A Tutorial on Bayesian Optimization

Darian Nwankwo

Introduction

Problem motivation

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where f is a black-box. Subject to:

- evaluation is expensive
- observations may be noisy
- may only observe the function value (no gradients)

Real-world examples

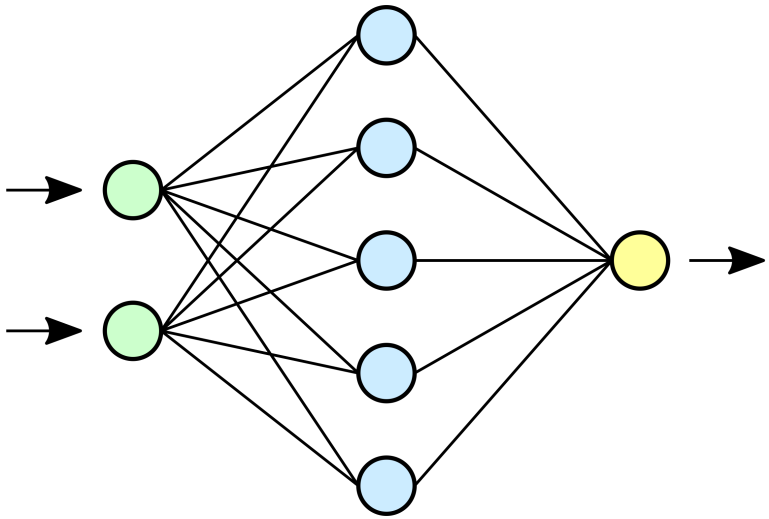


Figure: Neural Network

Hyperparameter configuration for deep neural networks

Real-world examples

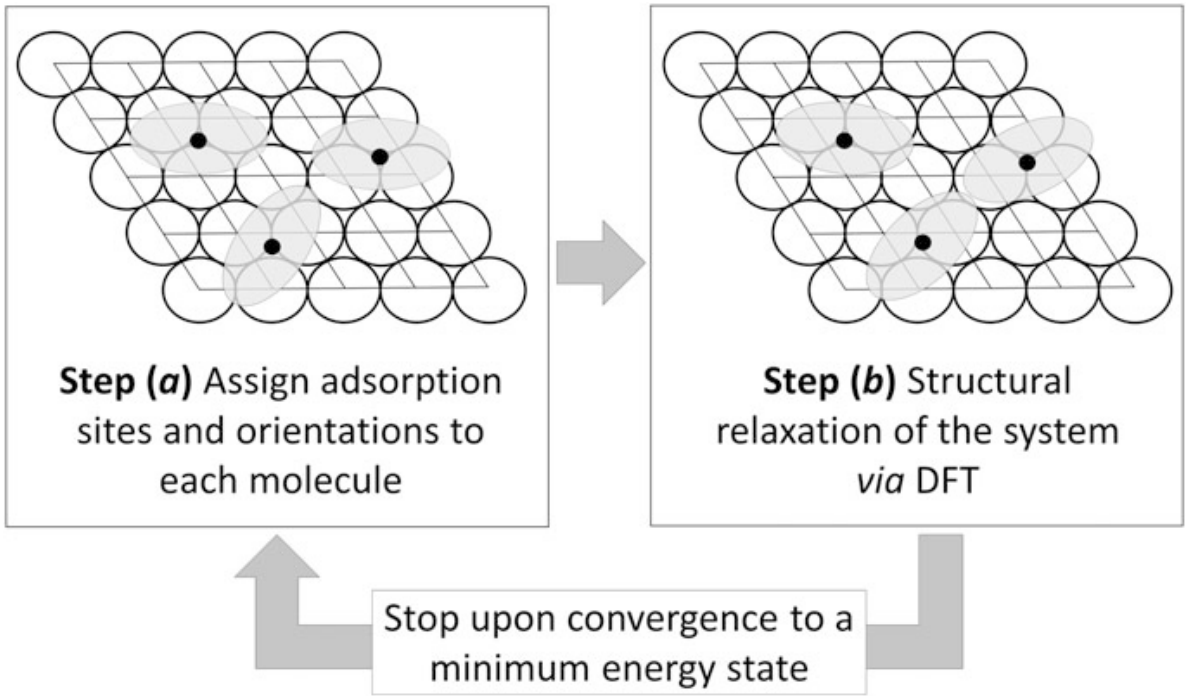


Figure: Conformation of molecules absorbed to a surface

Optimization of absorption sites and orientations for molecules in material science

