A tutorial on Bayesian Optimization

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Challenges in Engineering Design

The society demands new products of better quality, functionality, usability, etc.!

   

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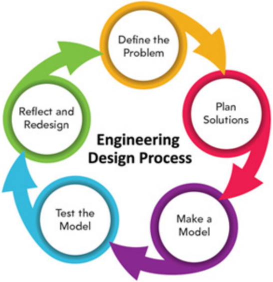

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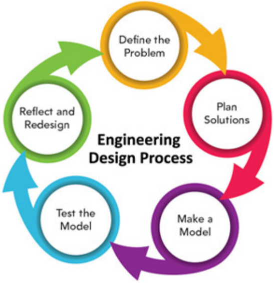

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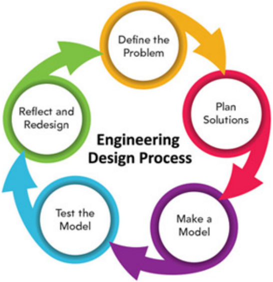

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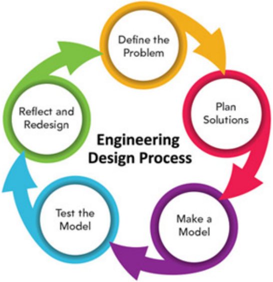

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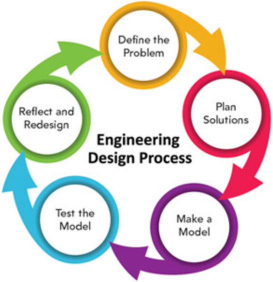

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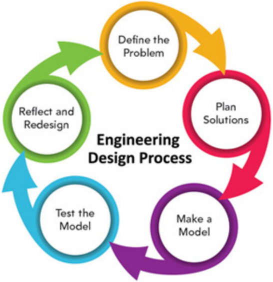

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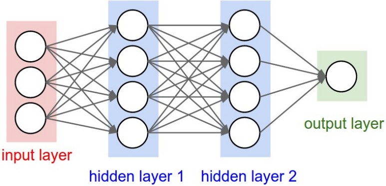
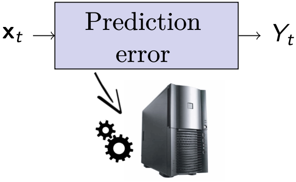
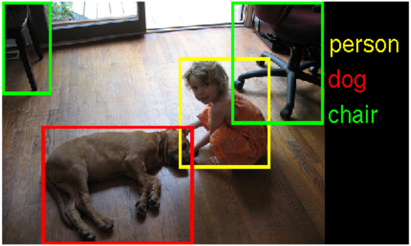
Optimization is a challenging task in new products design!

Example: **Deep Neural Network** for object recognition.







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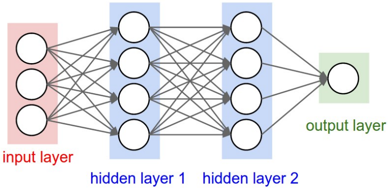
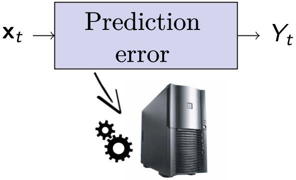
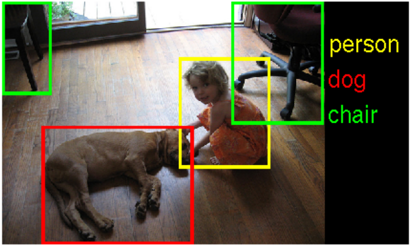
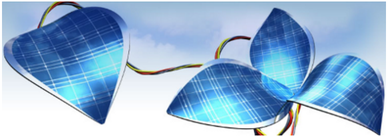


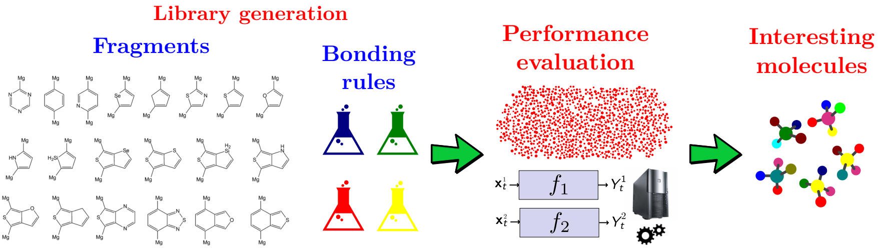




Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc.

Example: new **plastic solar cells** for transforming light into electricity.





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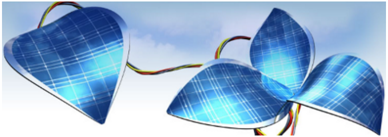
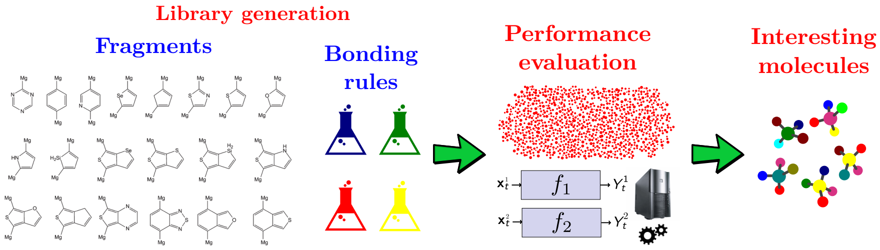
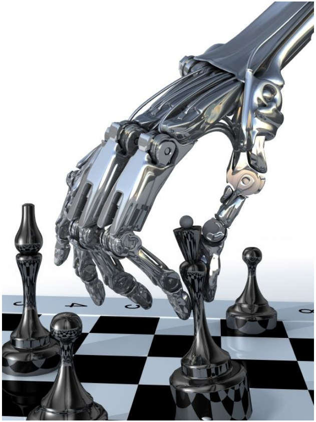




Explore **millions of candidate molecule structures** to identify the compounds with the best properties.

Example: **control system** for a robot that is able to grasp objects.



Finger Joint Trajectories

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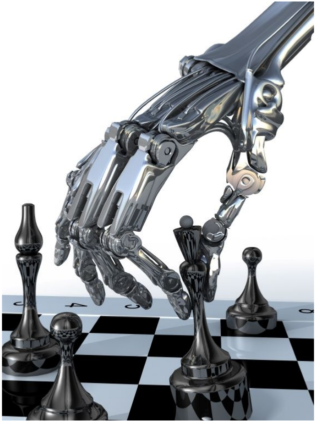
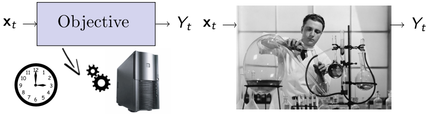


Parameters to tune: initial pose for the robot's hand and finger joint trajectories.

Optimization Problems: Common Features

- Very expensive evaluations.



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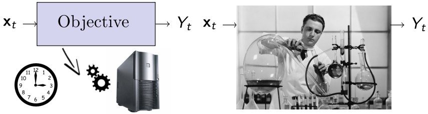
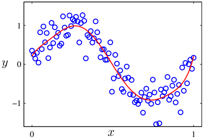


- The objective is a black-box.

- The evaluation can be noisy.

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



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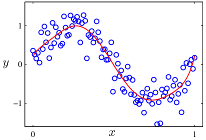
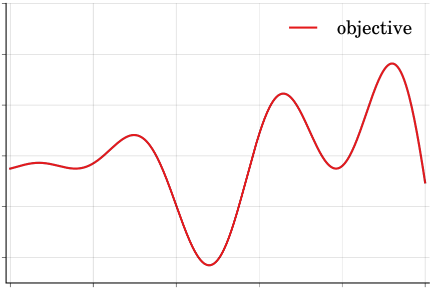


Bayesian optimization methods can be used to solve these problems!

Bayesian Optimization in Practice



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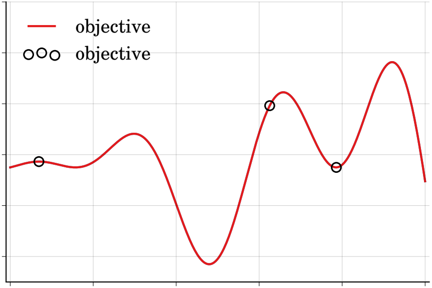

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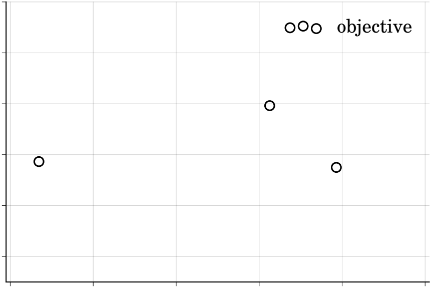

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2. Fit a model to the data:
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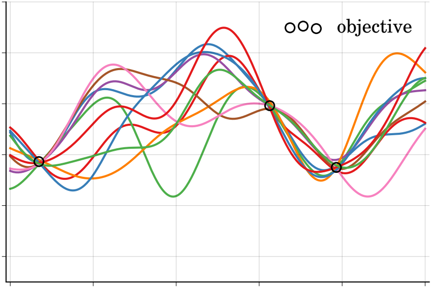

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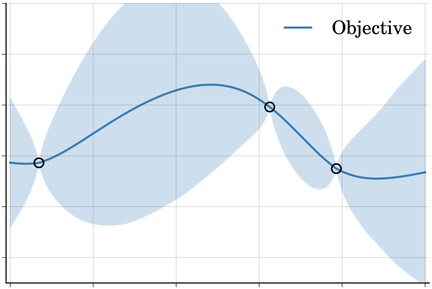

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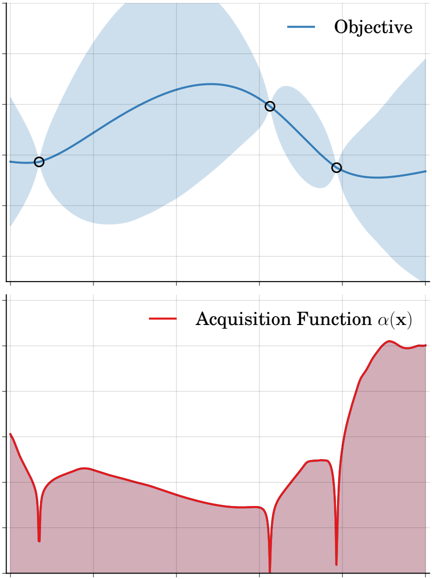

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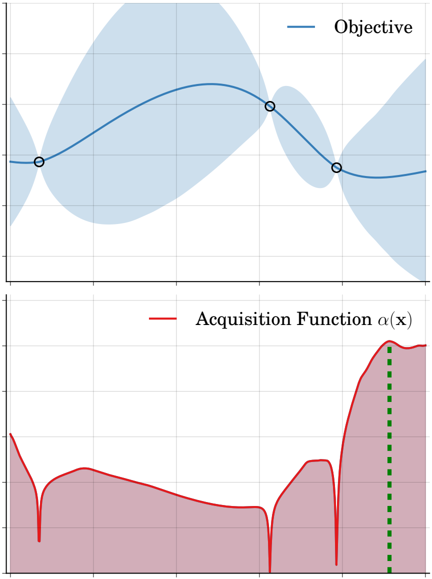

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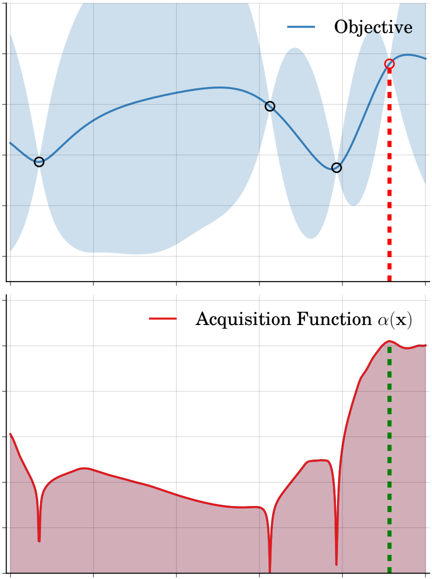

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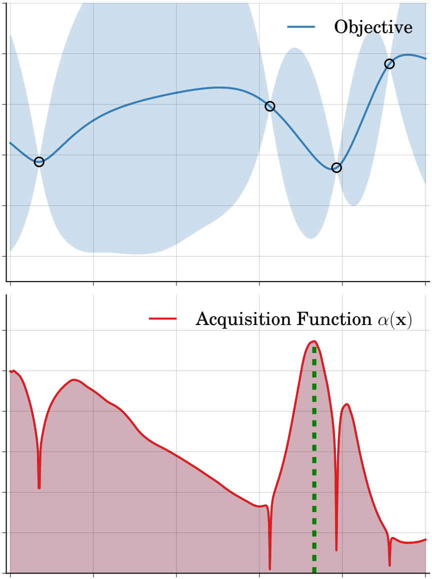

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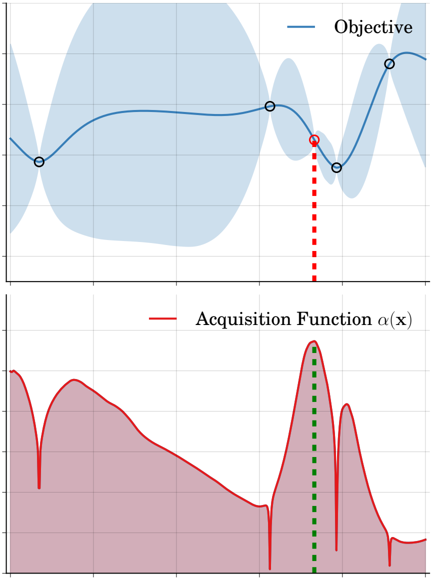

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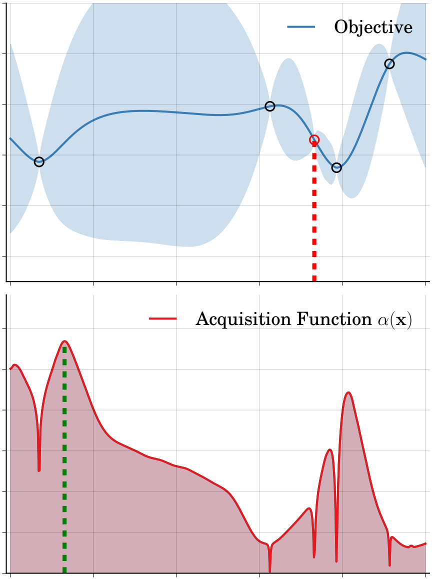

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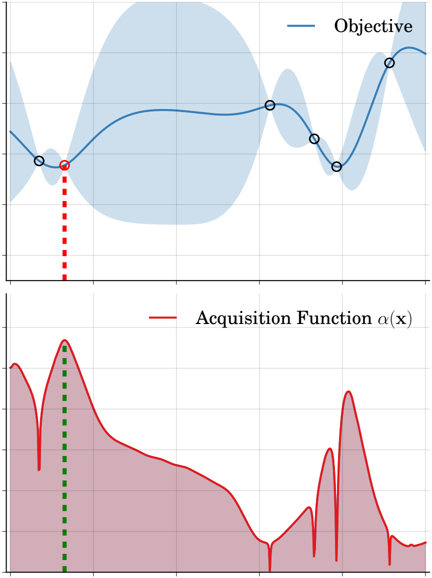

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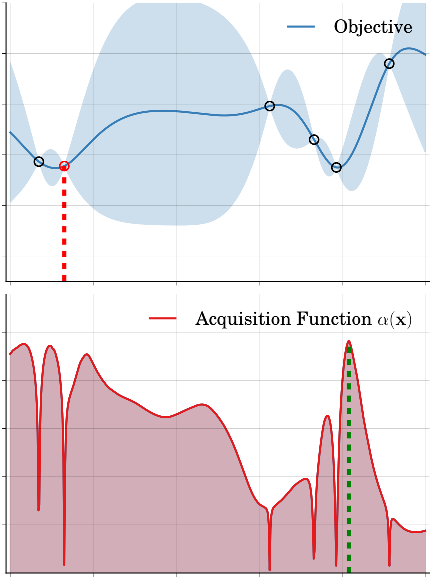

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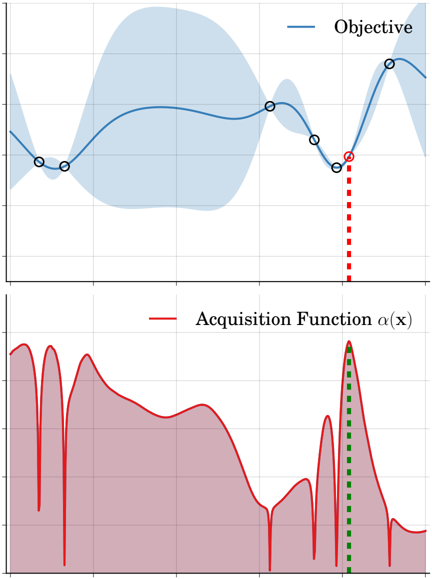

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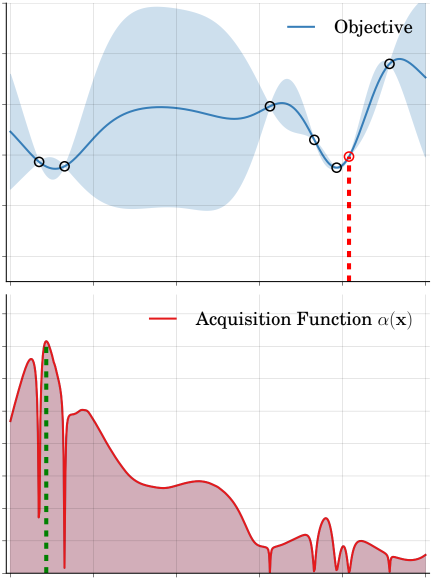

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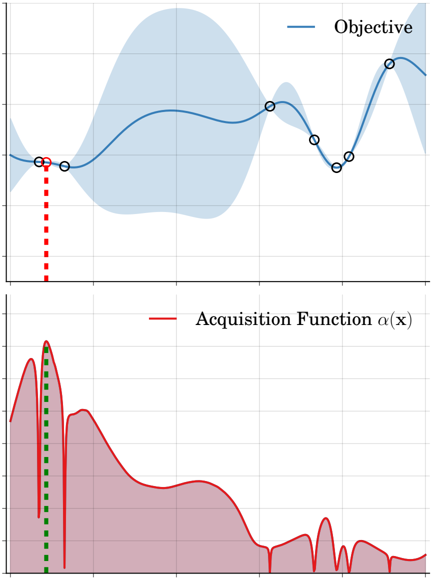

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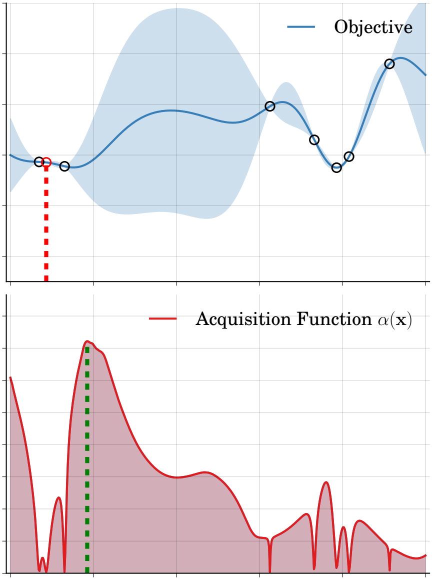

