Zero-Order Methods

Derivative-Free Search, Bayesian Optimization, Surrogate Modeling

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Outline

- Introduction to NLP
- Necessary and Sufficient Conditions for Optimality
- Convex Programming
- Methods for Solving NLP
    - One-Dimensional, Unconstrained NLP
    - Multivariable, Unconstrained NLP
    - **Zero-order**, First-order, Second-order Methods
    - Constrained NLP

A Taxonomy of NLP Solvers

Zero-order Methods

Derivative-free, black-box

- Grid Search / Exhaustive Search
- Random Search
- Nelder-Mead Simplex

- Metaheuristic Search
  - Genetic Algorithms
  - Particle Swarm
  - Simulated Annealing
  - Differential Evolution
  - CMAES

- **Bayesian Optimization / Surrogate-based**

First-order Methods

Second-order Methods

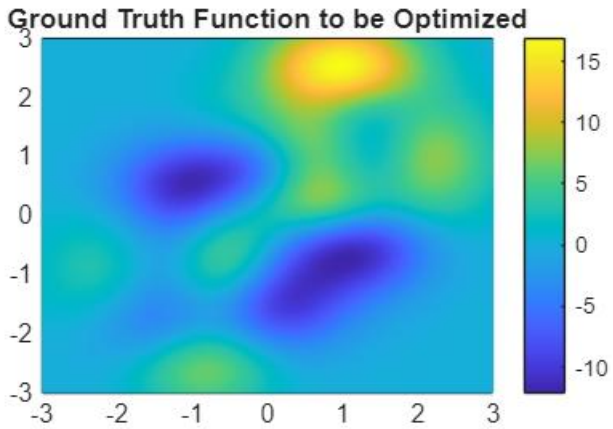
- **Zero-order methods** are good for objective functions whose
  - exact expression is unknown, or
  - it is known but hard / impossible to differentiate.

- If we know the exact expression and it is differentiable, then it is better to use first-order / second-order methods.

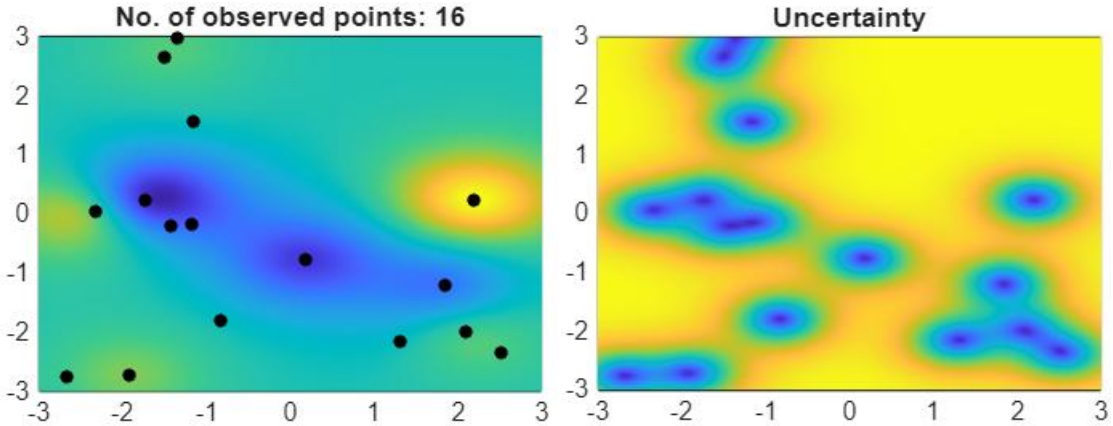
- **Scenarios where zero-order methods are useful:**
  - Design of Experiments → Self-driving labs!
  - Fast prototyping of a product / material design → Materials Discovery!
  - Optimization of machine learning hyper-parameters or architectures
  - Surrogate optimization in chemical plants

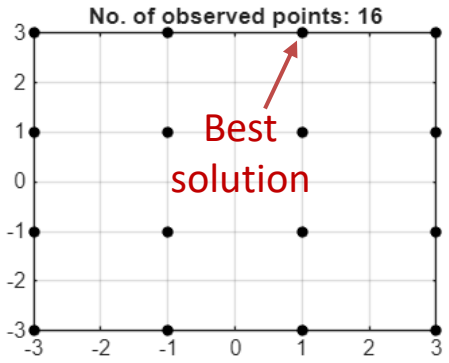
Zero-Order Methods

Find the maximum point in this surface. Assume it is unknown and you can only sample it 50x.

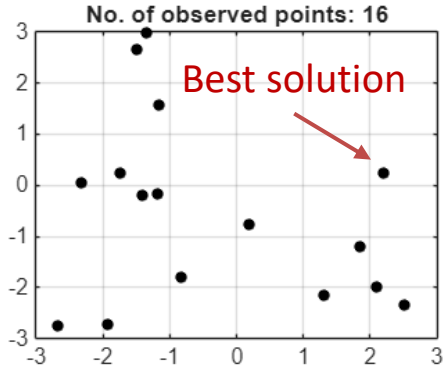


[Step 1] Surrogate Modelling





Grid Search



Random Search

Bayesian Optimization

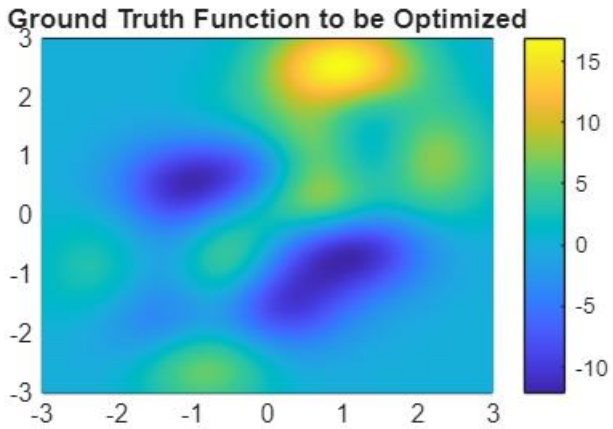
- We will use the rest of the 14 trials left only.
- Need: *Surrogate model* + *Acquisition function*

Evolutionary Search

- Takes N x G no. of more samples
- N = no. of iterations
- G = population size

Bayesian Optimization

Find the maximum point in this surface. Assume it is unknown and you can only sample it 50x.



