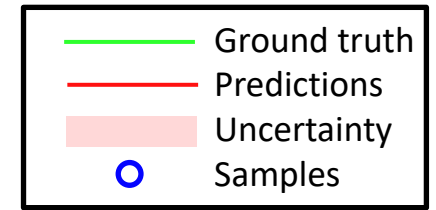


The GP places a prior Gaussian distribution over the weights,  $\mathbf{w}$ .

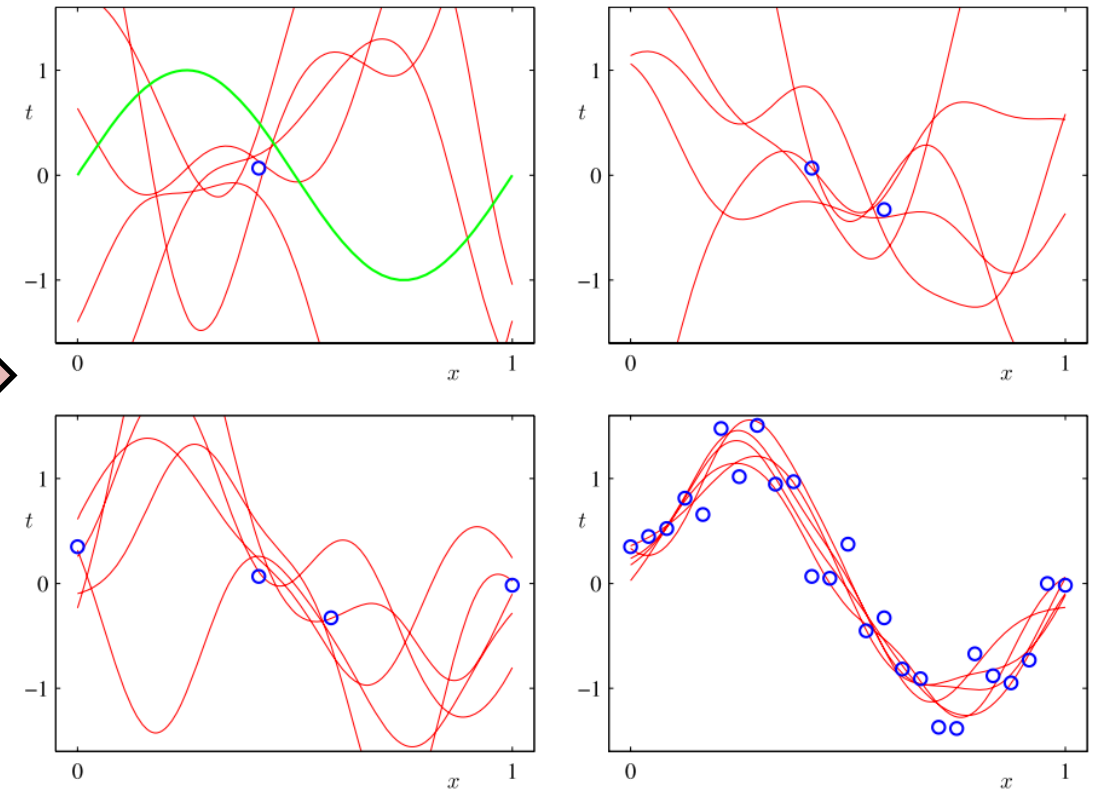


# Motivation for Gaussian Processes

Having a *predictive distribution* is important in understanding the **uncertainty** of the model.



Functions sampled from the distribution:



# Bayesian Statistics

## Notation:

If  $X$  is a random variable that is Gaussian or *normally* distributed, then:

$$p(X) = \mathcal{N}(\mu, \sigma^2)$$

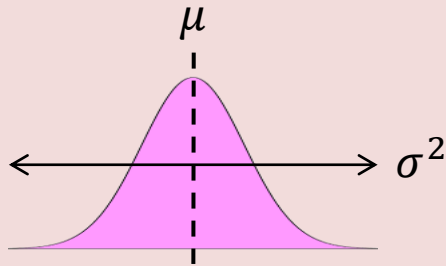
or

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

where  $\mathcal{N}$  stands for “*normal*”.

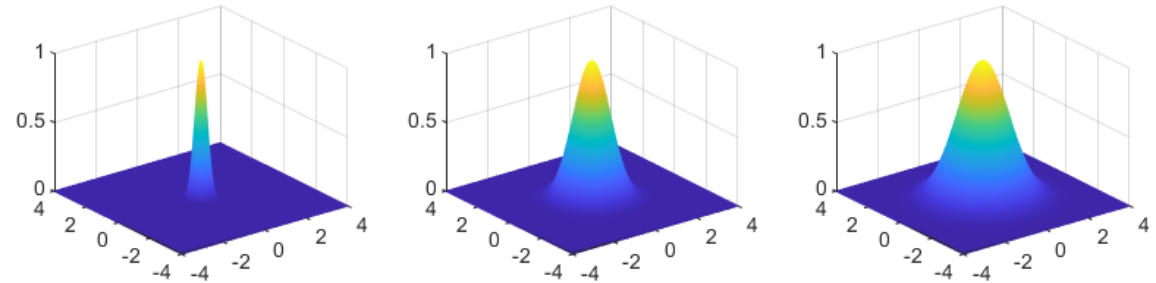
The normal distribution is parametrized by a mean,  $\mu$ , and a variance  $\sigma^2$ :

$$\mathcal{N}(X|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(X - \mu)^2}{2\sigma^2}\right)$$



**Multivariate**  
Normal  
Distribution:

$$\mathcal{N}(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{X} - \boldsymbol{\mu})\right)$$



$\boldsymbol{\mu} \in \mathbb{R}^D$       mean vector (D-dimensional)

$\boldsymbol{\Sigma} \in \mathbb{R}^{D \times D}$       covariance matrix (D-by-D)

$|\boldsymbol{\Sigma}| \in \mathbb{R}$       determinant of the covariance matrix

In order to understand Bayesian statistics, let's turn to an example involving discrete events...

# Bayesian Statistics

## The Coffee Meet-up Example



For the sake of example, let  $Y$  be the *weather condition* and  $X$  be the event that your friends *come* to meet you for coffee:

$y_1$  = the weather is sunny

$y_2$  = slightly raining

$y_3$  = a storm is coming

$x_1$  = Friend 1 comes

$x_2$  = Friend 2 comes

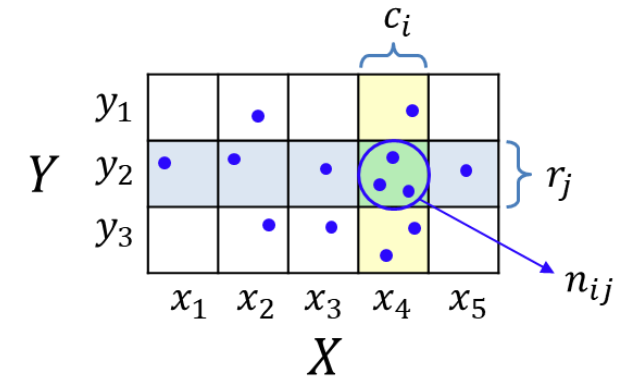
$x_3$  = Friend 3 comes

$x_4$  = Friend 4 comes

$x_5$  = Friend 5 comes

$X$  and  $Y$  are two random variables that can take on values  $\{y_j\}$  and  $\{x_i\}$ .