Real-world examples

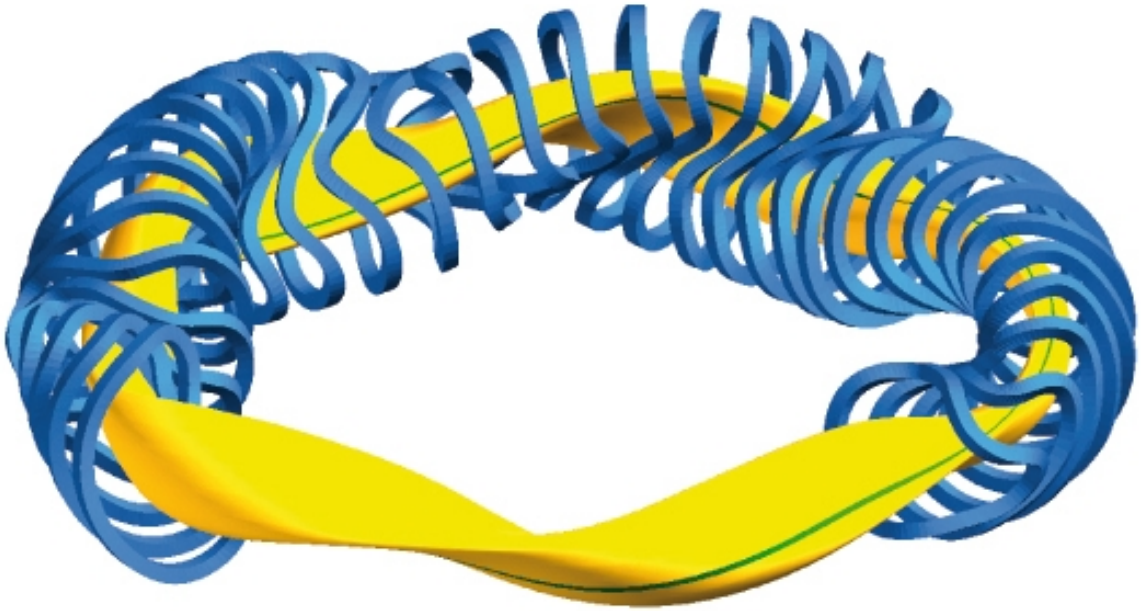
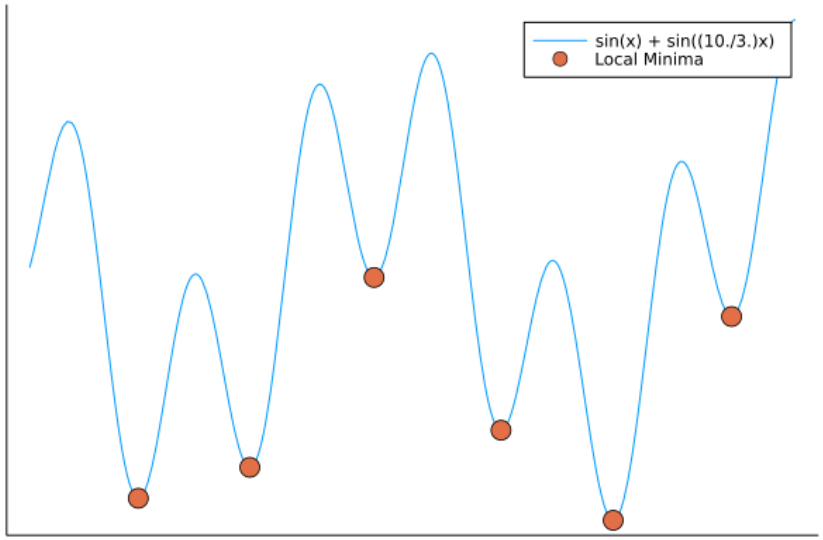


Figure: Stellarator Configuration

Optimal geometry of stellarators in plasma physics for fusion energy

Local and Global Optimization

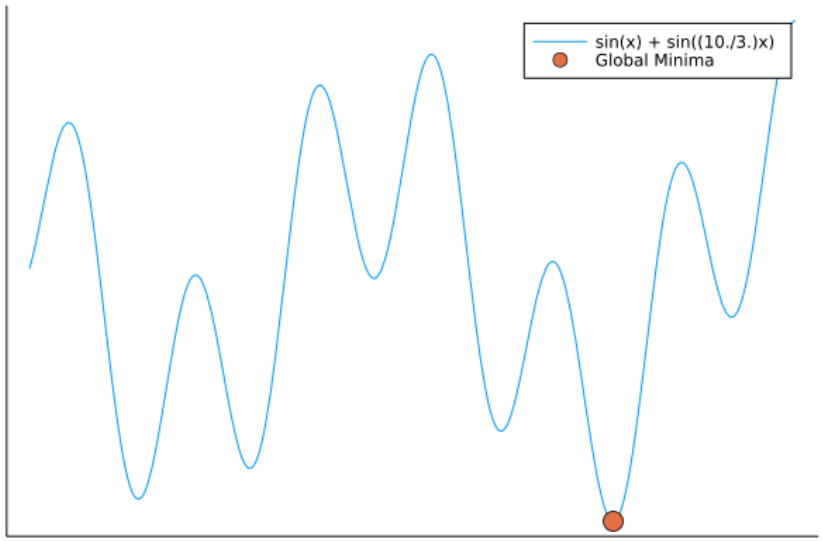
Local optimization



The point x^* is a strong local minimum of F if there exists $\delta > 0$ such that

- $F(x)$ is defined on $N(x^*, \delta)$
- $F(x^*) < F(y)$ for all $y \in N(x^*, \delta)$, $y \neq x^*$

Global optimization



The point x^* is a global minimum of F if

- $F(x^*) < F(y)$ for all $y \in D$, $y \neq x^*$

Recap and takeaways

- Characterizing local optima is easy

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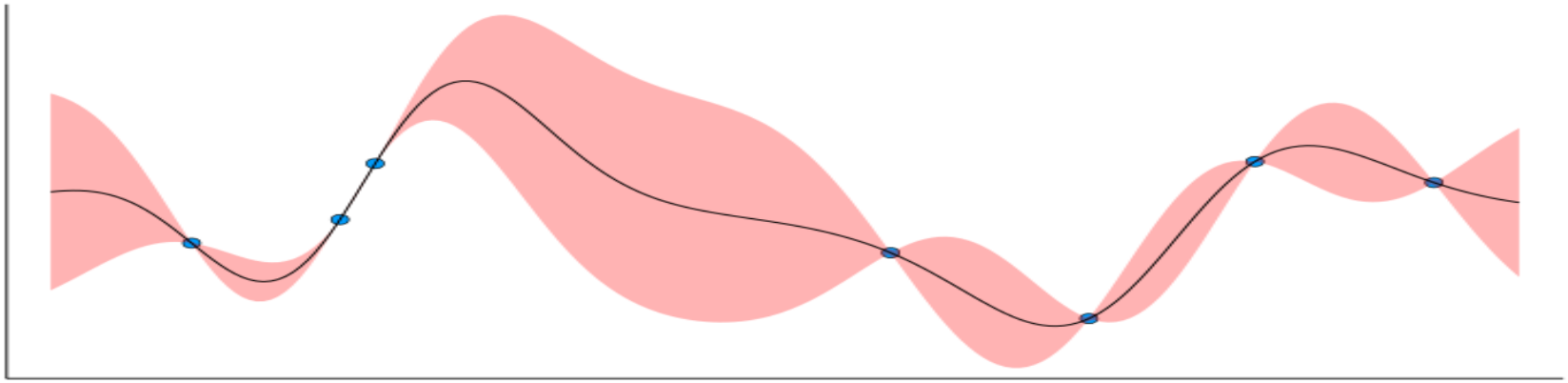
- Characterizing local optima is easy
- Characterizing global optima is harder

Gaussian Processes

Definition of a Gaussian process



A Gaussian process (GP) is a collection of random variables, any finite number of which have a joint Gaussian distribution.

