Tutorial on Bayesian Optimization

Johannes Kirschner and Mojmír Mutný

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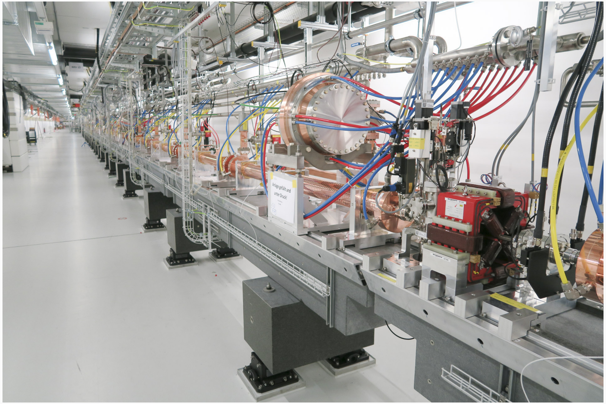
ICFA ML Workshop, PSI

ETH zürich

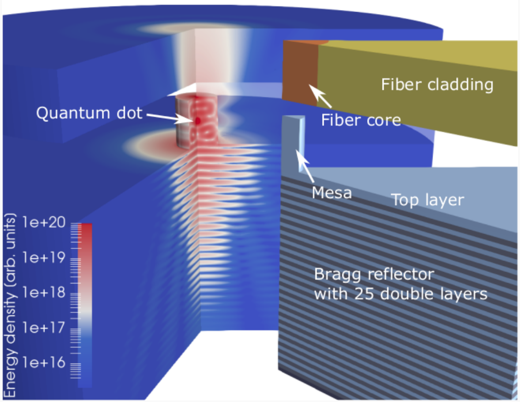
Motivating Application: Parameter Tuning of Accelerator

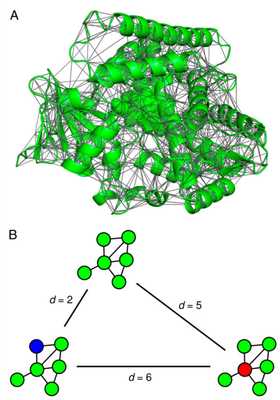


Maximize (photon) signal, minimize losses, . . .

[McIntire et al., 2016, Kirschner et al., 2019]

Motivating Application: Experimental Design

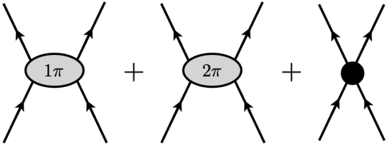




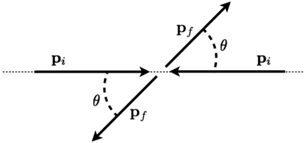
Optimize design parameters, e.g. nano materials, molecules,...

[Schneider et al., 2018, Romero et al., 2013]

Motivating Application: Fitting Physical Models



χEFT model for the NN interaction



Experimental data on NN scattering

Optimize model parameters to fit observational data

[Ekström et al., 2019]

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Maximize a Black box function:

$$\mathcal{X} \longrightarrow f \rightsquigarrow f(x) + \epsilon$$

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Only get (noisy) evaluations $y = f(x) + \epsilon$

- Evaluations of f are 'expensive'

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Prior data set: $\mathcal{D}_0$

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Part I: Gaussian Process Regression

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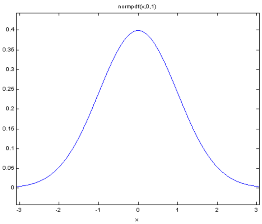
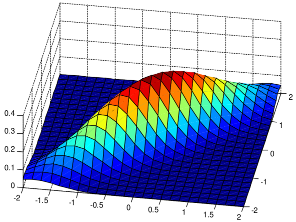
Posterior distribution: $\mathcal{P}(f|D_t) = \dfrac{\mathcal{P}(D_t|f)\mathcal{P}(f)}{\mathcal{P}(D_t)}$

- ▷ Bayes' theorem
- ▷ The posterior distribution captures our belief in f after seeing the data.

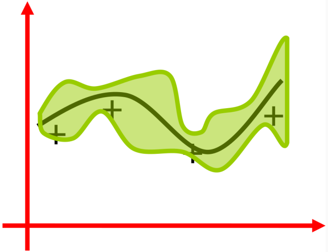
Gaussian Processes



Normal dist.
(1-D Gaussian)



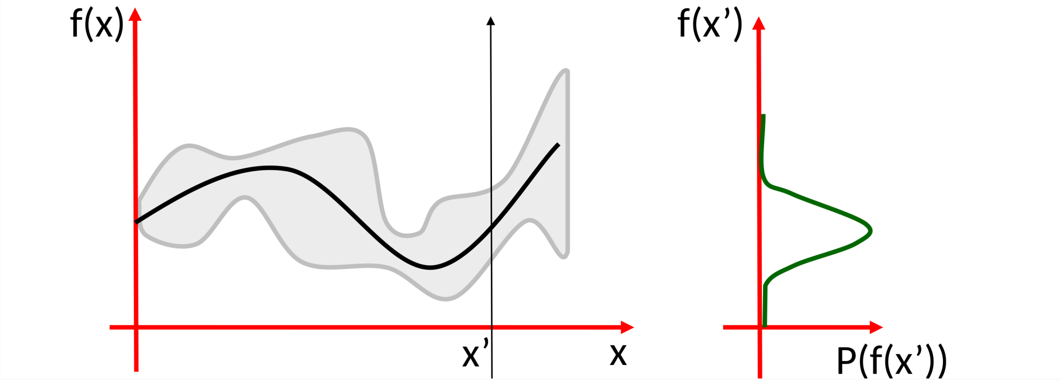
Multivariate normal
(n-D Gaussian)



Gaussian process
(∞-D Gaussian)

- ▷ **Gaussian process (GP)** $=$ normal distribution over *functions*

Gaussian Processes



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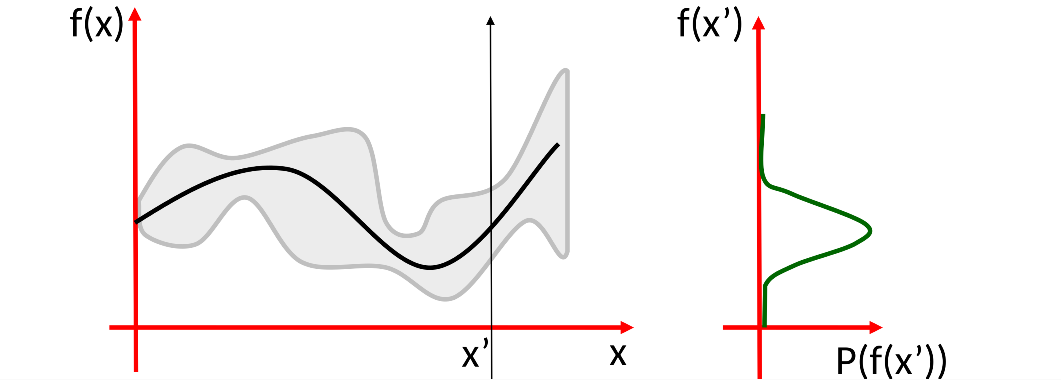

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- Finite marginals $f(x_1), \ldots, f(x_n)$ are multivariate Gaussians
- Parameterized by covariance function (kernel) $k(x, x') = Cov(f(x), f(x'))$

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Finite domain: $\mathcal{X} = \{x_1, \ldots, x_n\}$

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Denote $f \sim GP(m, k)$.