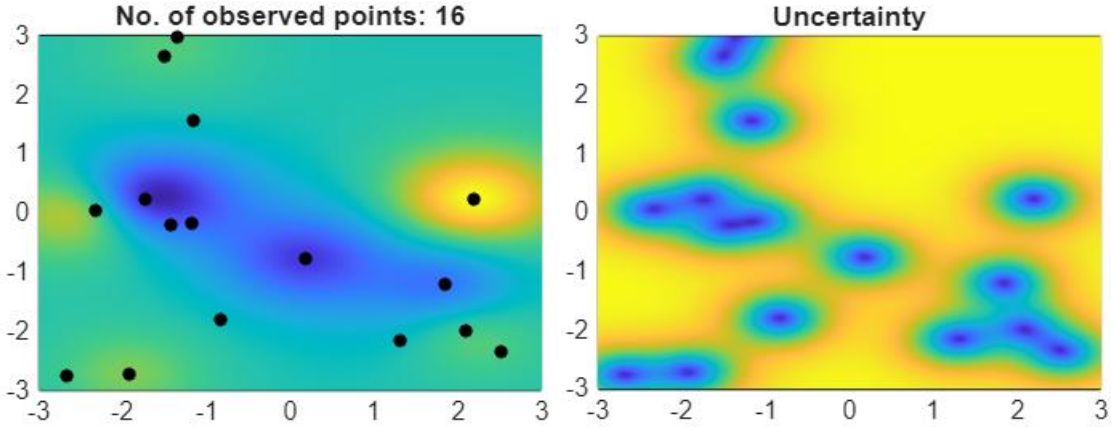
Surrogate Model

- Any regression model that can output a *mean* and *uncertainty* estimate over the search space.
- A **proxy** for the unknown *objective function* that is *sequentially fitted* to new samples using **Bayesian inference**.
- Typically, **Gaussian process regression** is used:

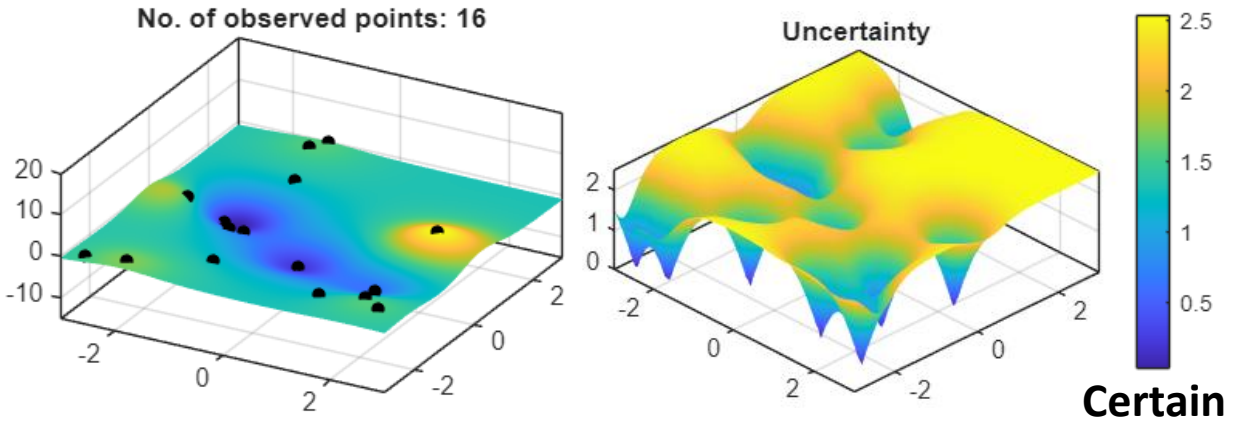
$$\text{mean}(y|x^*) = k(x^*, \boldsymbol{x})^T [\boldsymbol{K} + \sigma^2 \boldsymbol{I}]^{-1} \boldsymbol{y}$$

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

[Step 1] Surrogate Modelling



In another viewpoint…

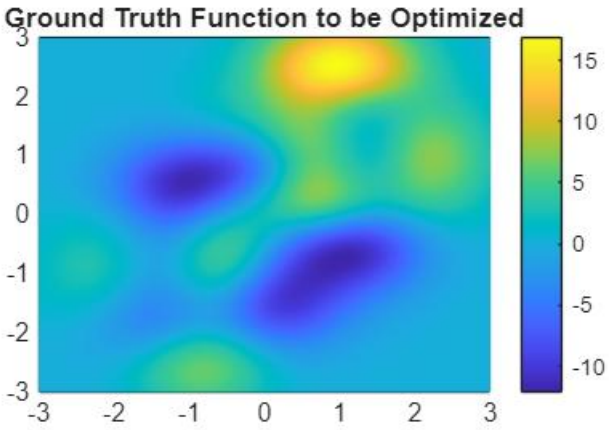


Mean estimate

Uncertainty estimate

Bayesian Optimization

Find the maximum point in this surface. Assume it is unknown and you can only sample it 50x.

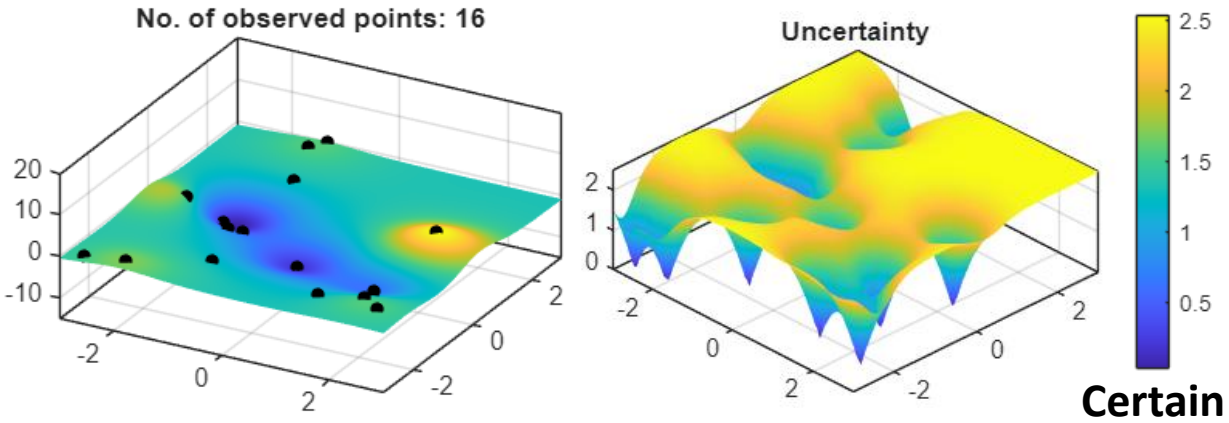


Acquisition Function

- A **policy** that evaluates the surrogate model output to find the best place to sample the objective function **next**.
- The next best trial is where the policy surface is **maximum**.
- Typically, **Upper Confidence Bound** (**UCB**) is used:

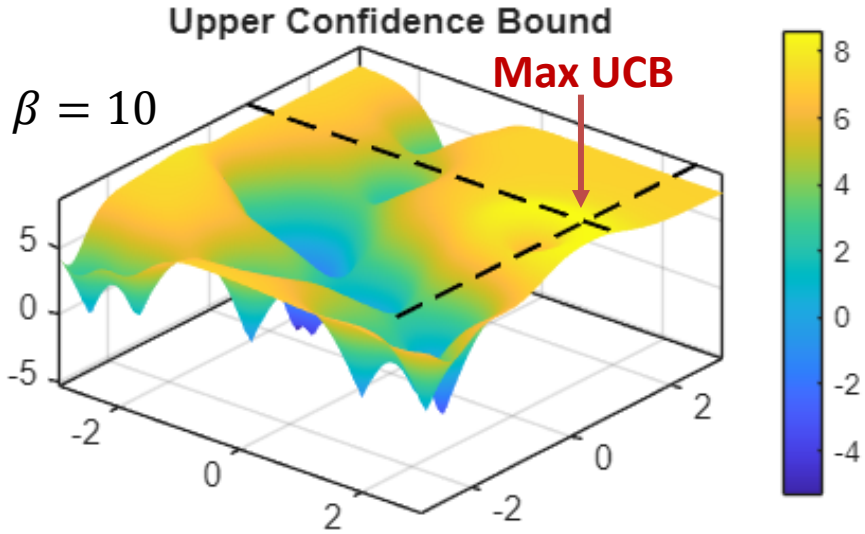
$$\mathrm{UCB}_n(x) = \underbrace{\mu_n(x)}_{\textit{Mean estimate}} + \beta^{1/2}\underbrace{\sigma_n(x)}_{\textit{Uncertainty estimate}}$$

[Step 1] Surrogate Modelling



Mean estimate *Uncertainty estimate*

[Step 2] Calculate Acquisition Function



Bayesian Optimization

Find the maximum point in this surface. Assume it is unknown and you can only sample it 50x.

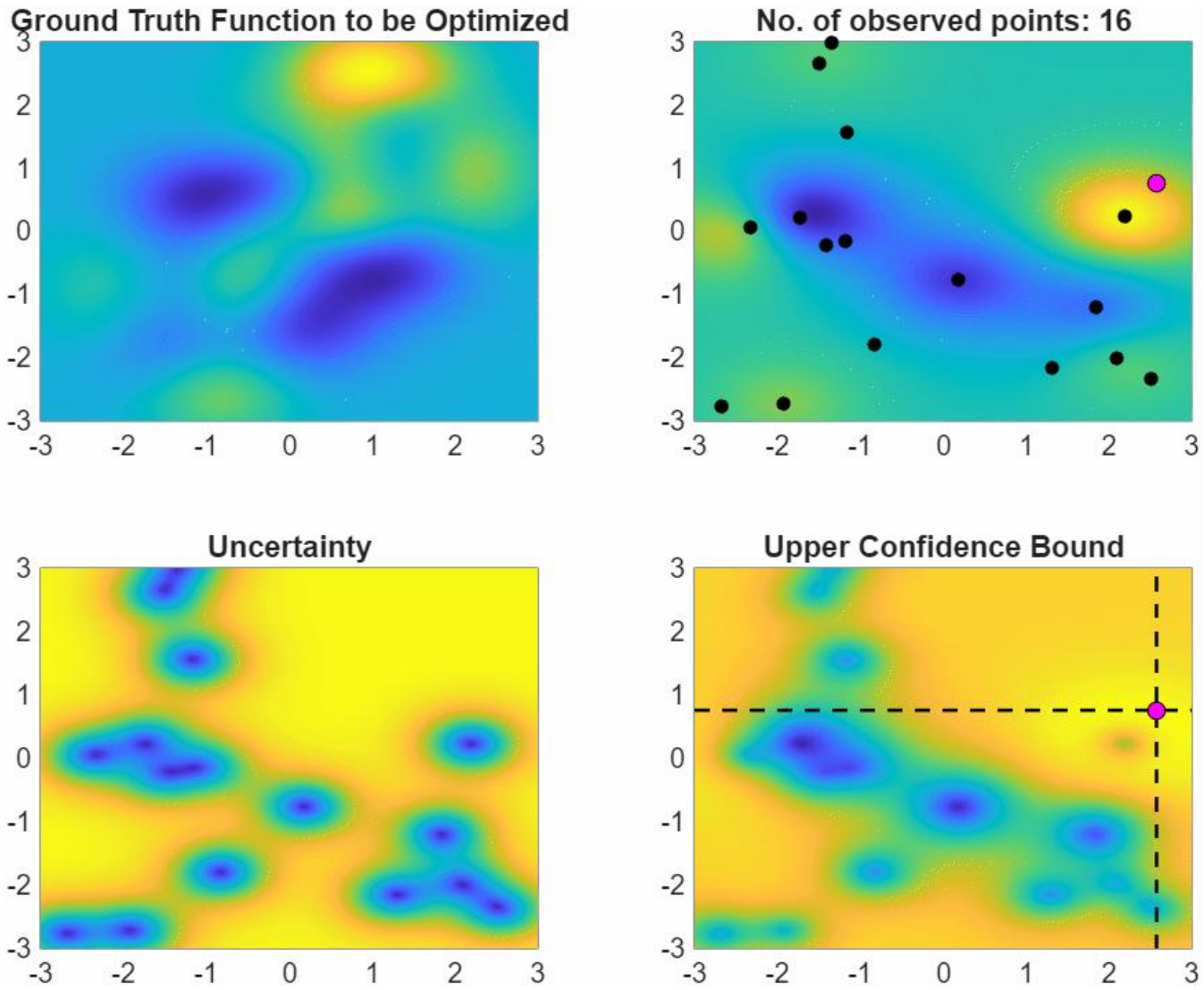
Observations:

1. Maximum already found in the 30th trial.

2. Non-promising regions may not be explored anymore.

3. Next best trial is guided by knowledge from all past trials. **Sample-efficient!**

Solution: (Top View)



Bayesian Optimization

Find the maximum point in this surface. Assume it is unknown and you can only sample it 50x.