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

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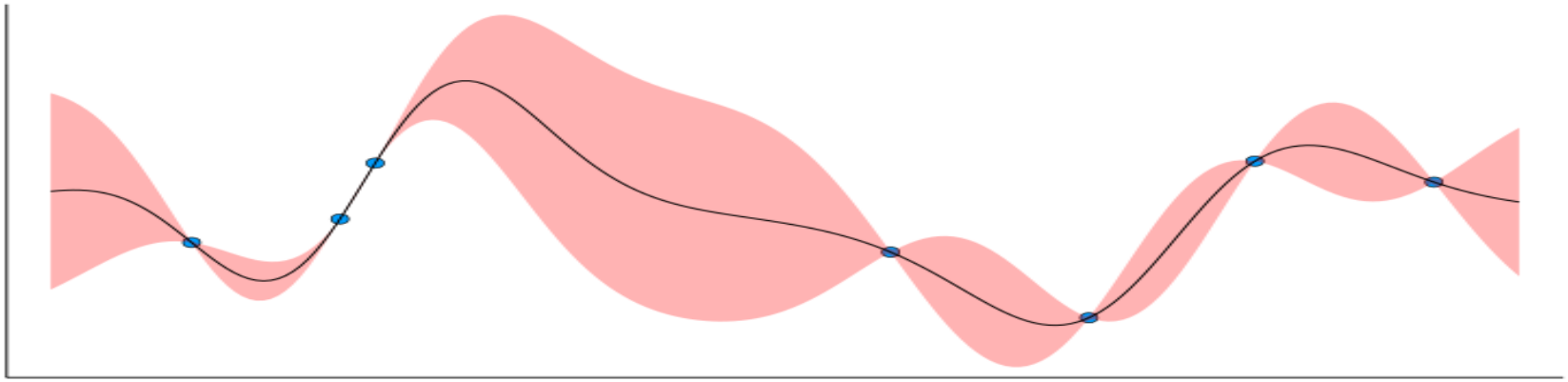

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$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')\right)$$

where $m(\cdot)$ is the mean function and $k(\cdot, \cdot)$ is the covariance function.

$$\begin{aligned} m(\mathbf{x}) &= \mathbb{E}\left[f(\mathbf{x})\right] \\ k(\mathbf{x}, \mathbf{x}') &= \mathbb{E}\left[\left(f(\mathbf{x}) - m(\mathbf{x})\right)\left(f(\mathbf{x}') - m(\mathbf{x}')\right)\right] \end{aligned}$$

Kernels as a measure of covariance

Kernel	Formula
Squared Exponential (SE)	$s^2 \exp(-\frac{r^2}{2\ell^2})$
Matern 3/2	$s^2(1+\frac{\sqrt{3}r}{\ell})\exp(-\frac{\sqrt{3}r}{\ell})$
Linear	$x^T x'$

Figure: A few popular RBF kernels.

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- Each kernel has hyperparameters θ

Learning optimal kernel hyperparameters

- To learn hyperparameters in kernel, we need values and gradients of:

$$\mathcal{L}(y_X|\theta) = \mathcal{L}_y + \mathcal{L}_{|K|} - \frac{n}{2}\log(2\pi).$$

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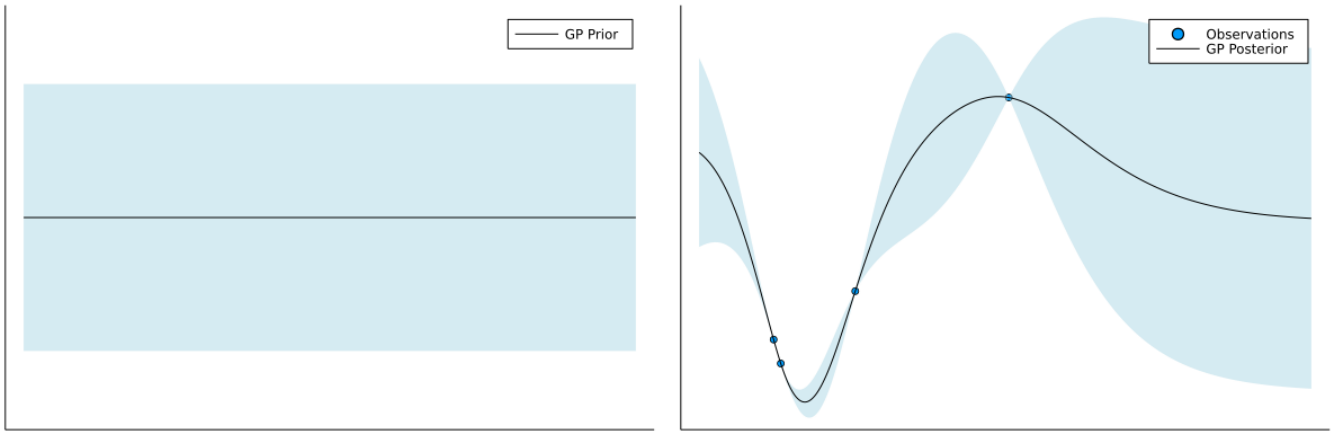
- Complexity penalty:

$$\mathcal{L}_{|K|} = -\frac{1}{2}\log|\widetilde{K}_{XX}|.$$

Gaussian process regression



- Suppose we have computed n potentially noisy samples $y_j = f(x^j) + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$
- $X = \begin{bmatrix} x^1 & x^2 & \dots & x^n \end{bmatrix}$ and values $y = \begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix}^T$