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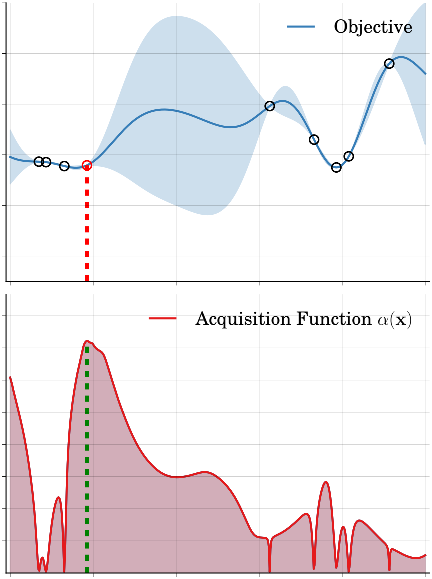

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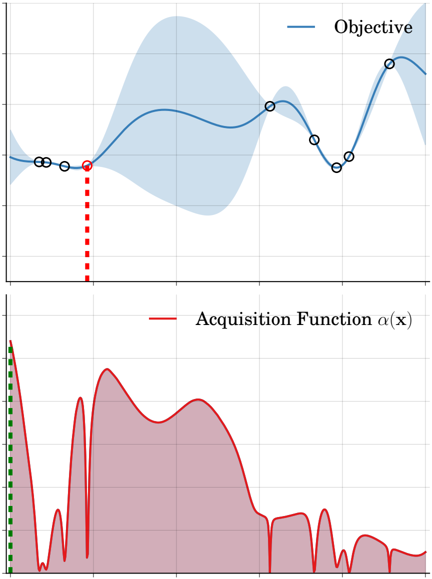

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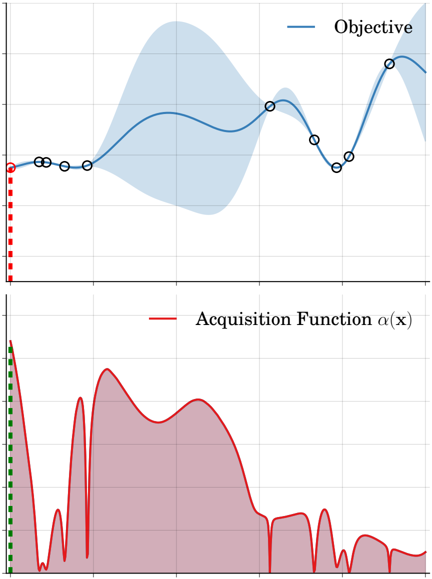

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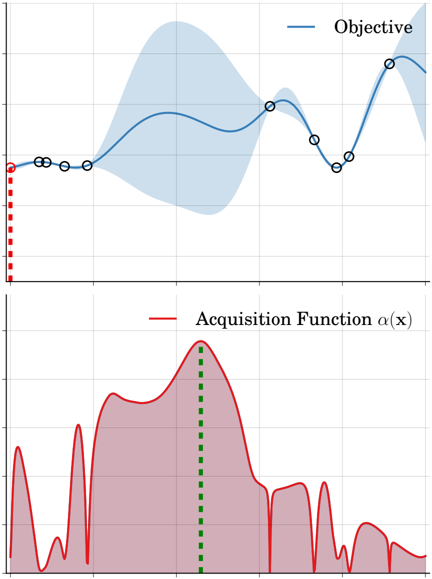

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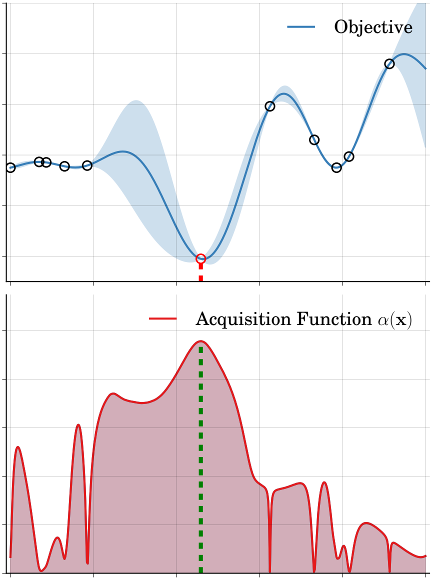

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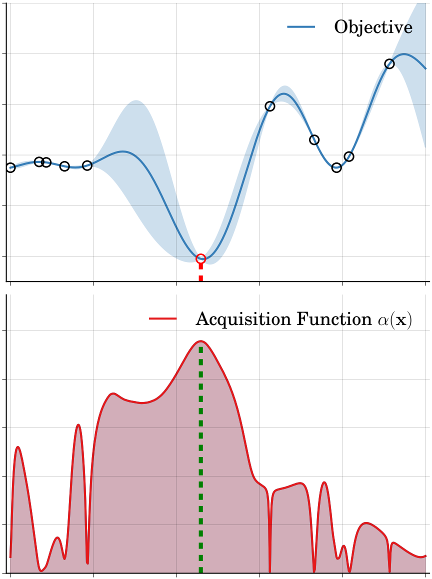

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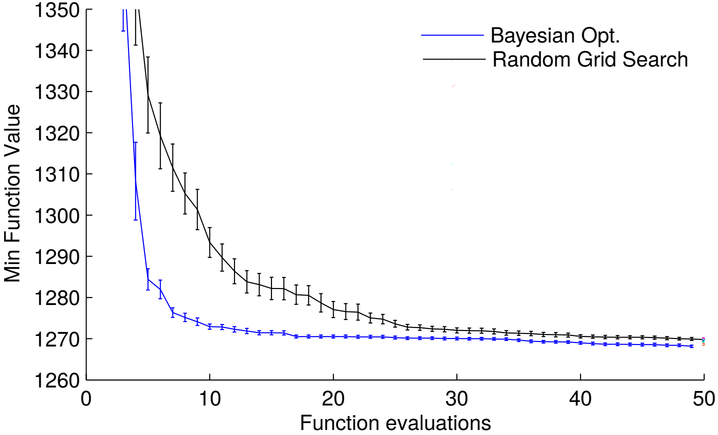
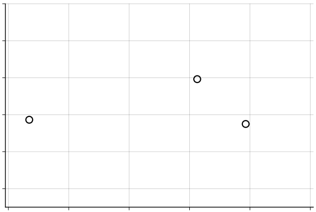
The model guides the search focusing on the most-promising regions of the input space!

Bayesian Optimization vs. Uniform Exploration



Tuning LDA on a collection of Wikipedia articles (Snoek *et al.*, 2012).

Fitting a Model to the Data



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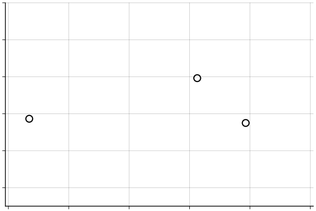

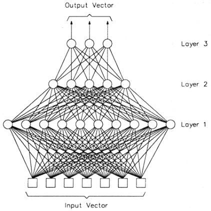

$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

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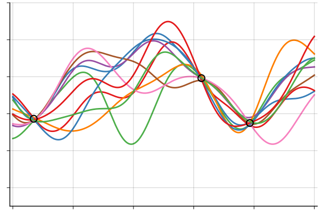

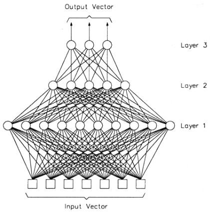

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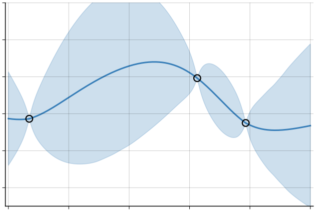

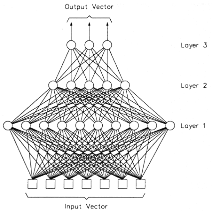

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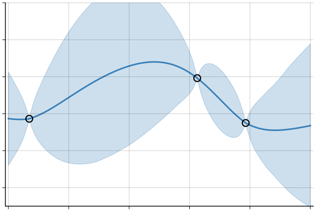

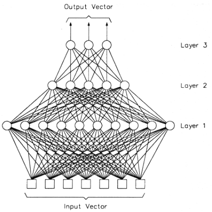

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Posterior Dist. $\quad p(\mathbf{W}|\mathrm{Data}) = p(\mathbf{W})p(\mathrm{Data}|\mathbf{W})/p(\mathrm{Data})$

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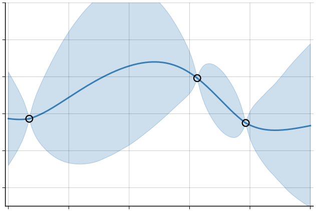

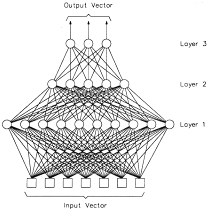

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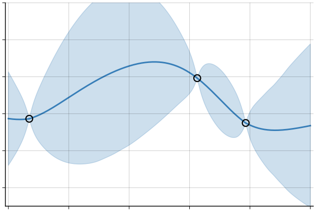

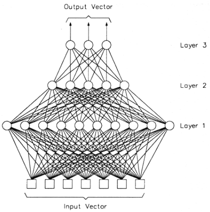

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Challenges: The model should be non-parametric (the world is complicated) and computing $p(\mathrm{Data})$ is intractable!

Solved by setting $p(\mathbf{W}) = \prod_{ij} \mathcal{N}(w_{ji}|0, \sigma^2 H^{-1})$ and letting $H \to \infty$!

Gaussian Processes

Distribution over functions $f(\cdot)$ so that for any finite $\{\mathbf{x}_i\}_{i=1}^N$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathsf{T}$ follows an N-dimensional Gaussian distribution.

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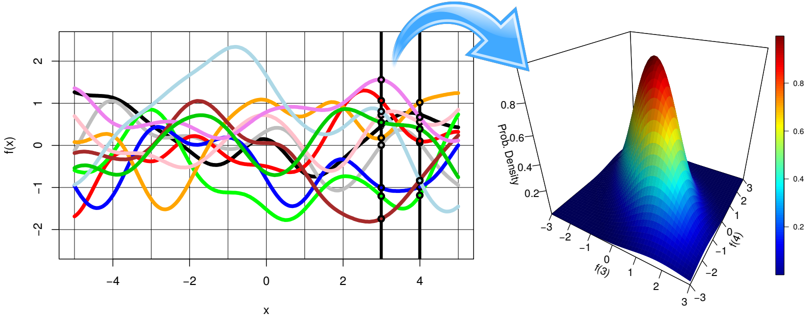

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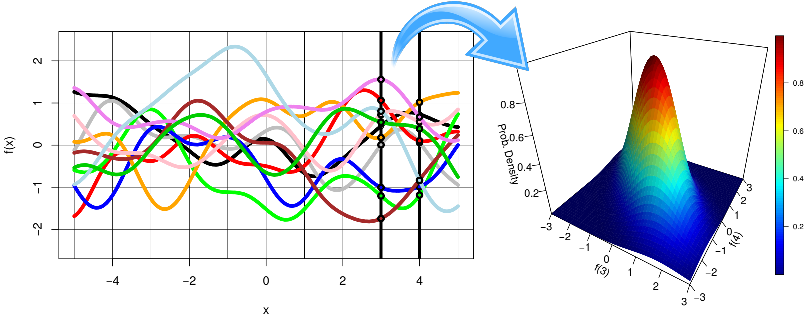

When $H \to \infty$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathsf{T}$ follows an N-dimensional Gaussian where $\mathbb{E}[f(\mathbf{x}_i)f(\mathbf{x}_k)] = \sigma^2\mathbb{E}[h_j(\mathbf{x}_i)h_j(\mathbf{x}_k)]$ by the **central limit theorem**.

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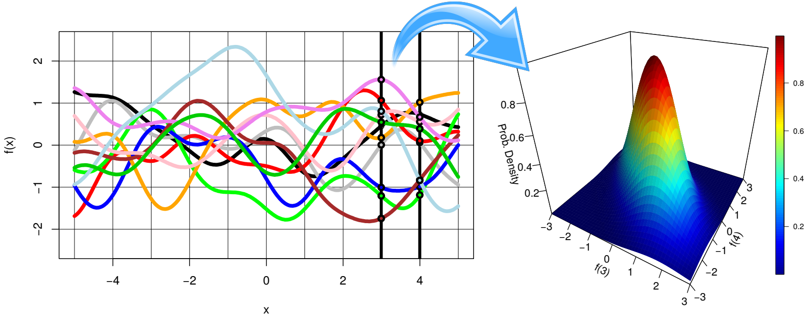

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Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.

Gaussian Processes

- The **joint distribution** for $\mathbf{y}^\star$ at test points $\{\mathbf{x}_m^\star\}_{m=1}^M$ and $\mathbf{y}$:

$$p(\mathbf{y}^\star, \mathbf{y}) = \mathcal{N}\left(\left[\begin{array}{c} \mathbf{0} \\ \mathbf{0} \end{array}\right], \left[\begin{array}{cc} \mathbf{k}_\theta & \mathbf{K}_\theta \\ \boldsymbol{\kappa}_\theta & \mathbf{k}_\theta^\mathsf{T} \end{array}\right]\right)$$

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- These **matrices** are computed from the covariance $C(\cdot, \cdot; \theta)$:

$$[\mathbf{K}_\theta]_{n,n'} = C(\mathbf{x}_n, \mathbf{x}_{n'}; \theta)$$
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- The **predictive distribution** for $\mathbf{y}^\star$ given $\mathbf{y}$, $p(\mathbf{y}^\star | \mathbf{y})$, is:

$$\mathbf{y}^\star \sim \mathcal{N}(\mathbf{m}, \boldsymbol{\Sigma})$$
$$\mathbf{m} = \mathbf{k}_\theta^\mathsf{T} \mathbf{K}_\theta^{-1} \mathbf{y}\,, \qquad \boldsymbol{\Sigma} = \boldsymbol{\kappa}_\theta - \mathbf{k}_\theta^\mathsf{T} \mathbf{K}_\theta^{-1} \mathbf{k}_\theta\,,$$

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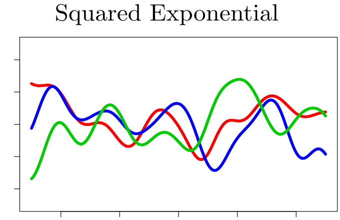
- The log of the **marginal likelihood**, $p(\mathbf{y}|\theta)$, is:

$$\log p(\mathbf{y}) = -\frac{N}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{K}_\theta| - \frac{1}{2} \mathbf{y}^\top \mathbf{K}_\theta^{-1} \mathbf{y}$$

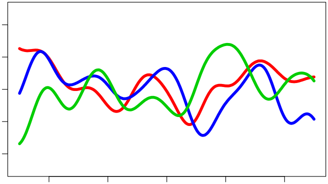
Some Covariance Functions



$$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left\{ \frac{1}{2} \sum_j \left(\frac{x_j - x_j'}{l_j} \right)^2 \right\}$$

Some Covariance Functions

Squared Exponential



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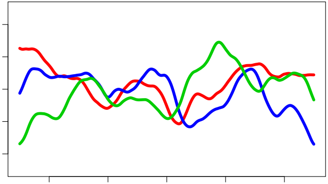
Matérn



$$C(\mathbf{x},\mathbf{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\sqrt{2\nu}r}{l}\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}r}{l}\right)$$

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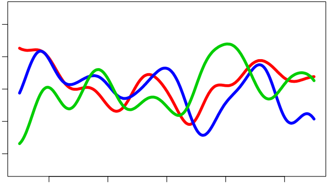

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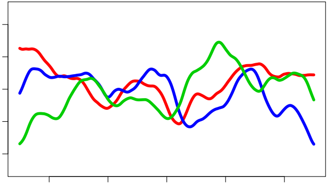

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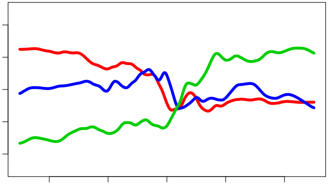
Neural Network



$$C(\mathbf{x},\mathbf{x}') = \frac{2}{\pi}\sin^{-1}\left(\frac{2\mathbf{x}^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{x}'}{\sqrt{(1+2\mathbf{x}^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{x})(1+2\mathbf{x}'^{\mathrm{T}}\boldsymbol{\Sigma}\mathbf{x}')}}\right)$$

Some Covariance Functions

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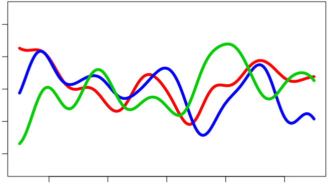

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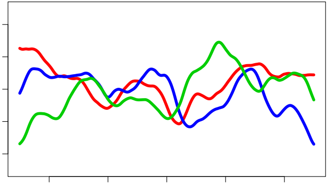

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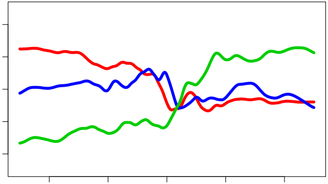

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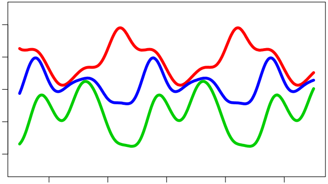
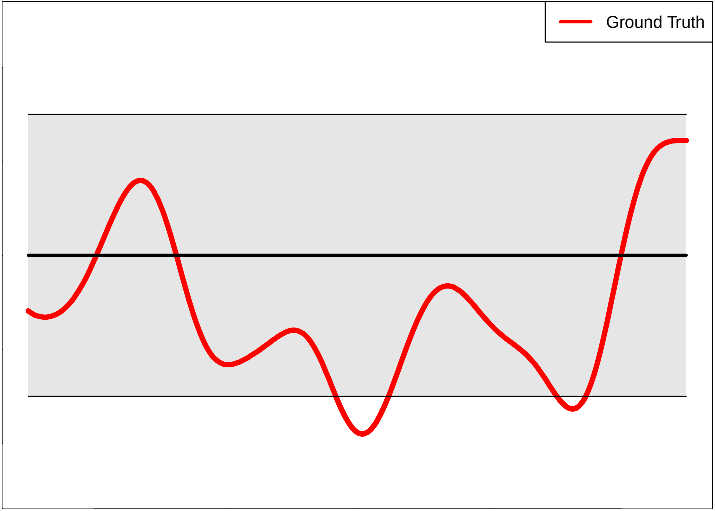
Periodic



$$C(\mathbf{x},\mathbf{x}') = \exp\left\{ - \frac{2 \sin^2 \left(\frac{|\mathbf{x}-\mathbf{x}'|}{2} \right)}{l^2} \right\}$$

From the Prior to the Posterior

GP regression provides a **closed-form** posterior distribution for $f(\cdot)$.



