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Optimization for Industrial Applications

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Optimization

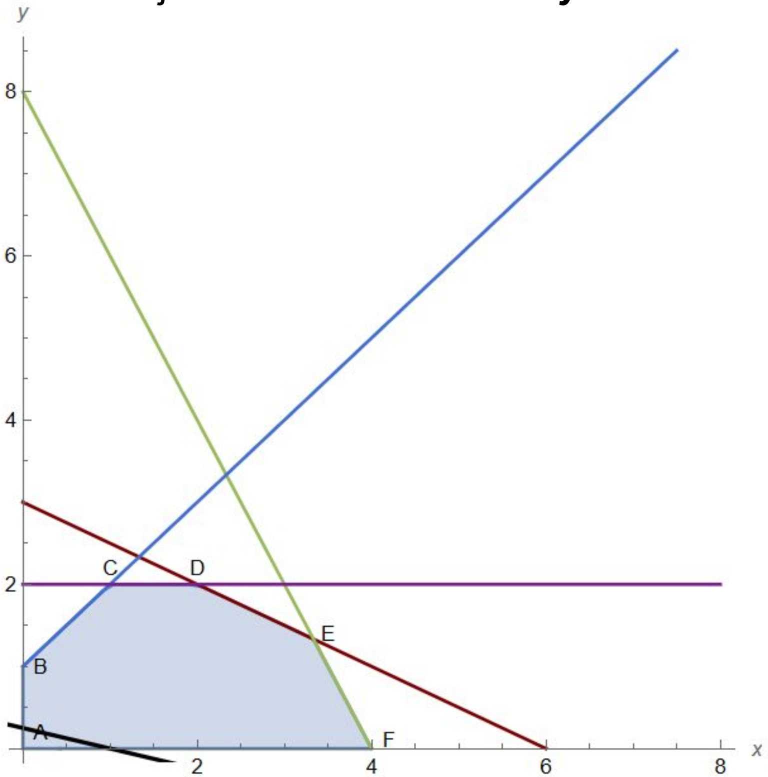
- Finding the **optimum** value of an **objective** given some **constraints**

$$\theta^* \in arg\,max\ f(\theta)$$

$$\theta \in R^d$$

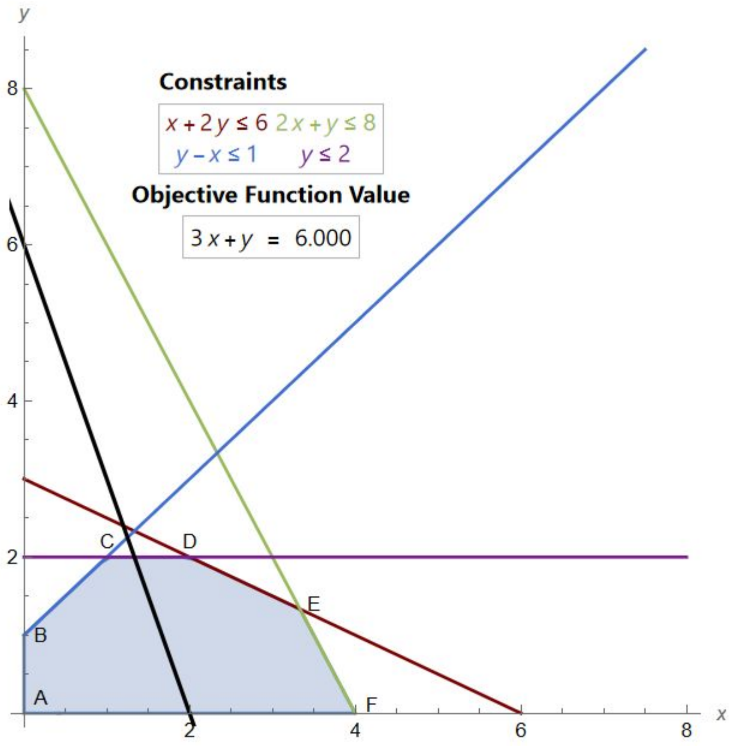
Linear Optimization

Objective Function = ***3*x + y***



Source: https://demonstrations.wolfram.com/GraphicalLinearProgrammingForTwoVariables/

Linear Optimization



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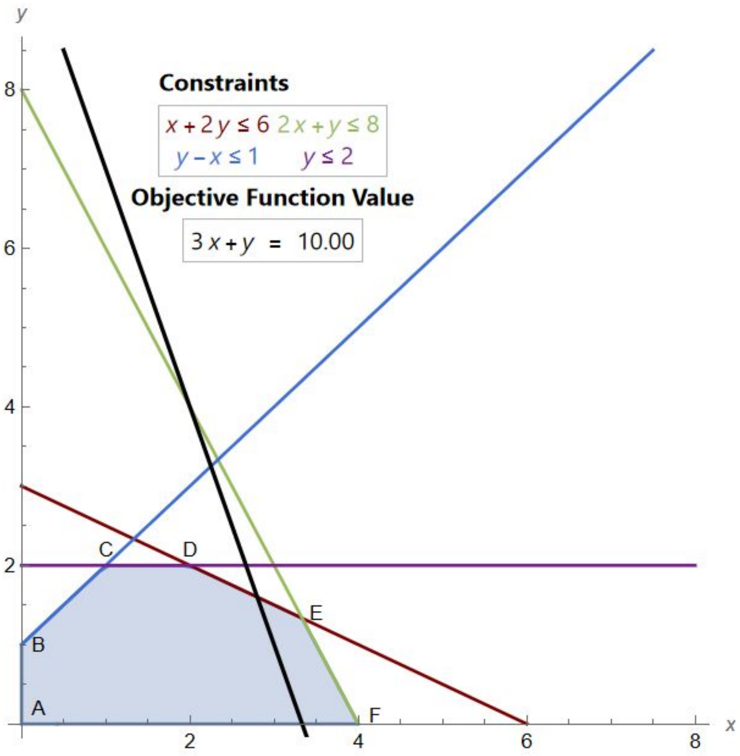
Linear Optimization



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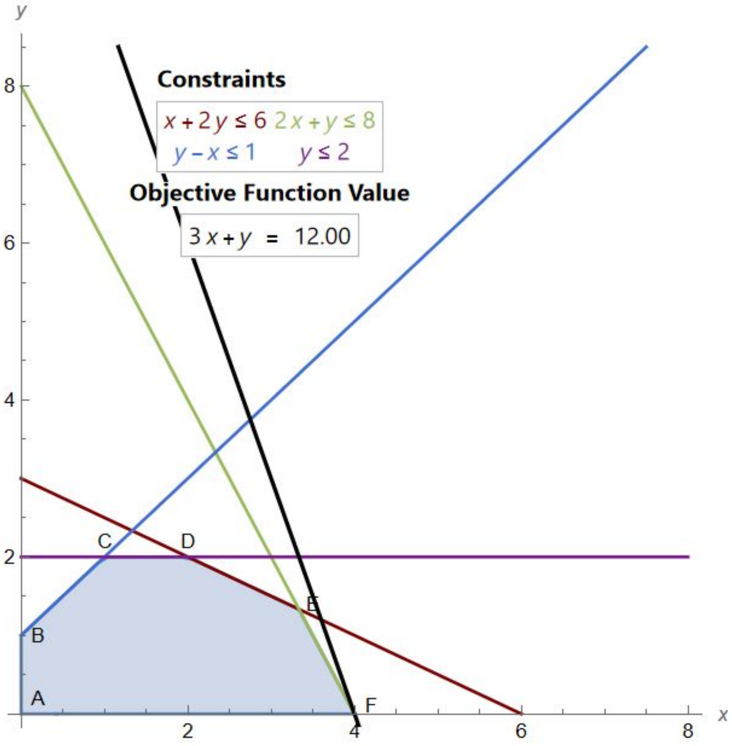
Linear Optimization



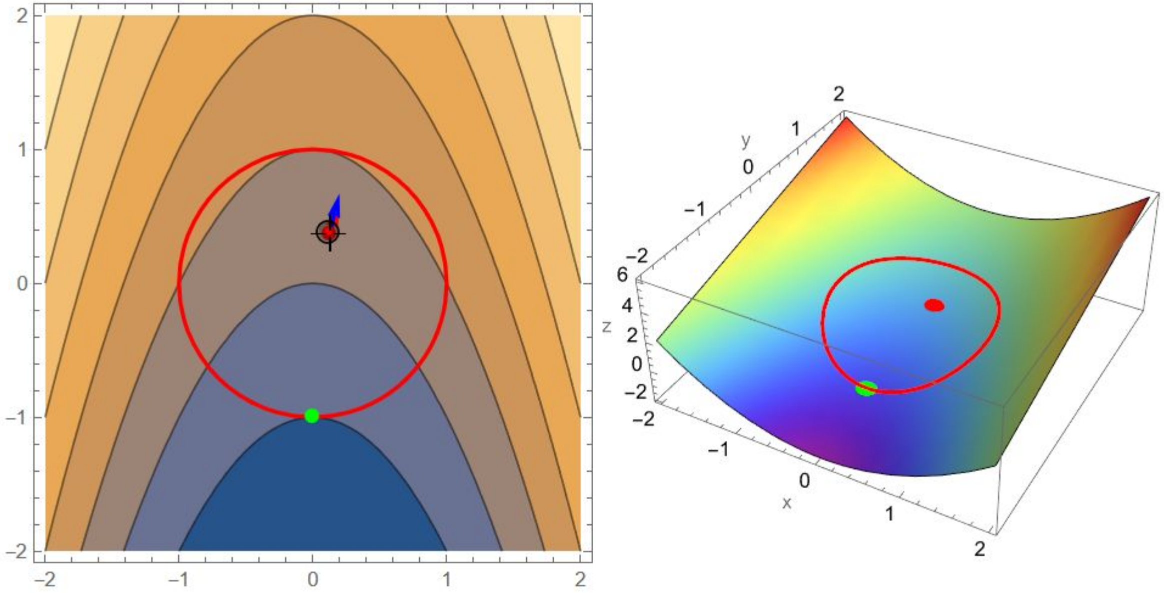
Source: https://demonstrations.wolfram.com/GraphicalLinearProgrammingForTwoVariables/