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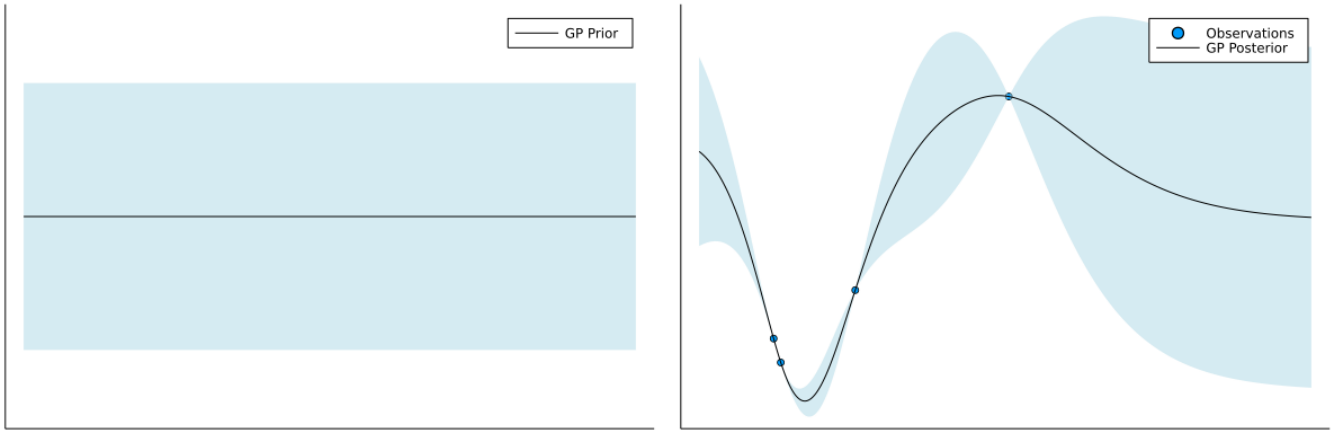

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- Posterior prediction at $\bar{x}$ is $\hat{f}(\bar{x}) \sim \mathcal{N}(\mu_{\bar{x}}, \hat{K}_{\bar{x}\bar{x}})$:

$$\mu_{\bar{x}} = K_{X\bar{x}}^T c \ , \ \hat{K}_{\bar{x}\bar{x}} = K_{\bar{x}\bar{x}} - K_{X\bar{x}}^T \widetilde{K}_{XX}^{-1} K_{X\bar{x}}$$

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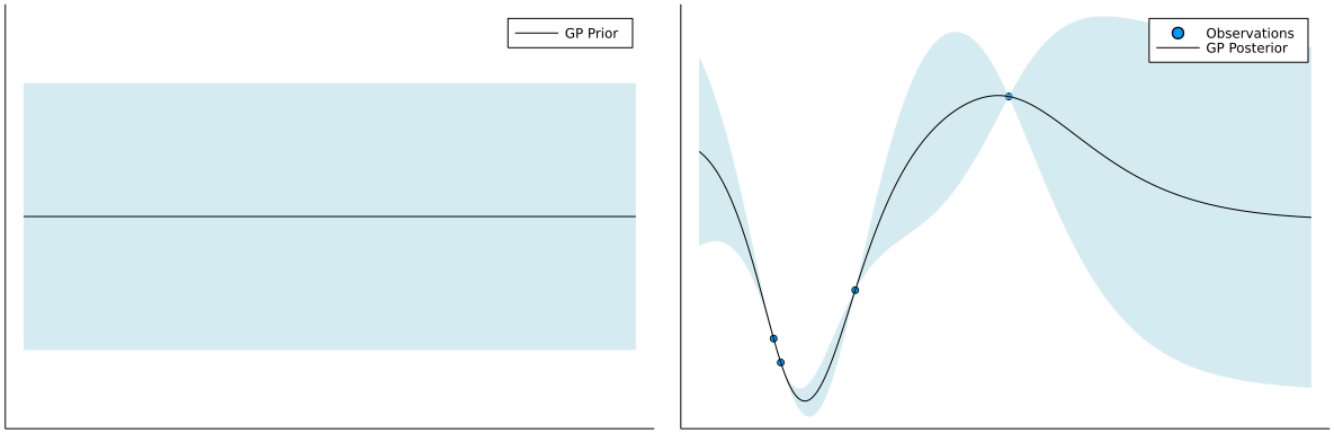

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- Where the coefficients c are the solution to this system of equations:

$$\widetilde{K}_{XX} c = y, \widetilde{K}_{XX} = K_{XX} + \sigma_n^2 \mathcal{I}$$

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- Our choice of kernel defines the function space
- GPs allow us to perform inference while quantifying our uncertainty

Bayesian Optimization

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6. Repeat until the budget is exhausted
7. Make final recommendation

BO: 1. Gather Initial Samples (if any)

Gathering our initial samples is trivial and we denote the collection of covariates and their respective observations as such:

$$X = \begin{bmatrix} x^1 & x^2 & \dots & x^n \end{bmatrix}$$
$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix}^T$$

where $x^j \in \mathbb{R}^d$, $\forall \quad 1 \leq j \leq n$

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- Or, in the nomenclature of Bayesian statistics, computing the posterior probability distribution.

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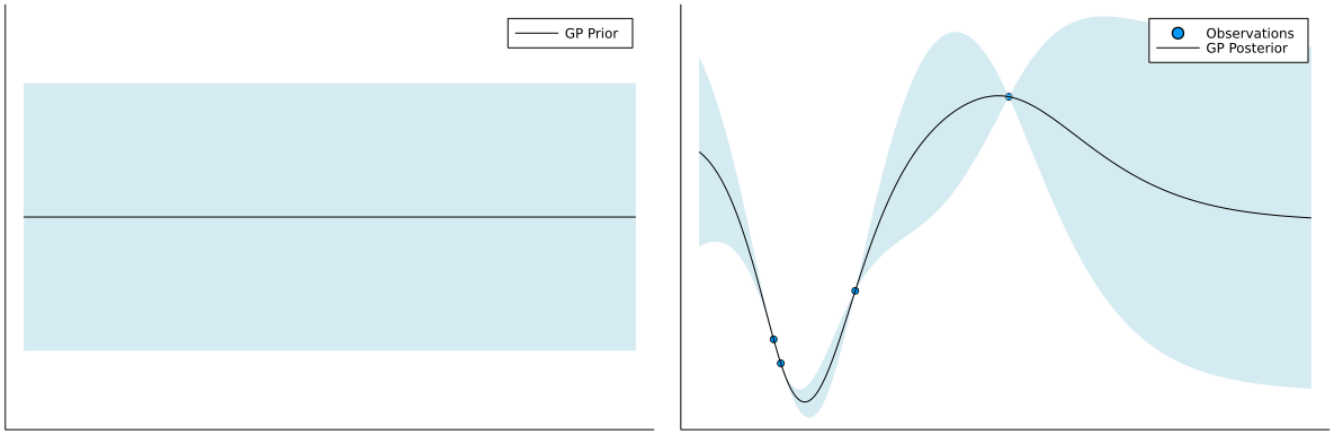