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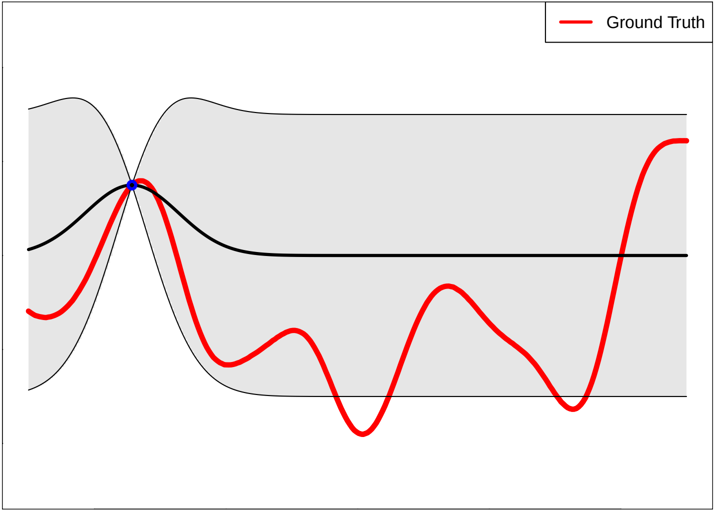

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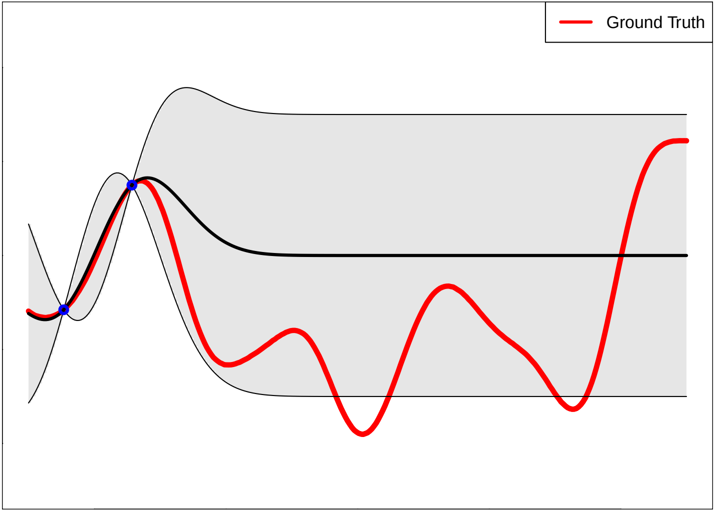

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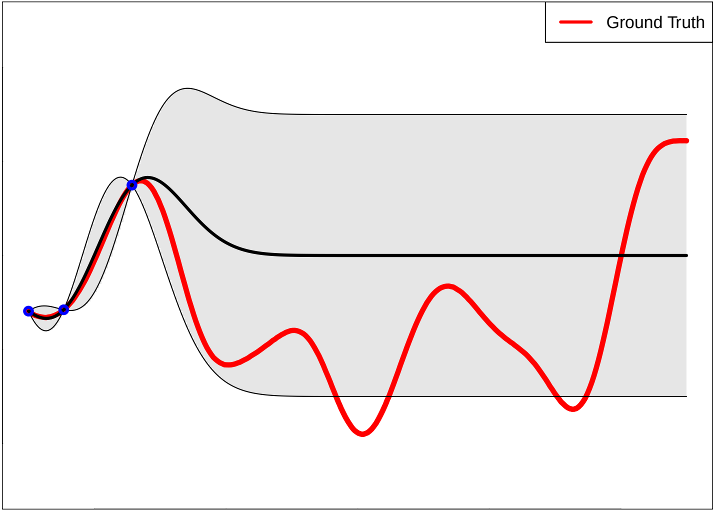

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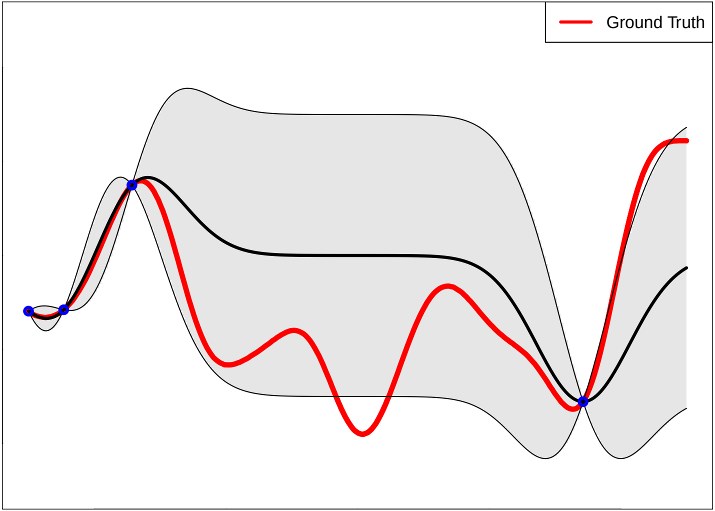

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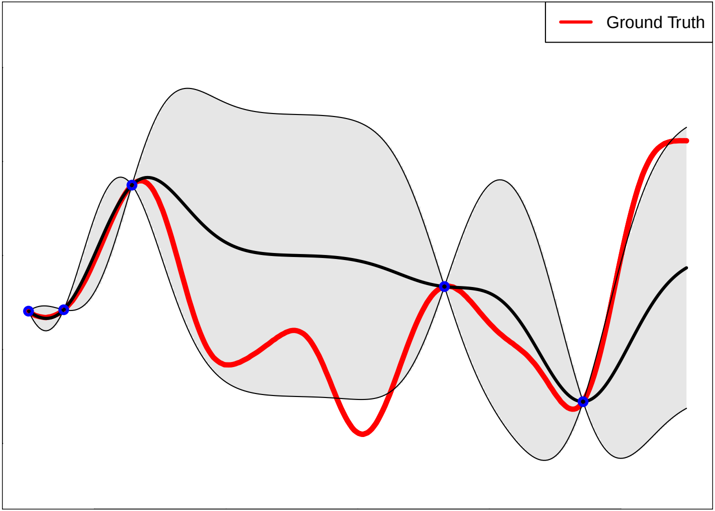

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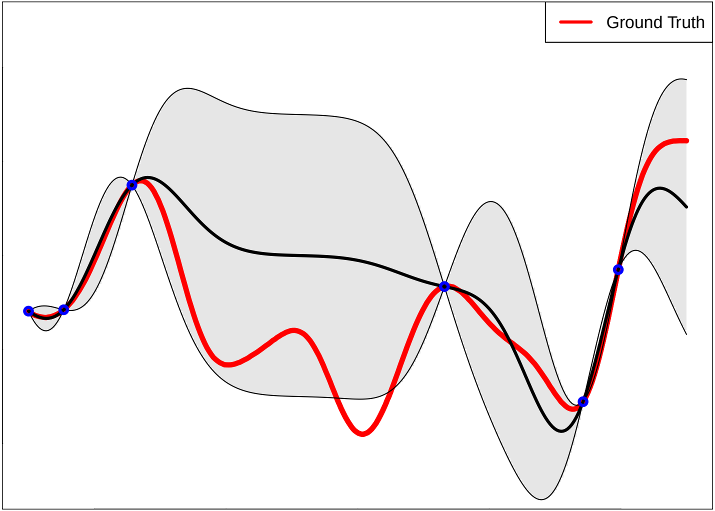

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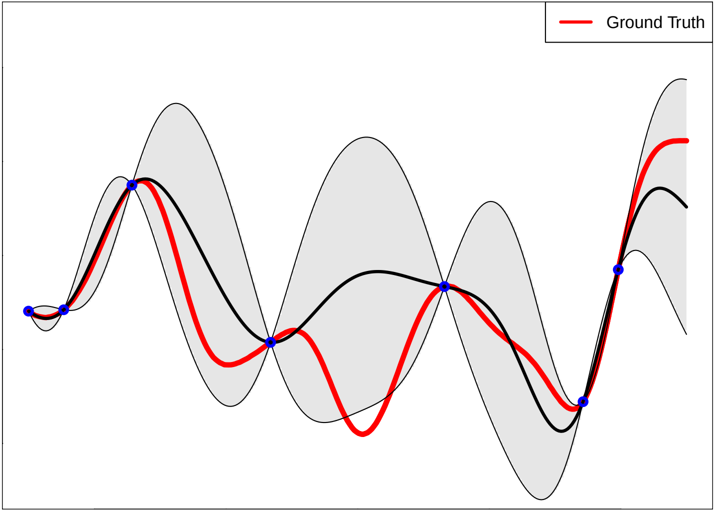

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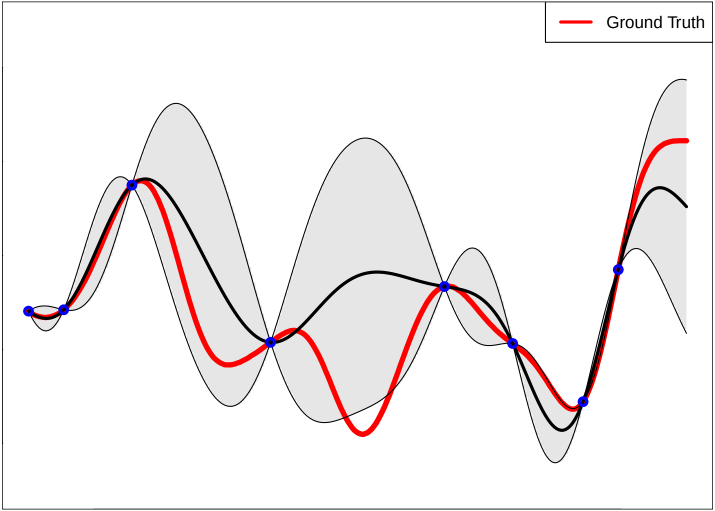

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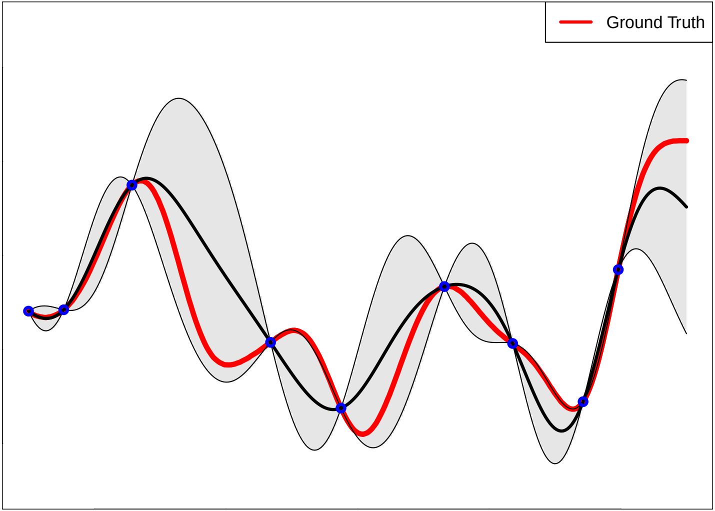

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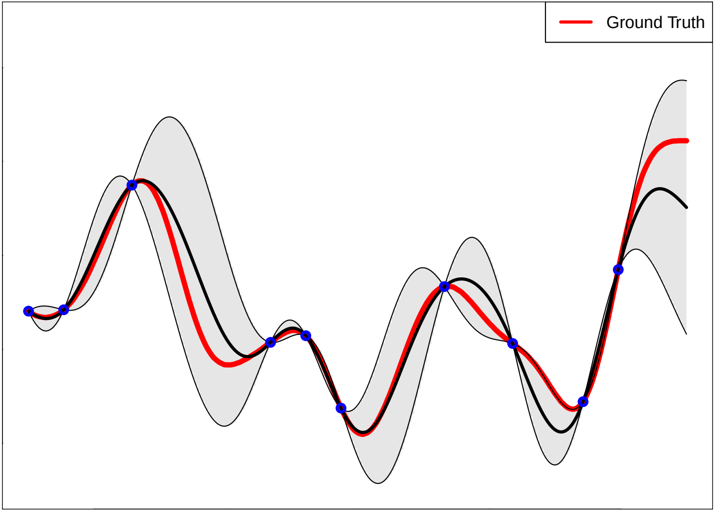

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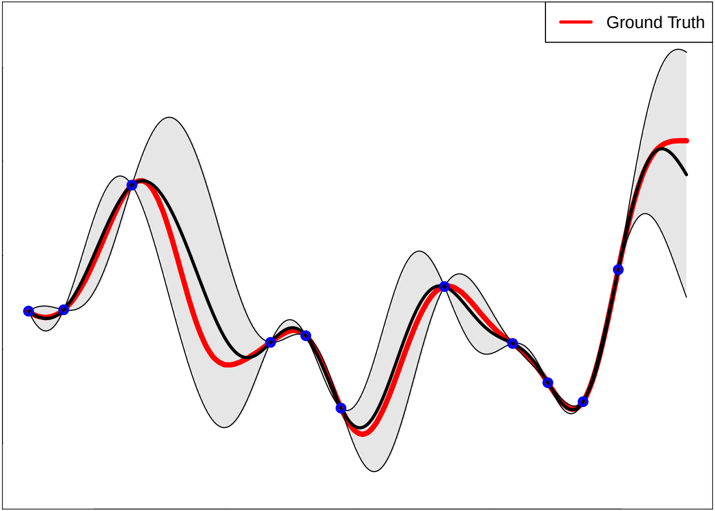

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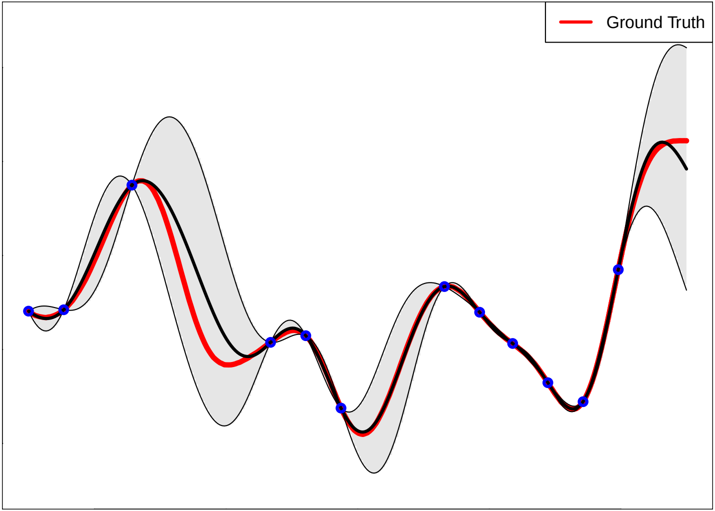

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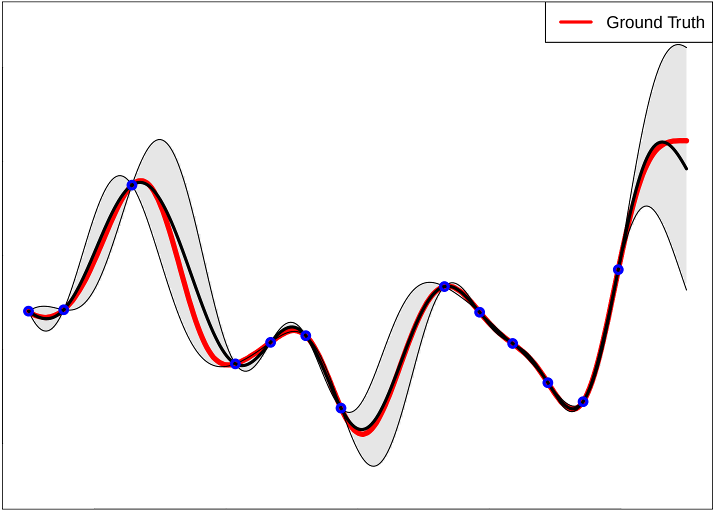

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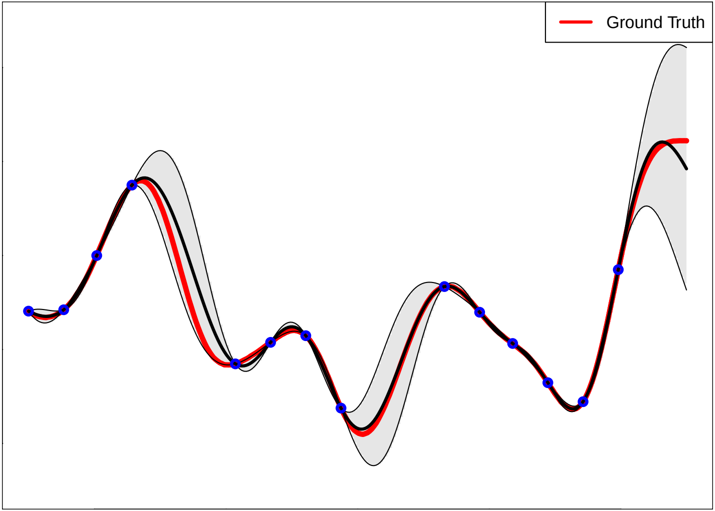

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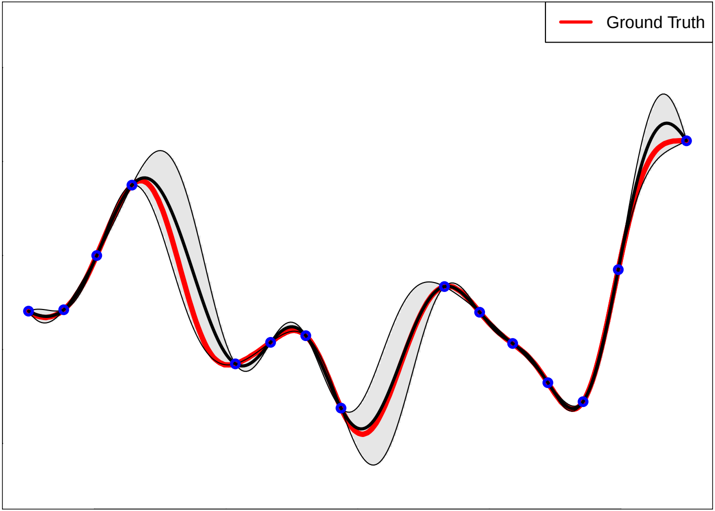

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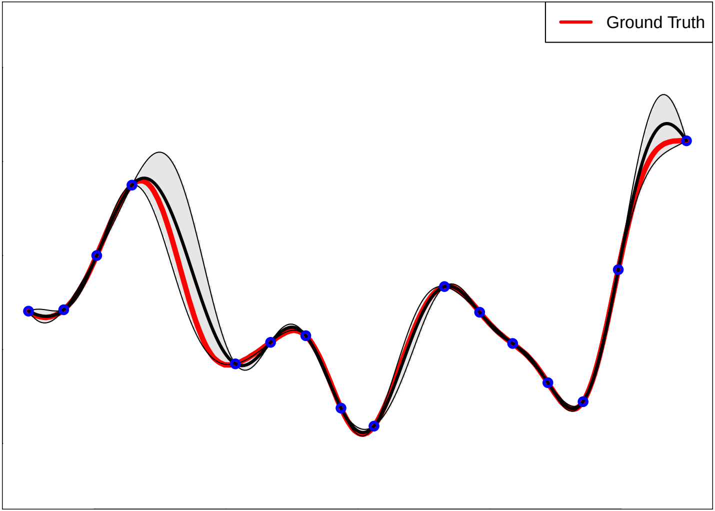