Linear Optimization

Objective Function = ***3*x + y***

Convex Optimization

Objective Function = $\boldsymbol{x^2 + y}$

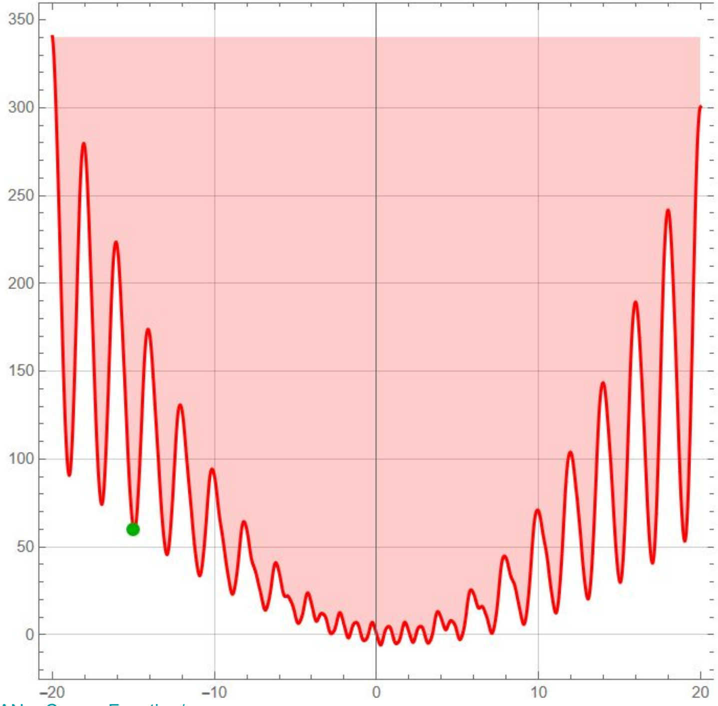


optimal solution at $(-1.17799 \times 10^{-9}, -1.)$

Source: https://demonstrations.wolfram.com/ConstrainedOptimization/

Non-Convex Optimization

Objective function = $\frac{1}{2}(x-\beta)^2 + \gamma x^2\cos(\pi x) - \lambda\sin(2\pi x) + \cos(4\pi x)\sin(\pi x)$



$\beta = 1.0$

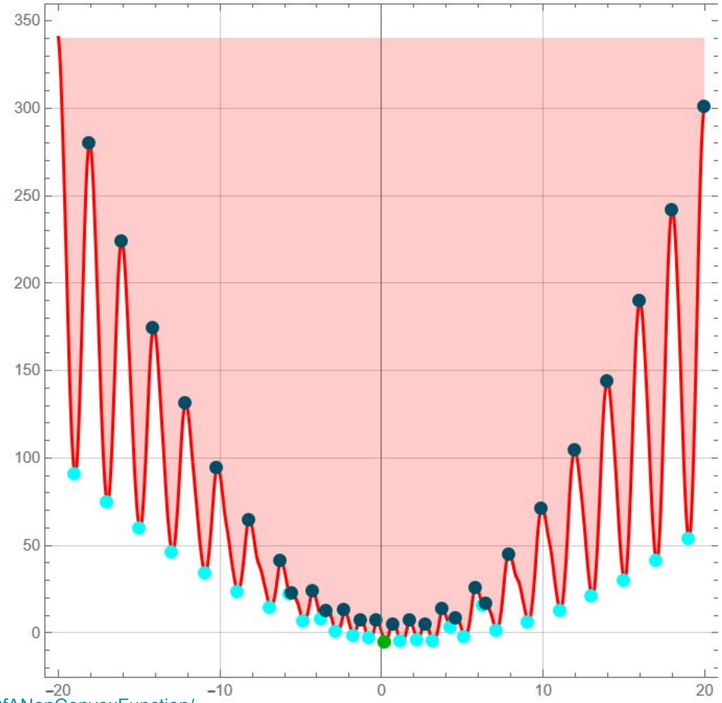
$\gamma = 0.3$

$\lambda = 5.5$

Source: https://demonstrations.wolfram.com/GlobalMinimumOfANonConvexFunction/

Non-Convex Optimization

Objective function = $\frac{1}{2}(x-\beta)^2 + \gamma x^2\cos(\pi x) - \lambda\sin(2\pi x) + \cos(4\pi x)\sin(\pi x)$



$\beta = 1.0$

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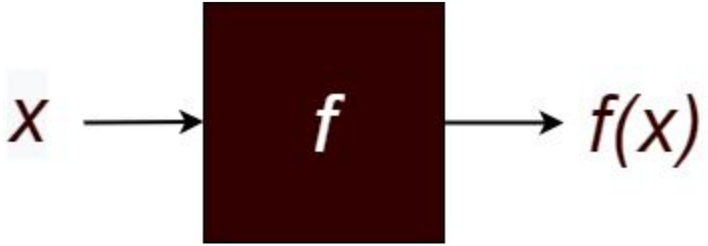
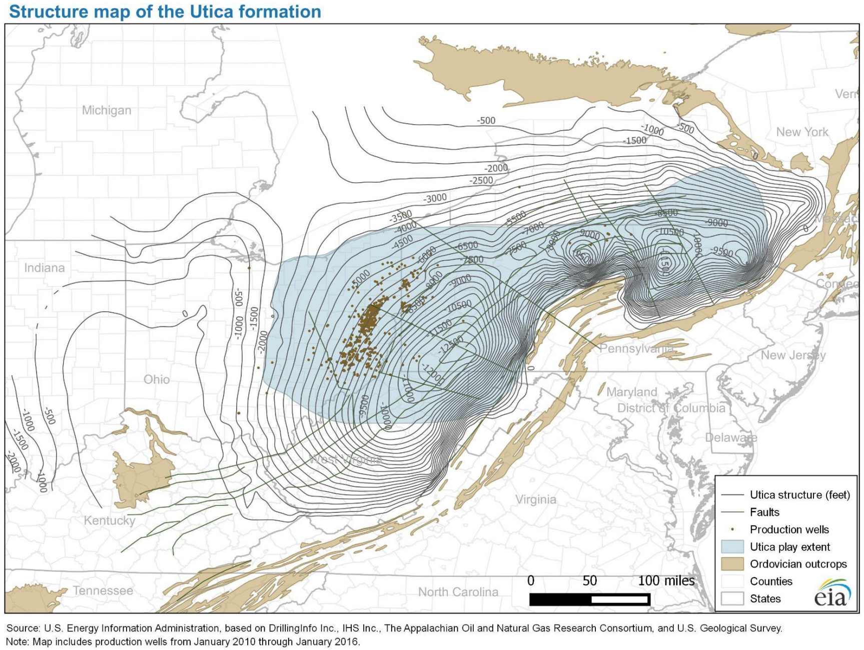
Black Box Functions

Objective Function = ***Analytic form not known***



- **cannot** access ***f***
- **observe** its outputs based on some given inputs

Black Box Functions



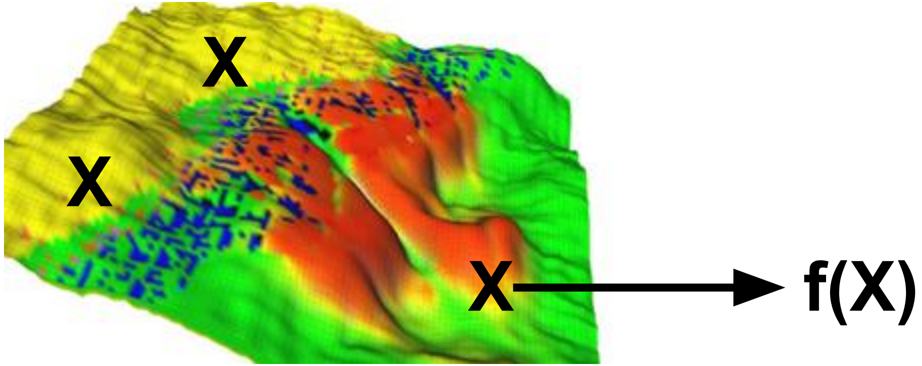
Source: [EIA produces new maps of the Utica Shale play]

Source: [Land Oil Rig 3D Model]

Black Box Functions

Objective Function = ***Analytic form not known***

Costly to evaluate!



Bayesian Optimization

Hence, if **function** is
Black box + Costly to evaluate = **Bayesian Optimization** is used

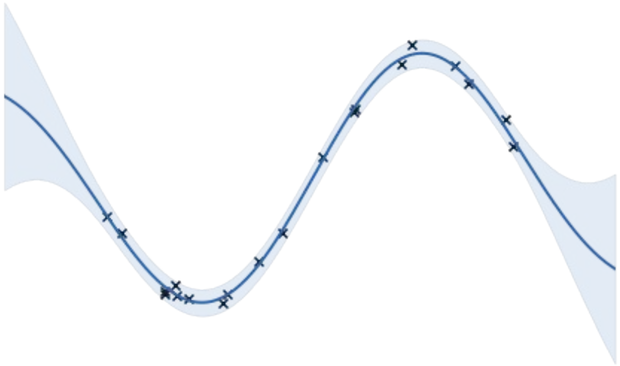
How?

Bayesian Optimization

What? When? Why? How? Where?

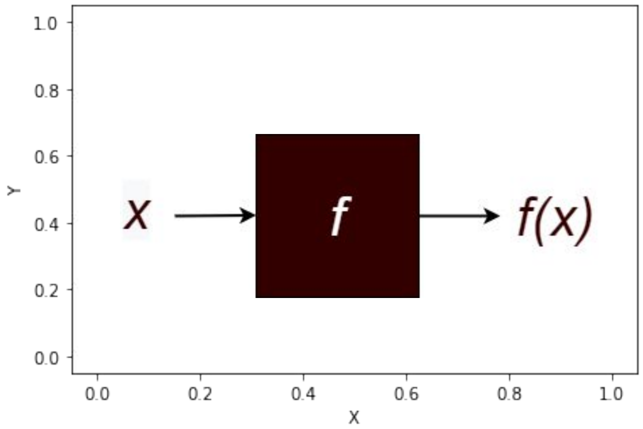
Bayesian Optimization - How?