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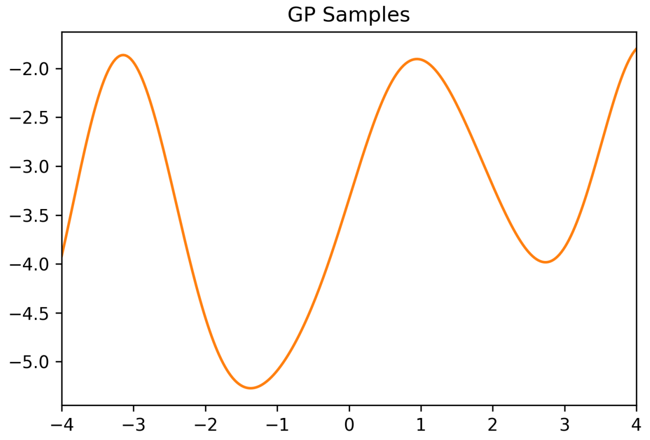
In practice we always evaluate/sample the GP on finite (grid) domains.

Samples from a Gaussian Process



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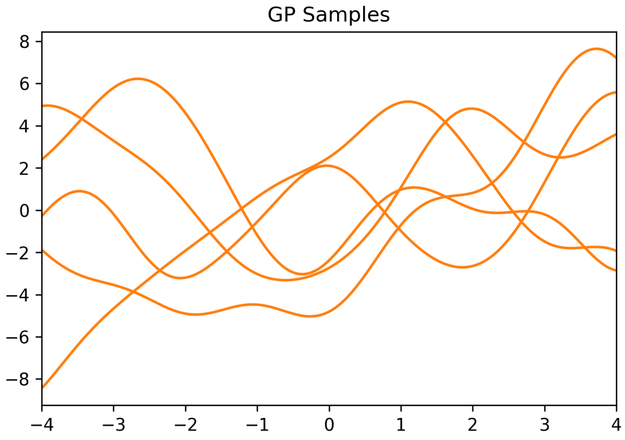

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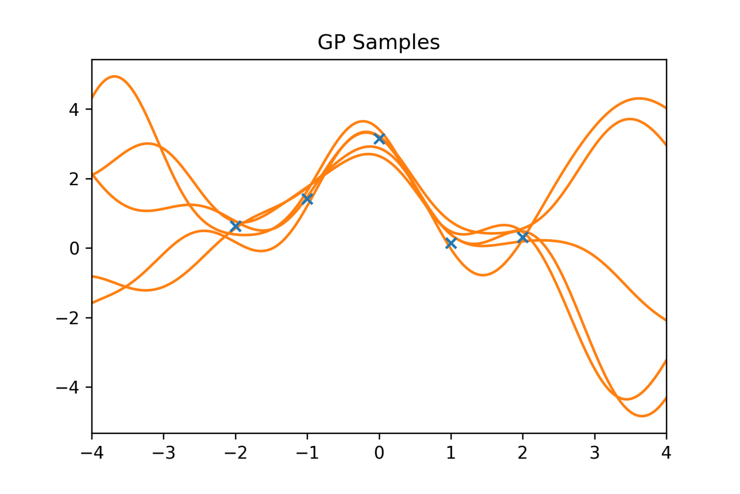

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Gaussian likelihood: iid Gaussian noise:

- ▷ $\mathcal{P}(\{y_1, \ldots, y_m\} | f(x_1), \ldots, f(x_n)) = \prod_i \mathcal{N}(f(x_i), \rho^2)$
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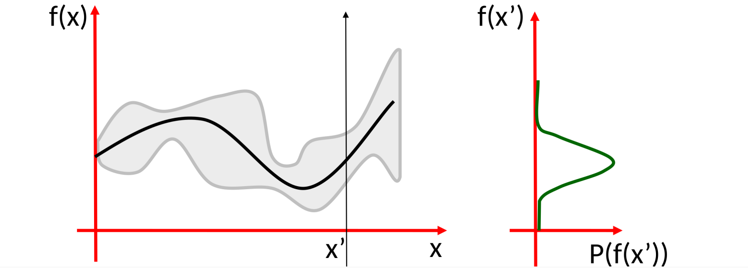
Posterior distribution: $\mathcal{P}(f | D_t) = GP(\mu_n, k_n)$

- Posterior distributions is a again a GP!
- Closed form updates exist.
- Excellent book (free pdf): [Rasmussen, 2004, Chapter 2]

Marginals

Posterior distribution: $\mathcal{P}(f|D_t) = GP(\mu_n, k_n)$

- *Remember:* Finite marginals are Gaussians!
- Marginal posterior distribution at any point x is $\mathcal{N}(\mu_n(x), k_n(x, x))$



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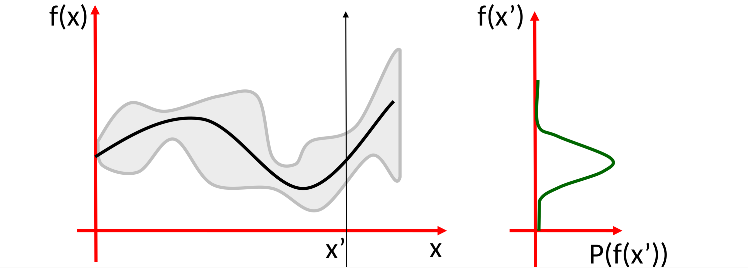

Posterior variance $\sigma_n(x)^2 = k_n(x,x)$ quantifies uncertainty

Kernel Functions

Kernel k needs to satisfy some technical assumptions:

- symmetric
- positive semidefinite.