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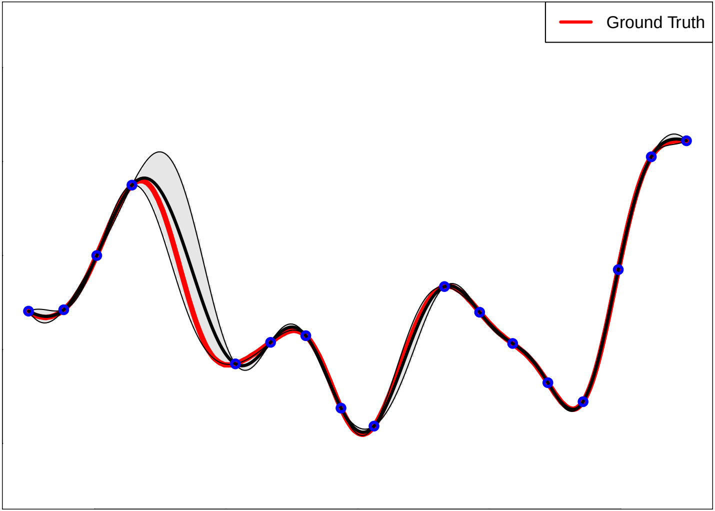

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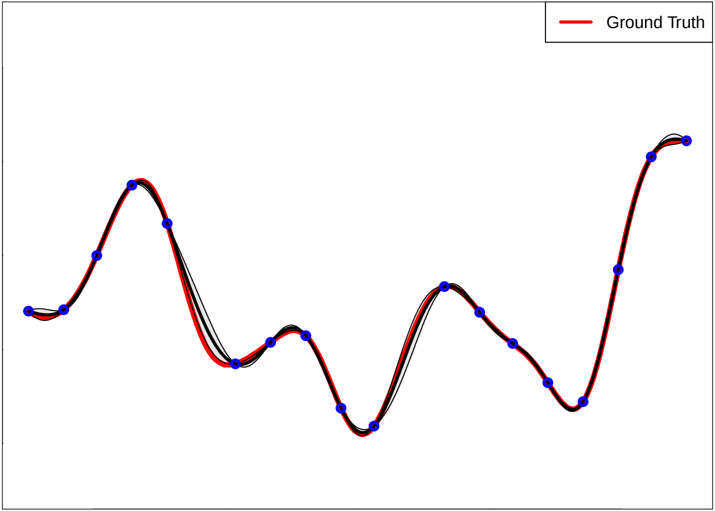

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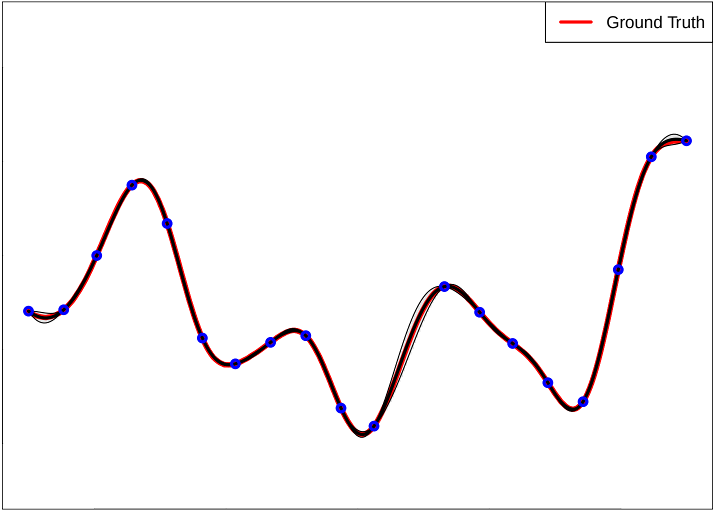

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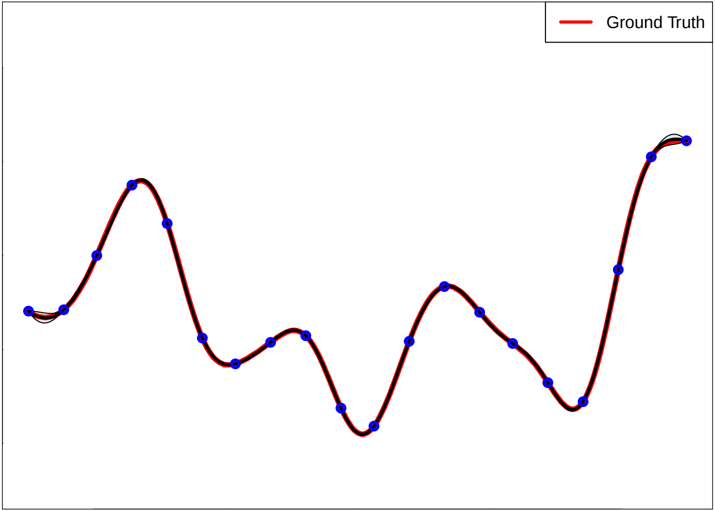

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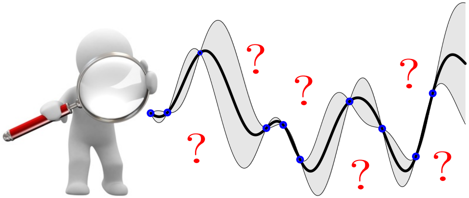

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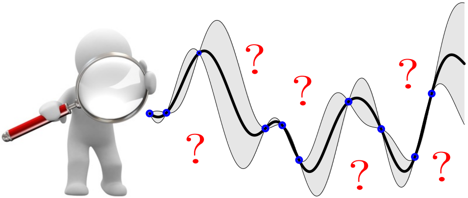

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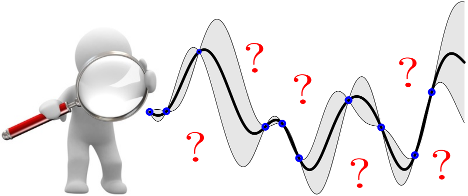

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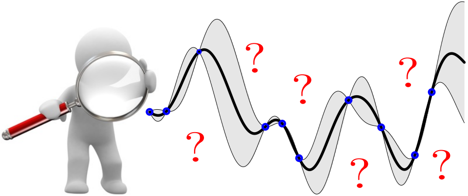

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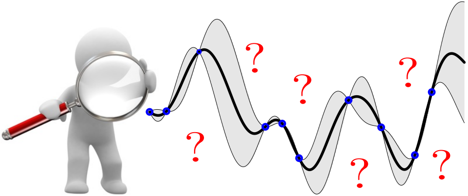

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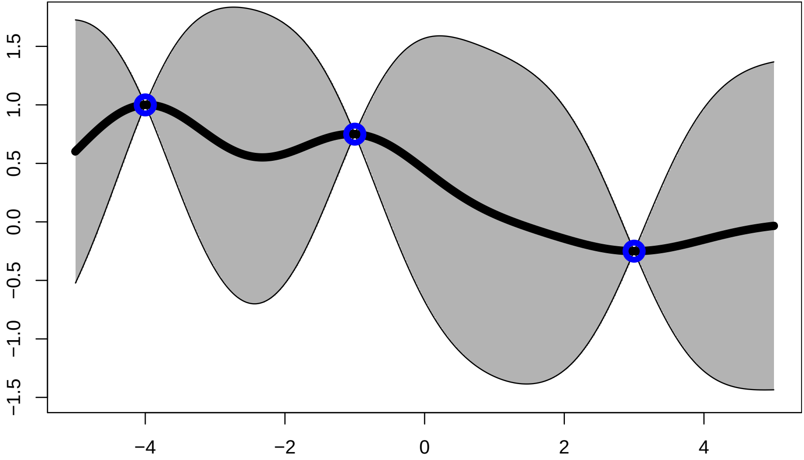

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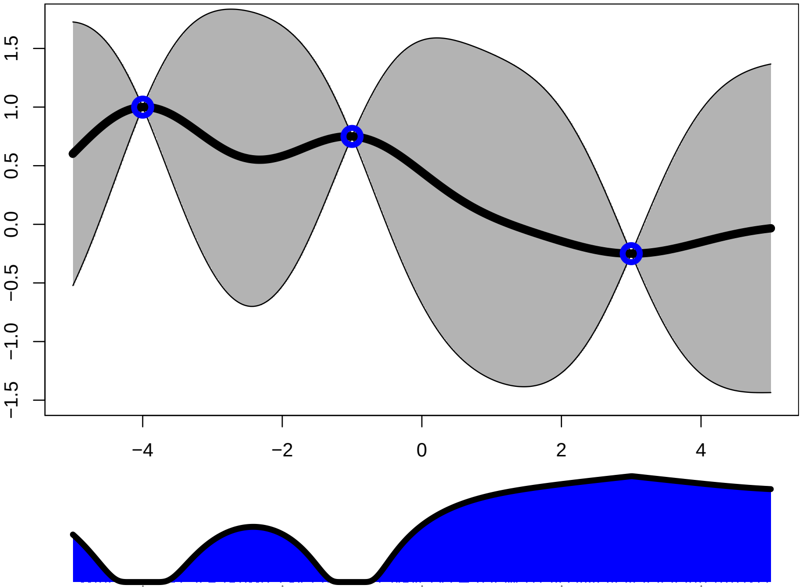

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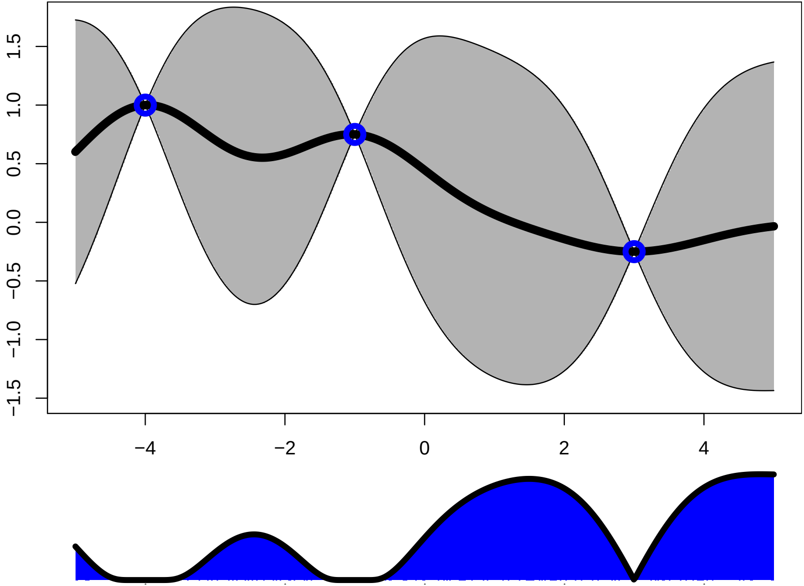

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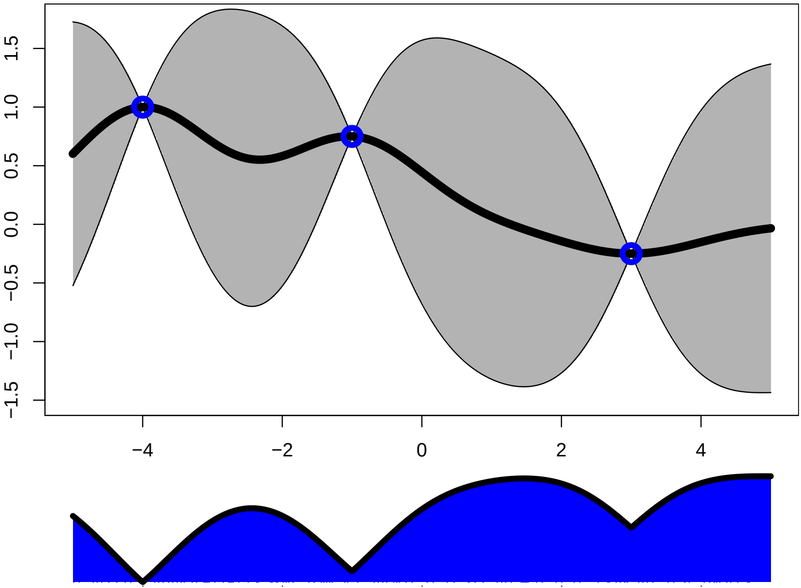

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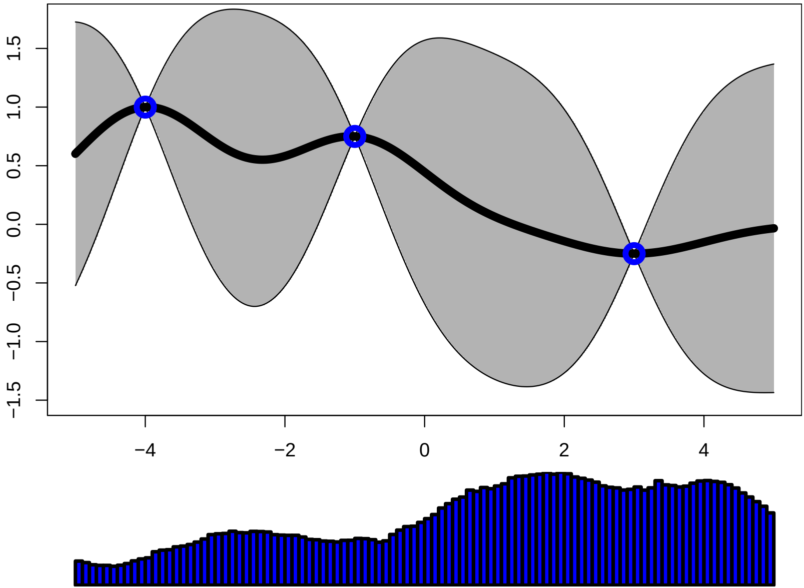

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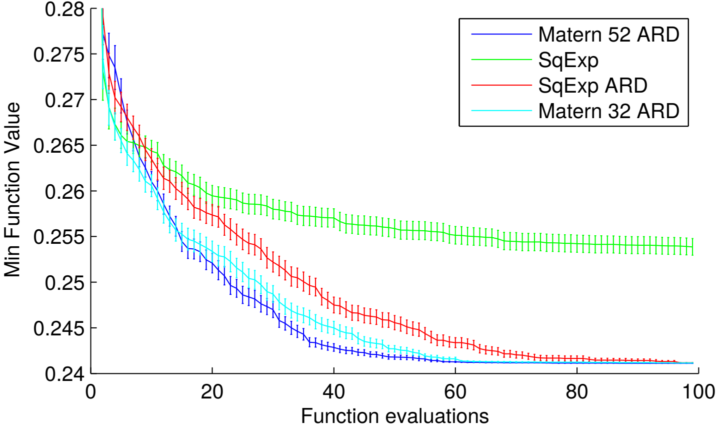

Structured SVM for protein motif finding (Snoek *et al.*, 2012).

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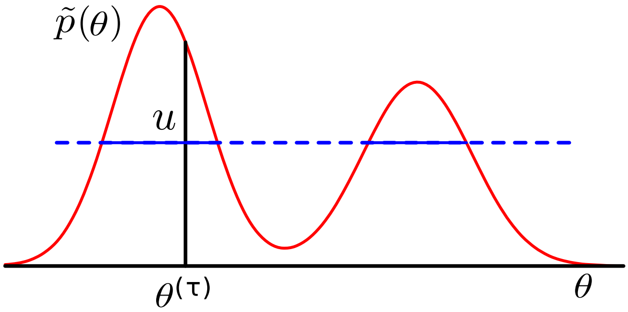

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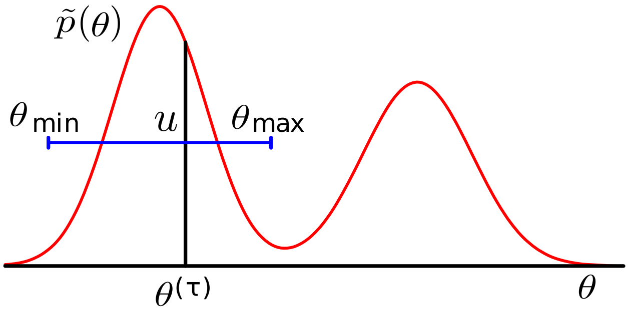

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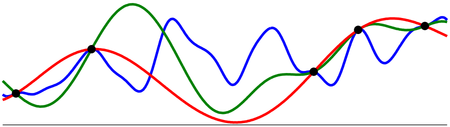

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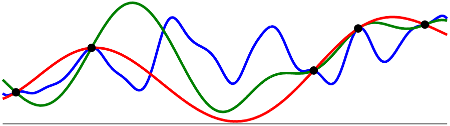
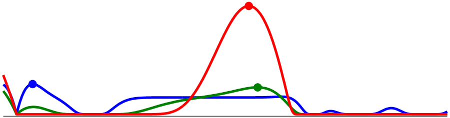


Length-scale specific expected improvement



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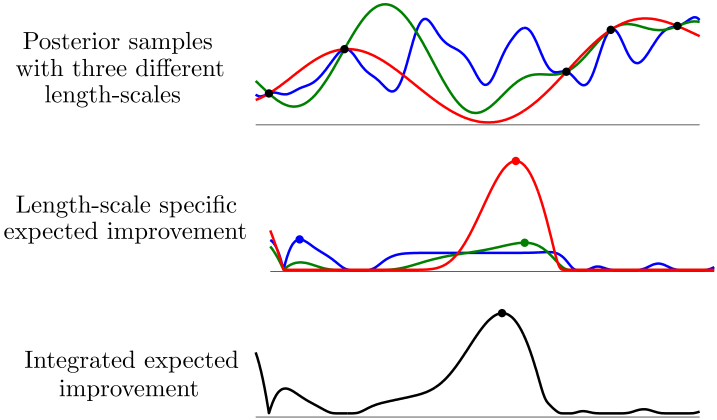

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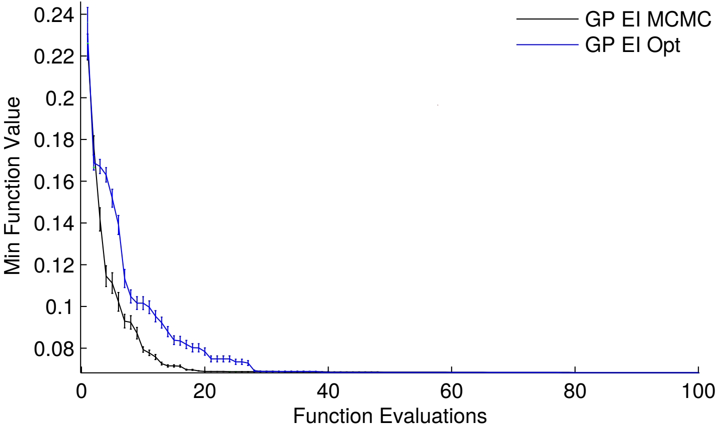
MCMC estimation vs. Maximization



Logistic regression on the MNIST (Snoek *et al.*, 2012).