Step 1- Surrogate Model

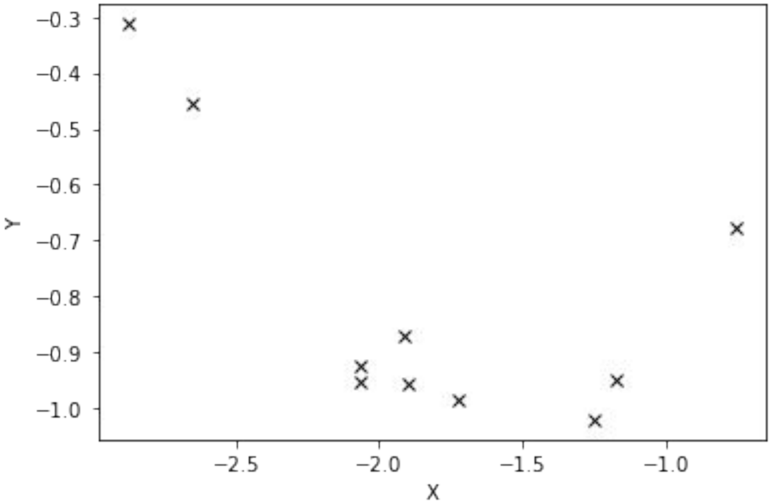


Step 2- Acquisition Functions

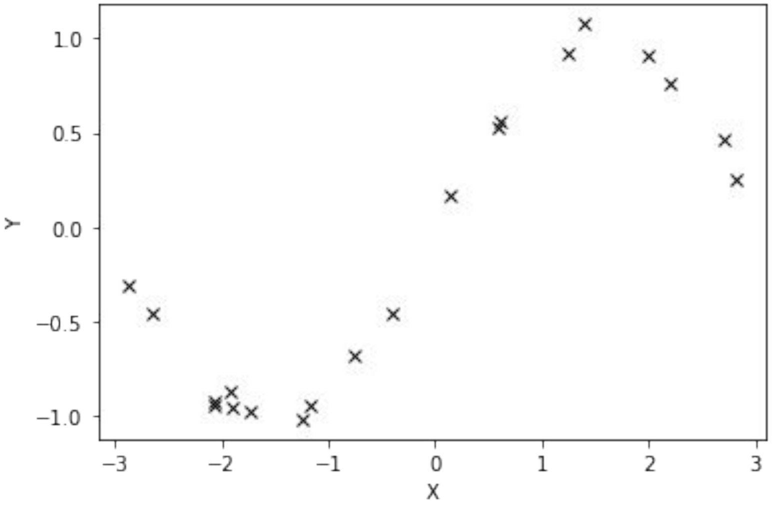
Dataset



Dataset



Dataset



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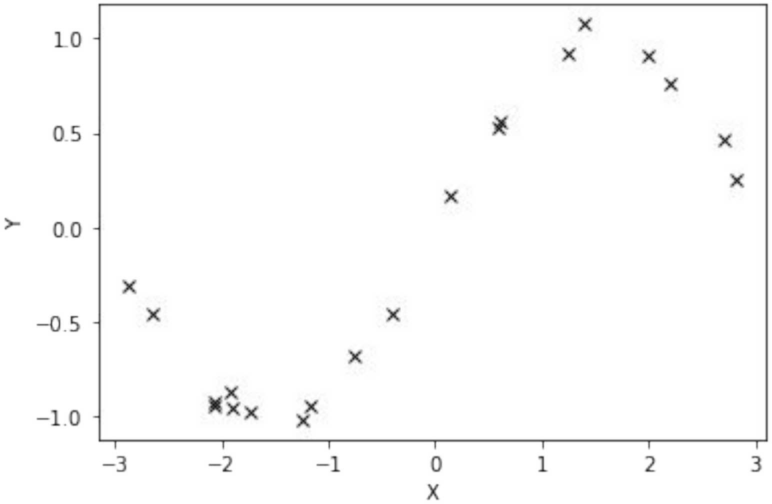
Gaussian Processes

$$\mathbf{X} = \{x_1, x_2, \ldots, x_n\} \qquad \mathbf{Y} = \{y_1, y_2, \ldots, y_n\}$$

$$\mathbf{X}_* = \{x_{n+1}, x_{n+2}, \ldots, x_m\} \qquad \mathbf{Y}_* = \{y_{n+1}, y_{n+2}, \ldots, y_m\}$$

Gaussian Processes



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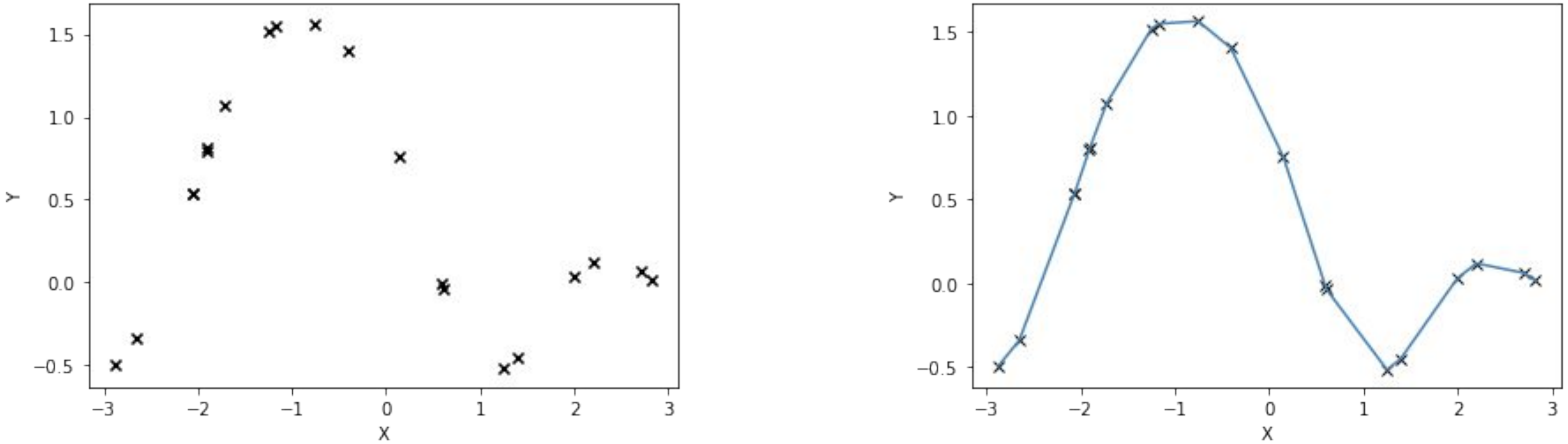
Gaussian Processes

$$p(Y|X) = \mathcal{N}(Y|\mu, K)$$

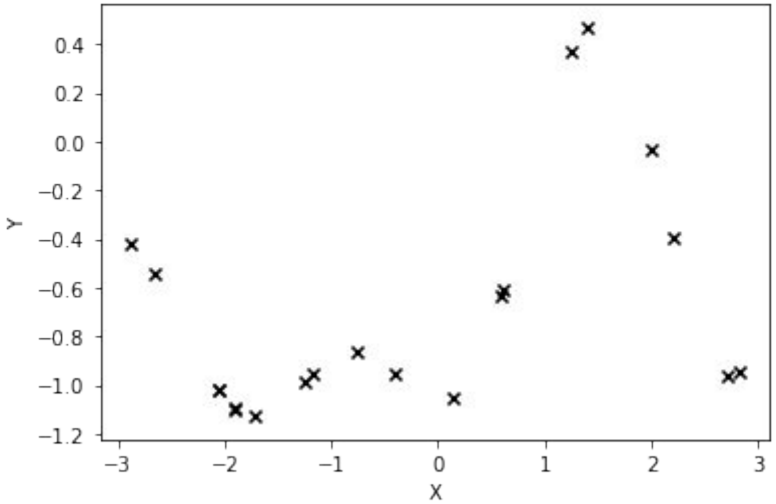
$$\mu = (m(x_1), m(x_2), \ldots, m(x_n))$$

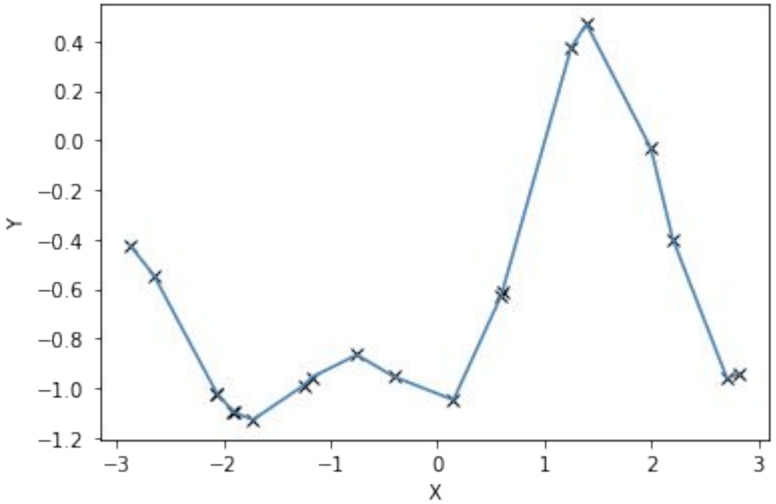
$$\mathbf{K} = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \ldots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \ldots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \ldots & k(x_n, x_n) \end{bmatrix}$$