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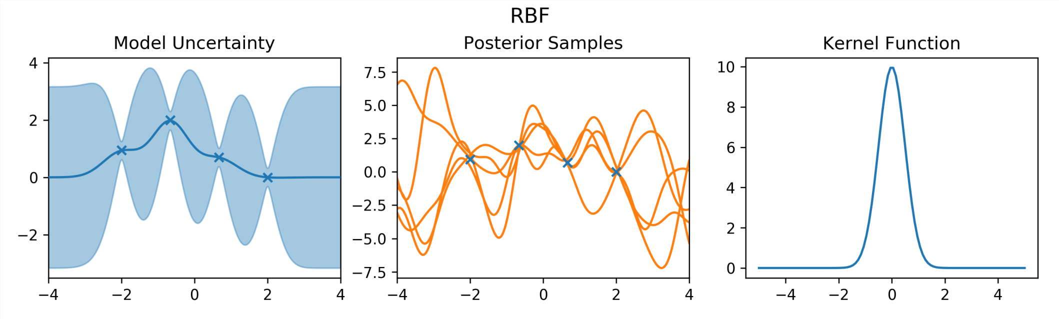
Kernels are similarity measures between points and encodes smoothness.

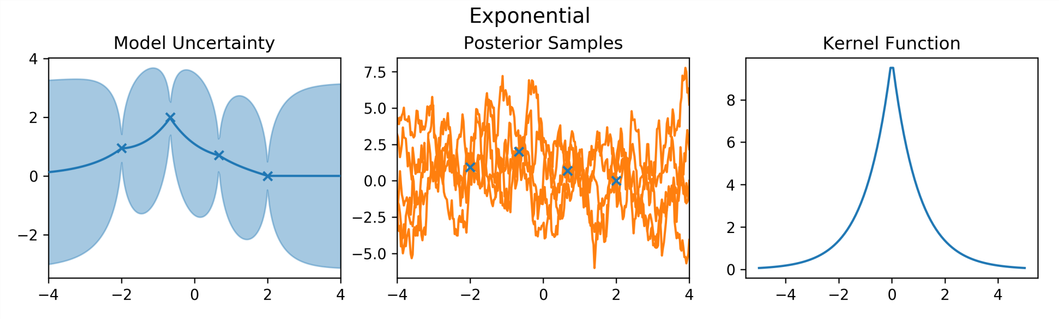
Kernel Functions: Squared Exponential (RBF)



Squared exponential kernel: $k(x, x') = \exp(-\|x - x'\|^2 / l^2)$

▷ l is called lengthscale (or bandwidth)

Kernel Functions: Exponential



Exponential kernel: $k(x, x') = \exp(-\|x - x'\|/l^2)$

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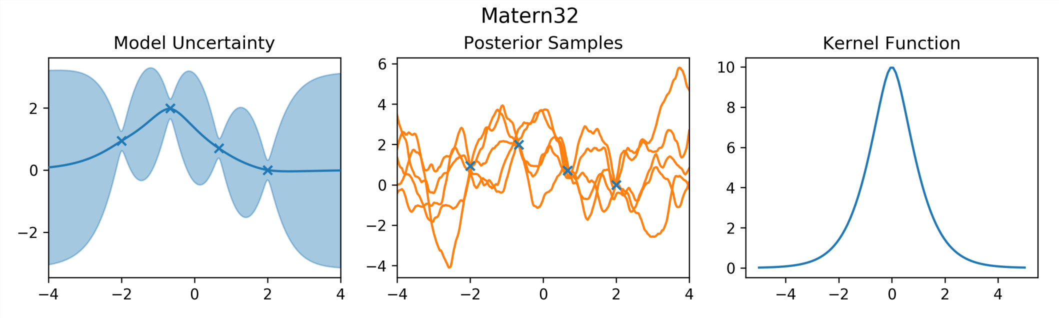
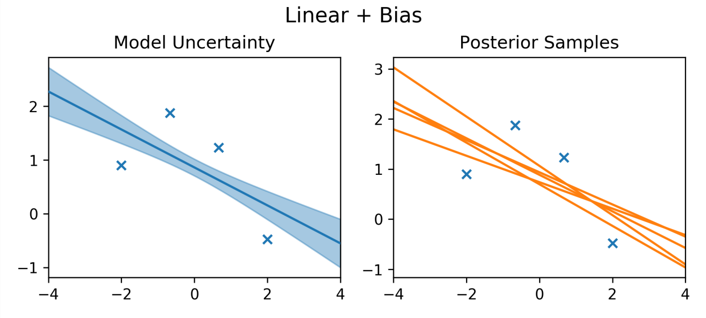
Kernel Functions: Matern



Matern32 kernel: $k(x, x') = \left(1 + \frac{\sqrt{3}\|x - x\|}{l}\right) \exp\left(-\frac{\sqrt{3}\|x - x'\|}{l}\right)$

- l is called lengthscale (or bandwidth)
- Matern52, etc: Family of kernels with increasing smoothness

Kernel Functions: Linear



Linear kernel: $k(x, x') = x^\top x'$

- ▷ Recovers (Bayesian) linear regression!

Feature kernel: $k(x, x') = \Phi(x)^\top \Phi(x')$

- ▷ E.g. polynomials $\Phi(x) = [1, x, x^2]$

Kernel Parameters I

Noise variance

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- ▷ Slightly larger value increases robustness

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Kernel

- Smoothness of function
- RBF smooth functions
- Matern32, Matern52, less smooth, often work well in pratice
- Can also combine kernels, e.g. RBF $+$ 5$\cdot$Matern32
- Each kernel has its own hyper-parameters

Kernel Parameters II

Normalizes objective (y-values)

Prior variance

- Expected range of objective values
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Normalizes domain (x-values)

Lengthscale

- Smoothness of function
- If too large, might not model the objective well
- Can pick different lengthscales for different dimensions (ARD)
- Normalizes the domain

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Try and error

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Point estimates

- Maximum a posteriori estimation: $\theta^* = \arg\max_\theta \mathcal{P}(D_t|\theta)\mathcal{P}(\theta)$
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Bayesian approach

- Define 'reasonable' prior distribution $\mathcal{P}(\theta)$ over θ
- Marginalize predictions over posterior $\mathcal{P}(\theta|D_t)$
- More expensive to compute, no closed form
- Eliminates hyperparameters

Notebook Session: GP Regression using GPy

Part II: Bayesian Optimization

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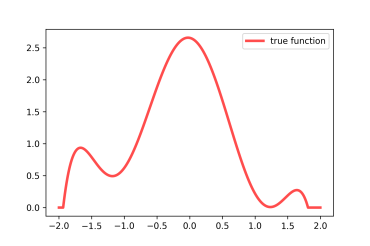

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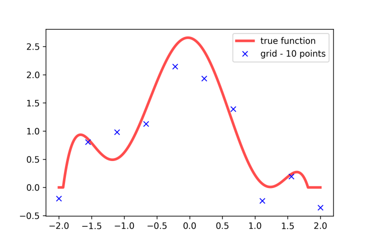

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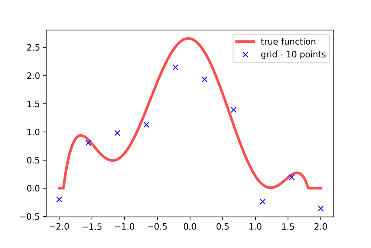

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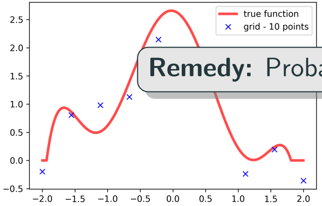

Remedy: Probabilistic model: Gaussian Processes!