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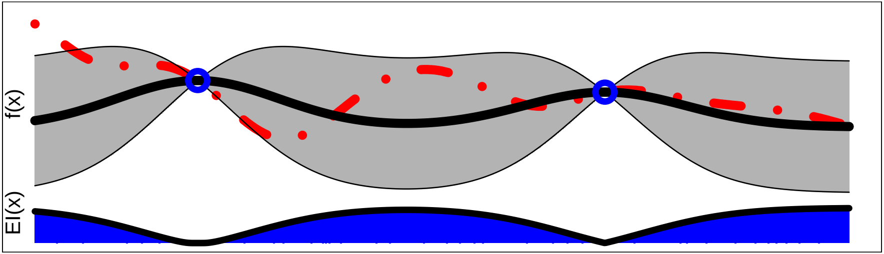

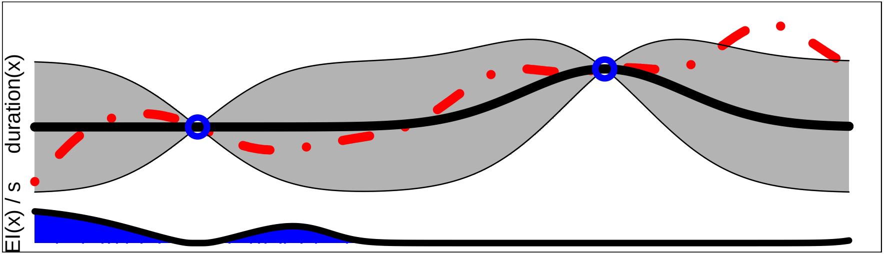

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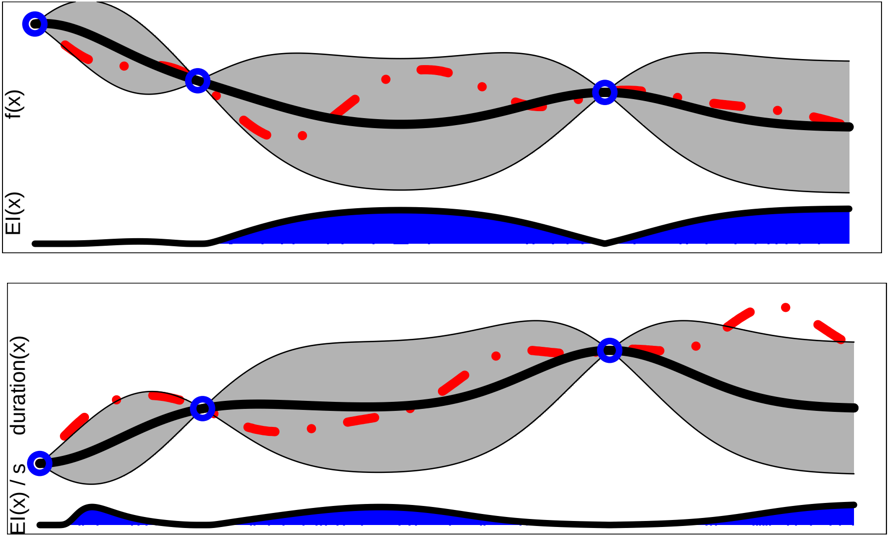

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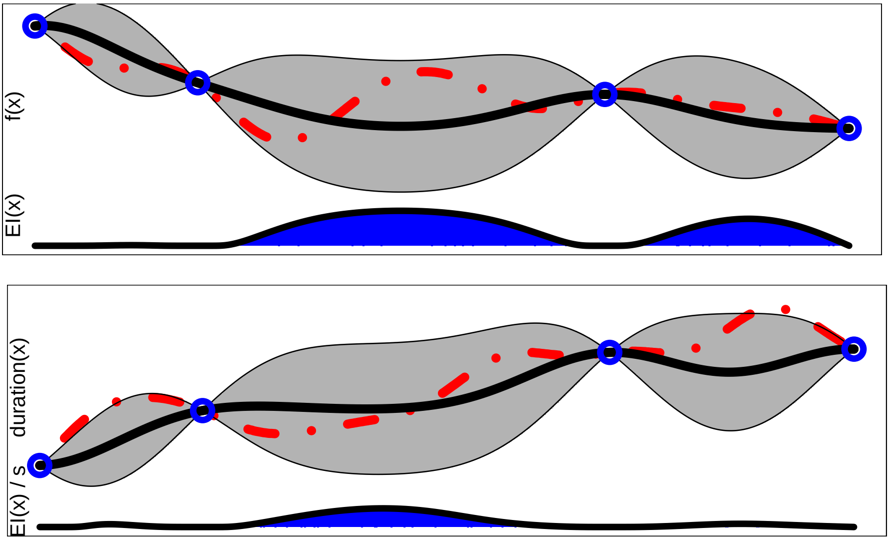

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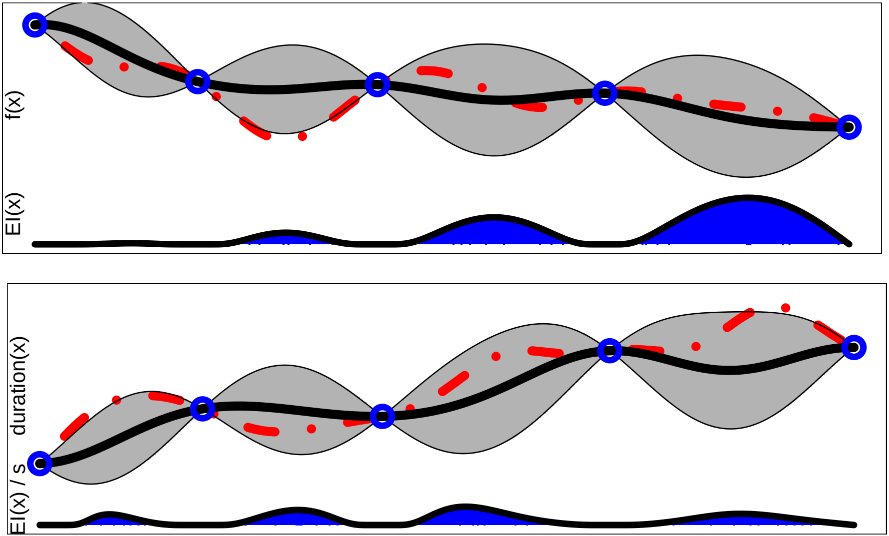

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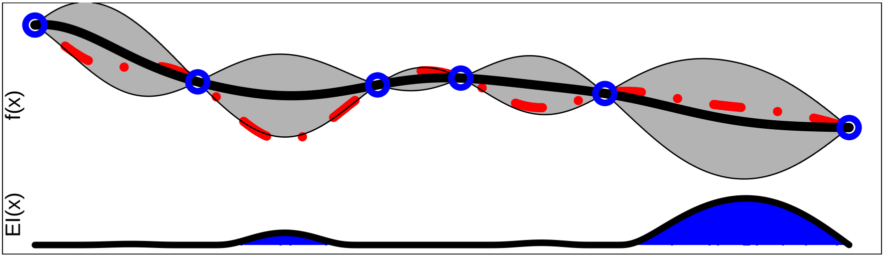

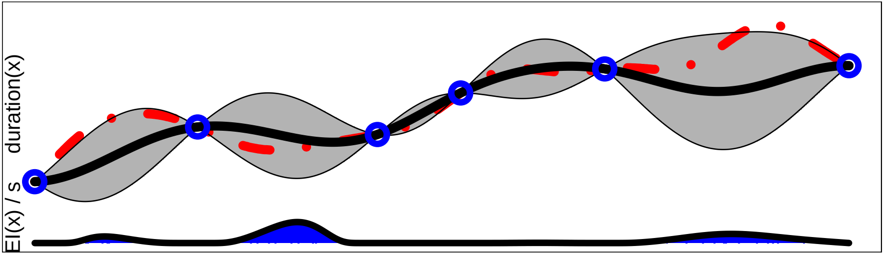

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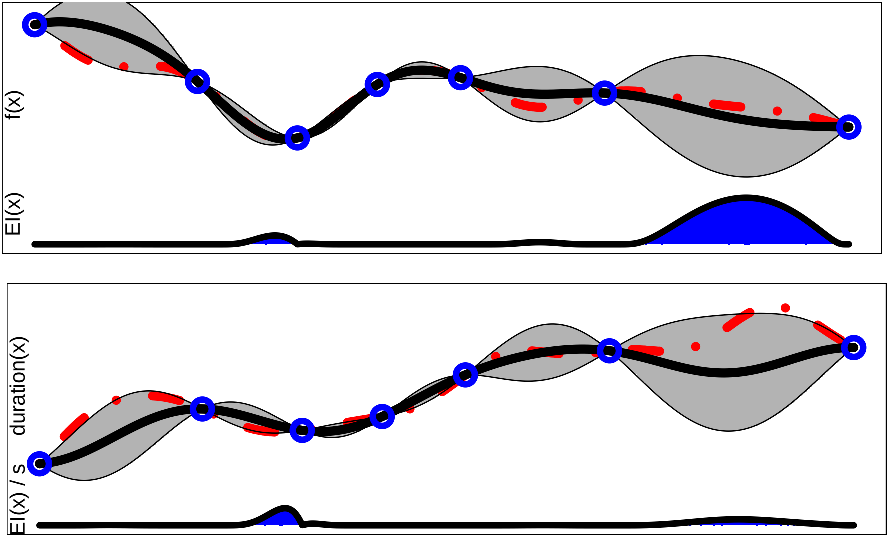

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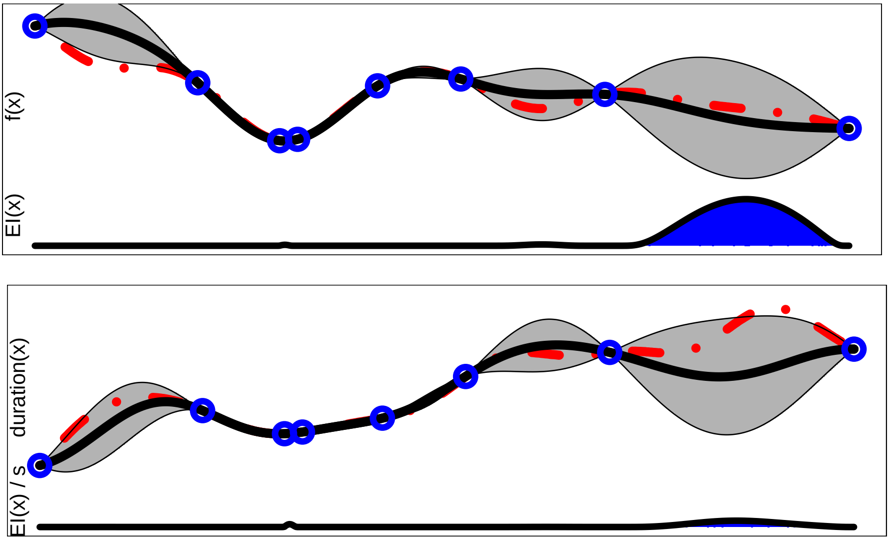

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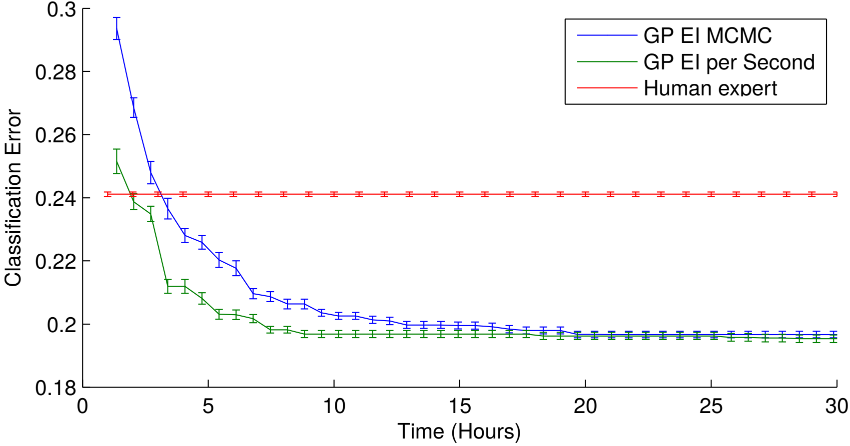
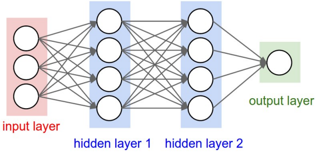
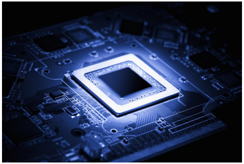


Deep neural network on the CIFAR dataset (Snoek *et al.*, 2012)

Several Objectives and Constraints

Optimal design of **hardware accelerator** for neural network predictions.





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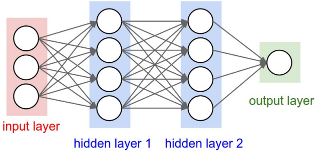

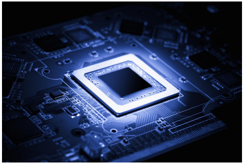

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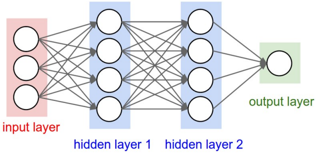

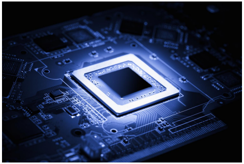

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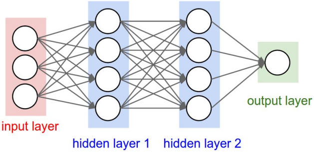

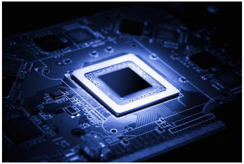

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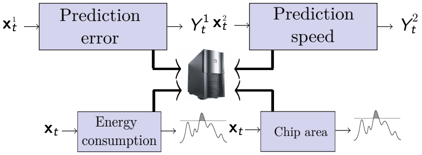

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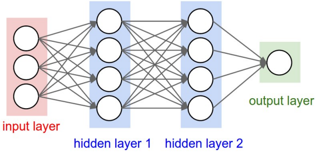

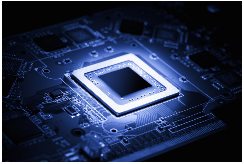

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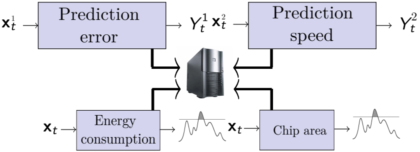
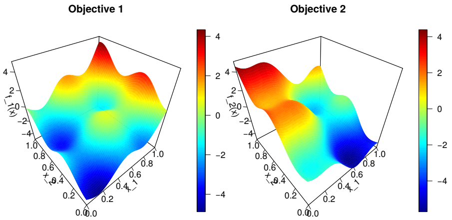


Challenges:

- **Complicated** constraints.
- **Conflictive** objectives.

Constrained Multi-Objective Optimization



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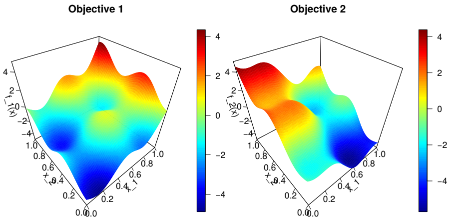

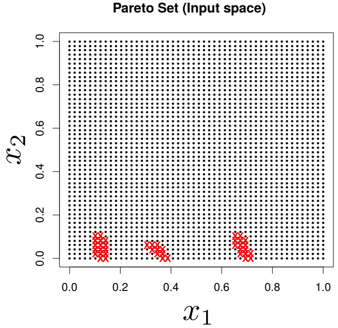

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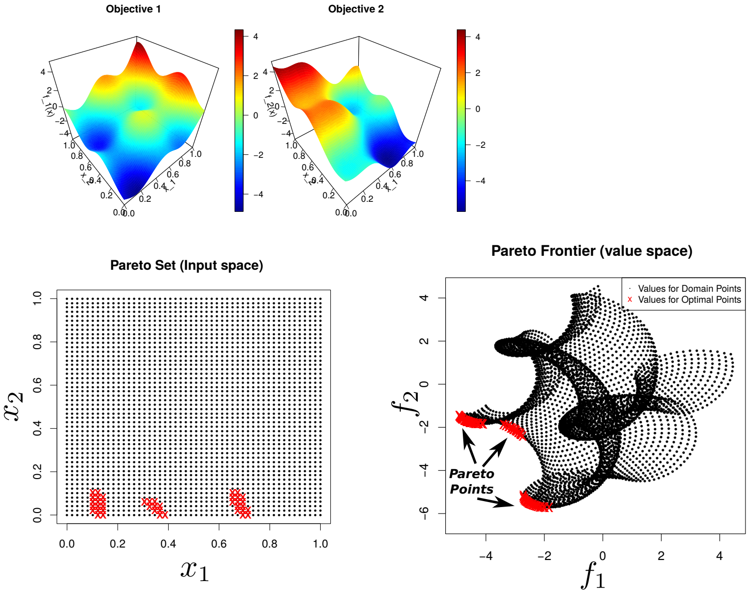

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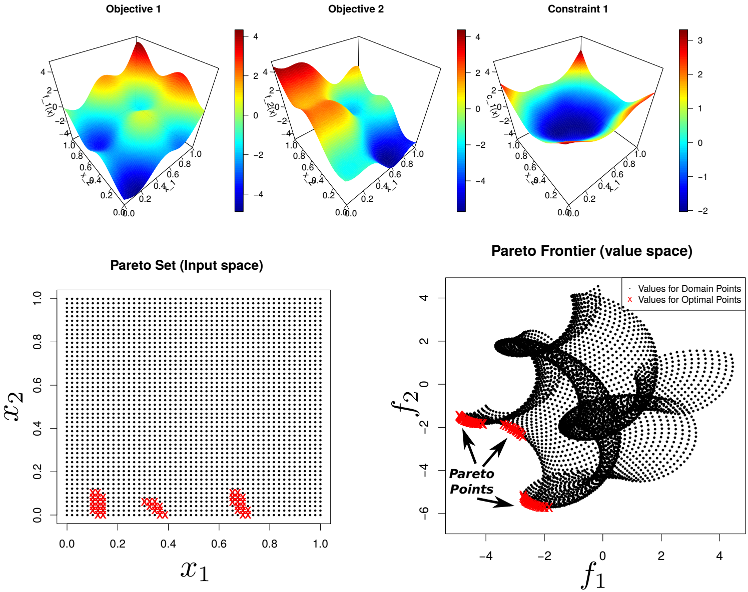