Gaussian Processes

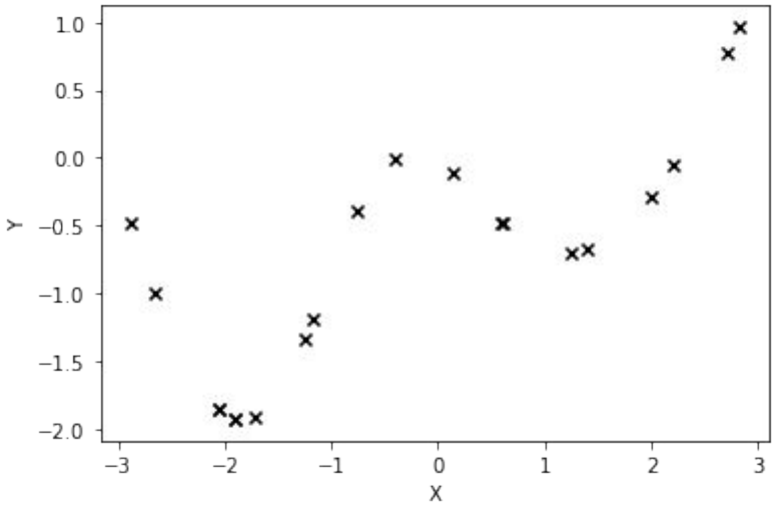


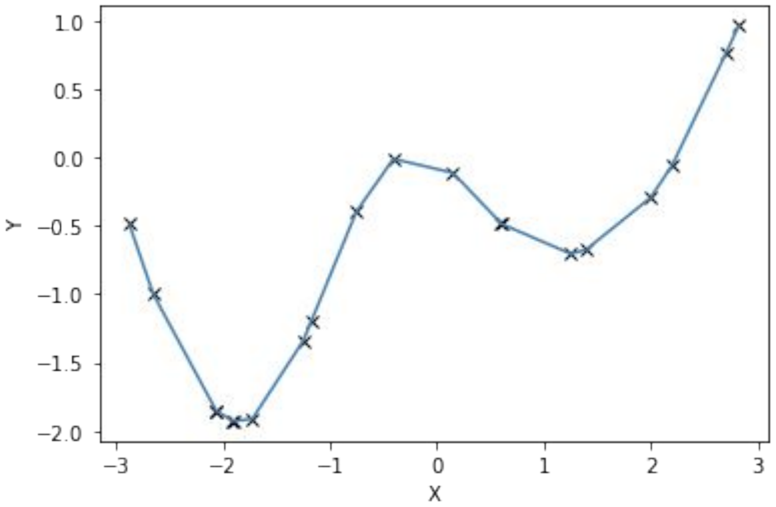
Gaussian Processes



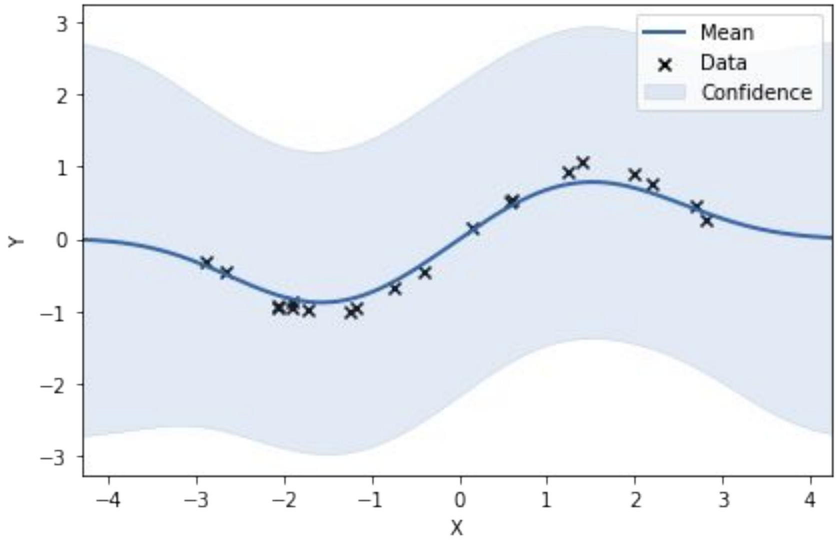


Gaussian Processes

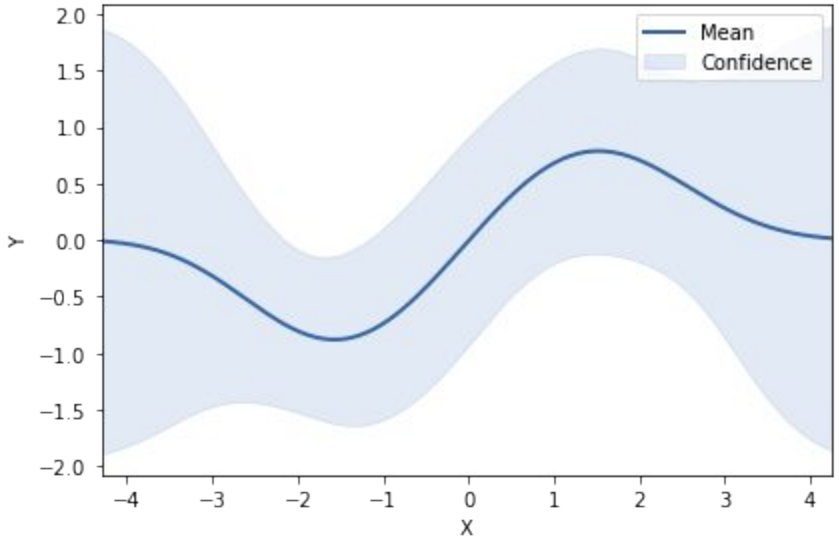




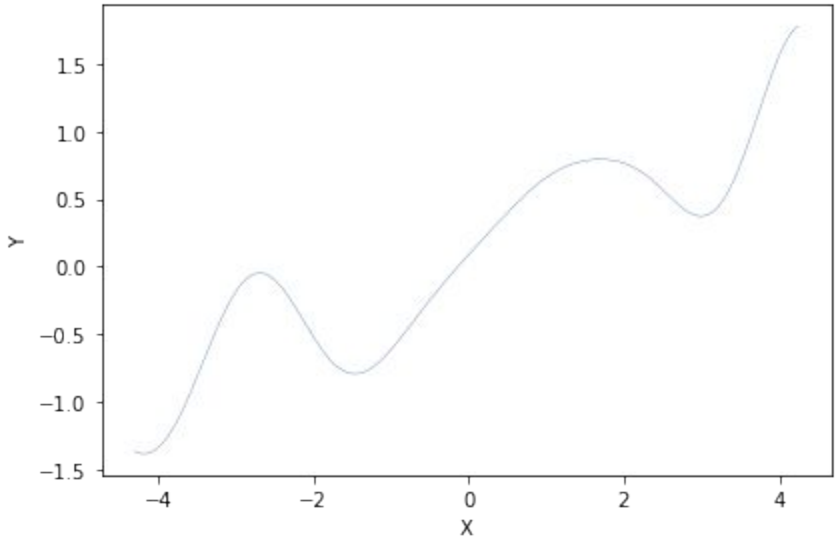
Gaussian Processes



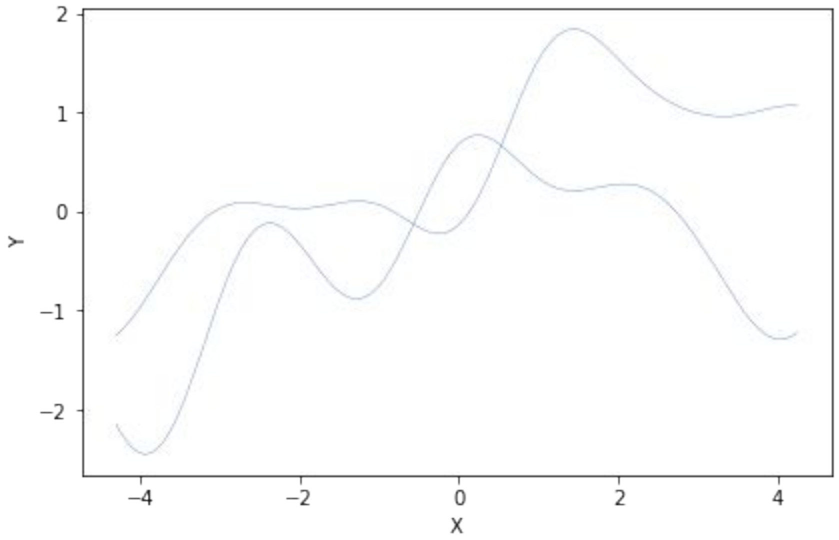
Gaussian Processes



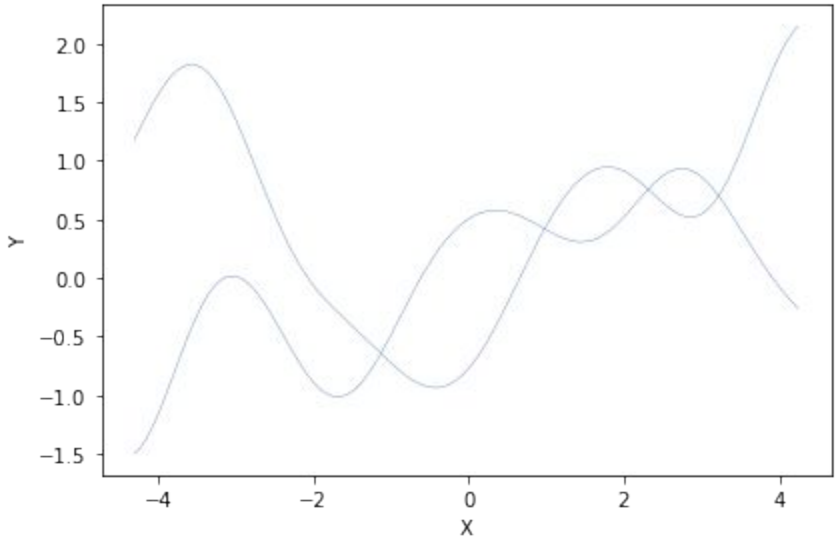
Gaussian Processes



Gaussian Processes

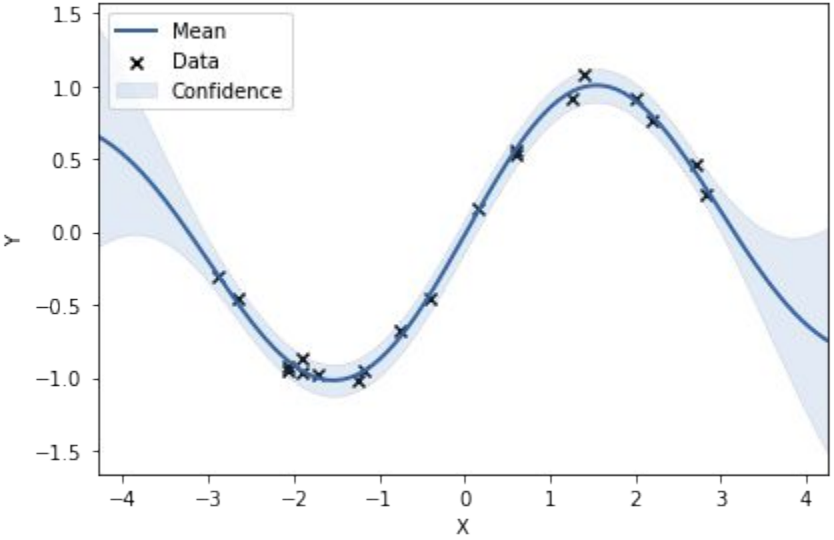


Gaussian Processes

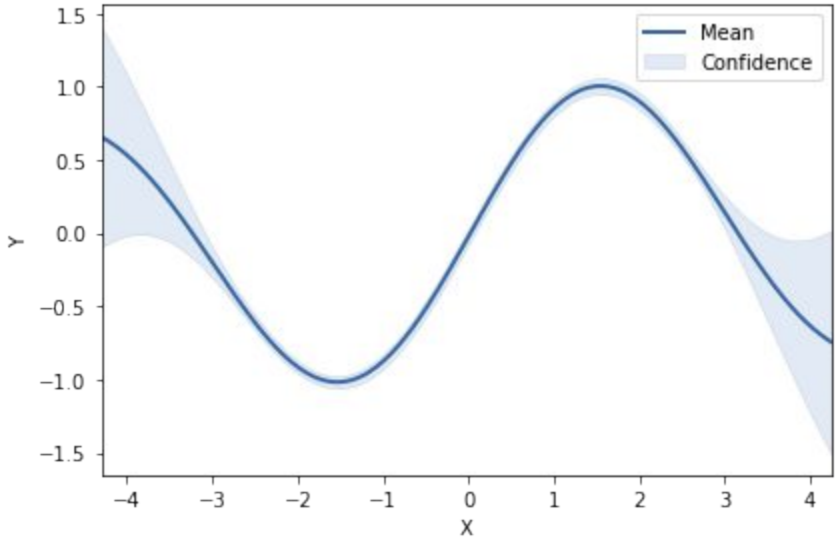


Gaussian Processes

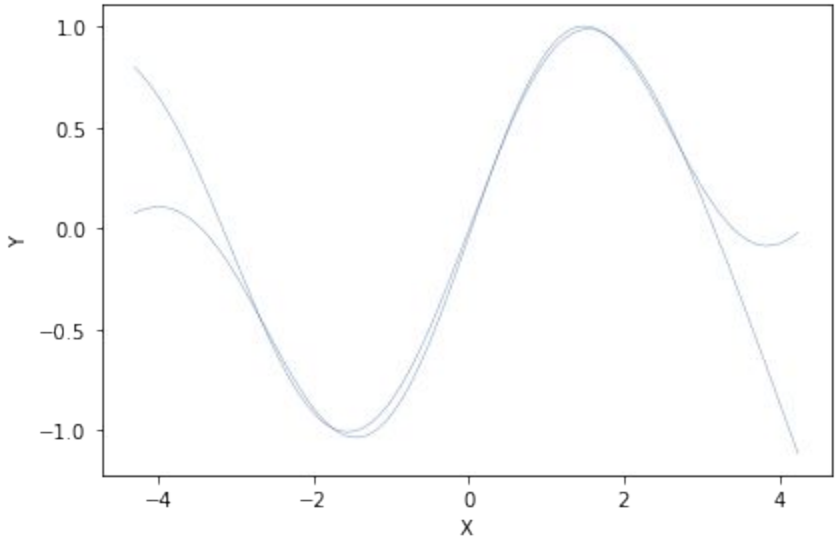
$$p(Y_*|X_*, X, Y) = \mathcal{N}(Y_*|\mu_*, K_*)$$