Therefore, predictions (f_*) at test locations (X_*) is computed as follows:

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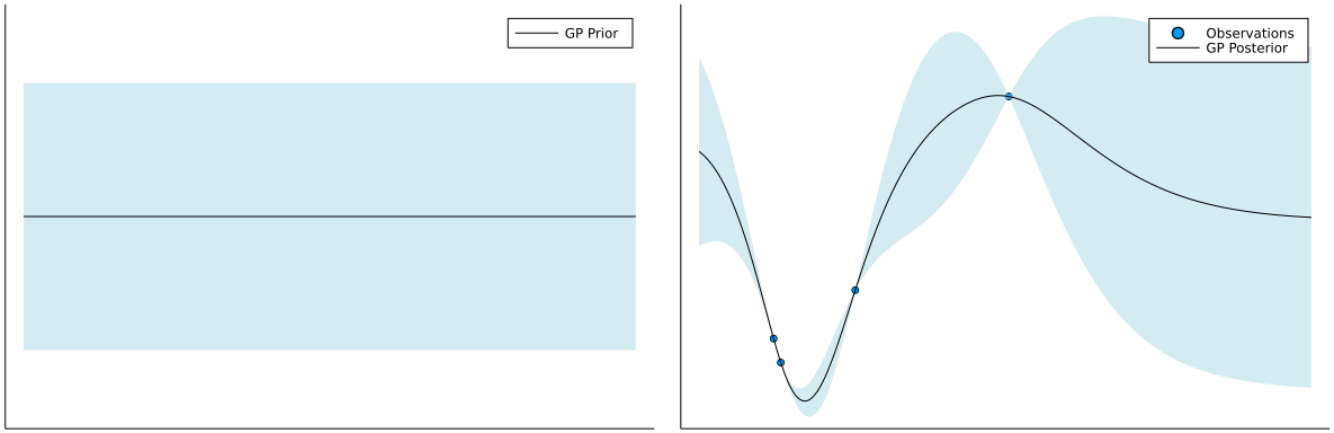

Therefore, predictions (f_*) at test locations (X_*) is computed as follows:

$$f_*|X, \mathbf{y}, X_* \sim \mathcal{N}(\bar{f}_*, cov(f_*)), \quad \textit{where}$$

$$\bar{f}_* \triangleq \mathbb{E}\left[f_*|X, \mathbf{y}, X_*\right]$$

$$= K(X_*, X)\left[K(X, X) + \sigma_n^2 \mathcal{I}\right]^{-1} \mathbf{y}$$

$$cov(f_*) = K(X_*, X_*) - K(X_*, X)\left[K(X, X) + \sigma_n^2 \mathcal{I}\right]^{-1} K(X, X_*)$$

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- The acquisition function drives our sampling process, i.e. where should we look next to update our beliefs so as to gain as much "information" as possible, while leveraging well known regions as well.

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  - We call this the "exploration-exploitation tradeoff".

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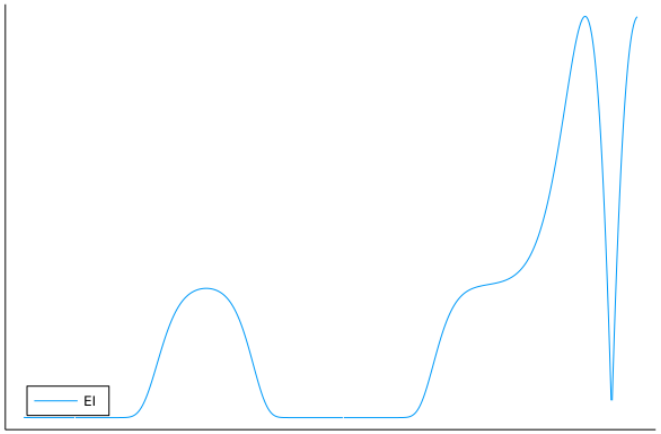

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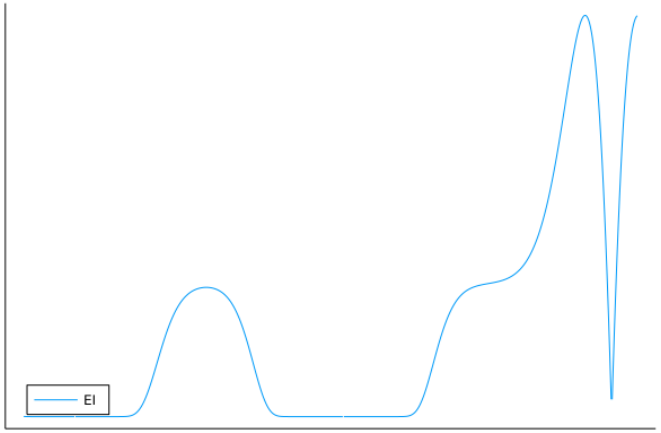

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$$EI(x) = z\sigma\Phi(z) + \sigma\phi(z)$$
$$POI(x) = \Phi(z)$$
$$UCB(x) = \mu + \kappa\sigma$$

where $z = \left(\mu - f^{+} - \xi\right)/\sigma$, μ, σ are functions of x, Φ is standard normal CDF and ϕ is standard normal PDF.

BO: 3. Construct Acquisition Function $\alpha(x)$

Regardless of the acquisition function, we denote it as:

$$\alpha(x)$$

which can be thought of as a scoring function on the viability of candidate location x.