In this example, events were recorded from the *history of past coffee meet-ups*.



Things that we can say for the next meet-up:

- The probability that  $X = x_4$  is

$$p(X = x_4) = \frac{c_i}{N} = \frac{6}{13}$$

$$p(X) = \left[ \frac{1}{13}, \frac{3}{13}, \frac{2}{13}, \frac{6}{13}, \frac{1}{13} \right]$$

- The joint probability,  $p(x_4, y_2)$ , is

$$p(X = x_4, Y = y_2) = \frac{n_{ij}}{N} = \frac{3}{13}$$

$$p(Y) = \left[ \frac{2}{13}, \frac{7}{13}, \frac{4}{13} \right]$$

- The conditional probability,  $p(y_2|x_4)$  is

$$p(Y = y_2|X = x_4) = \frac{n_{ij}}{c_i} = \frac{3}{6}$$

- The conditional probability,  $p(x_4|y_2)$  is

$$p(X = x_4|Y = y_2) = \frac{n_{ij}}{r_i} = \frac{3}{7}$$

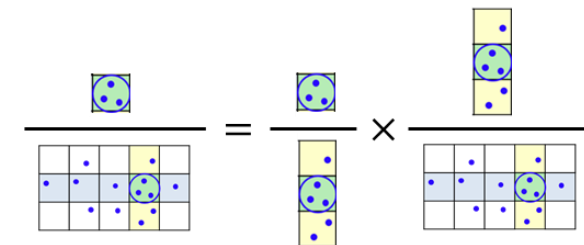
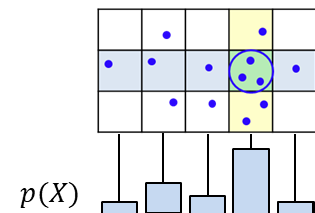
## Rules of Probability:

$$p(X) = \sum_Y p(X, Y)$$

$$p(X, Y) = p(Y|X)p(X)$$

A note in notation:

The quantity  $p(X = x_4)$  denotes the specific probability for event  $x_4$ , but the quantity  $p(X)$  is a distribution of probabilities on all events of  $X$ .



# Bayesian Statistics

**Rules of Probability:**

$$p(X) = \sum_Y p(X, Y) \quad p(X, Y) = p(Y|X)p(X)$$

(Sum Rule) (Product Rule)

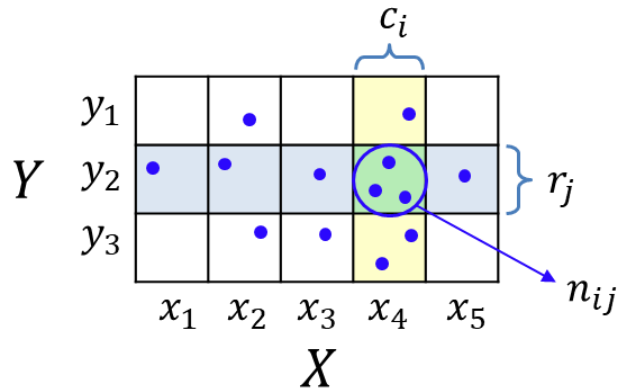
Based on the product rule and the symmetry of joint probabilities, i. e.  $p(X, Y) = p(Y, X)$ , we can derive the following:

**Bayes' Theorem**

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$



**Example:**



$$\left. \begin{aligned} p(Y = y_2|X = x_4) &= \frac{3}{6} \\ p(X = x_4|Y = y_2) &= \frac{3}{7} \\ p(Y = y_2) &= \frac{7}{13} \\ p(X = x_4) &= \frac{6}{13} \end{aligned} \right\} \frac{3}{6} = \frac{3/7 \times 7/13}{6/13}$$

If our random variables can take **continuous** values rather than discrete, then:

**(Sum Rule)**  $p(x) = \int p(x, y) dy$

**(Product Rule)**  $p(x, y) = p(y|x)p(x)$

Together, we have:  $p(x) = \int p(y|x)p(x) dy$

Upon substituting into Bayes' Theorem:

$$p(y|x) = \frac{p(x|y) p(y)}{\int p(y|x)p(x) dy}$$

posterior (pointing to  $p(y|x)$ )

likelihood (pointing to  $p(x|y)$ )

prior (pointing to  $p(y)$ )

Marginal likelihood (under the denominator)

# Bayesian Statistics: A Change of Perspective

**Bayes Theorem:**

$$p(y|x) = \frac{p(x|y) p(y)}{\int p(y|x)p(x) dy}$$

Diagram labels for the equation above:

- posterior:  $p(y|x)$
- likelihood:  $p(x|y)$
- prior:  $p(y)$
- Marginal likelihood:  $\int p(y|x)p(x) dy$

## Frequentists vs. Bayesians

In Frequentist statistics,  $p(x)$  refers to the **frequency** of occurrence of an event. In Bayesian statistics,  $p(x)$  refers to the **belief** that event  $x$  is true.

For Frequentists,  $p(x)$  is **fixed**, and its correct value can be approached with more and more data (evidence).

For Bayesians, beliefs  $p(x)$  **can change**, and there is no single correct value to aim for. New data will always cause the belief to change.

## Bayesian Inference in machine learning models:

Let:  $H$  = hypothesis (current belief of the world)  
 $D$  = new data

Belief that  $H$  is true, GIVEN the new data  $D$

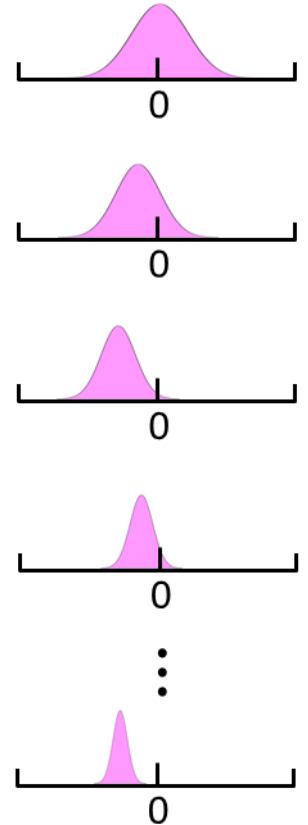
Belief that data  $D$  can exist GIVEN that  $H$  is true