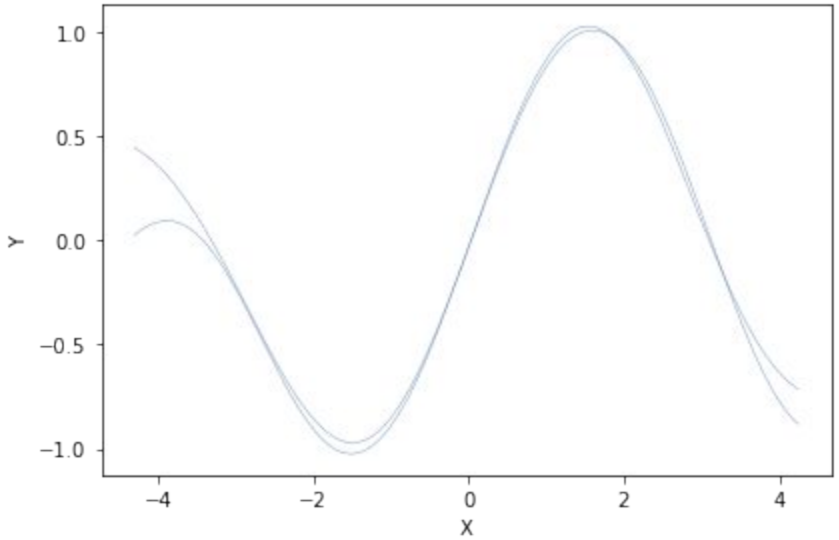
Gaussian Processes



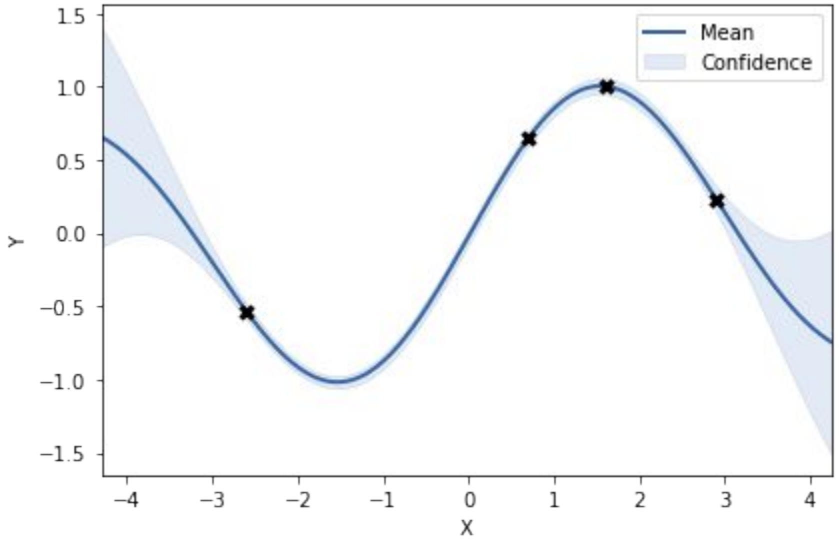
Gaussian Processes



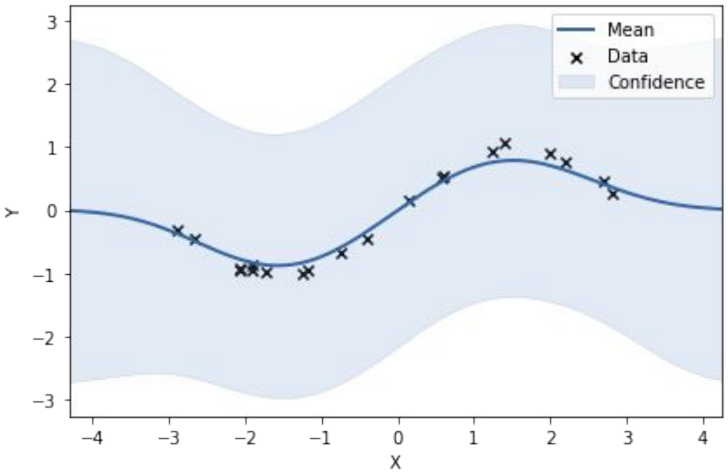
Gaussian Processes



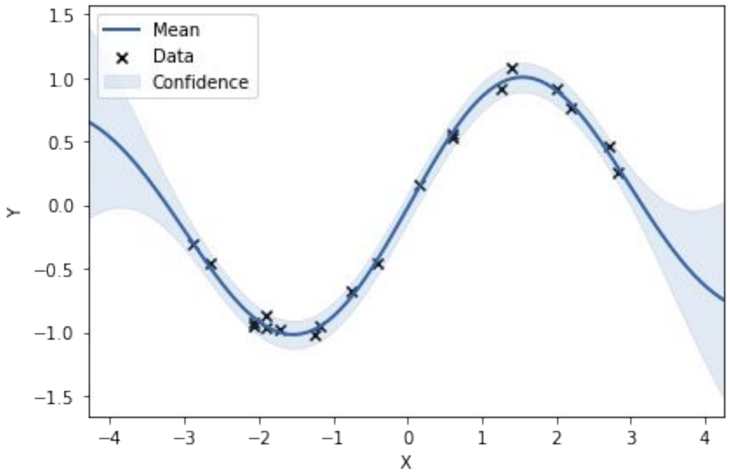
Gaussian Processes



Bayesian Inference



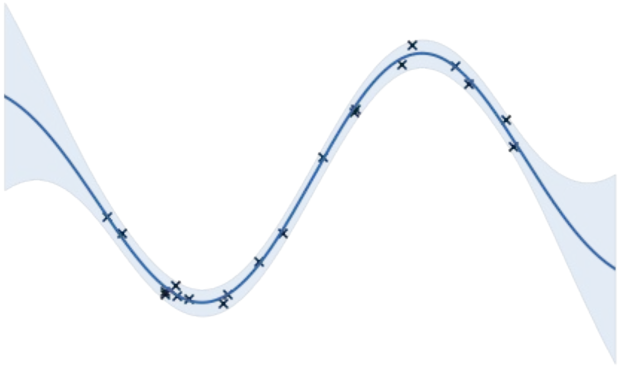
prior



posterior

Bayesian Optimization - How?

Step 1- Surrogate Model



Step 2- Acquisition Functions

Acquisition Functions

- Suggests **new points** which **can be** the **optimum**
- Uses the **mean** and **variance** from the **Gaussian Process posterior**
- Types-

Expected Improvement: $\mathrm{EI}(x) = (\mu - f(x^\star))\Phi\left(\frac{\mu - f(x^\star)}{\sigma}\right) + \sigma\varphi\left(\frac{\mu - f(x^\star)}{\sigma}\right)$

Probability of Improvement: $\mathrm{PI}(x) = \Phi\left(\frac{\mu(x) - f(x^\star)}{\sigma(x)}\right)$

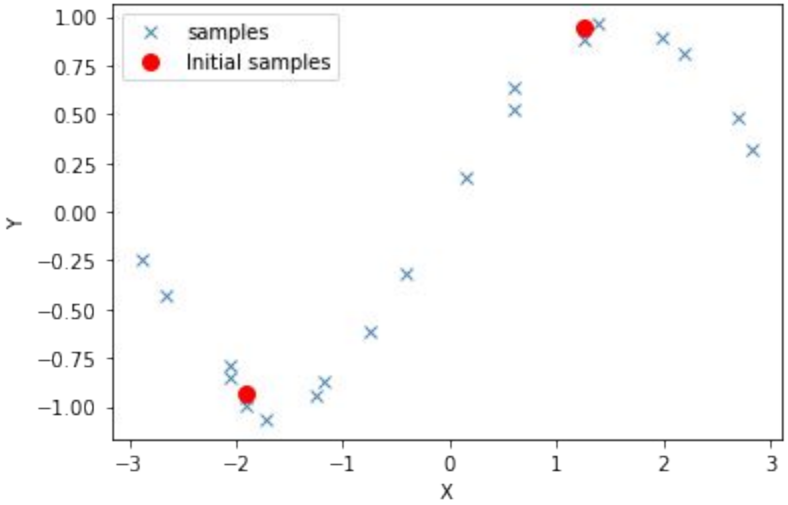
$$\Phi(z) \equiv \mathrm{CDF}(z) \qquad \varphi(z) = \frac{1}{\sqrt{2\pi}}\exp\left(-z^2/2\right)$$

Upper Confidence Bound: $a(x;\lambda) = \mu(x) + \lambda\sigma(x)$

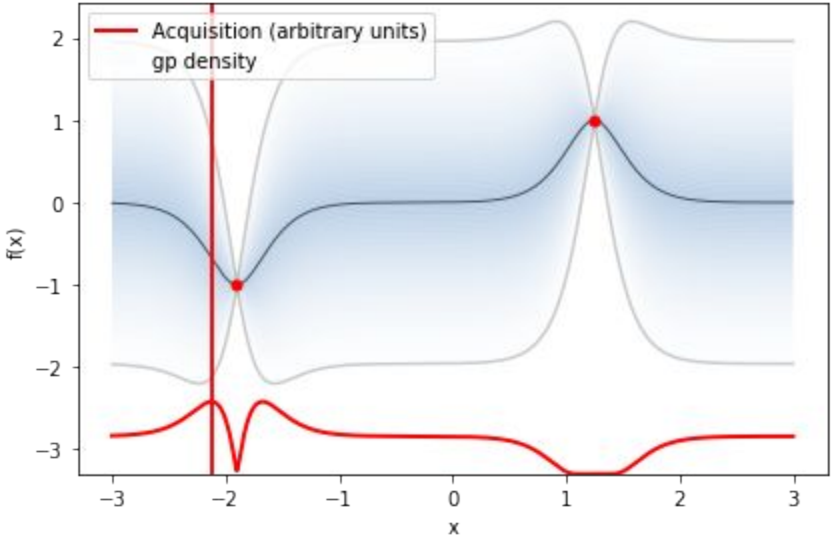
Algorithm

1. Select initial samples- X_i, Y_i
2. Obtain a Gaussian Process posterior
3. Acquisition Function suggests a new point x_{new}
4. Query **f** at x_{new} , get- y_{new}
5. Update gaussian process with (x_{new}, y_{new}) to obtain new posterior
6. Back to step 3
7. Repeat until optimum value