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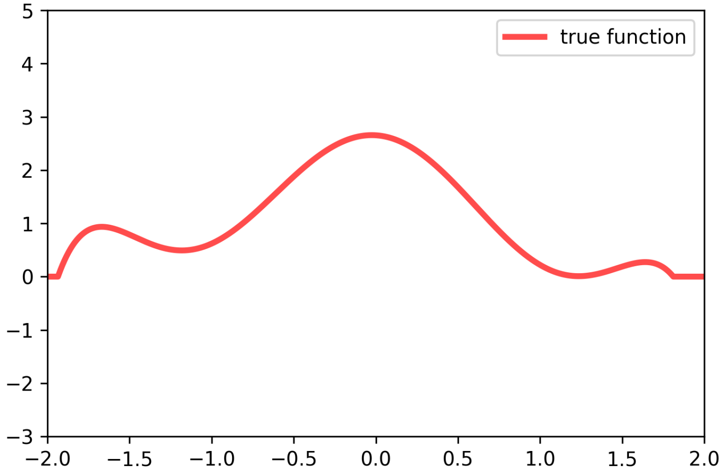
GPs: Avoid not necessary evaluations



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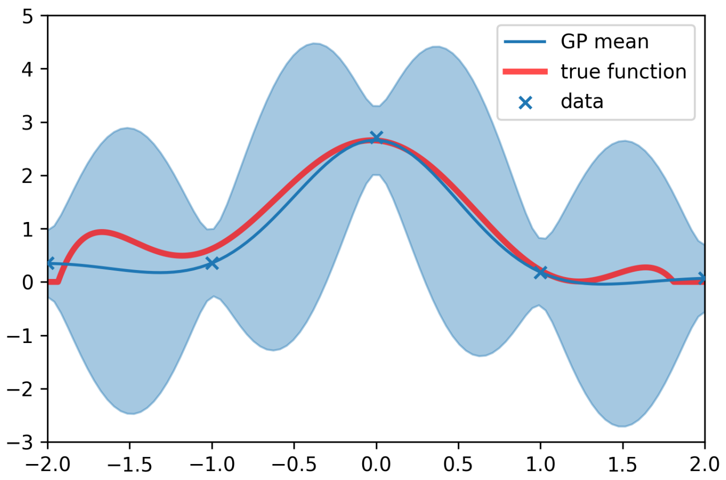

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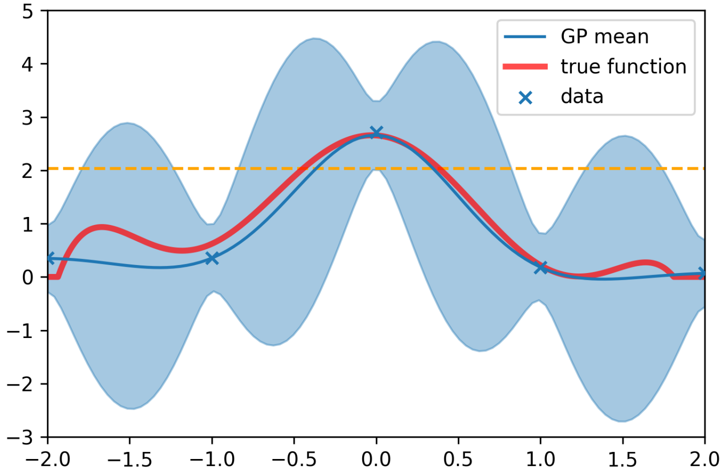

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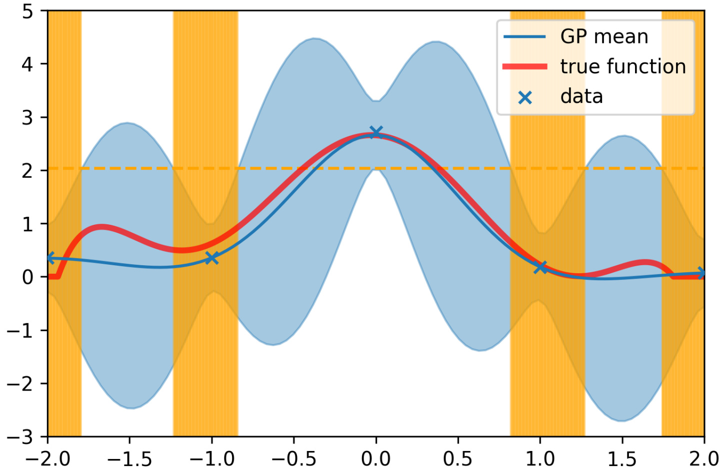

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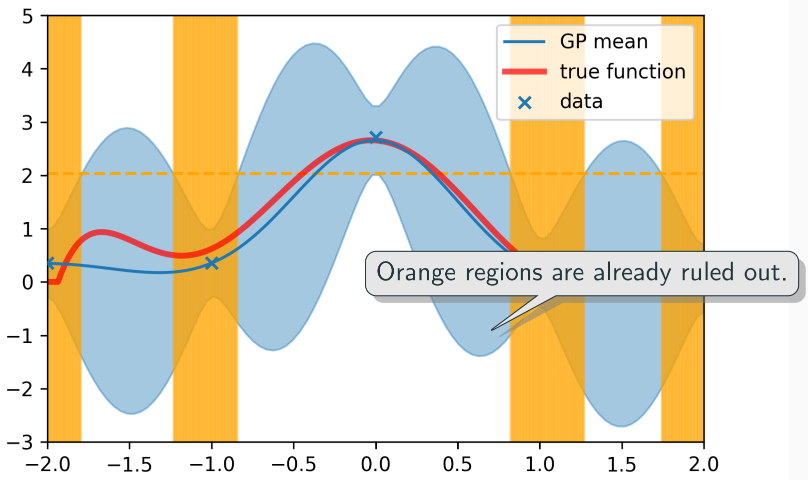

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Upper Confidence Bound (UCB)