Prior belief that  $H$  is true

$$p(H|D) = \frac{p(D|H) p(H)}{p(D)}$$

Total belief that data  $D$  can exist considering ALL possible hypotheses

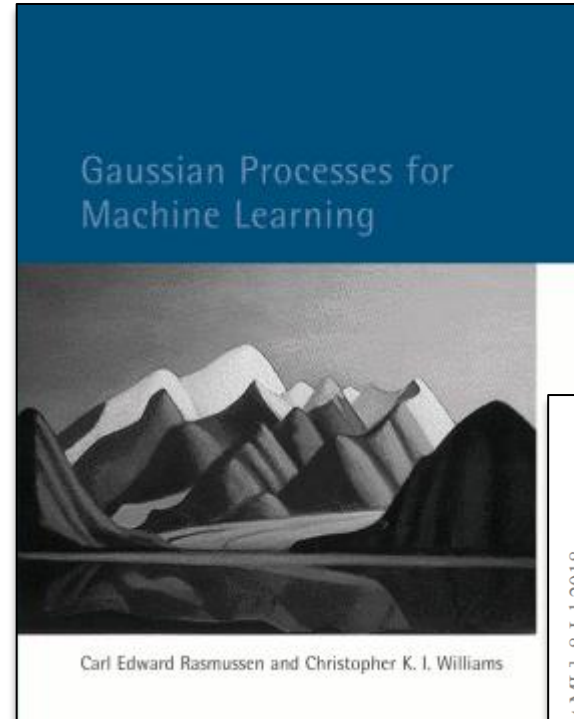
$$p(H) = p(w)$$





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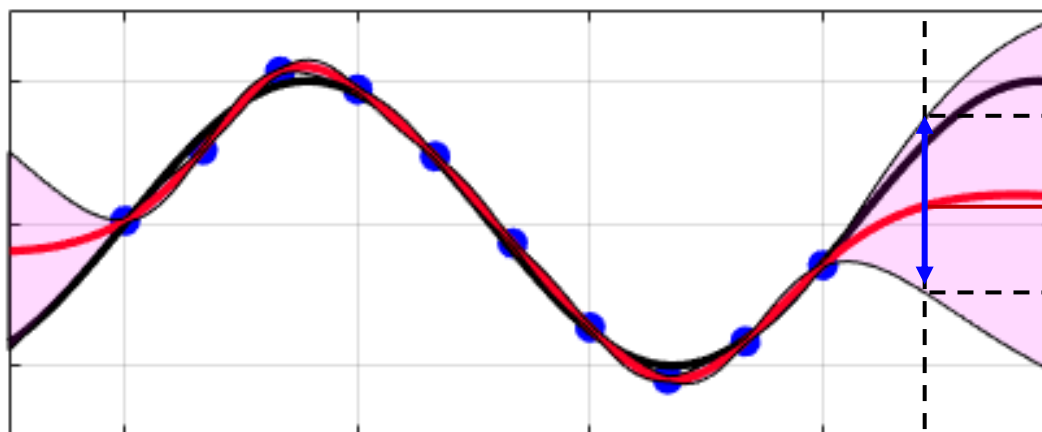
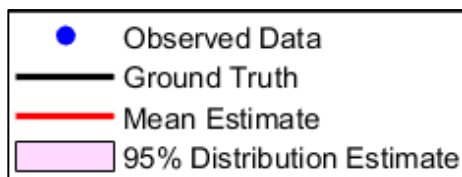
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# Gaussian Process Regression



$\text{var}(y^*|x^*)$   
 $\text{mean}(y^*|x^*)$

These are the quantities that we need to derive.

**Training Data:**  $\{x, y\}, \quad x \in \mathbb{R}^{N \times D}, \quad y \in \mathbb{R}^N$

**New Data:**  $x^*$

**Model ( $M$ ):**  $y = f(x) + \varepsilon$

**Desired prediction:**  $y^*$   $\begin{cases} \rightarrow \text{mean}(y^*|x^*) \\ \rightarrow \text{var}(y^*|x^*) \end{cases}$

## Assumptions:

1. The model is linear:  $y = w^T x + \varepsilon$
2. The noise is Gaussian:  $p(\varepsilon) = \mathcal{N}(\mathbf{0}, \sigma^2 I)$
3. The prior on  $w$  is Gaussian:  $p(w) = \mathcal{N}(\mathbf{0}, K)$
4. The likelihood is Gaussian:  $p(y|x, w) = \mathcal{N}(w^T x, \sigma^2 I)$

## Bayes Theorem:

$$\text{posterior } p(w|x, y) = \frac{\text{likelihood } p(y|x, w) \text{ prior } p(w)}{\int p(y|x, w) p(w) dw}$$

$$\text{Prediction, } y^* \quad y^* = w^T x^* + \varepsilon \quad \text{posterior}$$

$$p(y^*|x^*, x, y) = \int p(y^*|w, x^*) p(w|x, y) dw$$

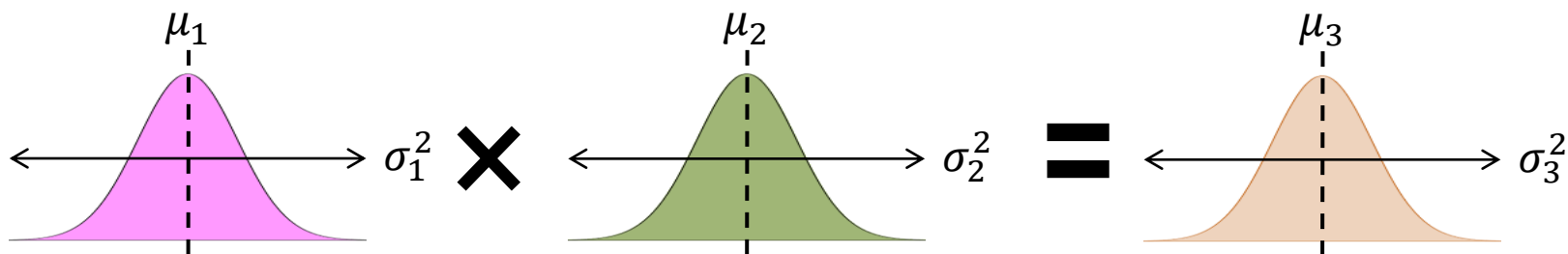
# Gaussian Process Regression

Bayes Theorem:

$$\overset{\text{posterior}}{p(\mathbf{w}|\mathbf{x}, \mathbf{y})} = \frac{\overset{\text{likelihood}}{p(\mathbf{y}|\mathbf{x}, \mathbf{w})} \overset{\text{prior}}{p(\mathbf{w})}}{\int p(\mathbf{y}|\mathbf{x}, \mathbf{w}) p(\mathbf{w}) d\mathbf{w}}$$

$$\overset{\text{Prediction, } y^*}{p(y^*|\mathbf{x}^*, \mathbf{x}, \mathbf{y})} = \int \overset{y^* = \mathbf{w}^T \mathbf{x}^* + \varepsilon}{p(y^*|\mathbf{w}, \mathbf{x}^*)} \overset{\text{posterior}}{p(\mathbf{w}|\mathbf{x}, \mathbf{y})} d\mathbf{w}$$

Using a Gaussian distribution makes the integration **tractable** because the result of multiplying two Gaussians is still a Gaussian.



$$\mu_3 = \frac{\mu_1 \sigma_2^2 + \mu_2 \sigma_1^2}{\sigma_1^2 + \sigma_2^2}$$

$$\sigma_3^2 = \frac{\sigma_1^2 \sigma_2^2}{\sigma_1^2 + \sigma_2^2}$$

## Prediction in GPR:

These are the main equations in GPR.

$$\text{mean}(y^*|\mathbf{x}^*) = \mathbf{k}(\mathbf{x}^*, \mathbf{x})^T [\mathbf{K} + \sigma^2 \mathbf{I}]^{-1} \mathbf{y}$$

$$\text{var}(y^*|\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) + \sigma^2 - \mathbf{k}(\mathbf{x}^*, \mathbf{x})^T [\mathbf{K} + \sigma^2 \mathbf{I}]^{-1} \mathbf{k}(\mathbf{x}^*, \mathbf{x})$$

$\{\mathbf{x}, \mathbf{y}\}$  = Training data

$\mathbf{x}^*$  = New Data

$y^*$  = Desired prediction

$\sigma^2$  = variance of noise,  $\varepsilon$

$\mathbf{K}$  = prior covariance kernel on  $\mathbf{w}$

$k(\cdot, \cdot)$  = kernel function

# Gaussian Process Regression

**Definition of a GP:** A Gaussian Process is a collection of random variables any finite number of which have (consistent) joint Gaussian distributions.