BO: 4. Optimize Acquisition Function

Optimizing our acquisition functions informs us of where we should sample next:

$$x_{opt} = \underset{x \in A}{\text{argmax}}\, \alpha(x) \implies \nabla \alpha(x_{opt}) = \mathbf{0}$$

BO: 5. Update Surrogate w/New Data

Condition our model on our new observation:

$$X_{update} = \begin{bmatrix} x^1 & x^2 & \dots & x^n & x_{opt} \end{bmatrix}$$
$$\mathbf{y}_{update} = \begin{bmatrix} y_1 & y_2 & \dots & y_n & y_{opt} \end{bmatrix}^T$$

where $x^j \in \mathbb{R}^d$, $\forall \quad 1 \leq j \leq n+1$

BO: 6. Repeat Until Budget Is Exhausted

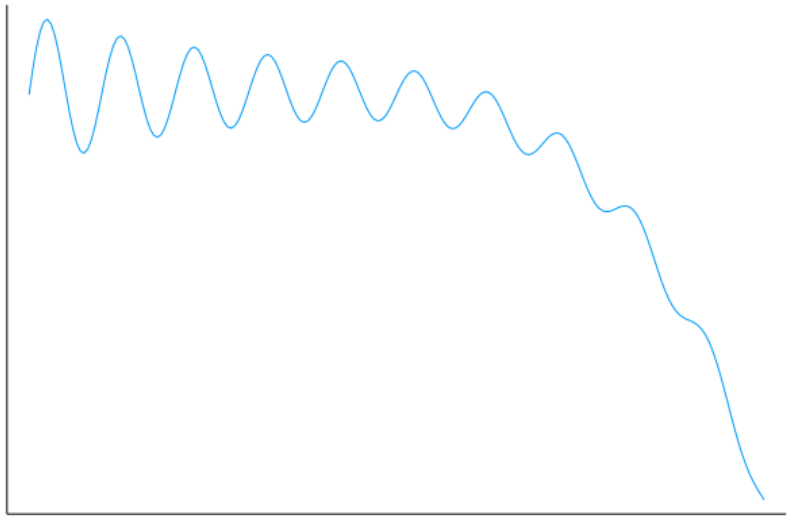
AND REPEAT

BO: 7. Make Final Recommendation

Once our budget is exhausted, we propose the best point we've seen thus far as our final recommendation.

Bayesian Optimization in 1D

7 Steps to Bayesian Optimization



Bayesian optimization steps:

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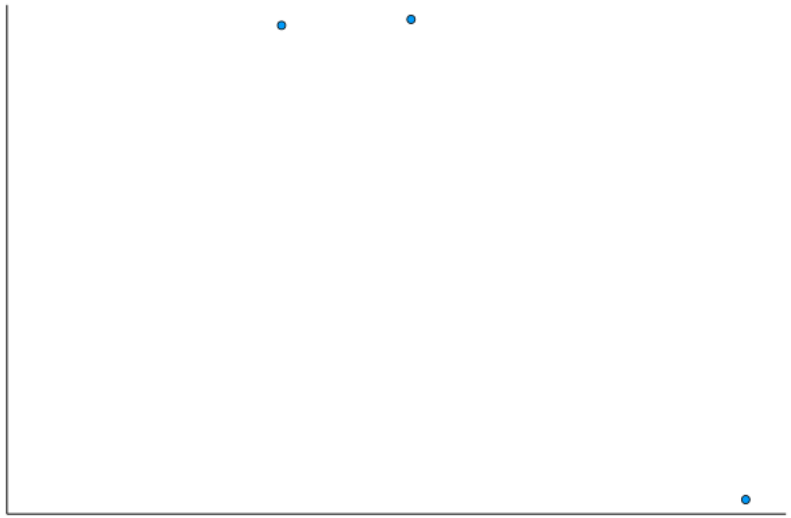

Bayesian optimization steps:

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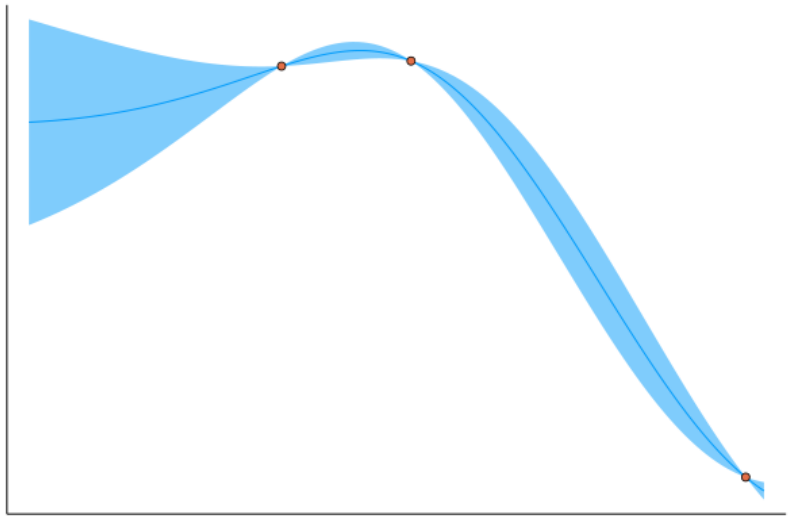

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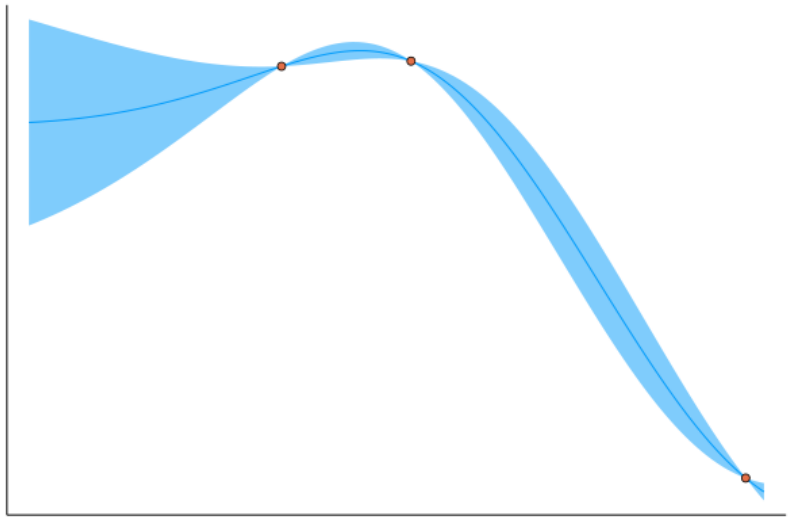