- $\mu_t \ldots$ *posterior mean* after seeing t points

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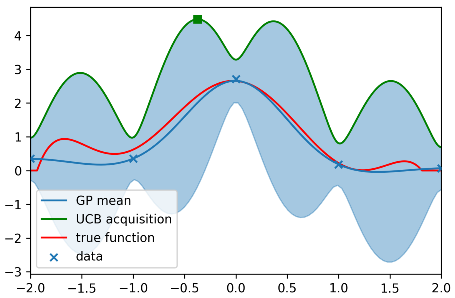

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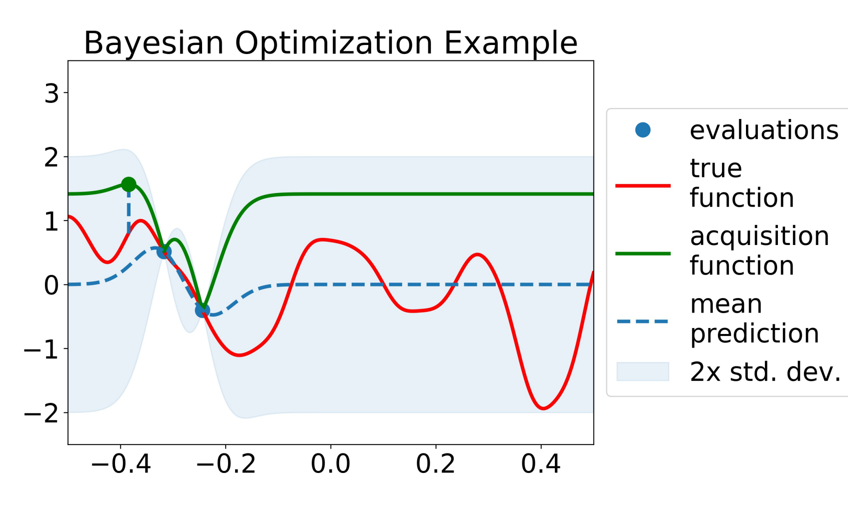

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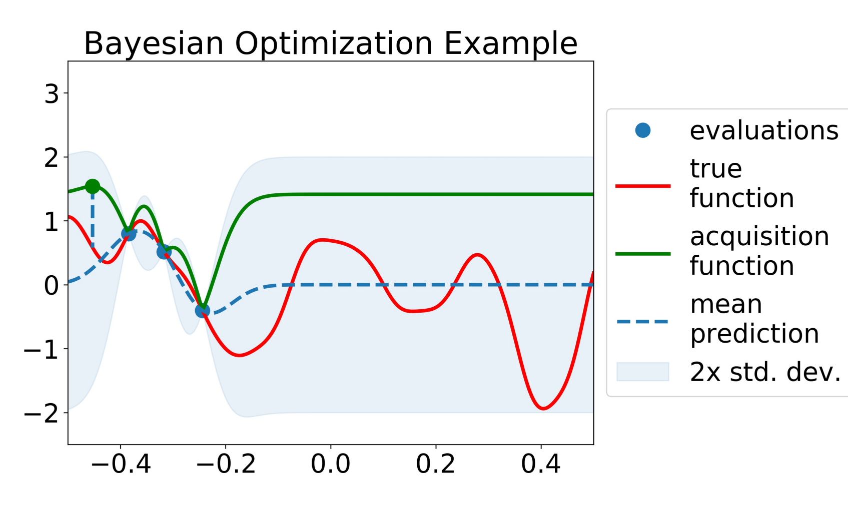

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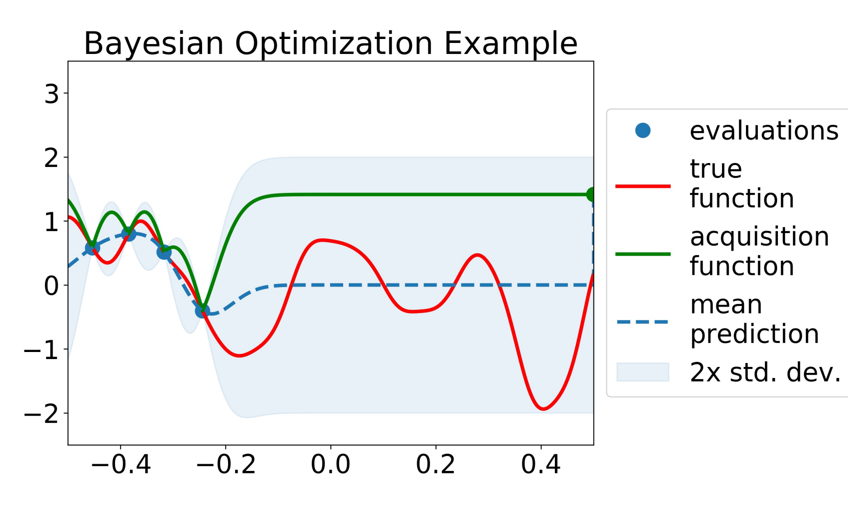

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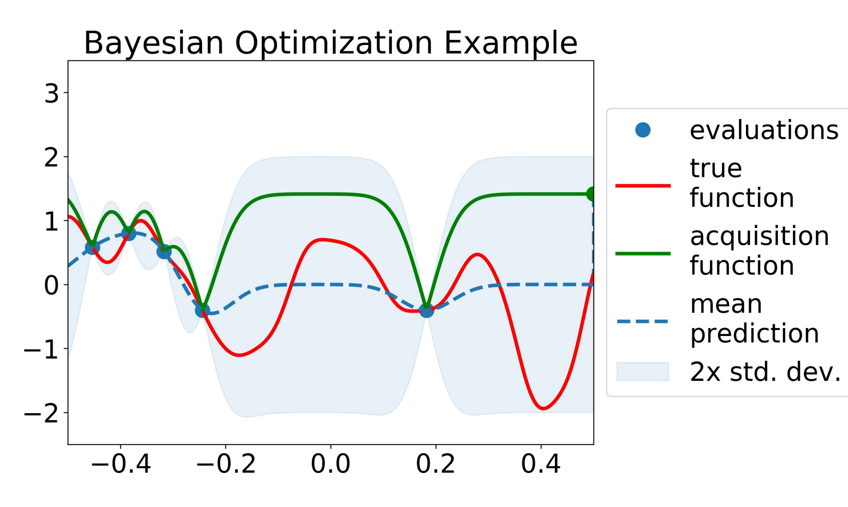