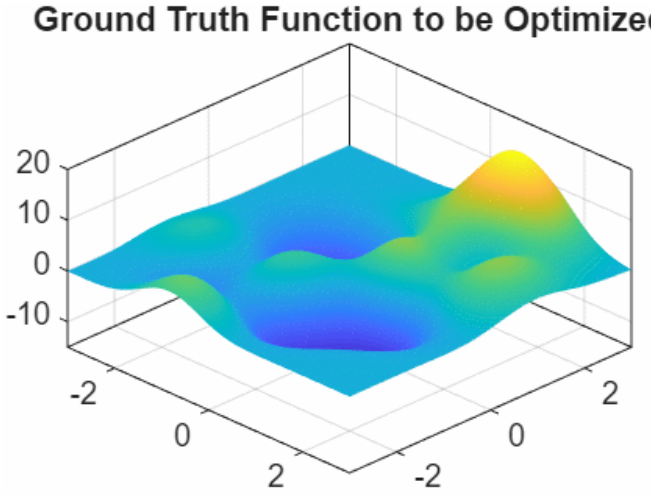
Observations:

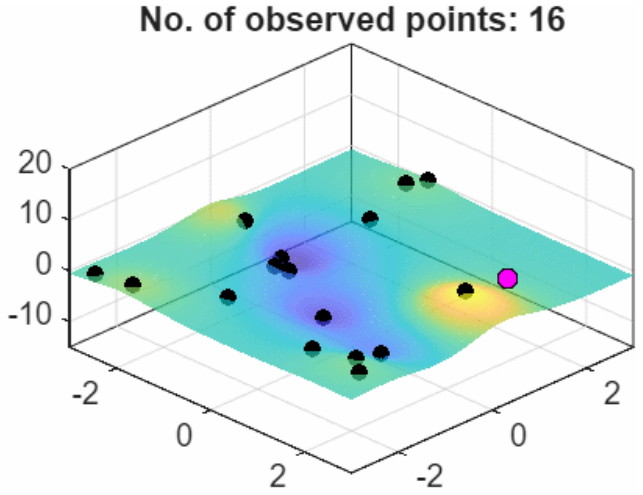
1. Maximum already found in the 30th trial.

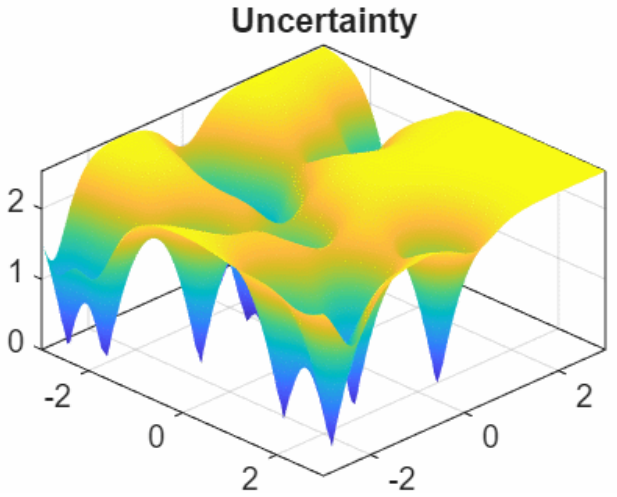
2. Non-promising regions may not be explored anymore.

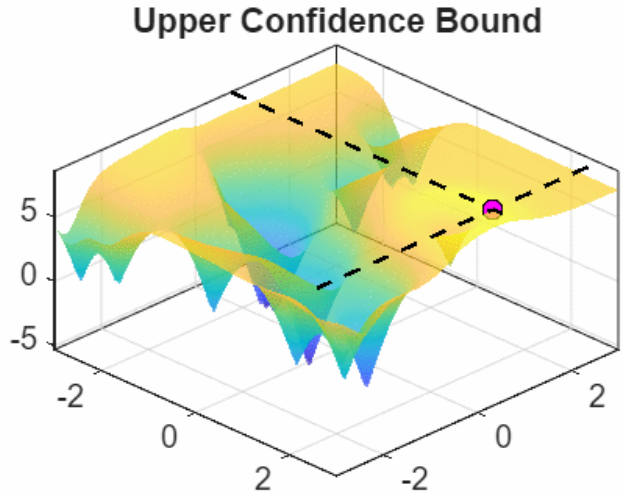
3. Next best trial is guided by knowledge from all past trials. **Sample-efficient!**

Solution: (Side View)



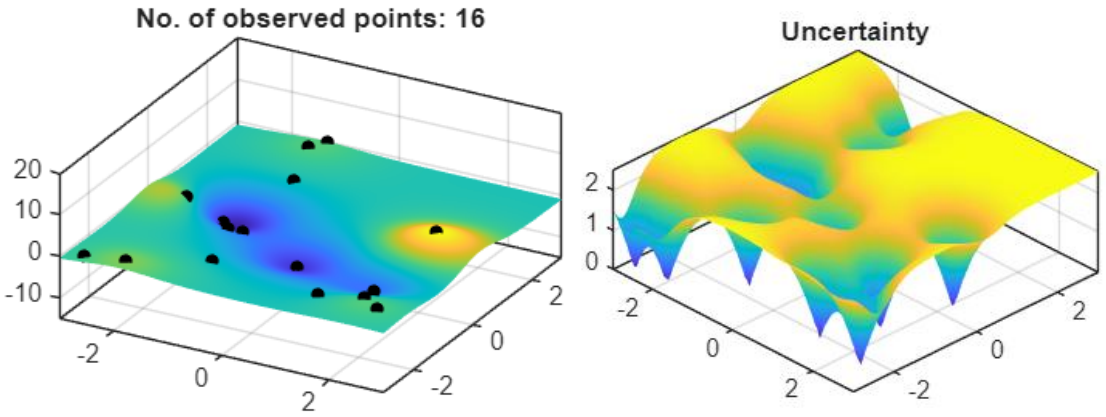






Bayesian Optimization: Acquisition Functions

Surrogate Model



Mean estimate $\mu_n(x)$

Uncertainty estimate $\sigma_n(x)$

Acquisition Function

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

Policy:
Sample where UCB is maximum.

High $\mu_n(x)$ **Exploitation**

High $\sigma_n(x)$ **Exploration**

β = exploration / exploitation parameter

Other Acquisition Functions:

Upper Confidence Bound

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

Expected Improvement

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

Probability of Improvement

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

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 nth iteration:

$\mu_n(x) = \mathrm{mean}(y|x)$ = surrogate mean estimate at x

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

y_n^* = max/min best observed so far (nth iteration)

ξ = exploration/exploitation parameter
(higher ξ, more exploration)

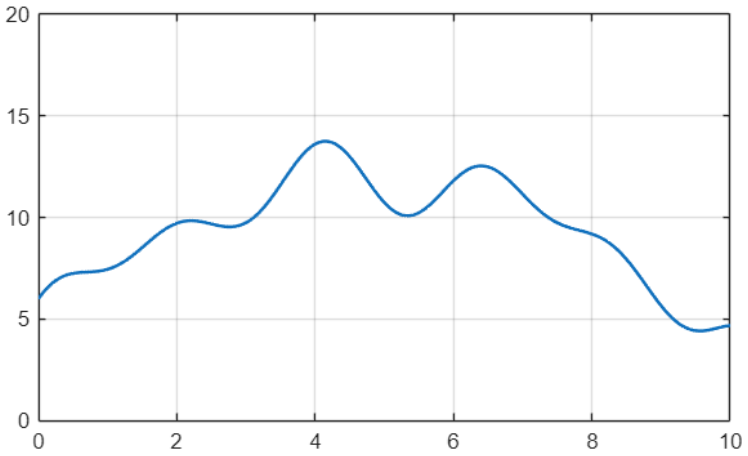
$\phi(\cdot)$ = normal cumulative density function (CDF)