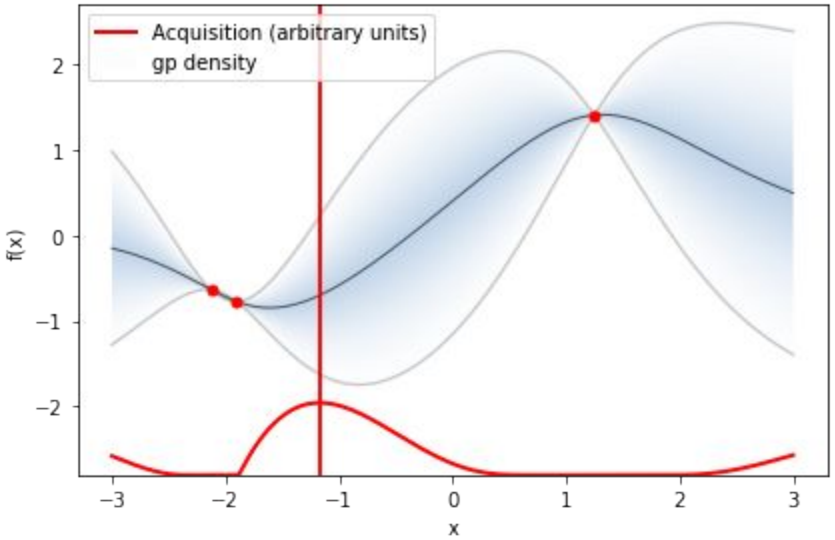
Acquisition Functions



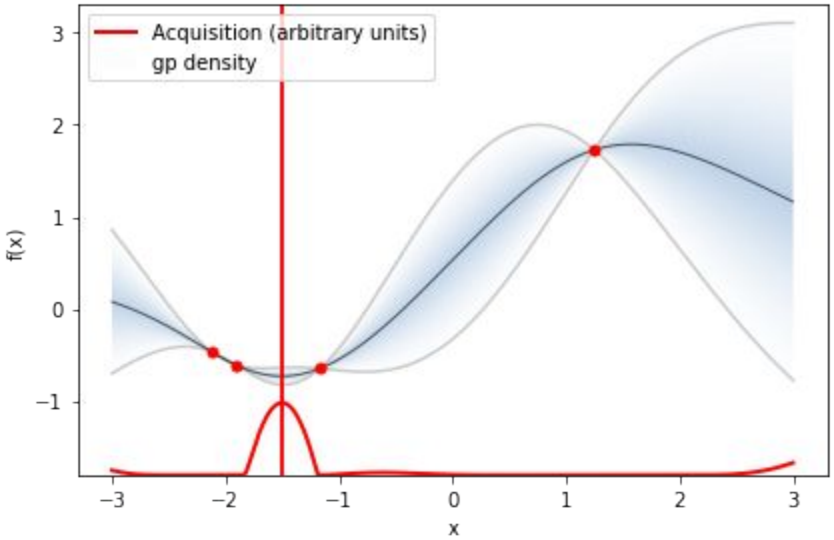
Acquisition Functions



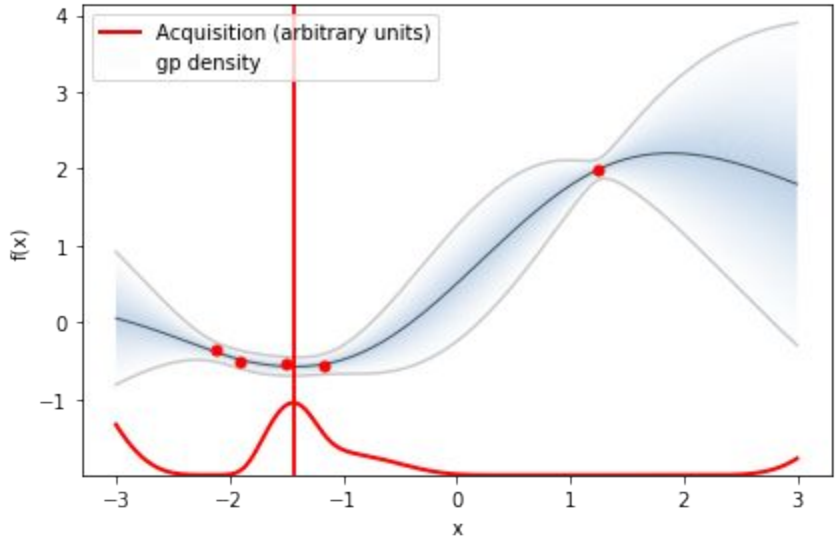
Acquisition Functions



Acquisition Functions



Acquisition Functions



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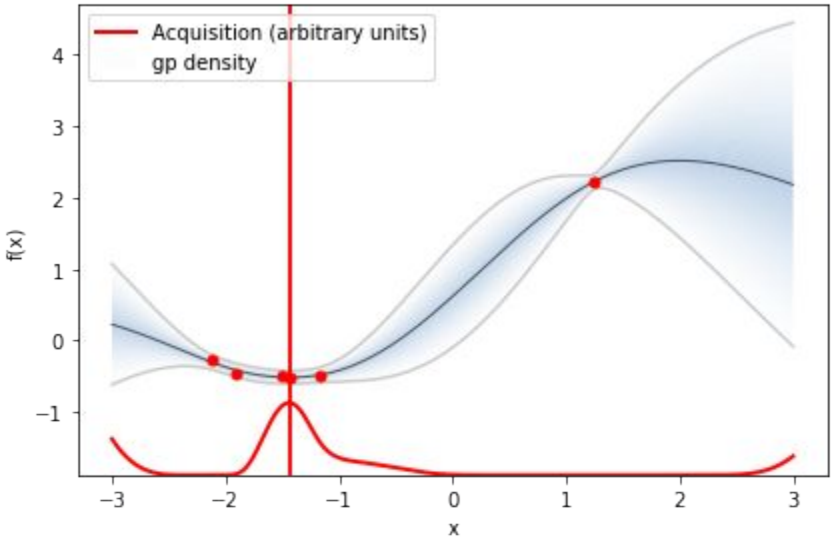


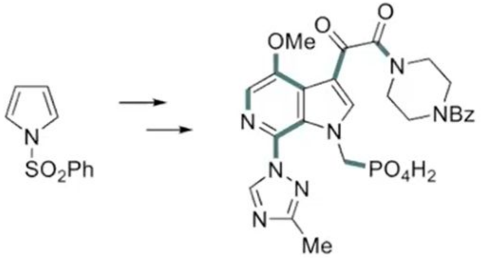
Applications

- Robotics
- Drug Development
- Astronomy
- Graphics and Animation
- Hyperparameter Optimization
- Autonomous Vehicles

Chemistry

Process Optimization

Late-stage synthesis and preparation scale



Experimental HIV inhibitor

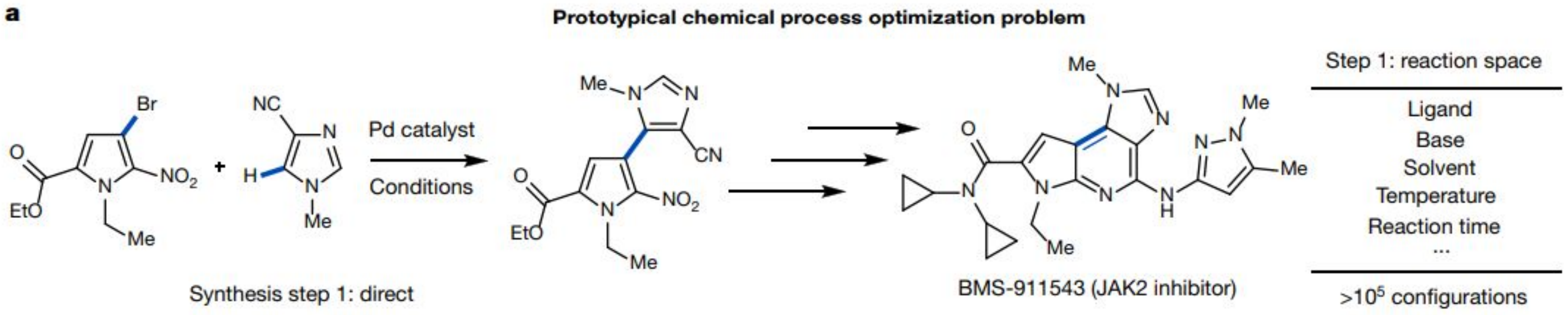
Optimize yield for a single target molecule

Important Experimental Parameters

Categorical
Catalyst (precat./ligand)
Acid/Base
Oxidant/Reductant
Solvent
Additive
...
Continuous
[Concentration]
Equivalents
Temperature
Pressure
Time
...