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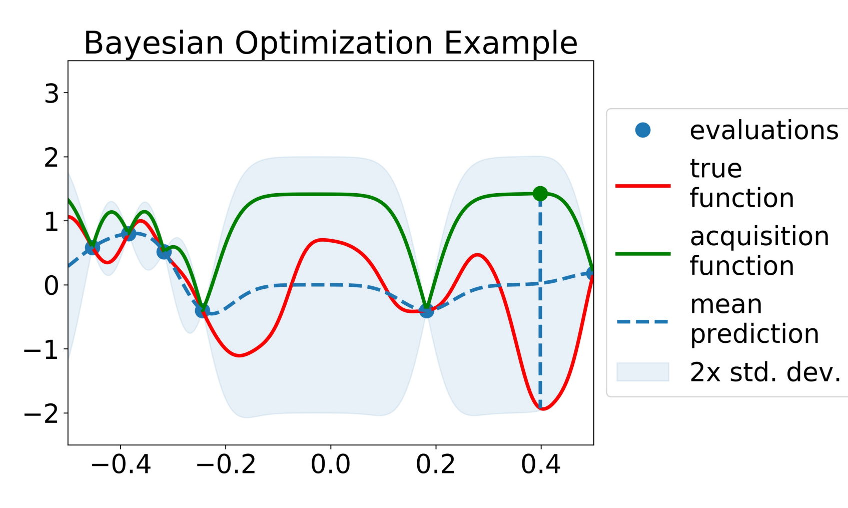

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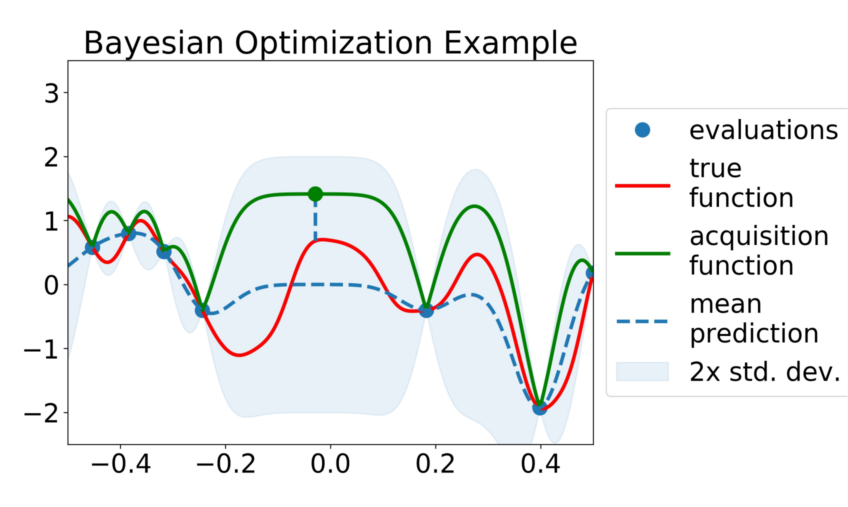

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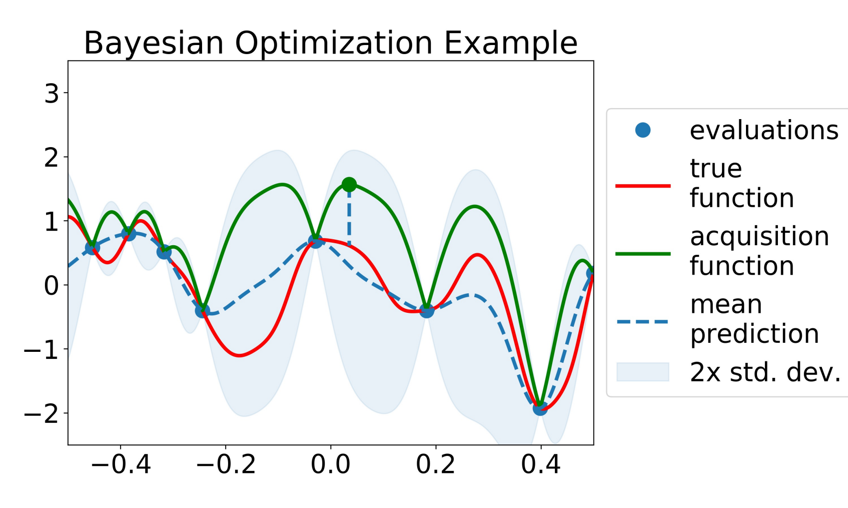

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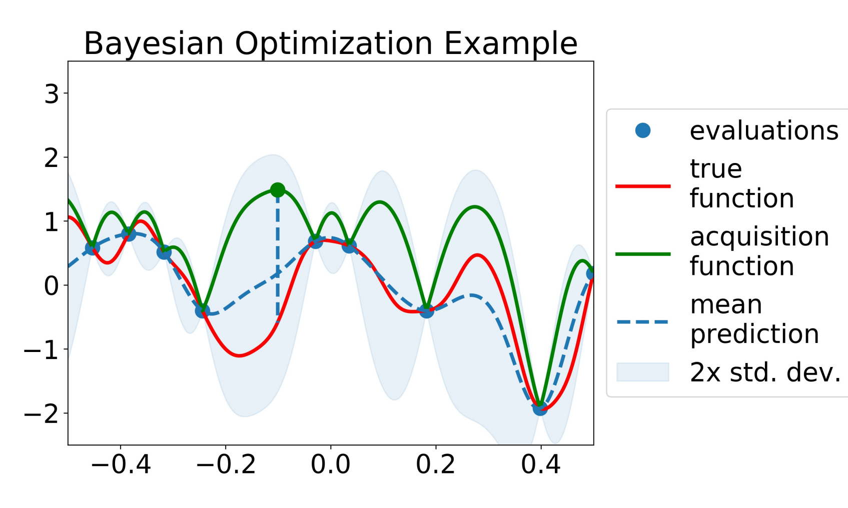

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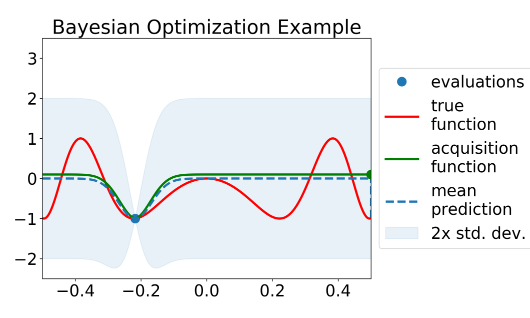

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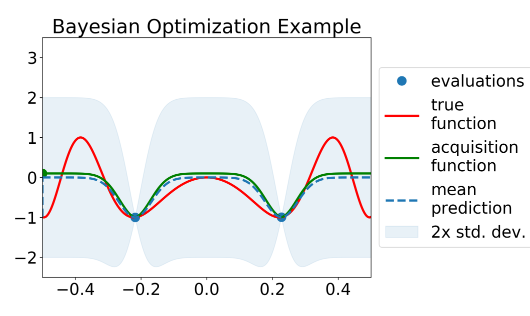