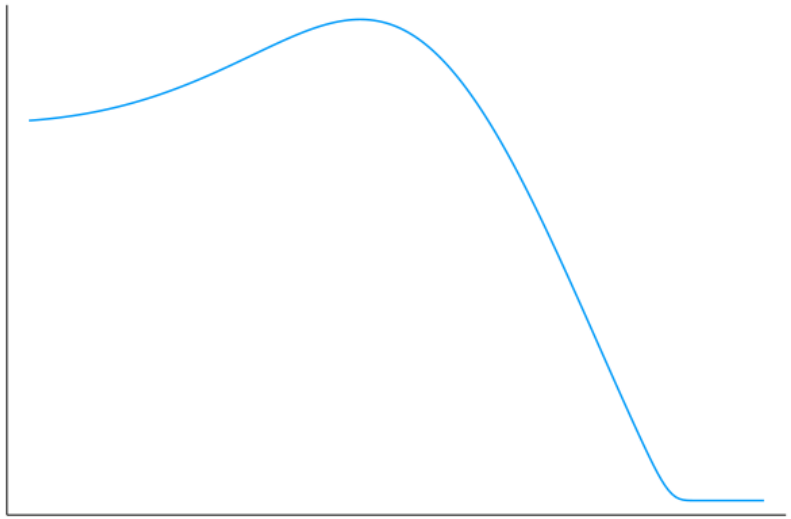

Bayesian optimization steps:

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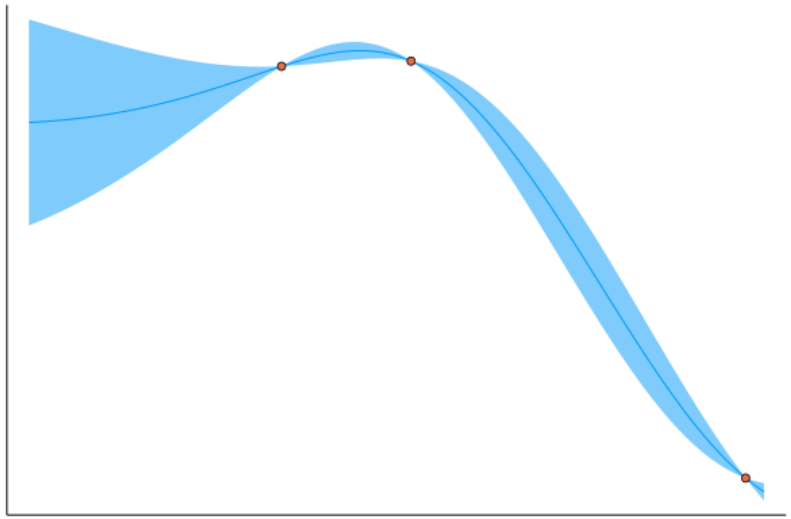

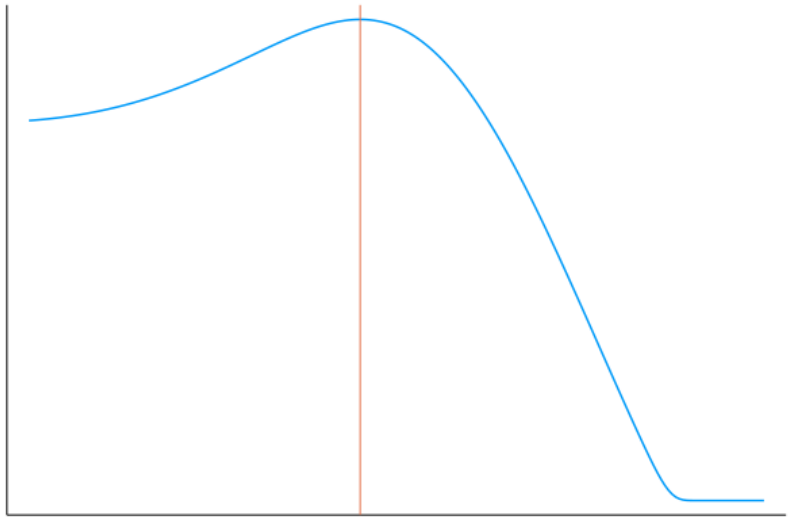

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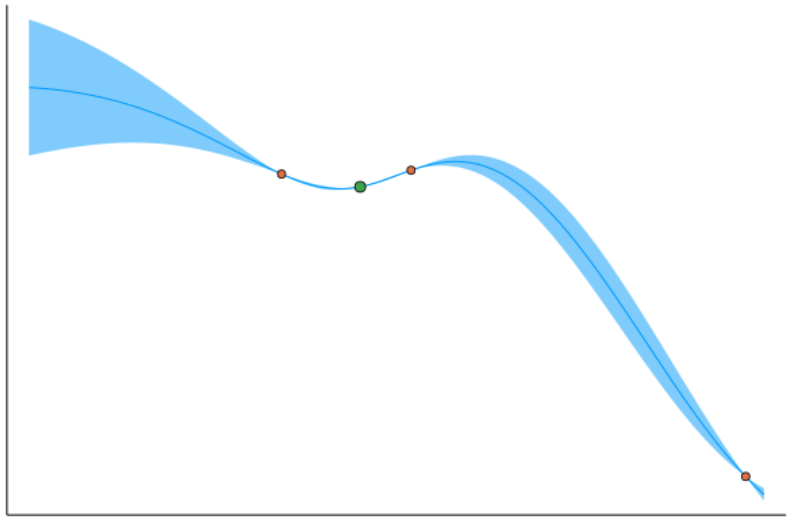