[Abigail Doyle, Princeton U & Jason Stevens, BMS: Bayesian Optimization for Chemical Synthesis]

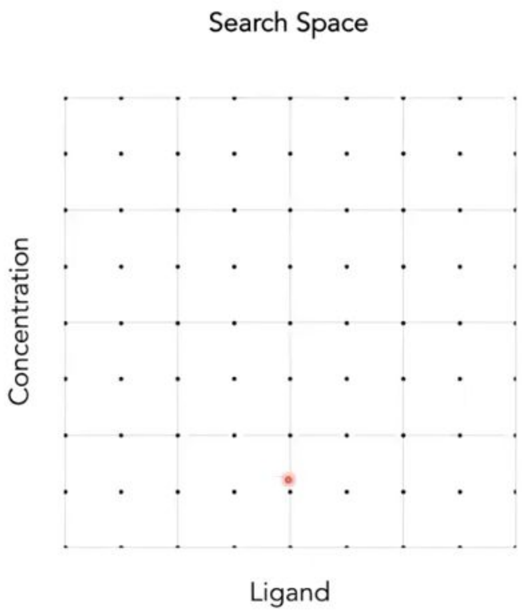
Drug Synthesis

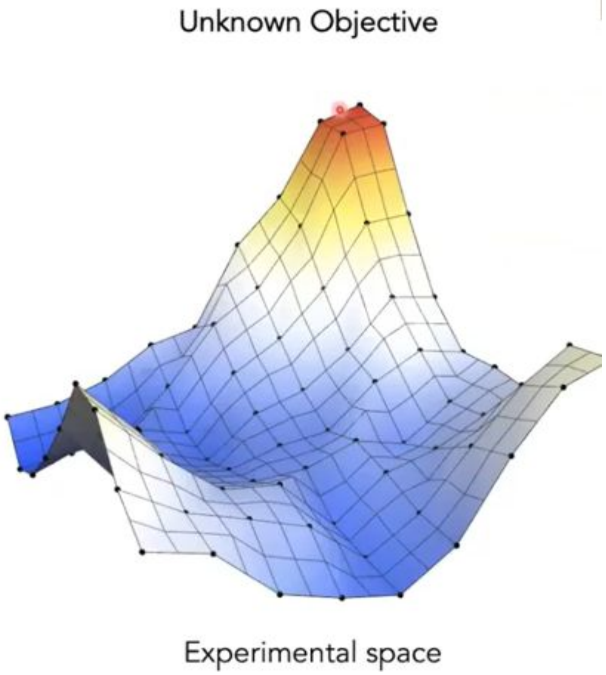


Synthesis of BMS-911543

Shields, B.J., Stevens, J., Li, J. *et al.* Bayesian reaction optimization as a tool for chemical synthesis. *Nature* 590, 89–96 (2021)

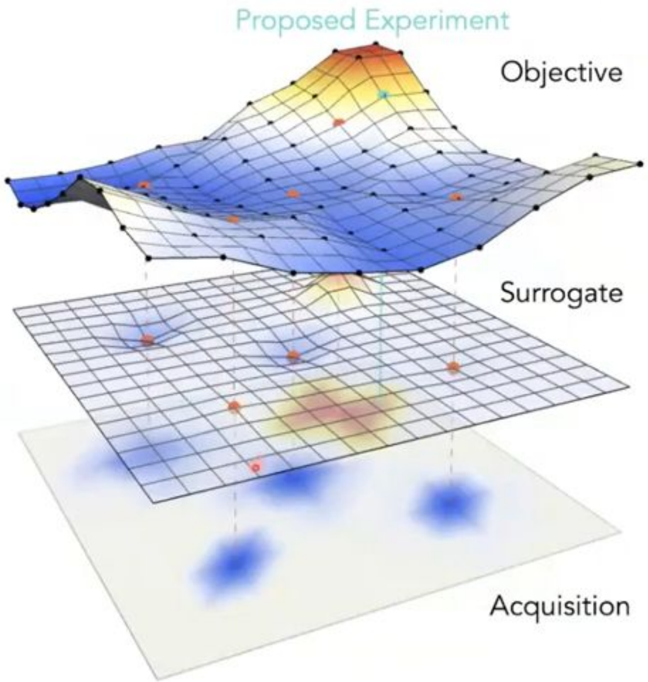
Drug Synthesis





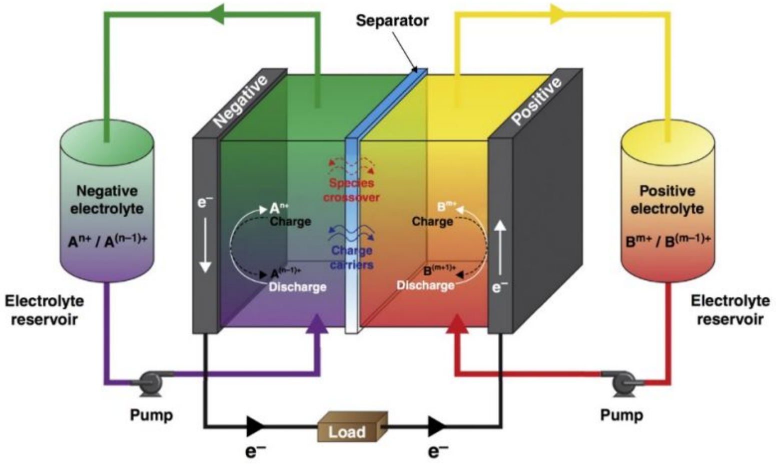
[Abigail Doyle, Princeton U & Jason Stevens, BMS: Bayesian Optimization for Chemical Synthesis]

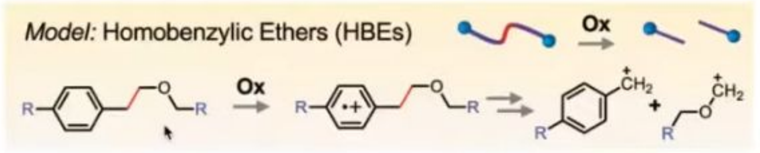
Drug Synthesis



[Abigail Doyle, Princeton U & Jason Stevens, BMS: Bayesian Optimization for Chemical Synthesis]

Materials Discovery





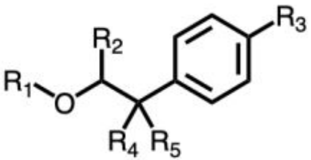
<u>Desirable HBEs' properties</u>:

- Suitable redox potential windows
- High solubility
- Ease of synthesis
- Electrochemical reversibility

[Hieu Doan, Garvit Agarwal, Active Learning via Bayesian Optimization for Materials Discovery](https://nanohub.org/resources/35144), https://nanohub.org/resources/35144

Materials Discovery

HBE scaffold



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SMILES (Simplified Molecular-Input Line Entry System)

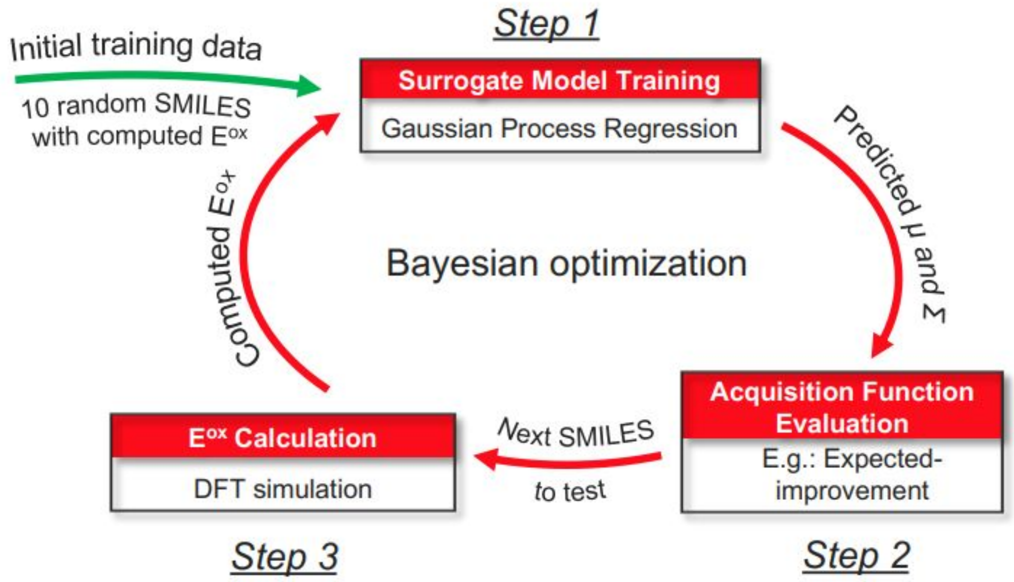
[**R3**]C1=CC=C(C([**R4**])([**R5**])C([**R2**])-[O][**R1**])C=C1

R_1 = -Me, -Et, -Pr, -Ph, -CN, -Eth, -COMe, -C(Me)Me, -CCOMe
R_2 = $-N(Me)_3^+$, -COMe, -Et, -OCMe, $N(Me)_2$, $-NO_2$, -C(=O), -Pr, -C(Me)Me, -CCOMe, -C(Me)OMe
R_3 = $-N(Me)_3^+$, -Me, -COMe, -Br, -C(=O), -OEth, -Pr, -C(Me)Me, -C(COMe), -C(Me)(OMe)
R_4 - R_5 = $-N(Me)_3^+$, -OMe, -COMe, -Br, -N(Me)Me, -Et, -OEt, $-NO_2$, -C(=O), -Pr, -C(Me)Me, -C(COMe), -C(Me)(OMe)

-> 10^5 molecules

[Hieu Doan, Garvit Agarwal, Active Learning via Bayesian Optimization for Materials Discovery]

Materials Discovery



[Hieu Doan, Garvit Agarwal, Active Learning via Bayesian Optimization for Materials Discovery]

Robotics

Action executed

Current state

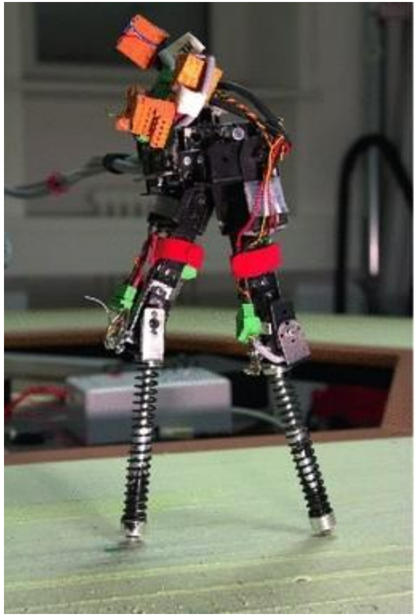
$$a_t = \pi(s_t, \theta)$$

Parameters of the policy

Policy (i.e., parametrized controller)