$\Phi(\cdot)$ = normal probability density function (PDF)

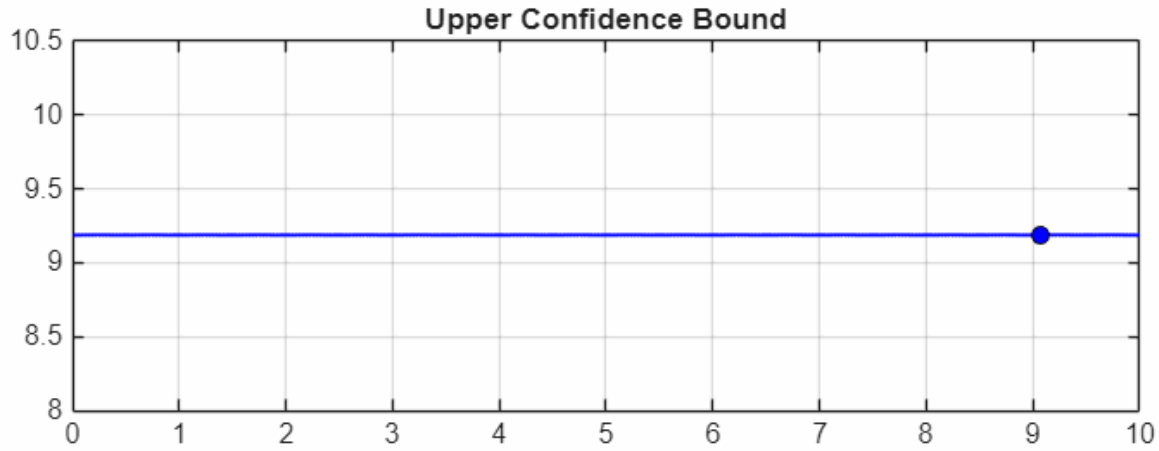
Bayesian Optimization

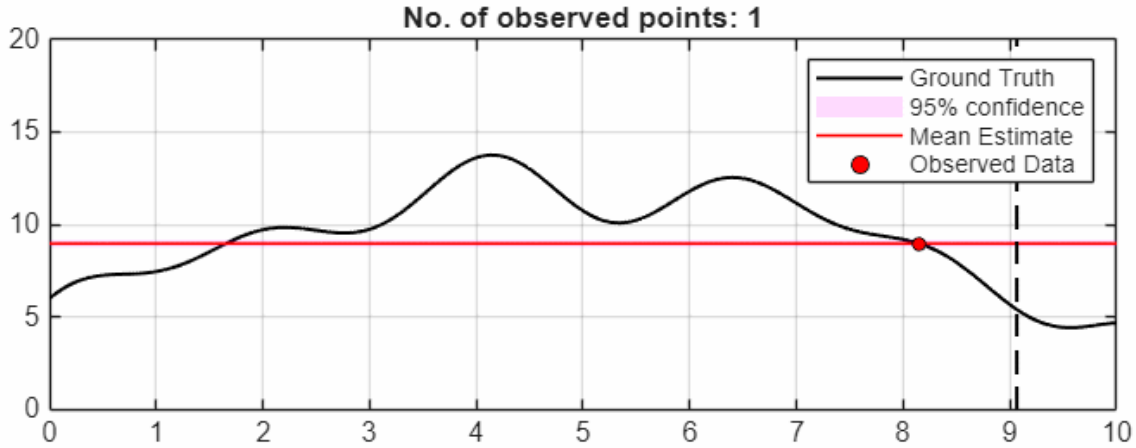
Find the maximum point in this unknown function within [0, 10] using only 20 trials.

- Start from only 1 random trial.
- Use the **UCB** with $\beta = 1$.



Solution:

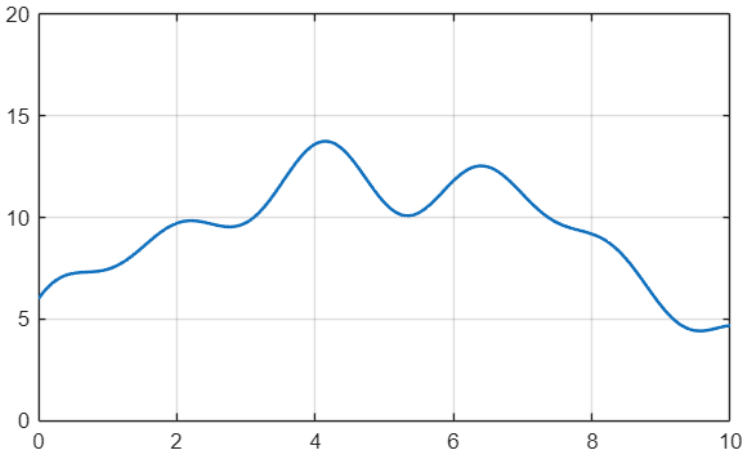




Bayesian Optimization

Find the maximum point in this unknown function within [0, 10] using only 20 trials.

- Start from only 1 random trial.
- Use the **Expected Improvement** Policy with $\xi = 0$.