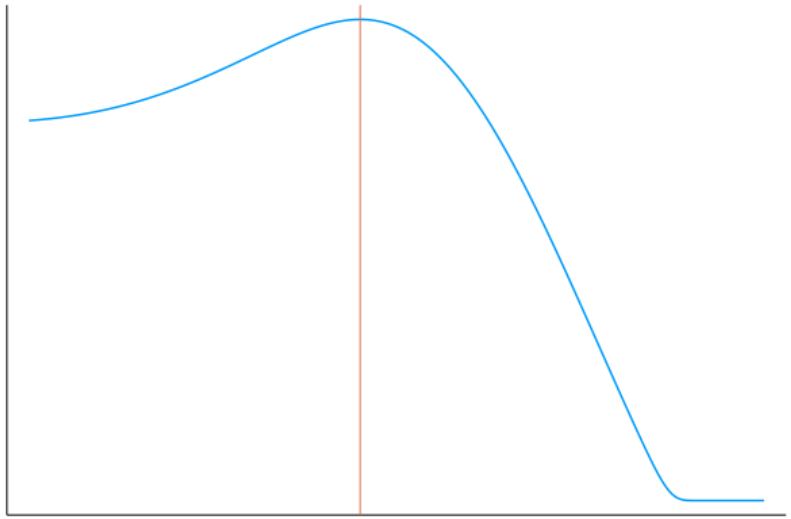

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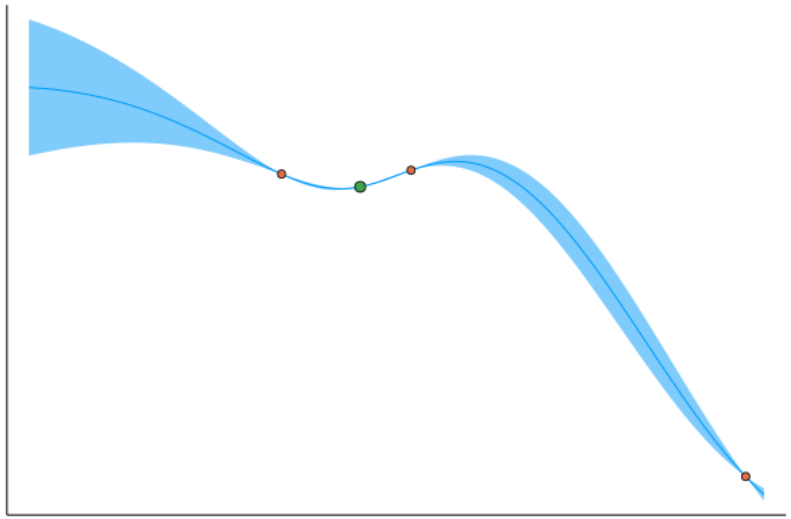

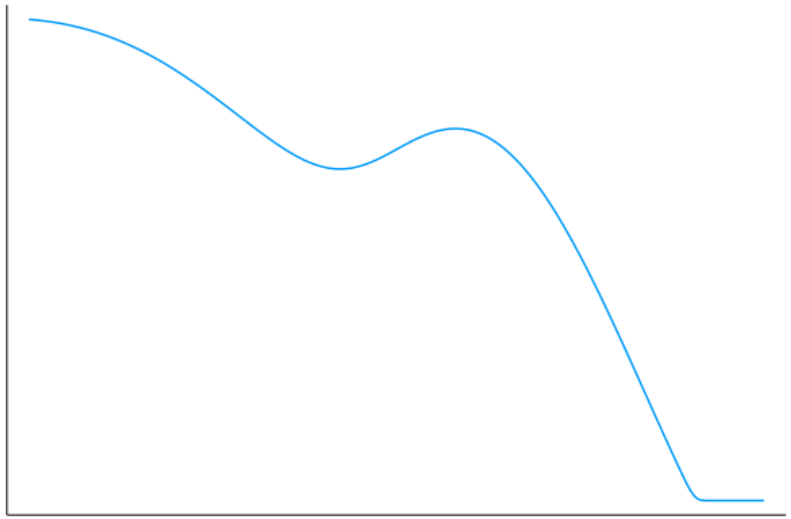

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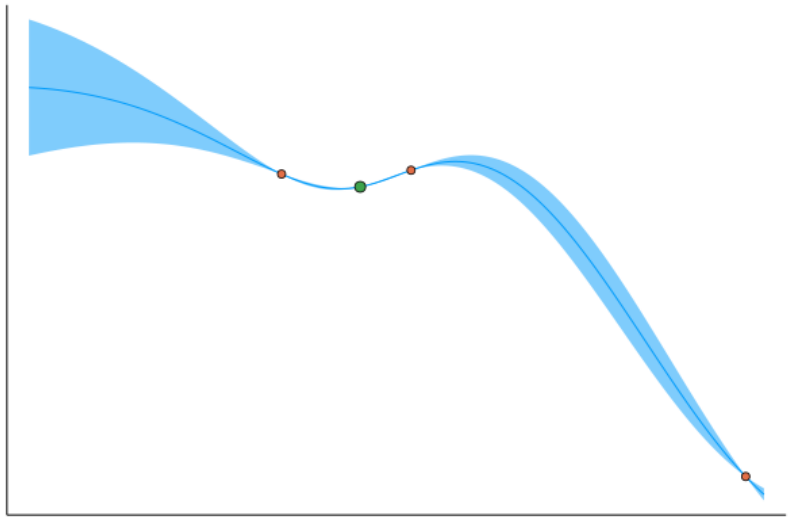

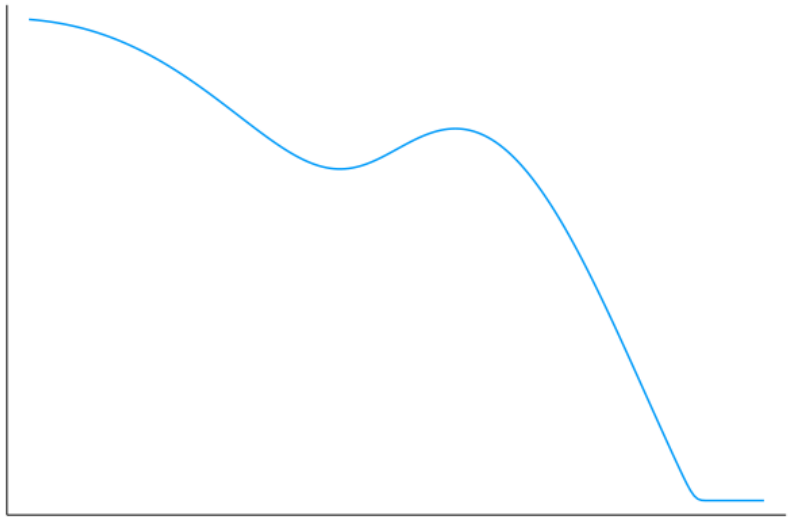

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5. Sample new data and update surrogate
6. Go to step 3 and repeat
7. Make final recommendation

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- When should I ignore regions of high uncertainty and exploit regions of low uncertainty but with a "reasonably" good reward?

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- How we construct the acquisition function directly influences what locations we try next
- Myopia is the tendency to focus on the short-term rather than the long-term implications of our actions

Additional Resources

1. (Paper) A Tutorial on Bayesian Optimization by Peter Frazier
2. (Book) Bayesian Optimization by Roman Garnett
3. (Book) Gaussian Processes for Machine Learning by Carl Rasmussen