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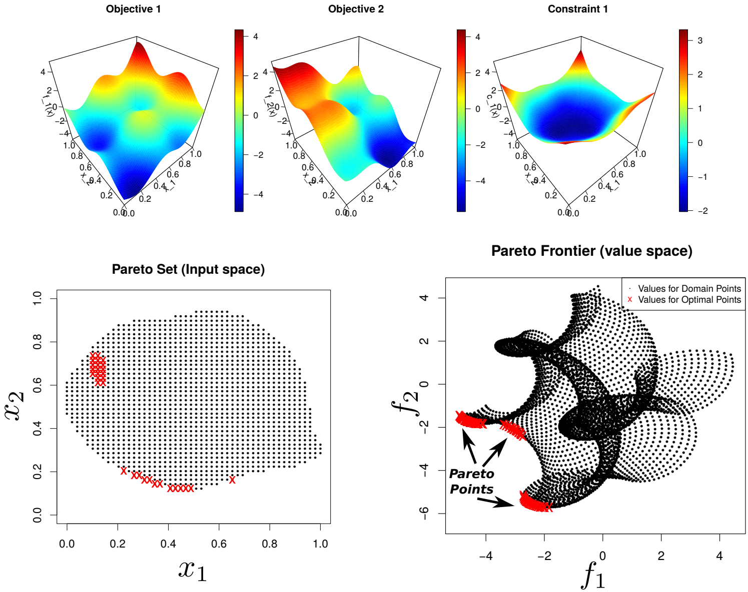

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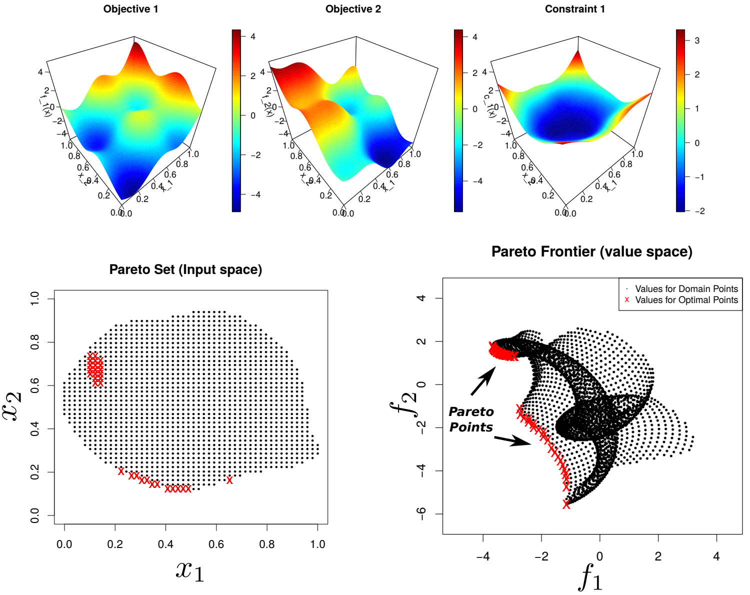

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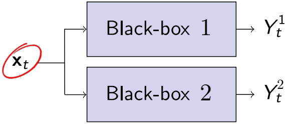

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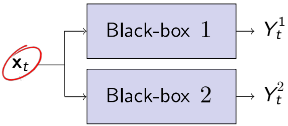

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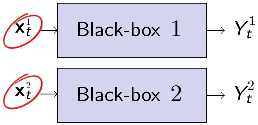

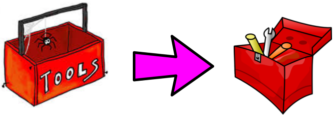

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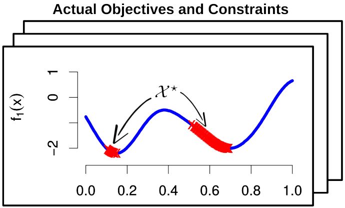

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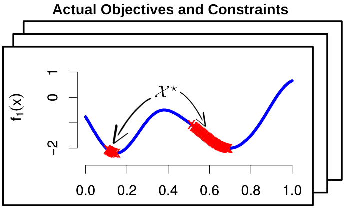

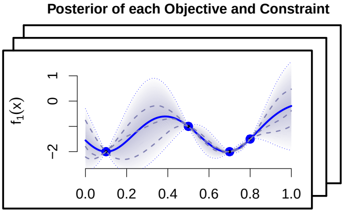

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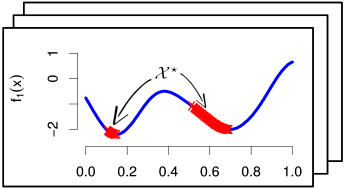

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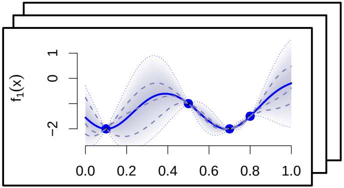

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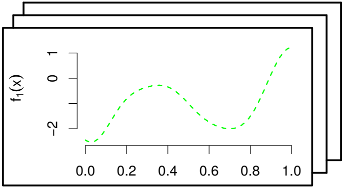

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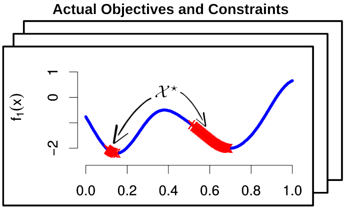

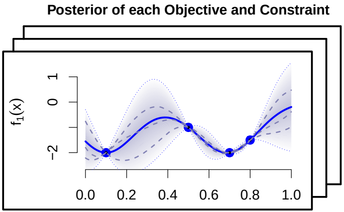

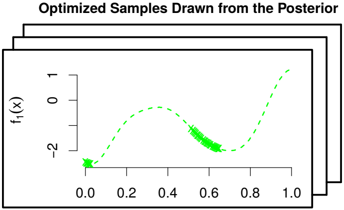

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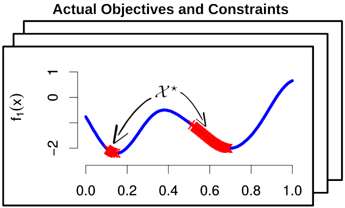

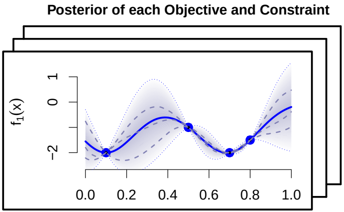

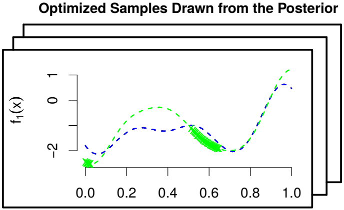

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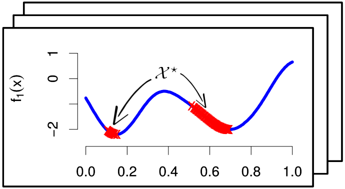

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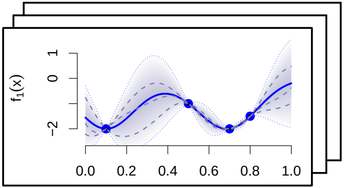

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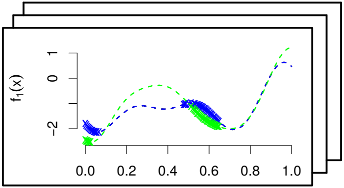

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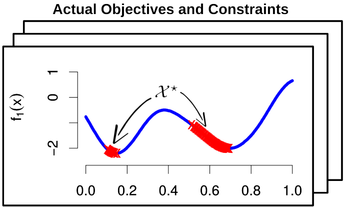

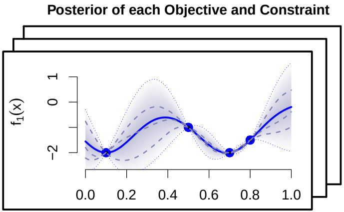

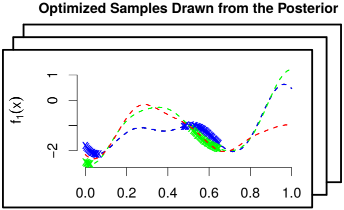

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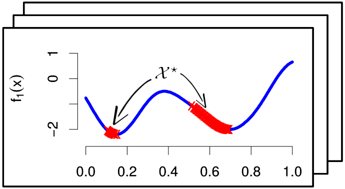

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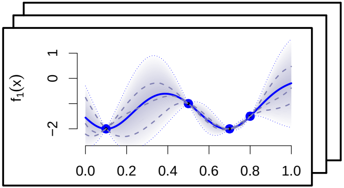

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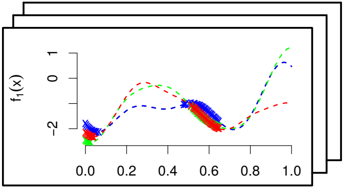

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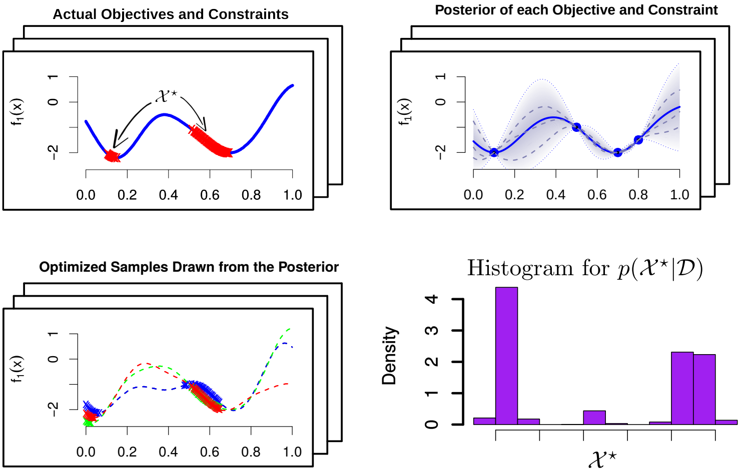

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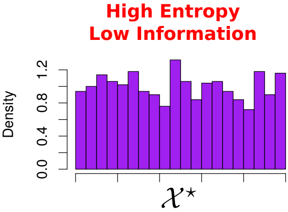

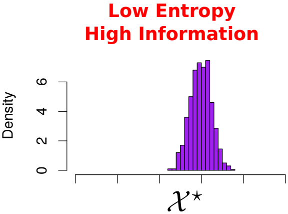

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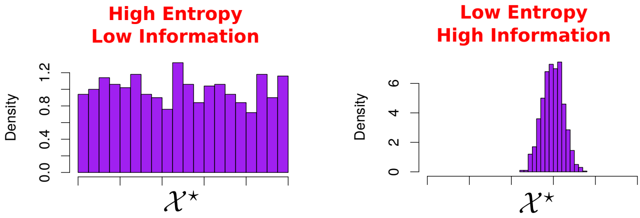

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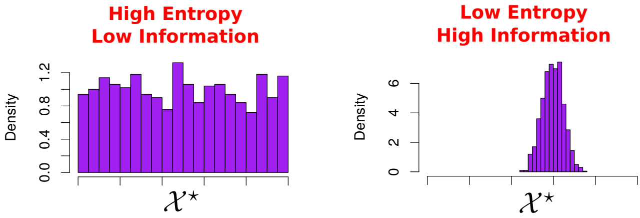

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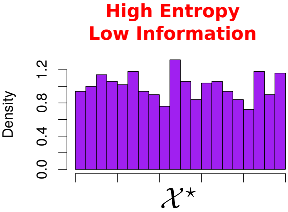

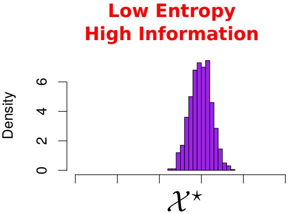

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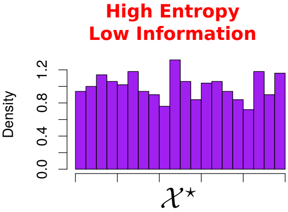

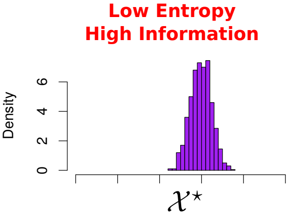

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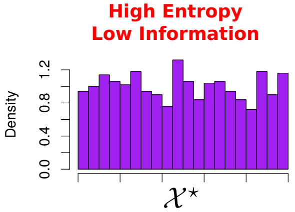

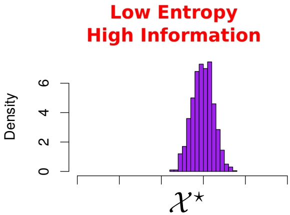

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Computing (1) is **very difficult in practice**!

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One acquisition per black-box

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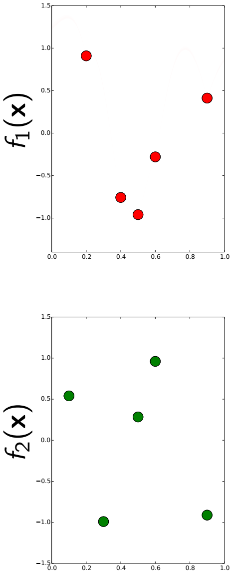
Example of PES' acquisition



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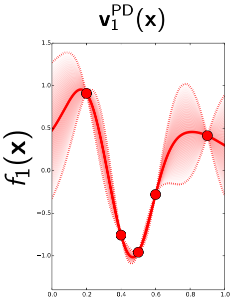

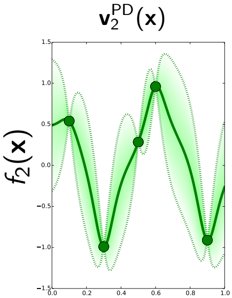

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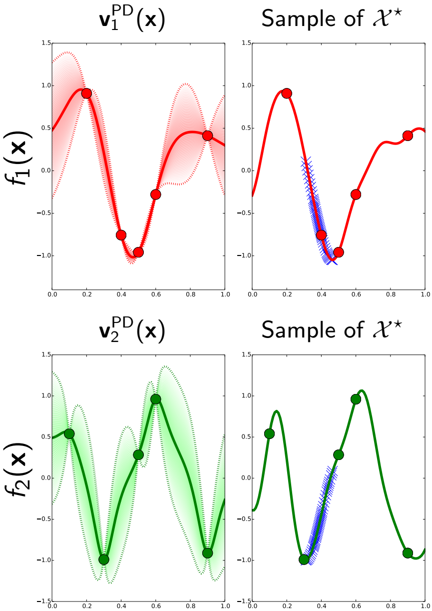

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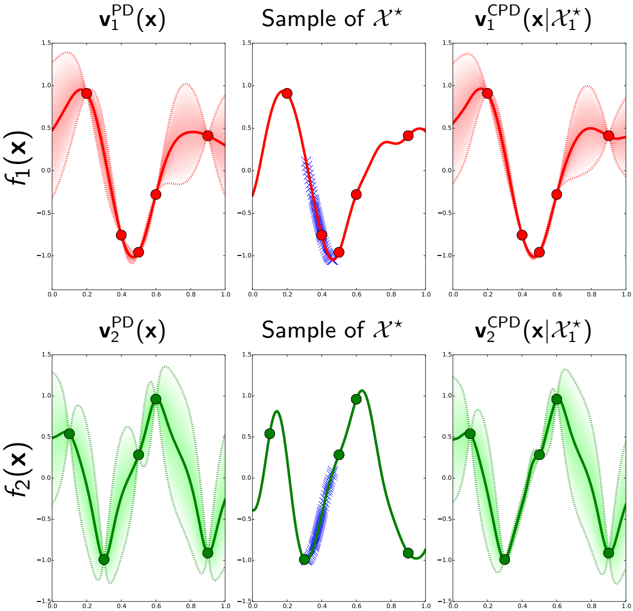

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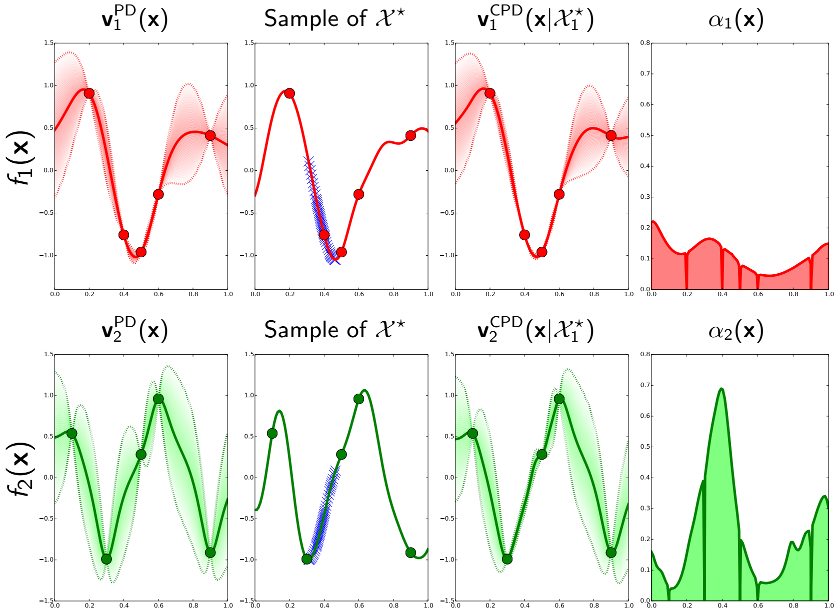

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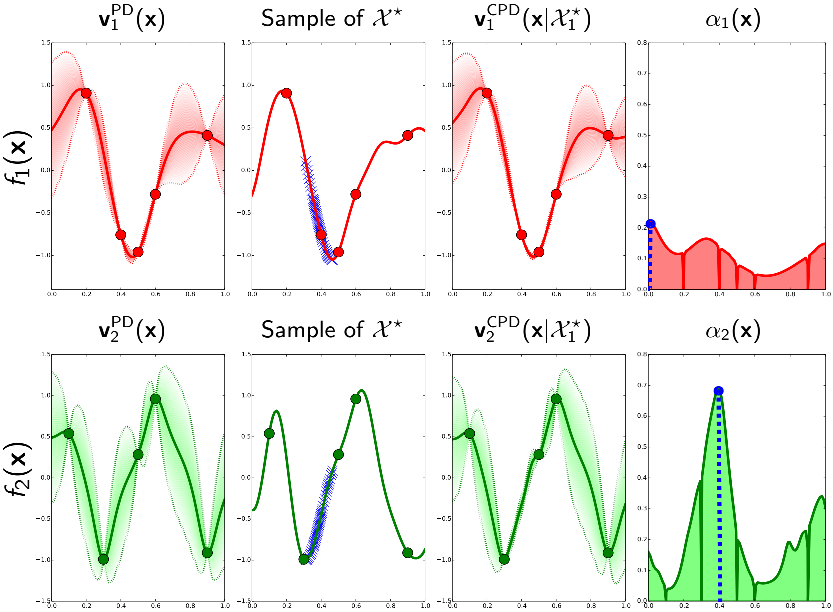
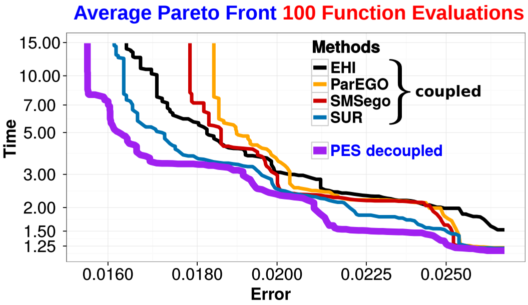