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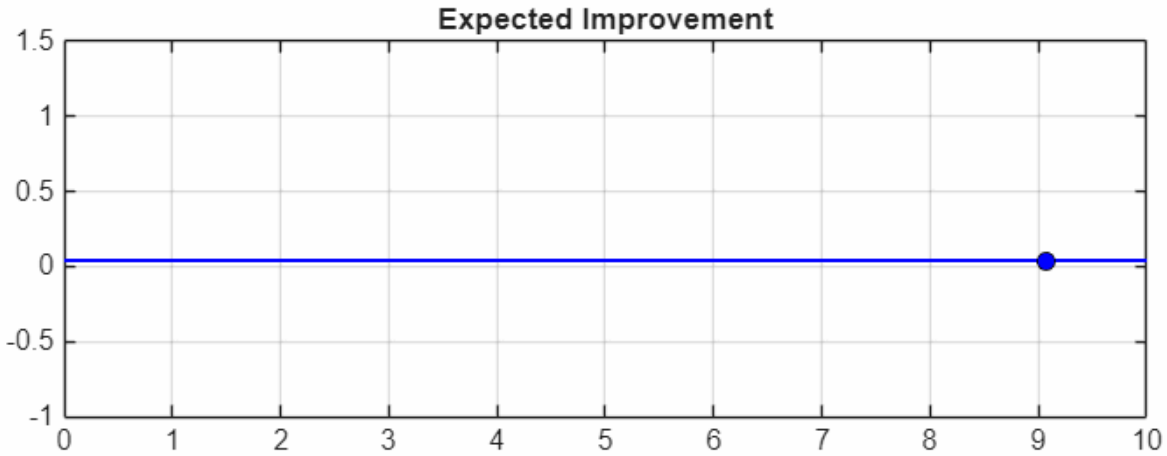
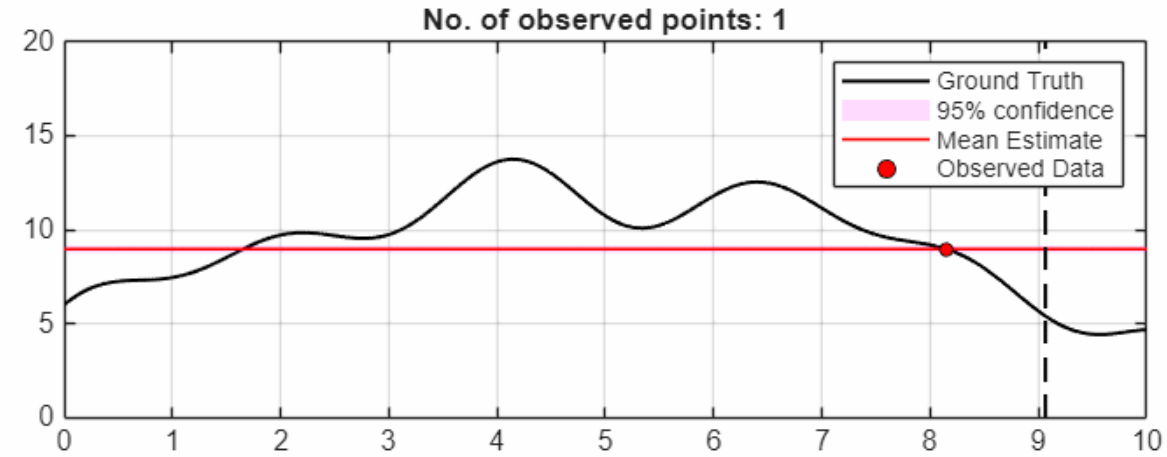




Bayesian Optimization: Gaussian Processes

*GPR outputs both a **mean and distribution** prediction.*

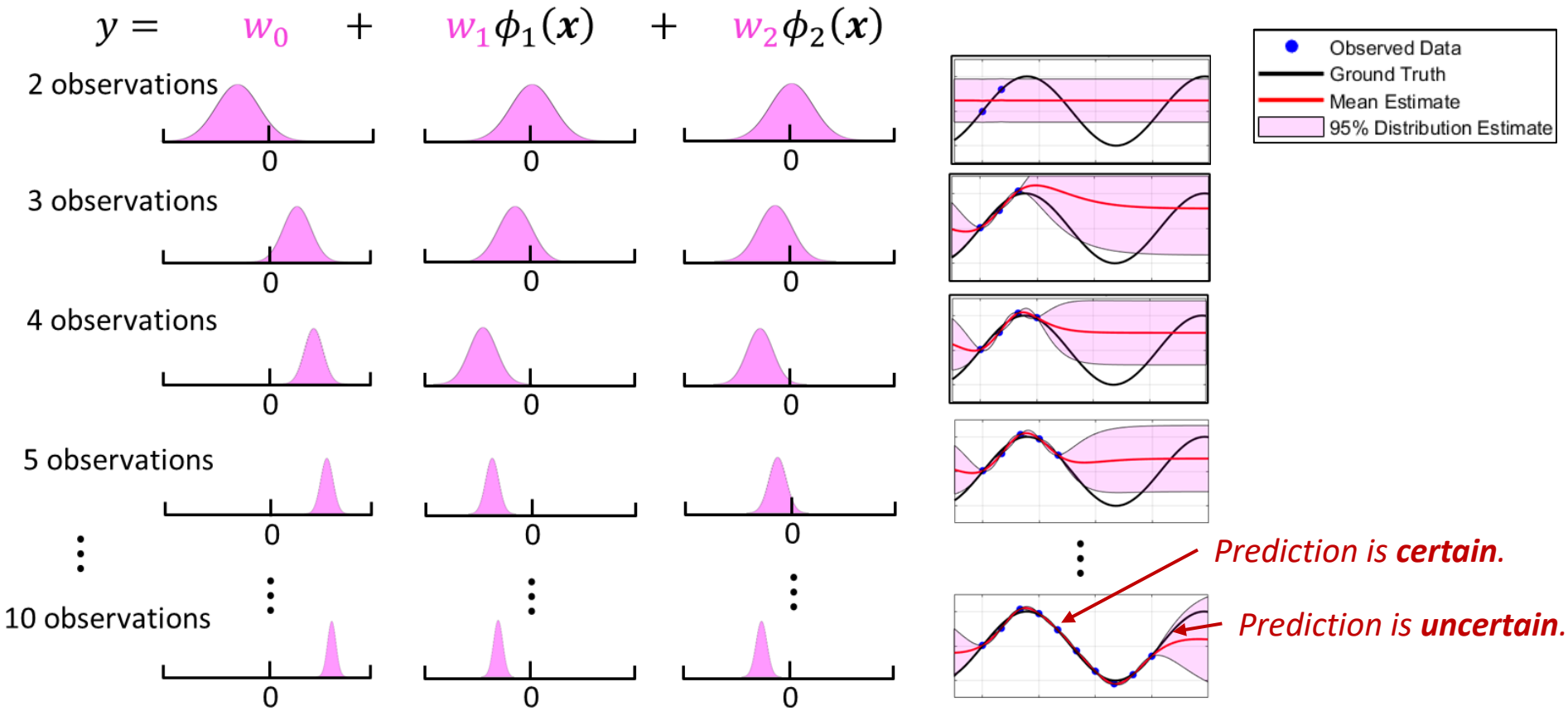
Gaussian Process Regression (GPR):

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

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

Derived using Bayes Theorem.