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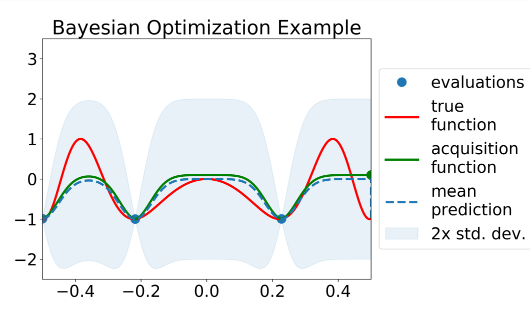

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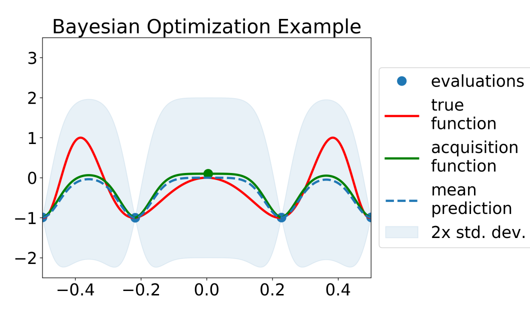

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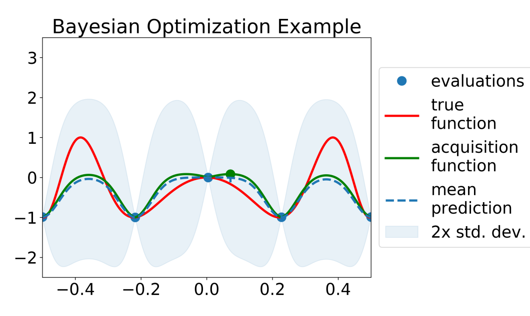

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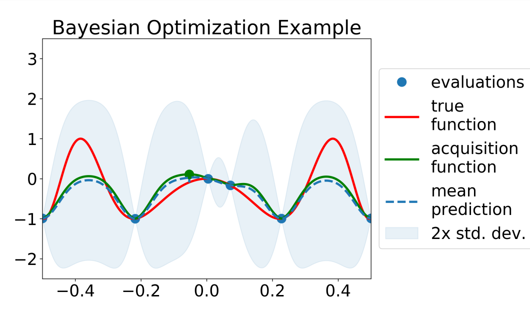

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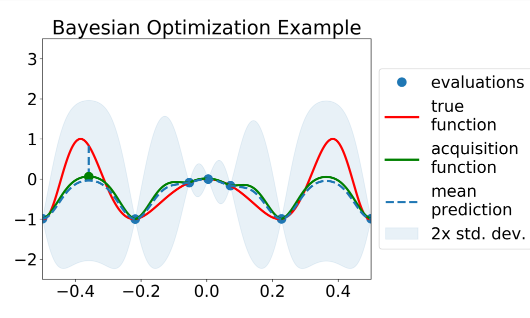

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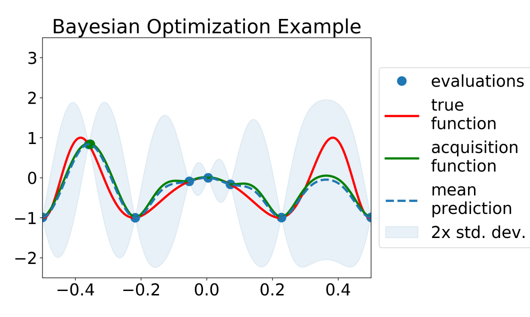

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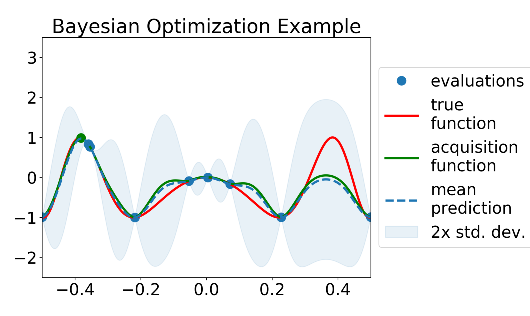

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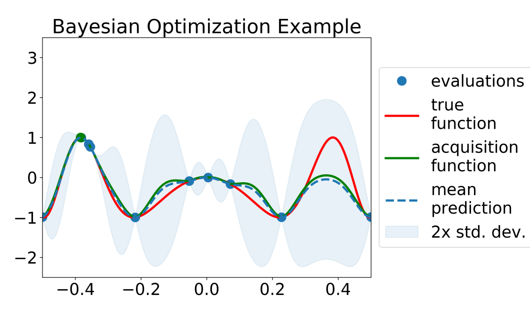

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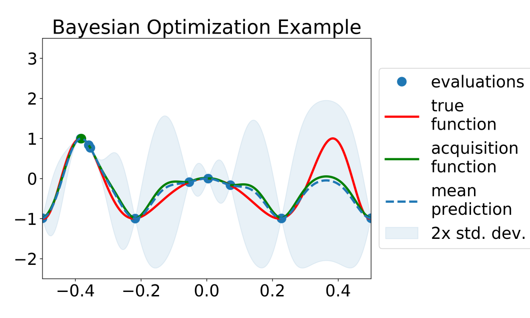

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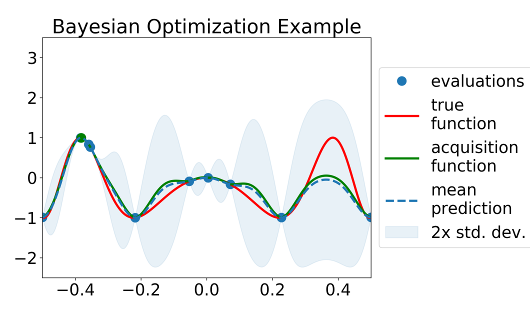

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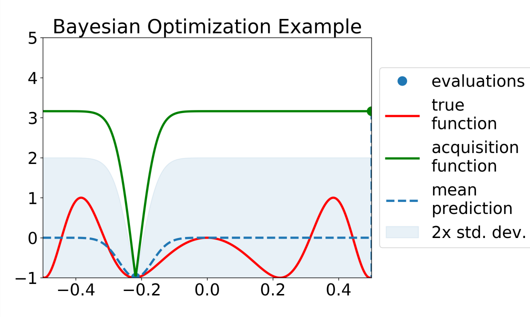

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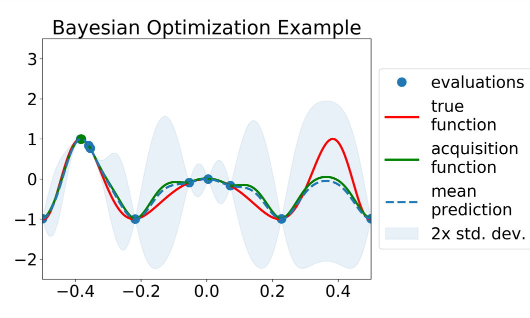