$$\mathbf{y} = f(\mathbf{x}) + \boldsymbol{\varepsilon}$$

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}) = \mathbf{0}, k(\mathbf{x}, \mathbf{x}'))$$

$$\text{mean}(\mathbf{y}^* | \mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x})^T [\mathbf{K} + \sigma^2 \mathbf{I}]^{-1} \mathbf{y}$$

$$\text{var}(\mathbf{y}^* | \mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) + \sigma^2 - k(\mathbf{x}^*, \mathbf{x})^T [\mathbf{K} + \sigma^2 \mathbf{I}]^{-1} k(\mathbf{x}^*, \mathbf{x})$$

Hyper-parameters in GPR:  $k(\mathbf{x}, \mathbf{x}'), \theta_i, \sigma^2$

To optimize hyper-parameters, GPR packages use gradient descent. The gradient can be calculated by:

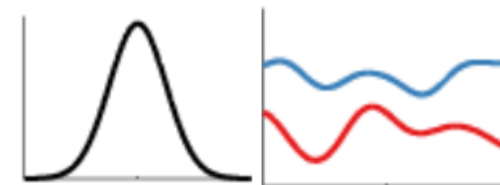
$$\frac{\partial}{\partial \theta_i} \ln p(\mathbf{y} | \boldsymbol{\theta}) = -\frac{1}{2} \text{tr} \left( \mathbf{C}^{-1} \frac{\partial \mathbf{C}}{\partial \theta_i} \right) + \frac{1}{2} \mathbf{y}^T \mathbf{C}^{-1} \frac{\partial \mathbf{C}}{\partial \theta_i} \mathbf{C}^{-1} \mathbf{y}$$

where  $\mathbf{C} = \mathbf{K} + \sigma^2 \mathbf{I}$ .

## Kernel Functions in GPR:

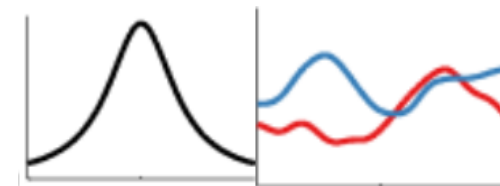
### Squared Exponential

$$k_{SE} = \sigma^2 \exp \left( -\frac{(\mathbf{x} - \mathbf{x}')^2}{2l^2} \right)$$



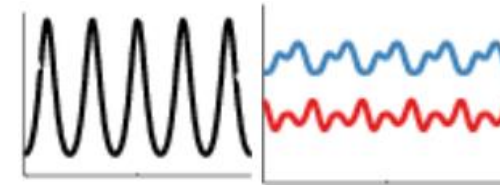
### Rational Quadratic

$$k_{RQ} = \sigma^2 \left( 1 + \frac{(\mathbf{x} - \mathbf{x}')^2}{2\alpha l^2} \right)$$



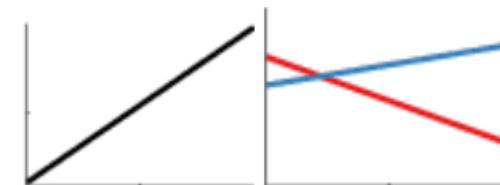
### Periodic

$$k_{PER} = \sigma^2 \exp \left( -\frac{2}{l^2} \sin^2 \frac{\pi |\mathbf{x} - \mathbf{x}'|}{p} \right)$$



### Linear

$$k_{LIN} = \sigma_b^2 + \sigma_v^2 (\mathbf{x} - c)(\mathbf{x}' - c)$$



- Matern 3/2 kernel
- Matern 5/2 kernel
- Automatic Relevance Determination kernels

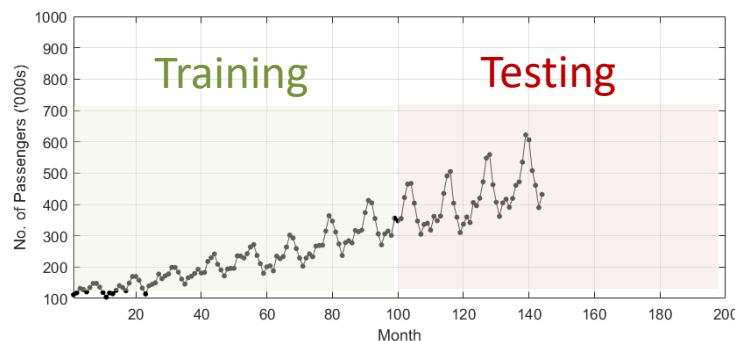
# Gaussian Process Regression

## Example:

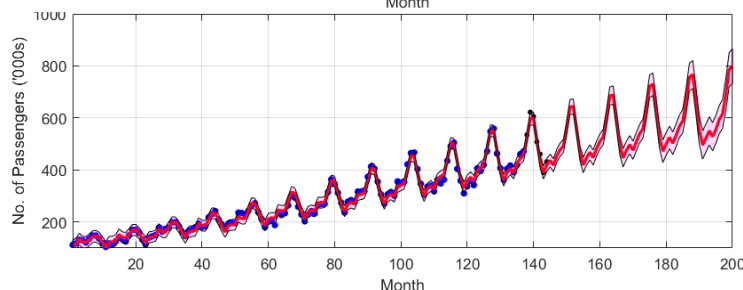
Find the mean and variance prediction of the Airline Passengers Data Set using the first 100 out of 144 data, and the following kernel function (**SE x Periodic**):

$$K(x, x') = \theta_1 \exp\left(-\frac{\|x - x'\|^2}{2\theta_2^2}\right) \times \exp\left(\frac{-2 \sin^2(\pi|x - x'|/\theta_3)}{\theta_4^2}\right)$$

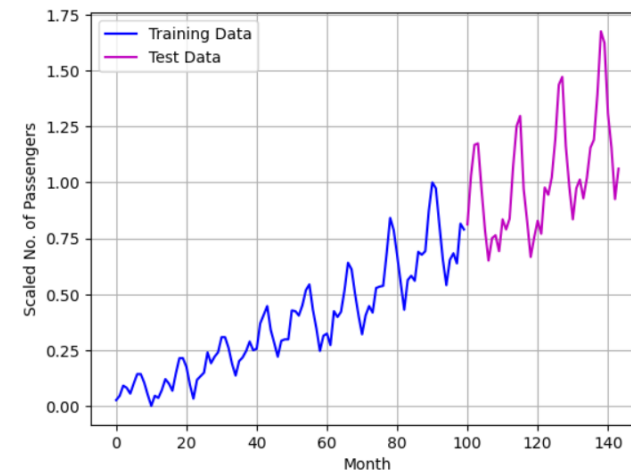
Given Data Set



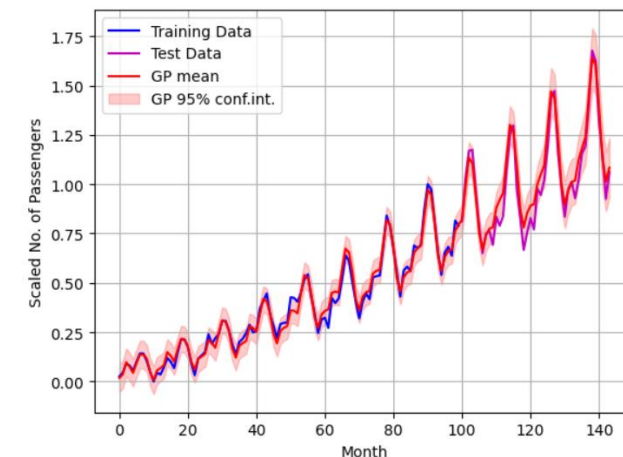
Given Data Set +  
GPR Predictions  
(**MATLAB**)