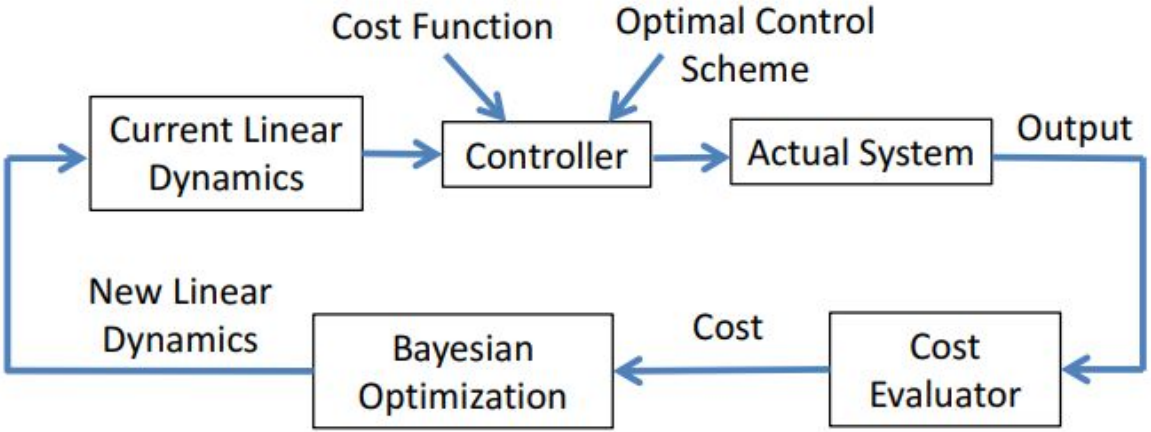
Learning a controller is equivalent to optimizing the parameters of the controller

$$\theta^* = \arg\max_\theta R[\pi(\theta)]$$



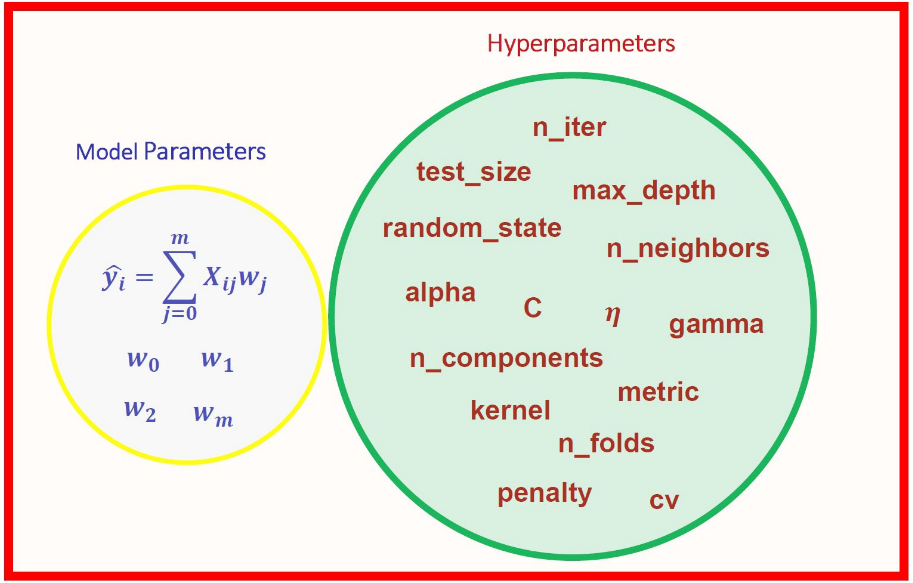
Calandra, R.; Seyfarth, A.; Peters, J. & Deisenroth, M. P. Bayesian Optimization for Learning Gaits under Uncertainty Annals of Mathematics and Artificial Intelligence (AMAI), 2015, 76, 5-23

Robotics



Somil Bansal, Roberto Calandra, Ted Xiao, Sergey Levine, and Claire J. Tomiin. 2017. Goal-driven dynamics learning via Bayesian optimization. In 2017 IEEE 56th Annual Conference on Decision and Control (CDC). IEEE Press, 5168–5173.

Hyperparameter Optimization



Jia Wu, Xiu-Yun Chen, Hao Zhang, Li-Dong Xiong, Hang Lei, Si-Hao Deng, Hyperparameter Optimization for Machine Learning Models Based on Bayesian Optimization,Journal of Electronic Science and Technology,Volume 17, Issue 1 ,2019,Pages 26-40

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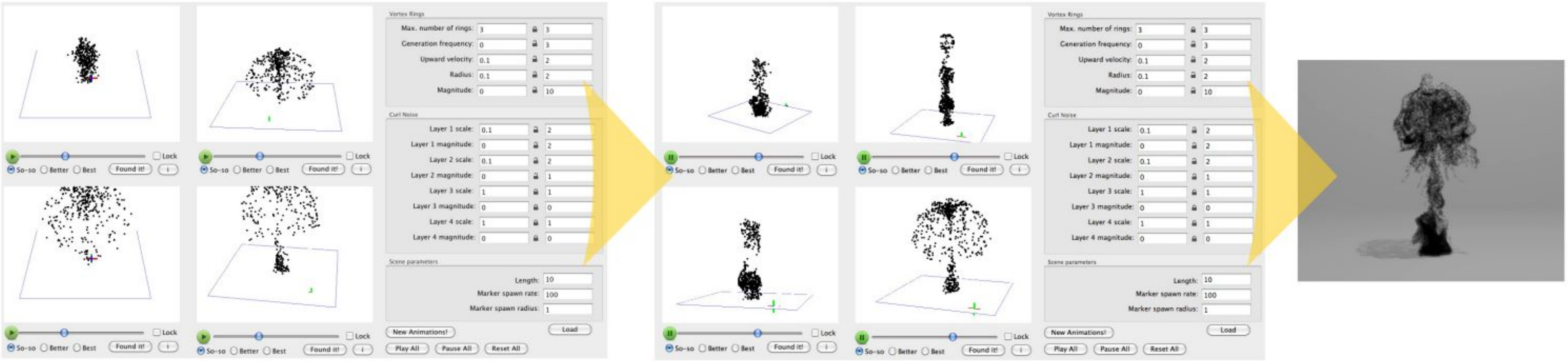
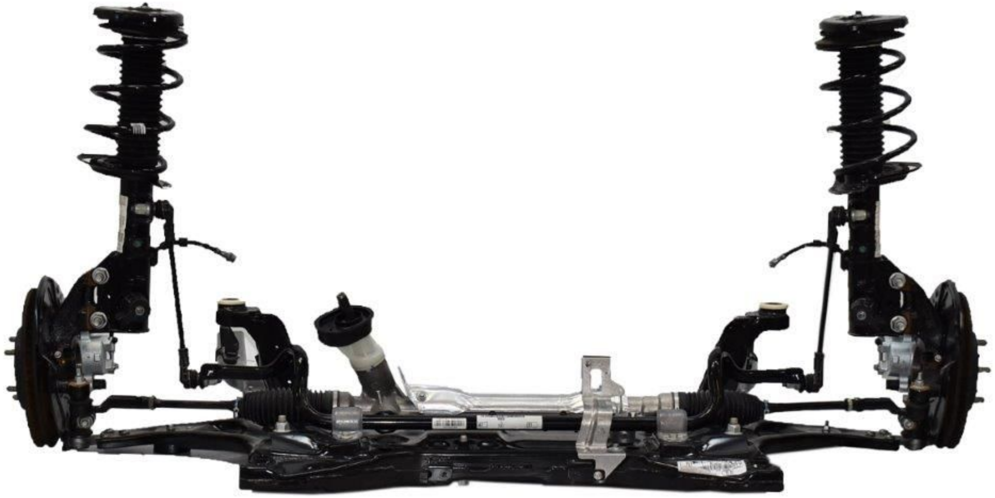
Computer Graphics and Visual Design



Eric Brochu, Tyson Brochu, and Nando de Freitas. 2010. A Bayesian interactive optimization approach to procedural animation design. In Proceedings of the 2010 ACM SIGGRAPH/Eurographics Symposium on Computer Animation (SCA '10). Eurographics Association, Goslar, DEU, 103–112.

MacPherson Architecture Front Suspension



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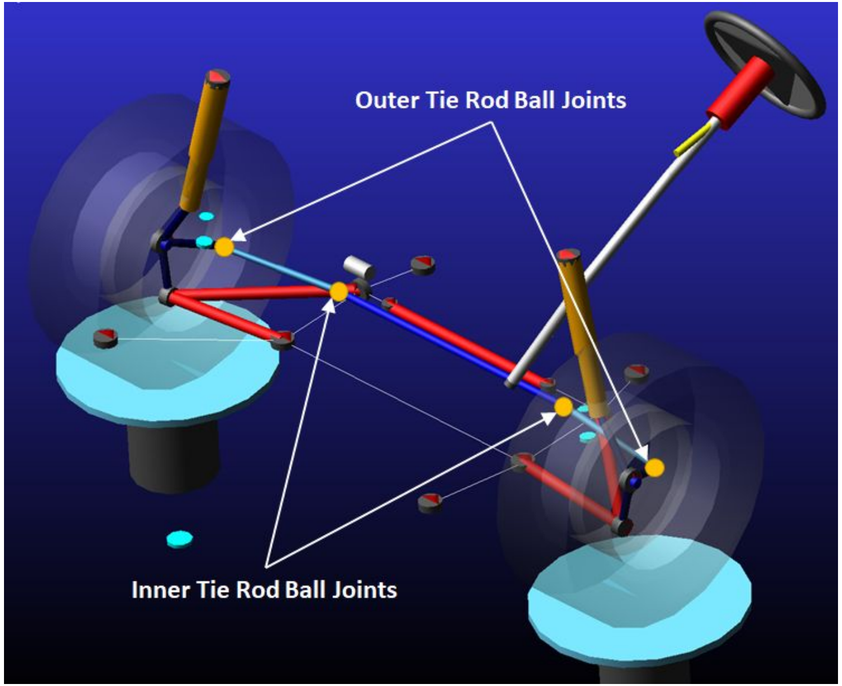
MacPherson Architecture Front Suspension



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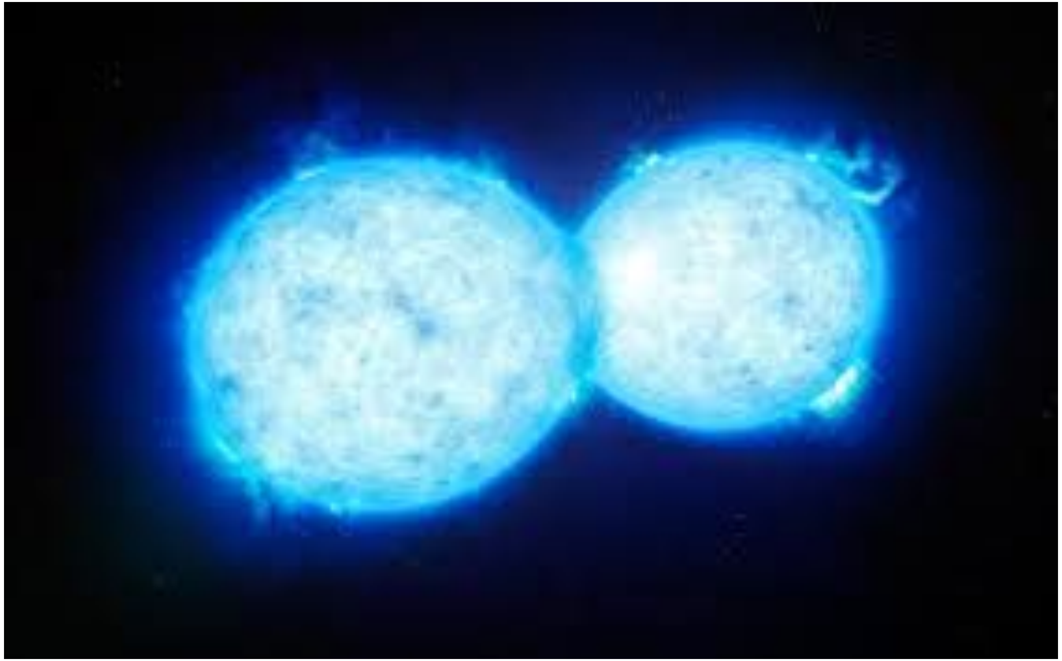
VFTS352 Stellar Parameter



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