To appreciate GPR, imagine that data points only arrive one at a time…



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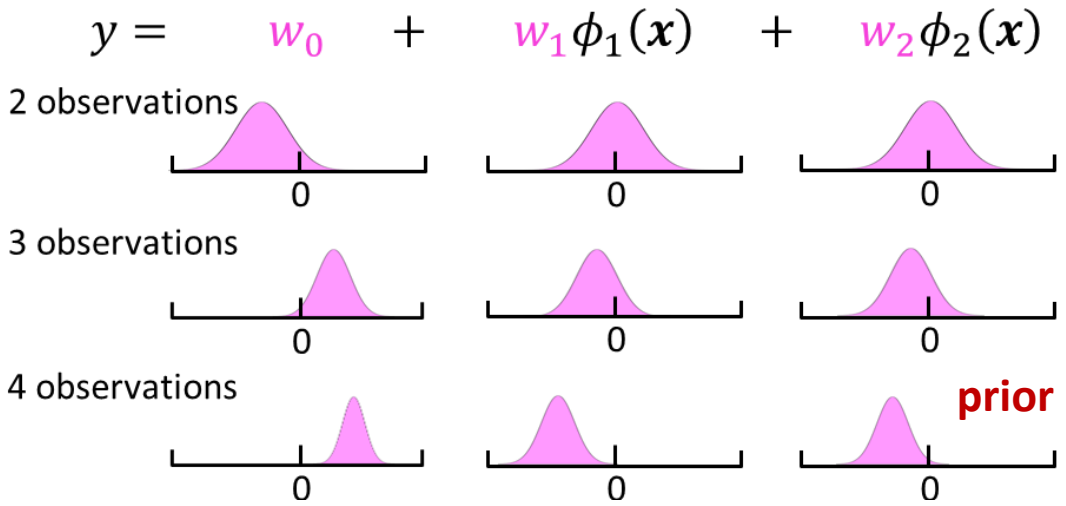
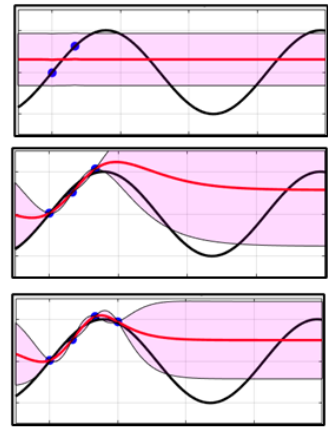
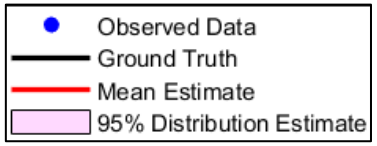


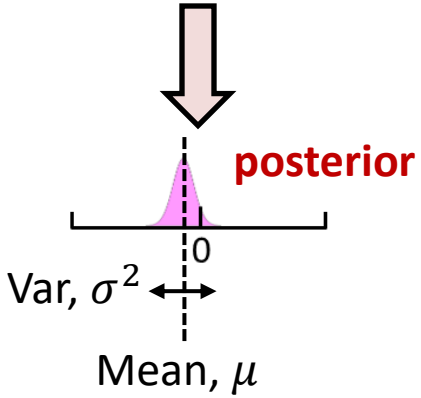




Bayes' Theorem:

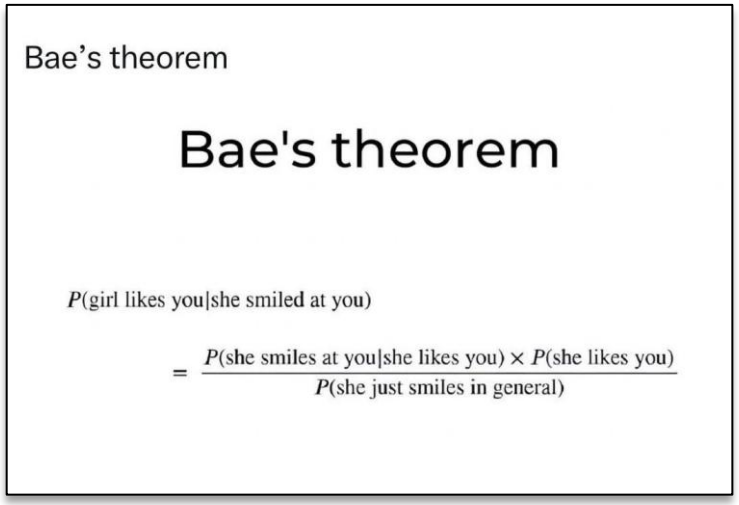
$$p(y|x) = \frac{p(x|y)\ p(y)}{\int p(y|x)p(x)\ dy}$$

posterior — likelihood — prior — Marginal likelihood



- In GPR, the prior, posterior, and likelihood are all **Gaussian** distributed.
- If they are not assumed Gaussian, Bayesian inference may be intractable.

Bayesian Statistics: A Change of Perspective



Bayes' Theorem:

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

posterior; likelihood; prior; Marginal likelihood

Bae's Theorem:

$$p(\text{girl likes you}|\text{she smiled at you}) = \frac{p(\text{she smiled at you}|\text{she likes you})\ p(\text{she likes you})}{P(\text{she just smiles in general})}$$

Bayesian Modeling:

Given what I just observed, how likely is this new model?

If this model were true, how likely is it that I would see this new observation?

Before observing anything new, how plausible did I think my current model was?

$$p(\text{model}|\text{observation}) = \frac{p(\text{observation}|\text{model})\ p(\text{model})}{P(\text{observation})}$$

Across all models I thought were possible, how likely was it to see this new observation?

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.

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

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

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

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

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

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

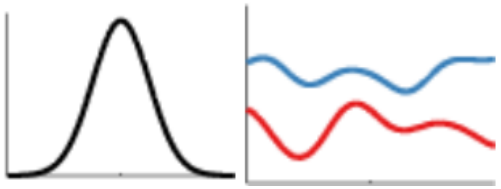
$$\frac{\partial}{\partial \theta_i} \ln p(\mathbf{y}|\boldsymbol{\theta}) = -\frac{1}{2}\text{tr}\left(\mathbf{C}^{-1}\frac{\partial \mathbf{C}}{\partial \theta_i}\right) + \frac{1}{2}\mathbf{y}^T \mathbf{C}^{-1}\frac{\partial \mathbf{C}}{\partial \theta_i}\mathbf{C}^{-1}\mathbf{y}$$

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

Kernel Functions in GPR:

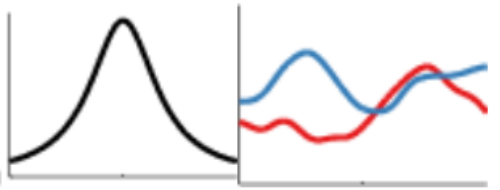
Squared Exponential

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



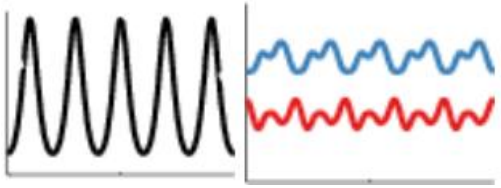
Rational Quadratic

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



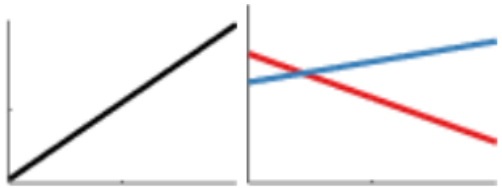
Periodic

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



Linear

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



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

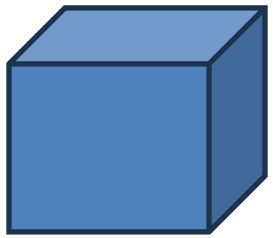
Bayesian Optimization: Initial Sampling

Depending on the constraints, various initial sampling methods are available.