Given Data Set



Given Data Set +  
GPR Predictions  
(**Python**)



## Optimized kernel:

RBf(length\_scale=179) \* ExpSineSquared(length\_scale=1.57, periodicity=12) + WhiteKernel(noise\_level=0.000967)

Training MSE: 0.0007858767229793949

Testing MSE: 0.004509114222736137

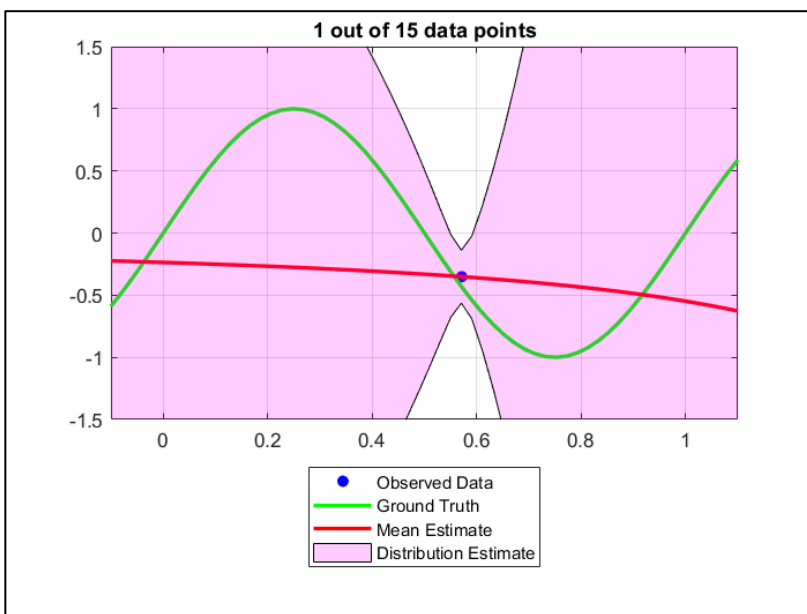
# Gaussian Process Regression

## Side Note on GPR:

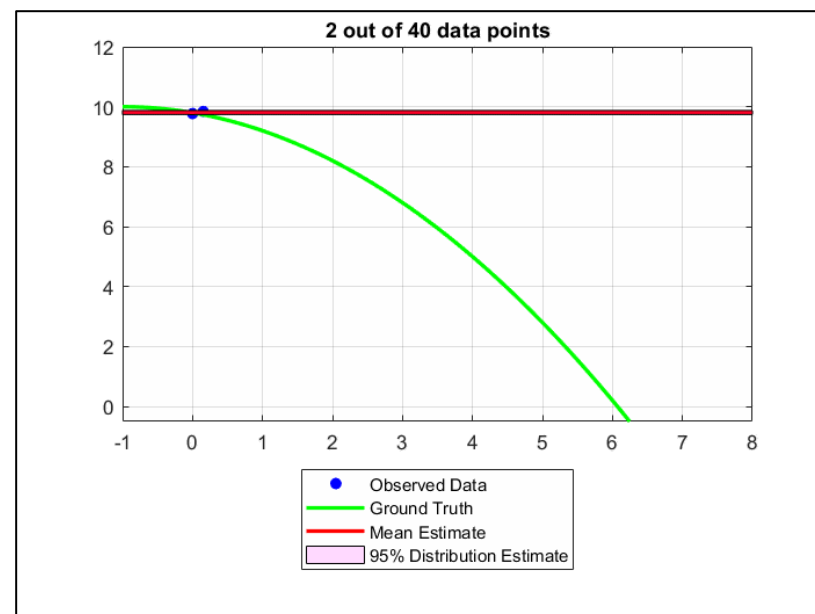
Neal (1996) has shown that for a broad class of prior distributions over  $w$ , the distribution of functions generated by a single-hidden-layer *neural network* will tend to a Gaussian Process as the number of hidden neurons tend to infinity.

## Other Notable Examples:

An example where data points from a sine wave arrive one at a time at random positions. The predictive distributions show which parts are **uncertain** to the model.

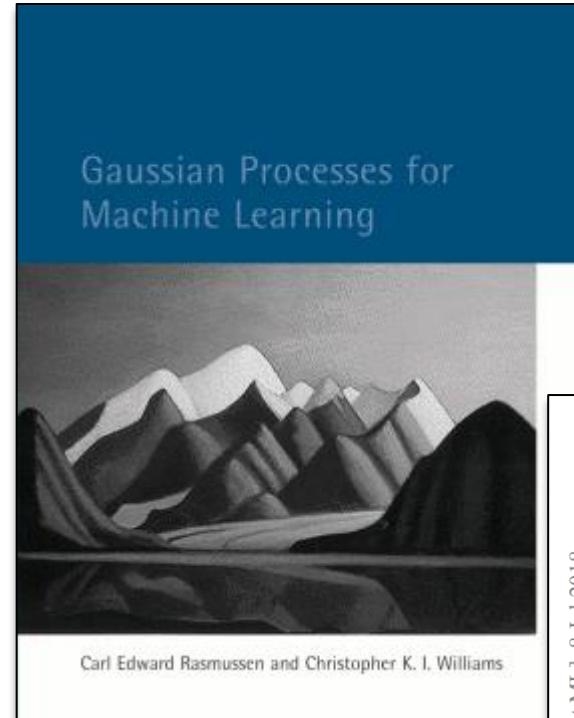


Prediction of **Battery Degradation** based on NASA data sets.



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  - Bayes Theorem
  - Bayesians vs. Frequentists
- Gaussian Processes
  - Derivation
  - Kernels
- Bayesian Optimization
  - Algorithm
  - Acquisition Functions



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## A Tutorial on Bayesian Optimization

Peter I. Frazier

July 10, 2018

### Abstract

Bayesian optimization is an approach to optimizing objective functions that take a long time (minutes or hours) to evaluate. It is best-suited for optimization over continuous domains of less than 20 dimensions, and tolerates stochastic noise in function evaluations. It builds a surrogate for the objective and quantifies the uncertainty in that surrogate using a Bayesian machine learning technique, Gaussian process regression, and then uses an acquisition function defined from this surrogate to decide where to sample. In this tutorial, we describe how Bayesian optimization works, including Gaussian process regression and three common acquisition functions: expected improvement, entropy search, and knowledge gradient. We then discuss more advanced techniques, including running multiple function evaluations in parallel, multi-fidelity and multi-information source optimization, expensive-to-evaluate constraints, random environmental conditions, multi-task Bayesian optimization, and the inclusion of derivative information. We conclude with a discussion of Bayesian optimization software and future research directions in the field. Within our tutorial material we provide a generalization of expected improvement to noisy evaluations, beyond the noise-free setting where it is more commonly applied. This generalization is justified by a formal decision-theoretic argument, standing in contrast to previous ad hoc modifications.