Finding a Fast and Accurate Neural Network



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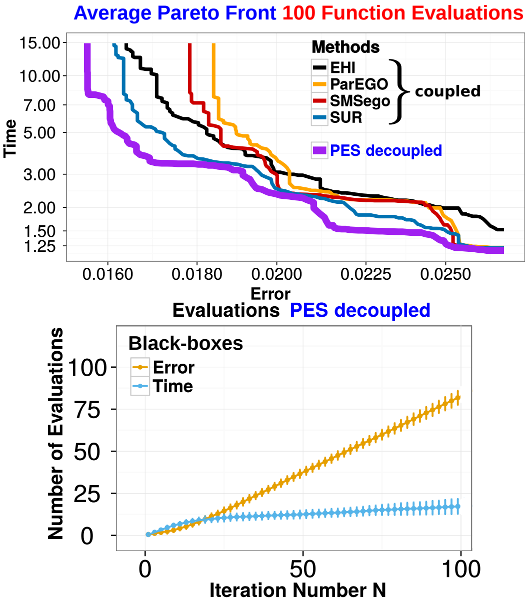

(Hernández-Lobato *et al.*, 2016)

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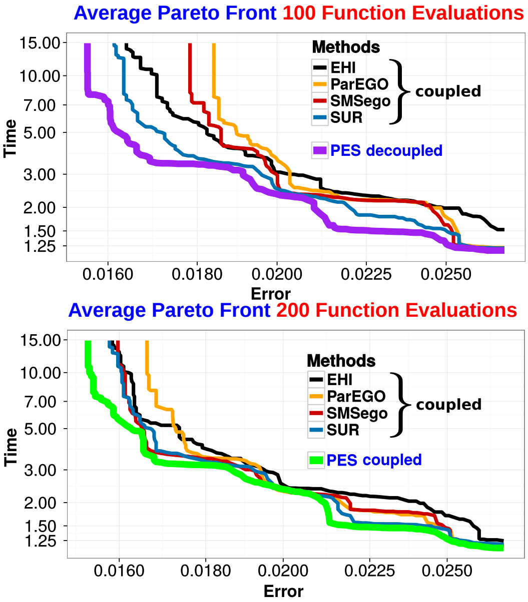

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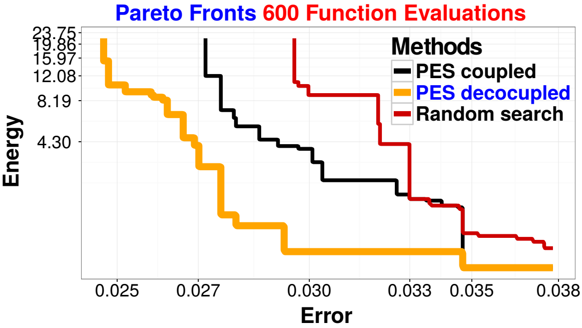
Low energy hardware accelerator



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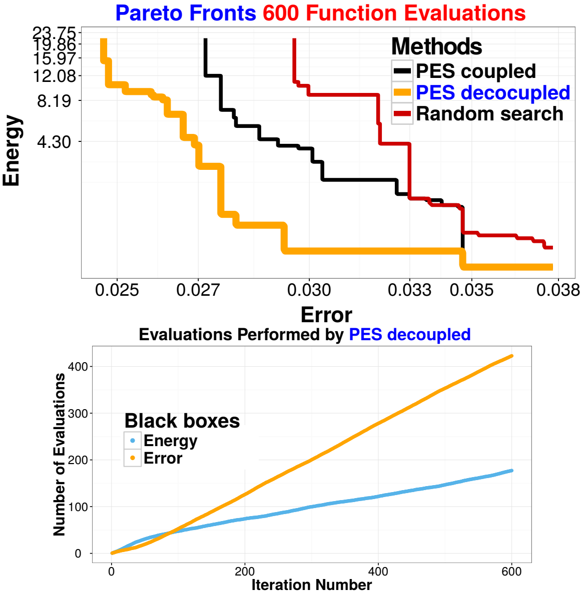

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Traditional Bayesian optimization is **sequential**!

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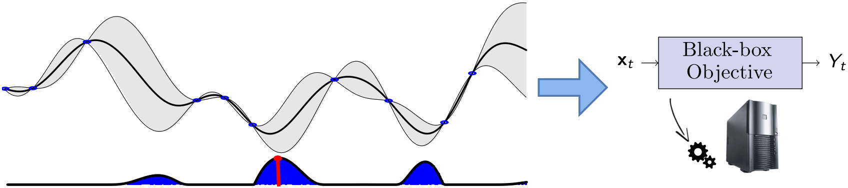

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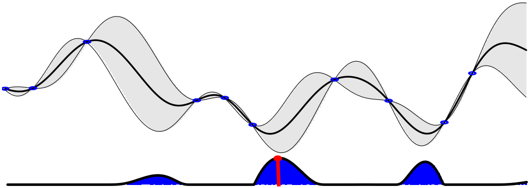

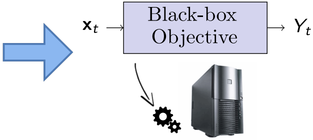

Computing clusters let us do **many things** at once!

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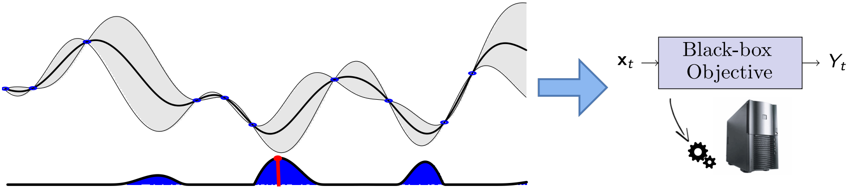

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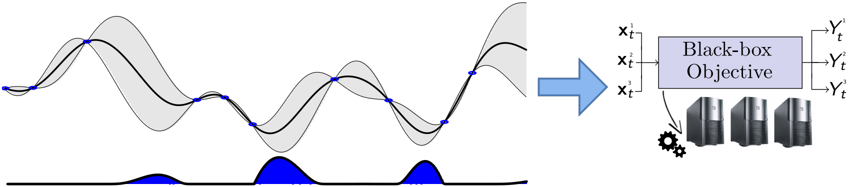

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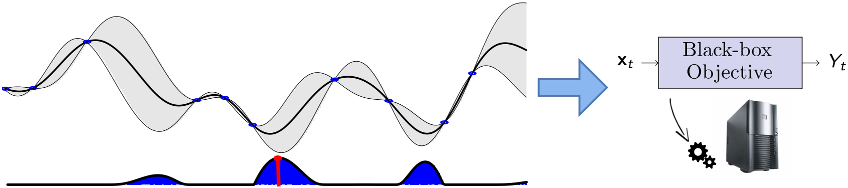

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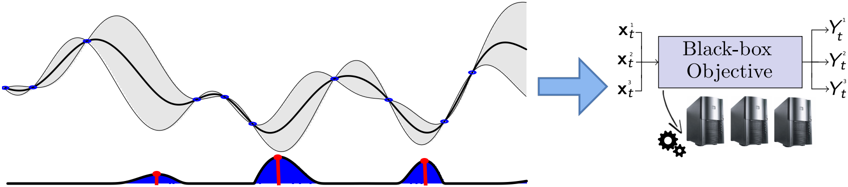

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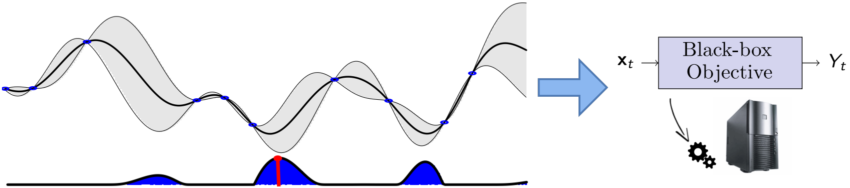

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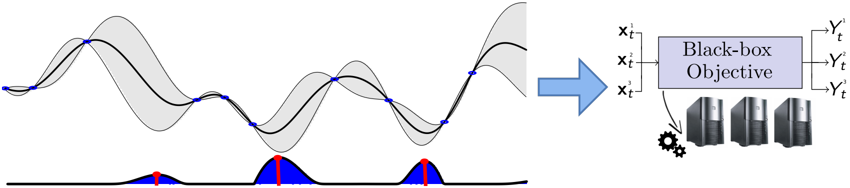

Parallel experiments should be highly informative but different!

Parallel Predictive Entropy Search

Choose a set Q points $\mathcal{S}_t = \{\mathbf{x}_q\}_{q=1}^{Q}$ to minimize the entropy of $\mathbf{x}^\star$.

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Multivariate Gaussian approximation with **expectation propagation**
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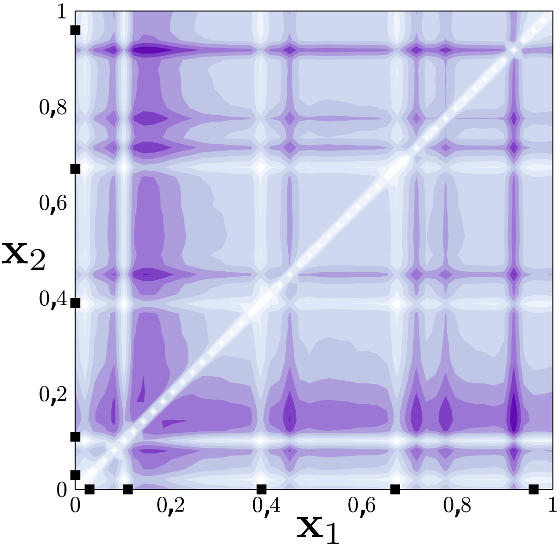
It is possible to compute the gradient of $\alpha(\cdot)$ w.r.t. each $\mathbf{x}_q \in \mathcal{S}_t$!

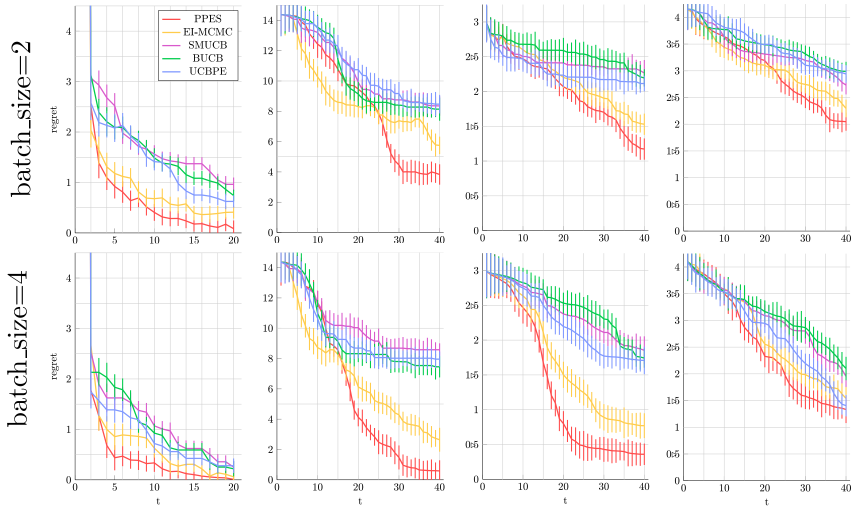
(Shah and Ghahramani, 2015)

Parallel Predictive Entropy Search: Level Curves



(Shah and Ghahramani, 2015)

Parallel Predictive Entropy Search: Results



(a) `boston` (b) `hydrogen` (c) `rocket` (d) `robot`

(Shah and Ghahramani, 2015)

BO with Integer-valued and Categorical Variables

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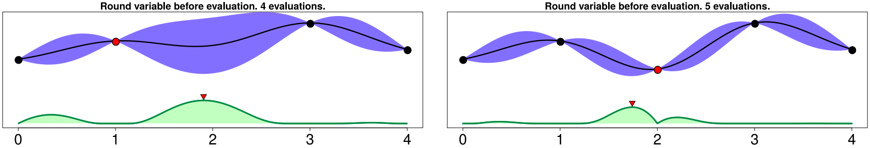

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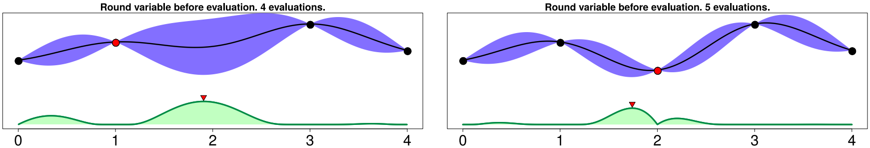
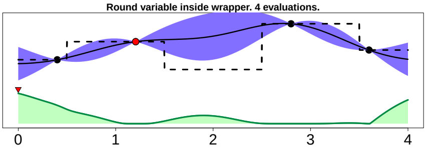
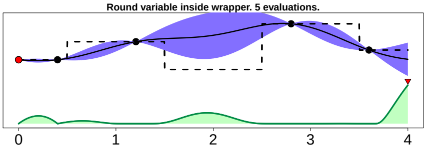


The BO algorithm may get stuck and may always perform the next evaluation at the same input location!

BO with Integer-valued and Categorical Variables

Rounding inside of the wrapper works but makes the objective flat!





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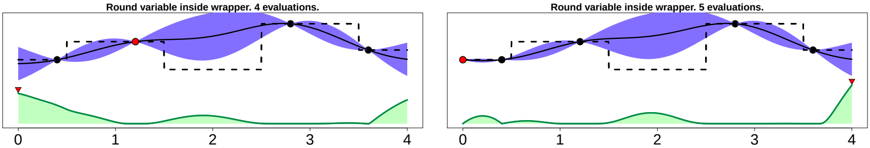

A modified GP covariance function accounts for this:

$$C_{\text{new}}(\mathbf{x}_n, \mathbf{x}_{n'}) = C(T(\mathbf{x}_n), T(\mathbf{x}_{n'}); \boldsymbol{\theta})$$

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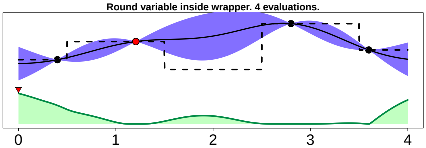

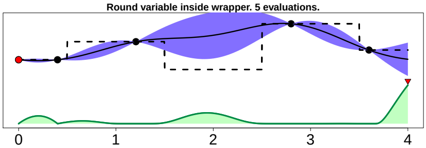

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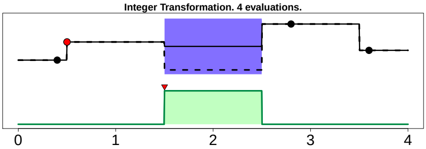

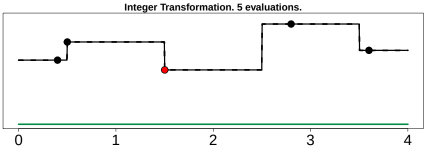

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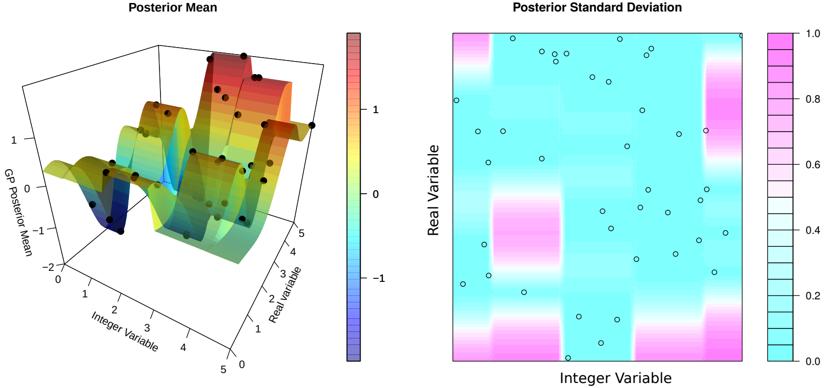

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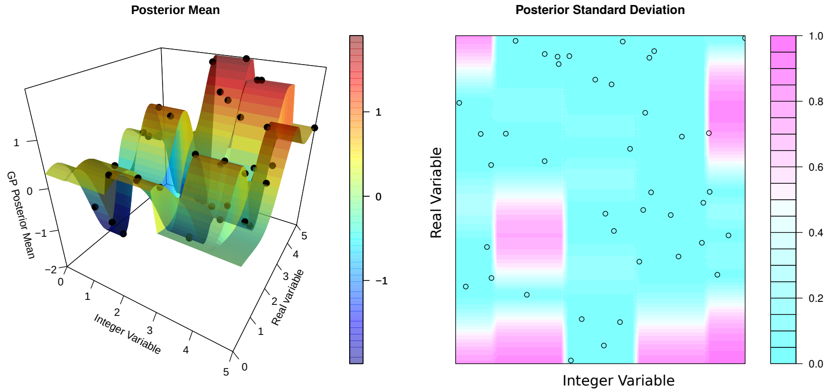
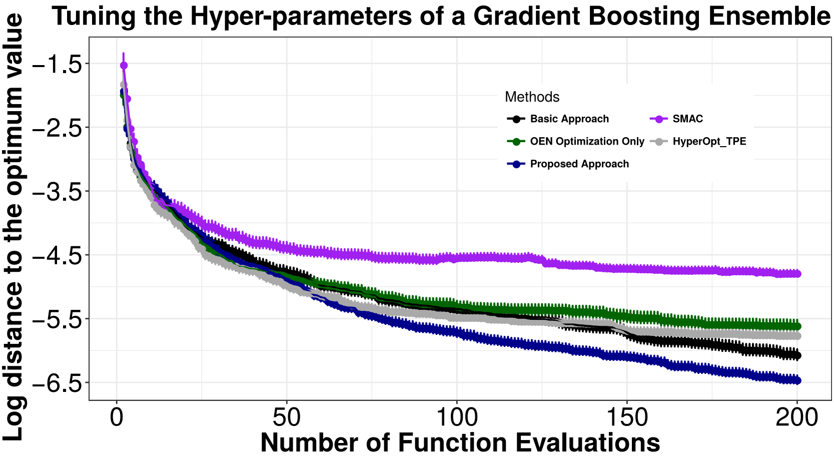


Similar results for categorical variables!

BO with Integer-valued and Categorical Variables



One continuous variable and two integer-valued variables.

Freeze-Thaw Bayesian Optimization

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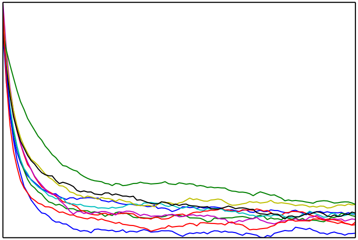

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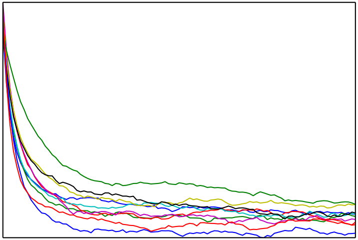

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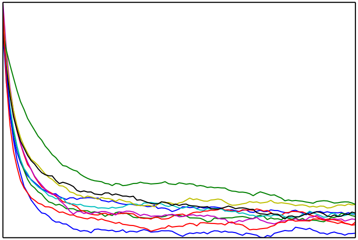

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Yes, that is precisely what Freeze-Thaw BO does!