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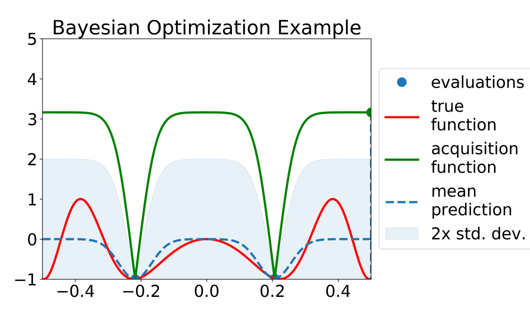

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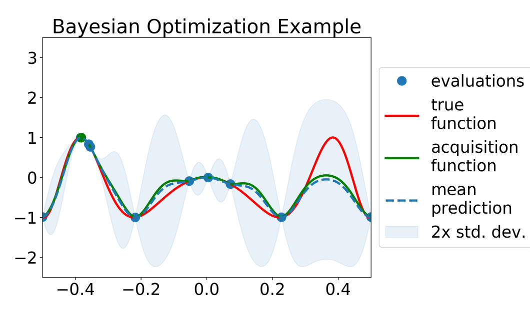

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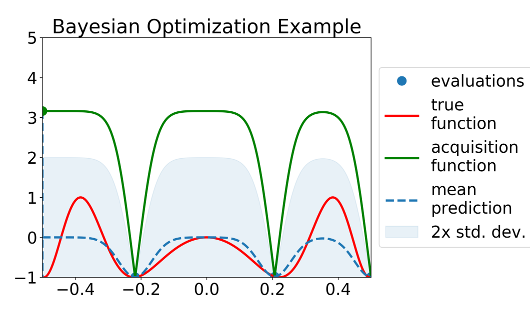

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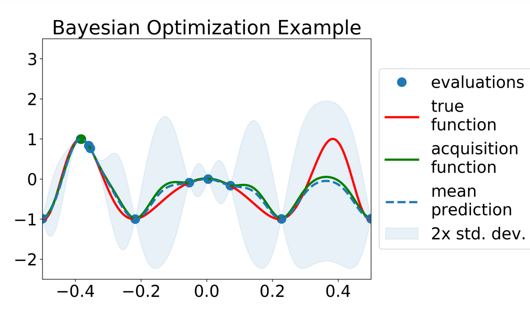

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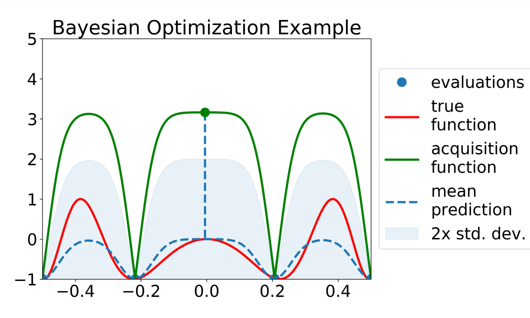

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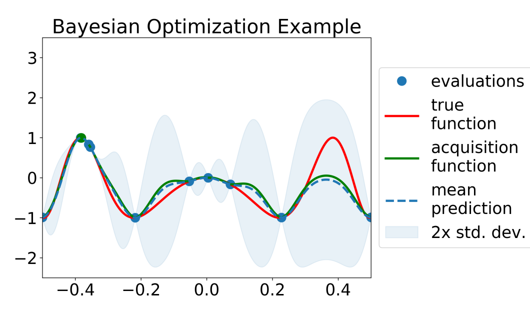

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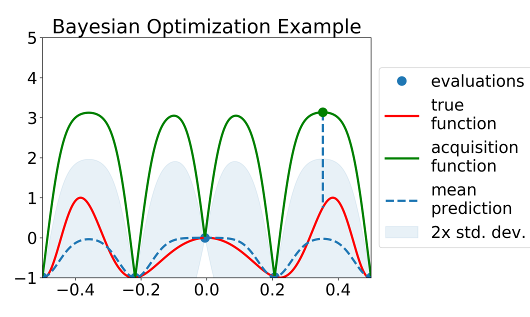

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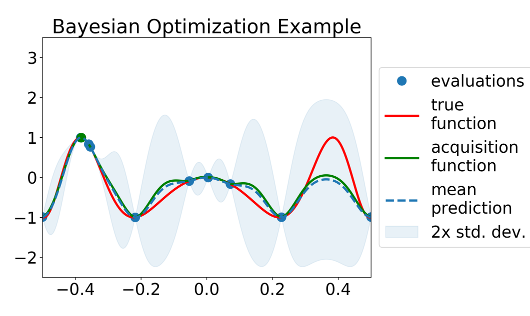

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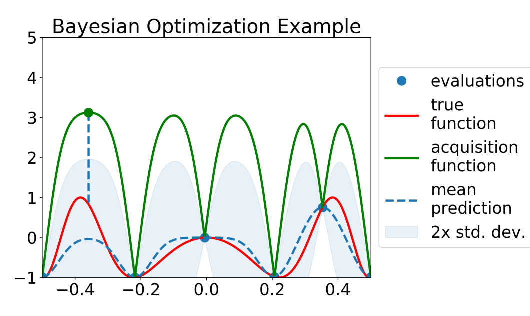

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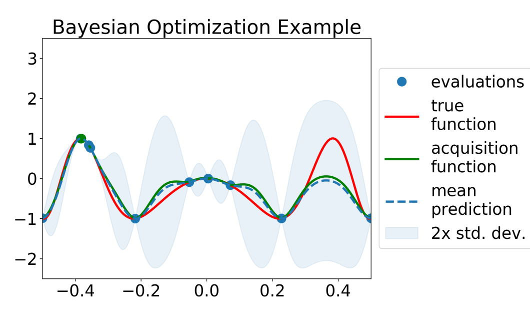

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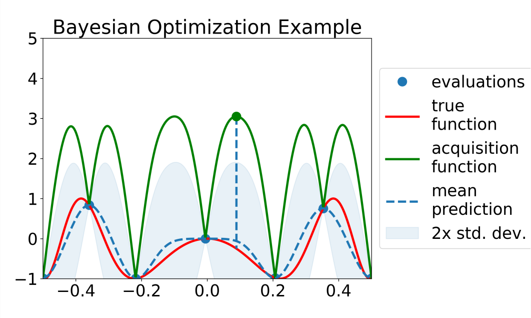

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Part II, Programming: Lets try it out.

Ekström, A., Forssén, C., Dimitrakakis, C., Dubhashi, D., Johansson, H., Muhammad, A., Salomonsson, H., and Schliep, A. (2019).
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