## 1 Introduction

Bayesian optimization (BayesOpt) is a class of machine-learning-based optimization methods focused on solving the problem

$$\max_{x \in A} f(x), \quad (1)$$

where the feasible set and objective function typically have the following properties:

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- The objective function  $f$  is continuous. This will typically be required to model  $f$  using Gaussian process regression.
- $f$  is “expensive to evaluate” in the sense that the number of evaluations that may be performed is limited, typically to a few hundred. This limitation typically arises because each evaluation takes a substantial amount of time (typically hours), but may also occur because each evaluation bears

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# Bayesian Optimization

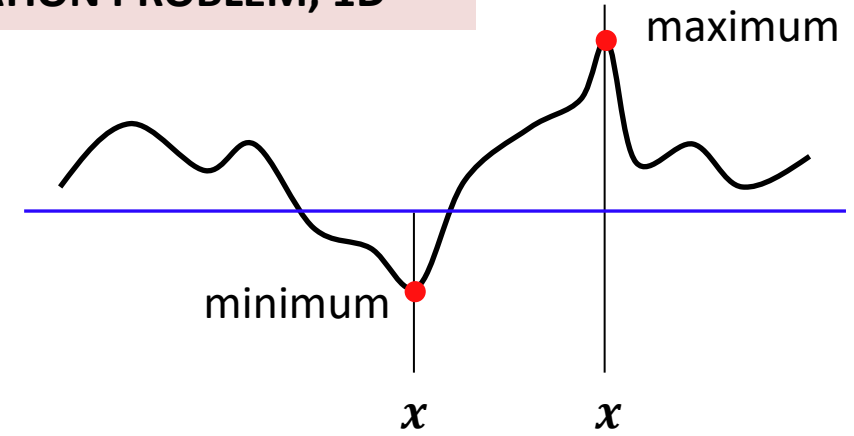
- An efficient algorithm for finding the optimum (minimum / maximum) of a function globally.

$$\min_x f(x)$$

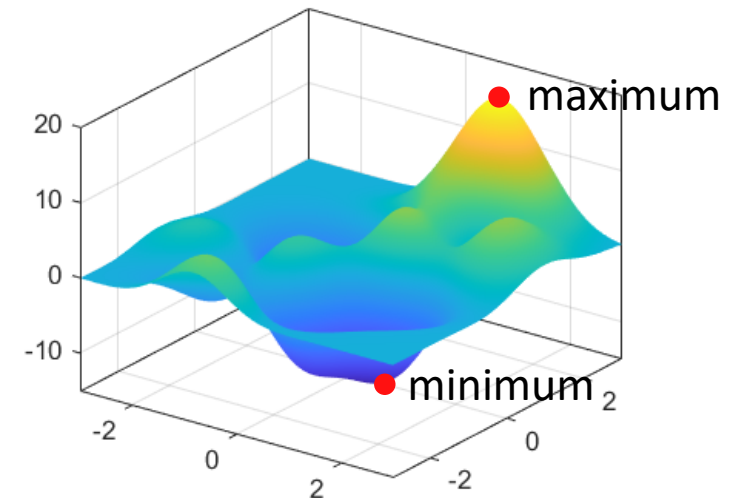
$$\max_x f(x)$$

- First popularized as **EGO** (Efficient Global Optimization) algorithm by Jones et al. (1998).
- Now widely used for optimizing hyper-parameters in machine learning algorithms.
- **Advantage:** Sample-efficient, gradient-free!
- **Disadvantage:** Good for low-dimensional  $x$  only
- Built on two basic components:
  - **Surrogate Model**
  - **Acquisition Function**

## OPTIMIZATION PROBLEM, 1D



## OPTIMIZATION PROBLEM, 2D





# Bayesian Optimization

## Surrogate Model (Gaussian Process)

$$\text{mean}(y|x^*) = k(x^*, x)^T [K + \sigma^2 I]^{-1} y$$

$$\text{var}(y|x^*) = k(x^*, x^*) + \sigma^2 - k(x^*, x)^T [K + \sigma^2 I]^{-1} k(x^*, x)$$

## Acquisition Functions

Expected Improvement

$$\text{EI}_n(x) = \Delta_n(x) \Phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right) + \sigma \phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right)$$

Probability of Improvement

$$\text{PI}_n(x) = \phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right)$$

Upper Confidence Bound

$$\text{UCB}_n(x) = \mu_n(x) + \beta^{1/2} \sigma_n(x)$$

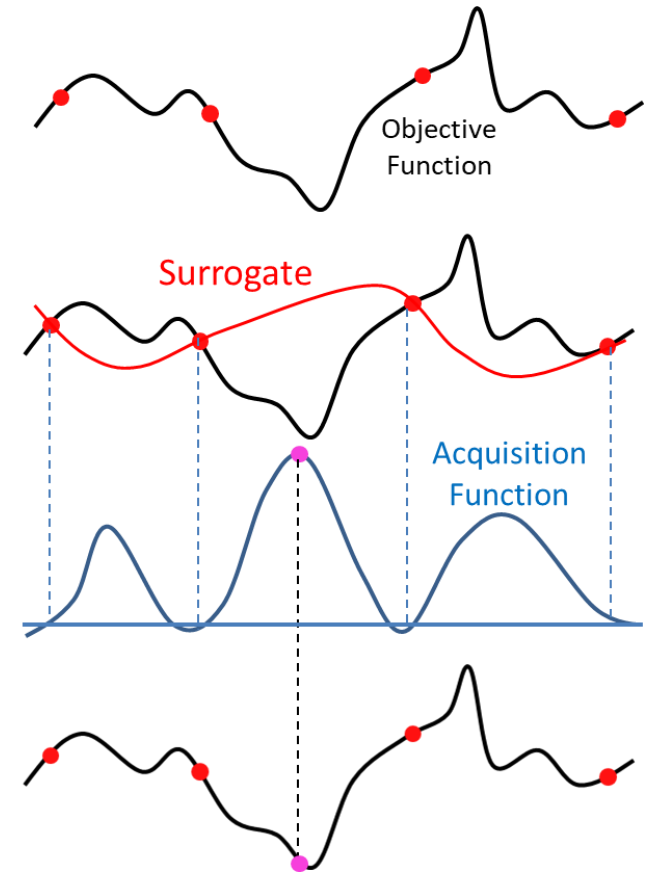
## Algorithm:

**Step 1.** Sample a few points from the objective function

**Step 2.** Fit the GP surrogate model on the observations.

**Step 3.** Compute the acquisition function then find its maximum. This is where we should sample next.

**Step 4.** Sample the objective function at the best point, then go back to **Step 1**.



# Bayesian Optimization

## Surrogate Model (Gaussian Process)

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## Acquisition Functions

Expected  
Improvement

$$\text{EI}_n(x) = \Delta_n(x) \Phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right) + \sigma \phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right)$$

Probability of  
Improvement

$$\text{PI}_n(x) = \Phi\left(\frac{\Delta_n(x)}{\sigma_n(x)}\right)$$

Upper Confidence  
Bound

$$\text{UCB}_n(x) = \mu_n(x) + \beta^{1/2} \sigma_n(x)$$

## Definitions:

$$\Delta_n(x) = \begin{cases} \mu_n(x) - y_n^* - \xi & \text{if maximization} \\ y_n^* - \mu_n(x) - \xi & \text{if minimization} \end{cases}$$