Independent Uniform Sampling

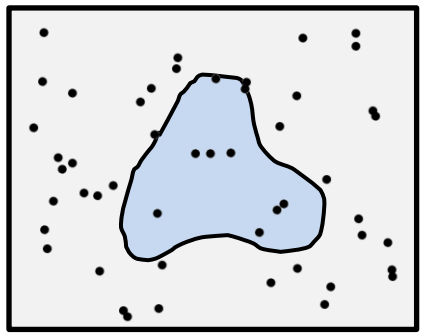
Used when we have box constraints:

$$0 \leq x_1 \leq 1$$
$$0 \leq x_2 \leq 1$$
$$0 \leq x_3 \leq 1$$



Rejection Sampling

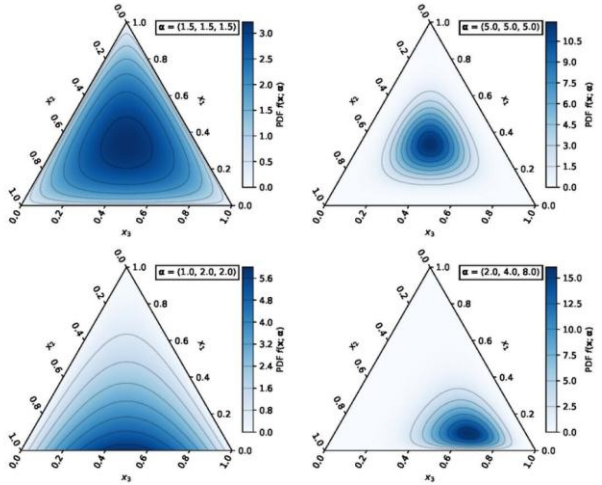
When constraints are nonlinear, just sample anywhere and reject if the constraints are violated.



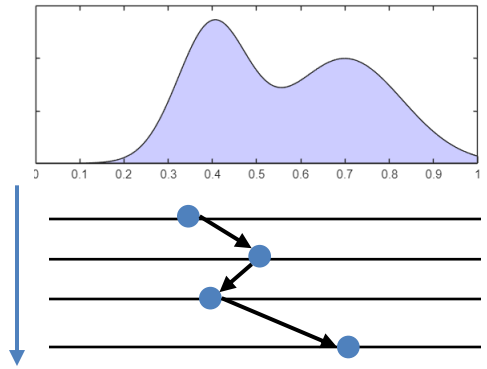
Dirichlet Sampling

Used when the constraint is a regular simplex:

$$0 \leq x_1 \leq 1$$
$$0 \leq x_2 \leq 1$$
$$0 \leq x_3 \leq 1$$
$$x_1 + x_2 + x_3 = 1$$



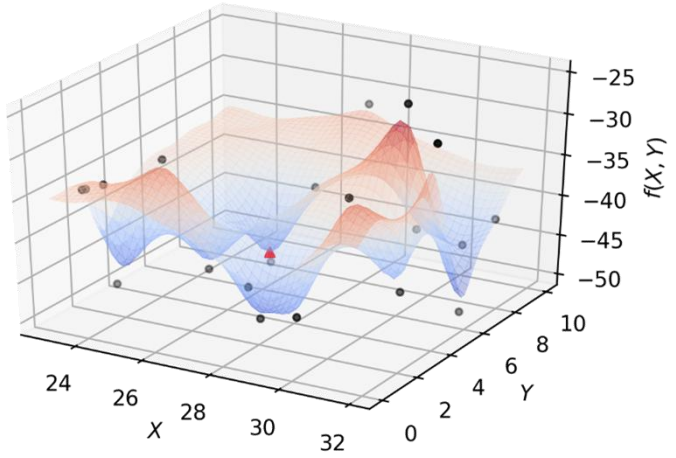
Markov Chain Monte Carlo (MCMC)



Specify a probability distribution, then draw samples using Markov chains, e.g. Metropolis-Hastings algorithm.

Reference: https://en.wikipedia.org/wiki/Dirichlet_distribution

Bayesian Optimization: Summary



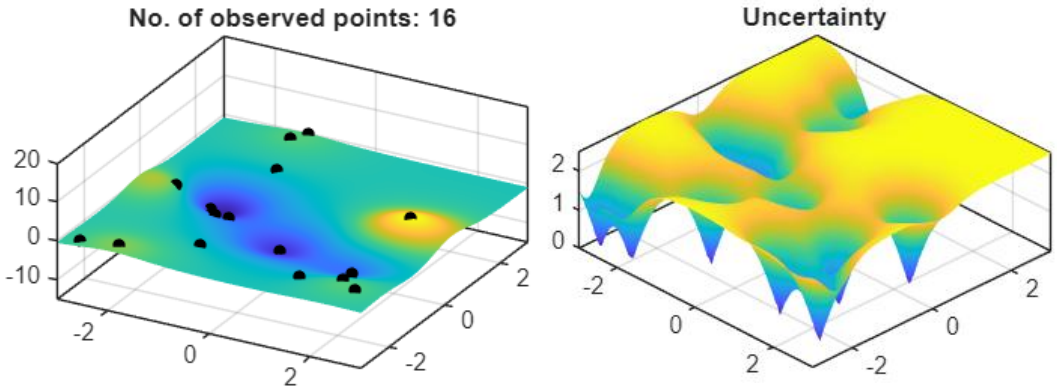
Algorithm:

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

Step 2. Fit a surrogate on the current samples.

Step 3. Compute the acquisition function then find its maximum.

Step 4. Sample the objective function at the best point, then go back to **Step 2**.



Surrogate-based Optimization

- The idea of replacing a hard-to-evaluate objective function with a surrogate model which is faster to evaluate.
- Initially, surrogate model is trained on a few samples of the objective function.
- Surrogate can be updated with more samples.

Reference: https://sksurrogate.readthedocs.io/en/latest/surrogate.html

A Taxonomy of NLP Solvers

Zero-order Methods

Derivative-free, black-box

- Grid Search / Exhaustive Search
- Random Search
- Nelder-Mead Simplex

- Metaheuristic Search
  - Genetic Algorithms
  - Particle Swarm
  - Simulated Annealing
  - Differential Evolution
  - CMAES

- **Bayesian Optimization / Surrogate-based**

First-order Methods

Second-order Methods

- **Zero-order methods** are good for objective functions whose
  - exact expression is unknown, or
  - it is known but hard / impossible to differentiate.

- If we know the exact expression and it is differentiable, then it is better to use first-order / second-order methods.

- **Scenarios where zero-order methods are useful:**
  - Design of Experiments → Self-driving labs!
  - Fast prototyping of a product / material design → Materials Discovery!
  - Optimization of machine learning hyper-parameters or architectures
  - Surrogate optimization in chemical plants