At the  $n$ th iteration:

$$\mu_n(x) = \text{mean}(y|x) = \text{surrogate value at } x$$

$$\sigma_n(x) = \sqrt{\text{var}(y|x)} = \text{uncertainty at } x \text{ (std. dev.)}$$

$$y_n^* = \text{max/min observed so far (} n\text{th iteration)}$$

$$\xi = \text{exploration/exploitation parameter} \\ \text{(higher } \xi, \text{ more exploration)}$$

$$\phi(a) = \text{normal cumulative density function (CDF)}$$

$$\Phi(a) = \text{normal probability density function (PDF)}$$

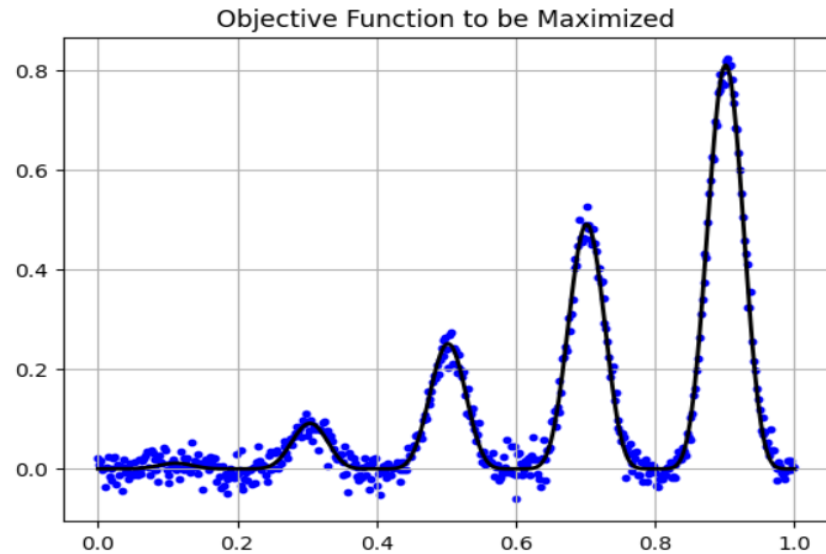
# Bayesian Optimization

## Example:

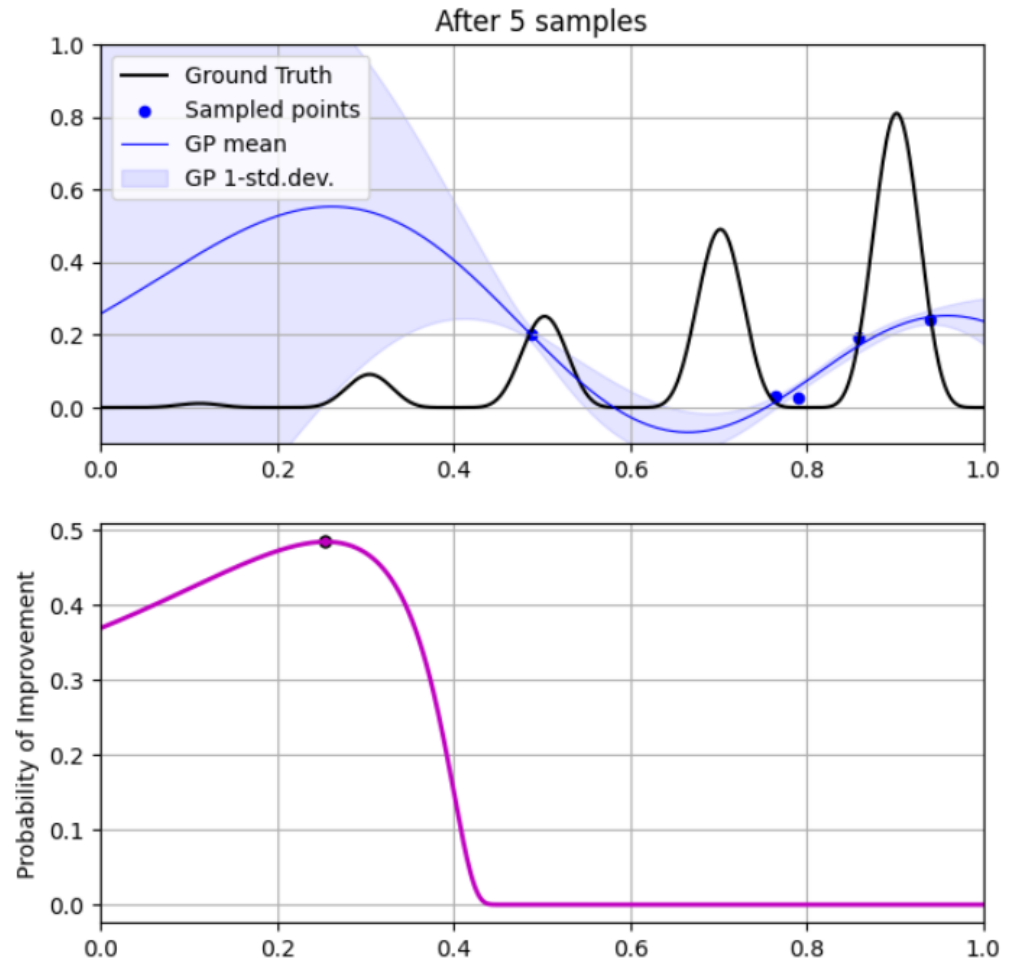
Find  $x$  within  $x \in [0, 1]$  such that

$$x^2 \sin^6(5\pi x) + \varepsilon$$

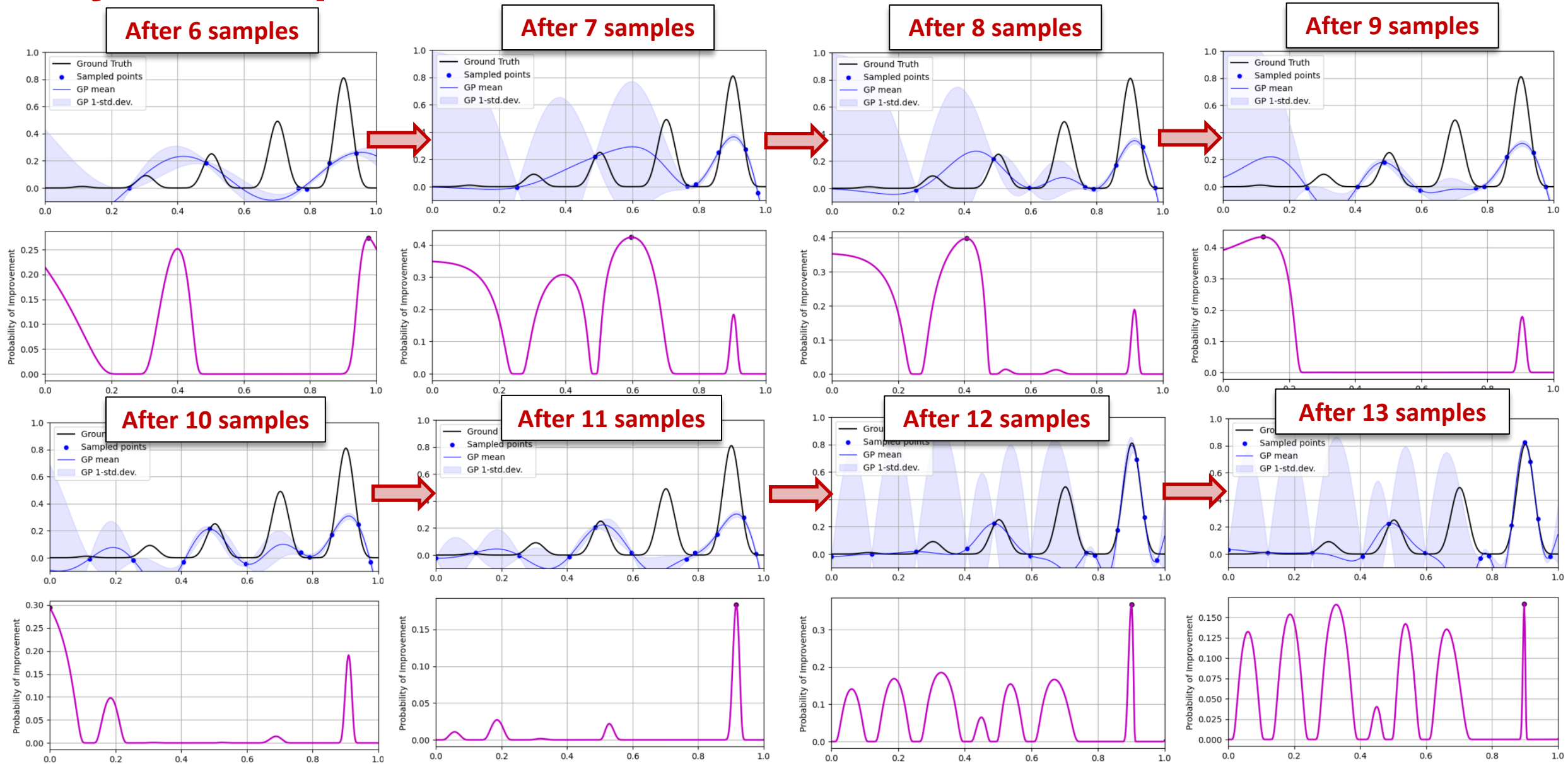
is maximum. The noise is distributed as  $\varepsilon \sim \mathcal{N}(0, 0.02)$ .  
Use BayesOpt with the *Probability of Improvement* acquisition function.



## Initialization:



# Bayesian Optimization



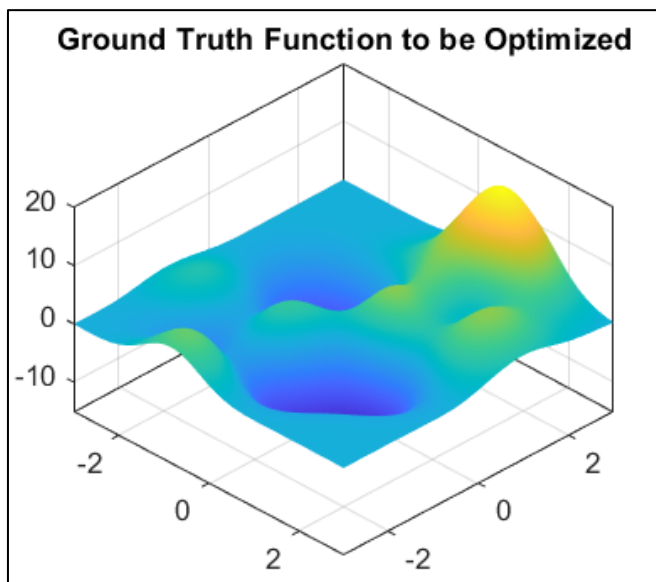
# Bayesian Optimization

## Example:

Find the point  $(x_1, x_2)$  that maximizes an *unknown* objective function given by the following surface.

Use Bayesian Optimization with the Expected Improvement policy and  $\xi = 0.2$ .

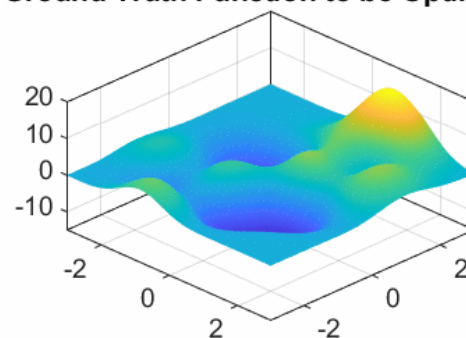
You can only sample the function **50 times**.



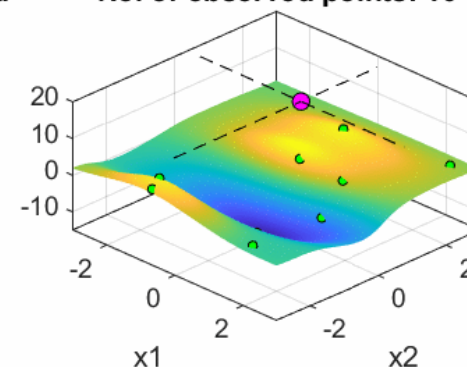
**Answer:** Maximum (estimated):  
 $(x_1, x_2) = (0.939394, 2.515152)$  Max point of the surrogate model  
 $f(x_1, x_2) = 16.795755$

Maximum (observed):  
 $(x_1, x_2) = (1.060606, 2.575758)$  Max point among all 50 samples observed  
 $f(x_1, x_2) = 16.619848$

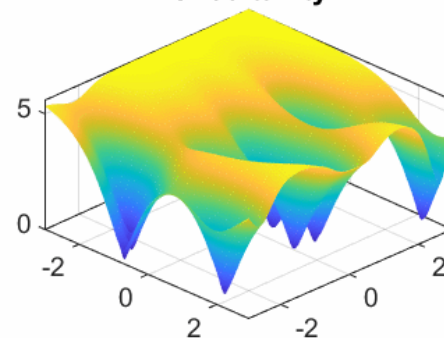
Ground Truth Function to be Optimized



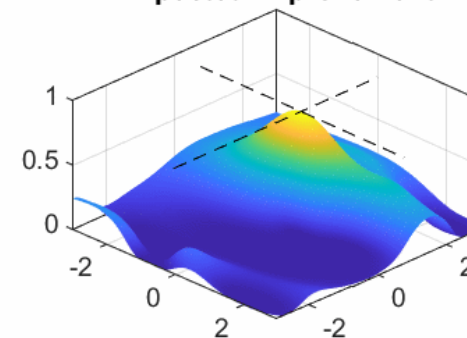
No. of observed points: 10



Uncertainty

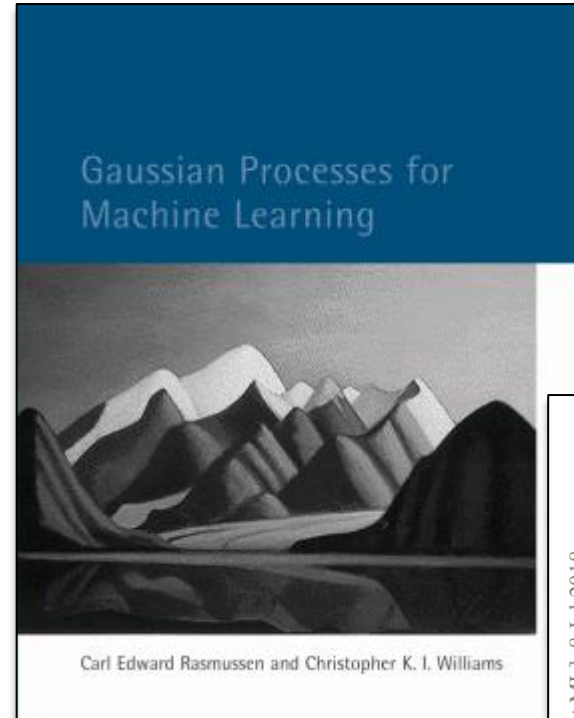


Expected Improvement



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# Further Reading

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