(Swersky et al., 2014)

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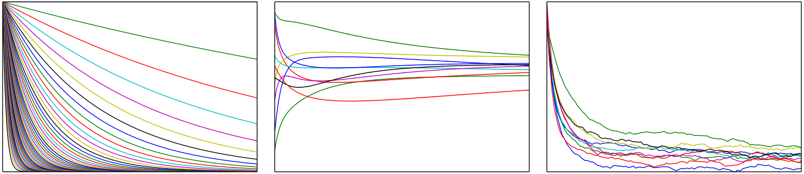

(a) Exponential Decay Basis (b) Samples (c) Training Curve Samples

Inference on Asymptotic Values

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where

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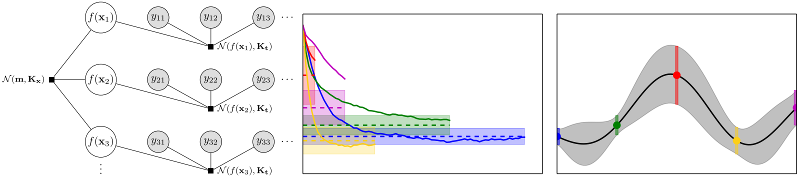
The joint distribution of $\{\mathbf{y}\}_{n=1}^N$ and $\mathbf{f}$ is Gaussian and hence so it the predictive distribution $p(\mathbf{f}|\{\mathbf{y}\}_{n=1}^N)$!

Inference on Asymptotic Values and BO



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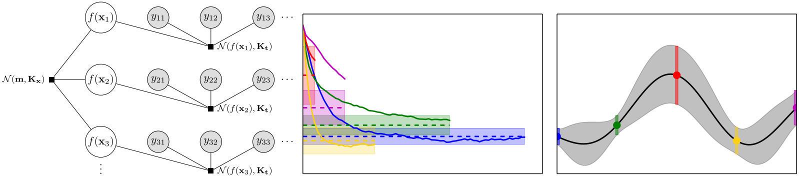

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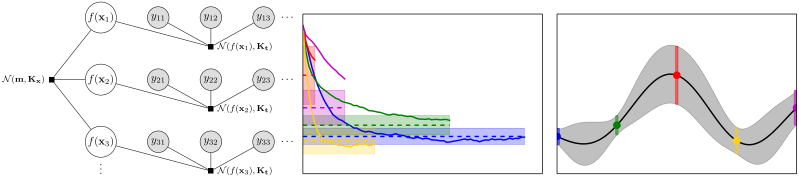

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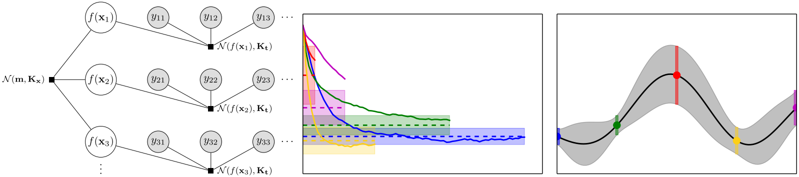

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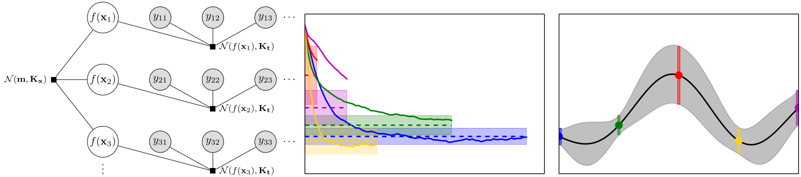

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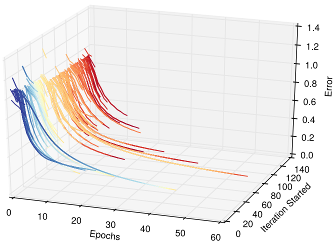
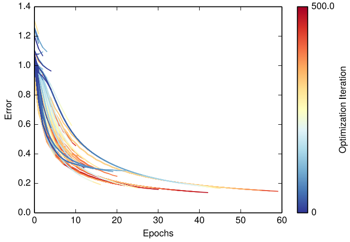
- A combination of EI and ES is used as the acquisition function.

(Swersky et al., 2014)

Freeze-Thaw BO in practice





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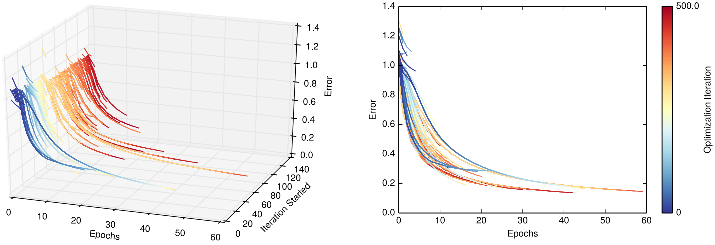

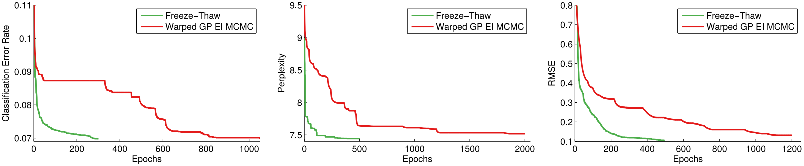

(a) Logistic Regression (b) Online LDA (c) PMF

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The computational cost is in $\mathcal{O}(nm^2)$!

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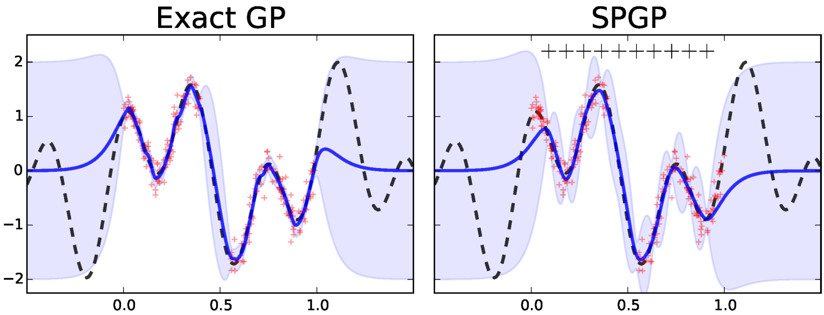

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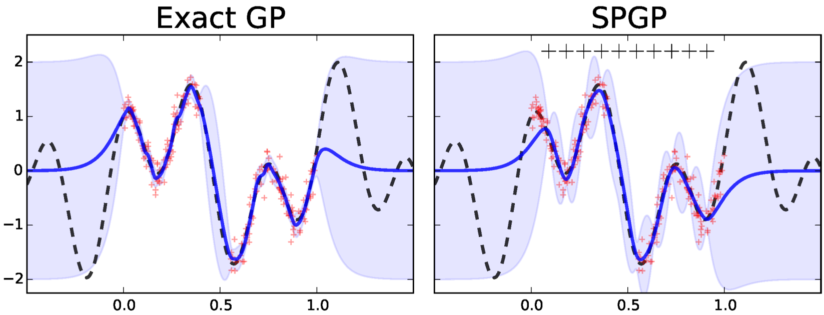

- Too small variance at the pseudo-inputs.
- Too big variance in between and away from pseudo-inputs.

(Shahriari et al., 2016)

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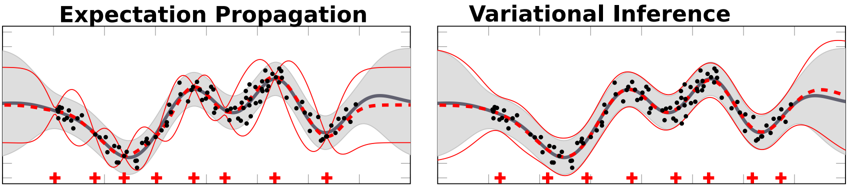

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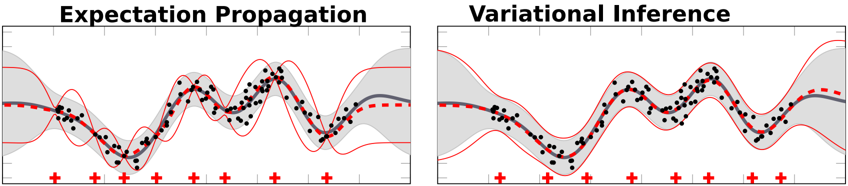

- EP: less local optima and easier to optimize, also less accurate.
- VI: more accurate, more local optima, more difficult to optimize.

(Bui et al., 2017) (Bauer et al., 2016)

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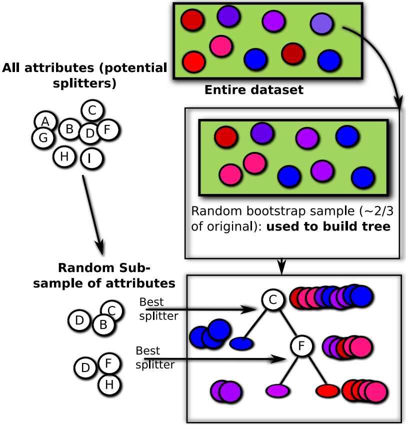

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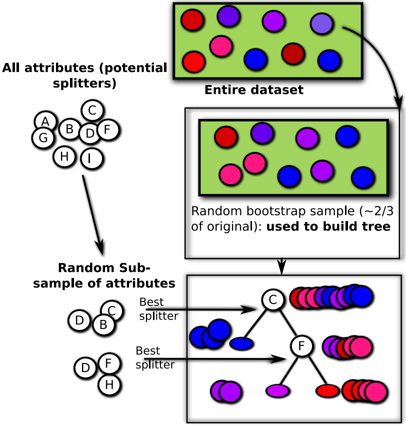

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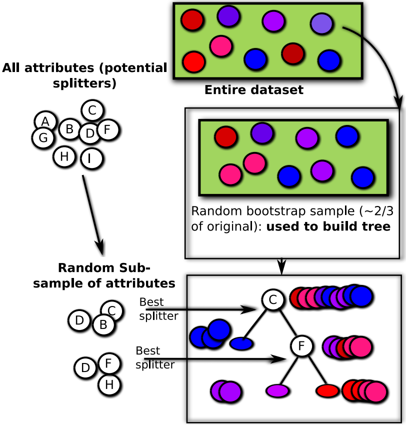

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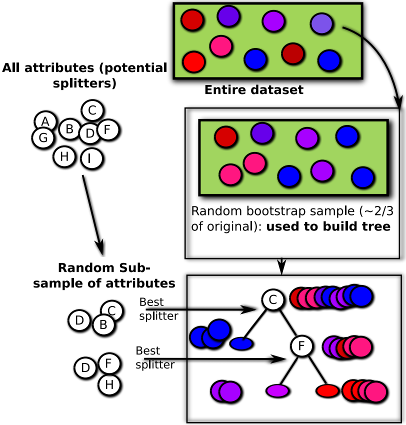

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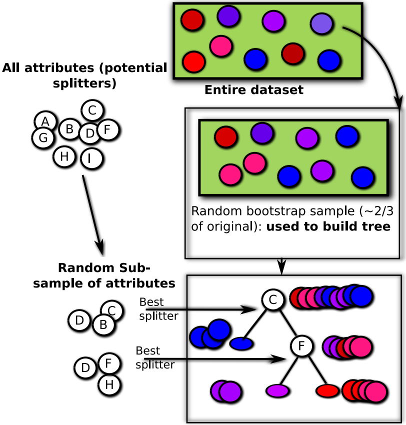

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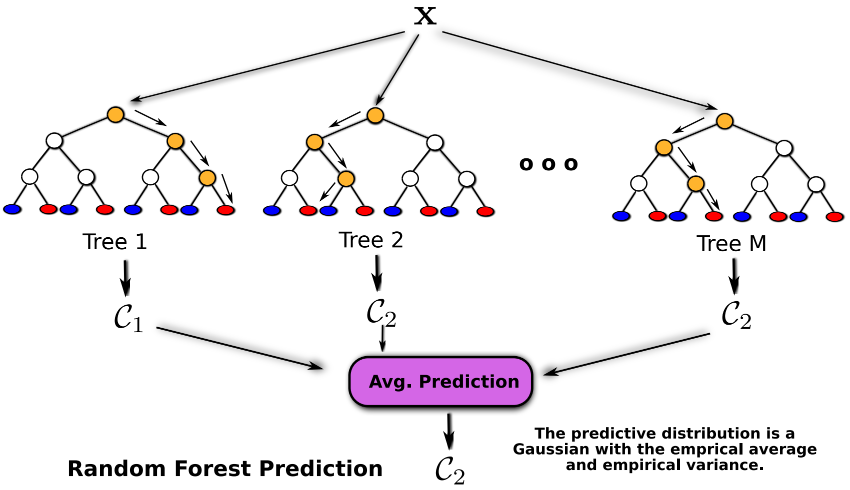
Very cheap to compute and massively paralelizable!

Random Forest: Predictive Distribution



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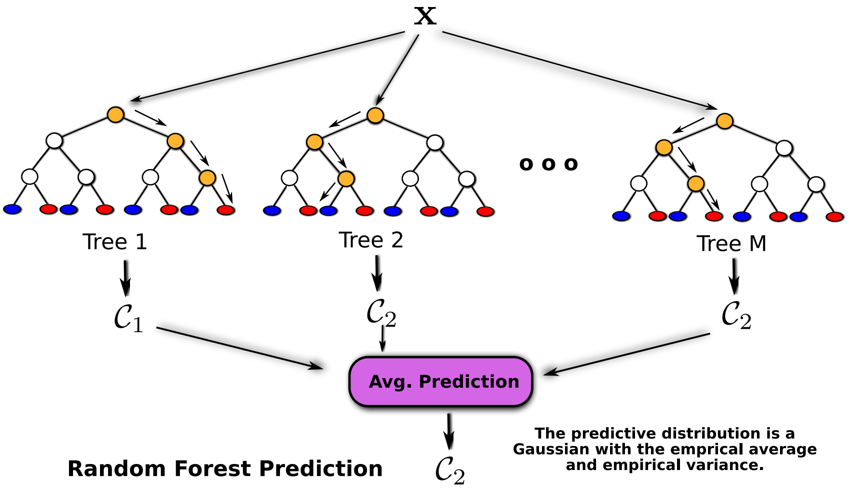
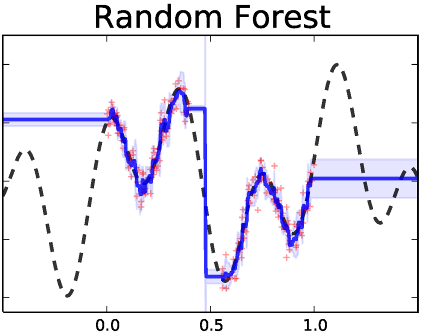


$$p(f^\star|\mathcal{D}_n) = \mathcal{N}(f^\star|\overline{\mu}, \overline{\nu}^2)$$

(Hutter et al., 2011)

Random Forest in Practice



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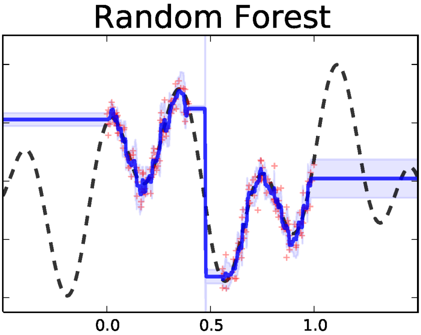

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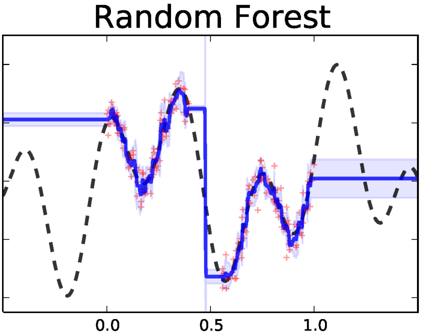

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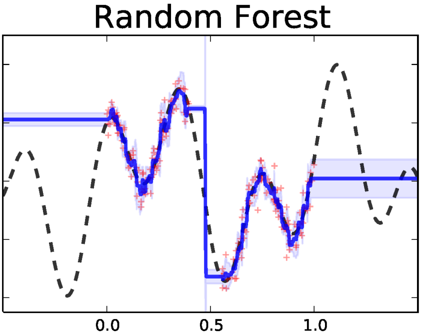

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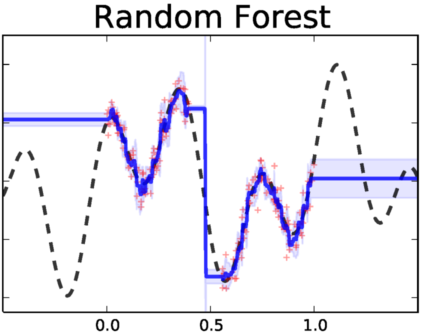

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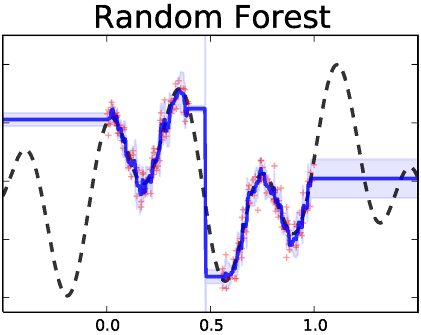

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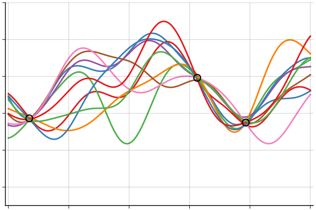

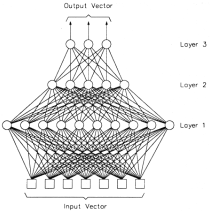

$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

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- Neural networks scale well to the training data (linear cost).

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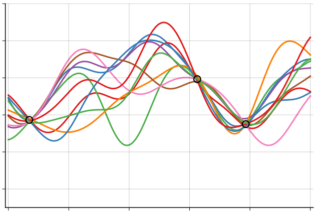

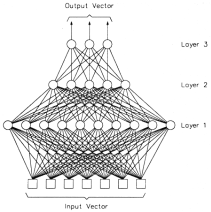

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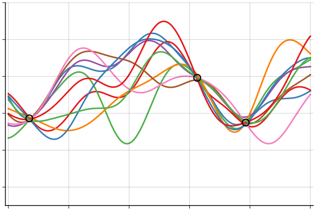

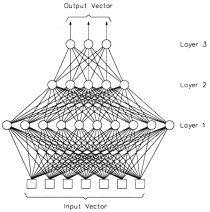

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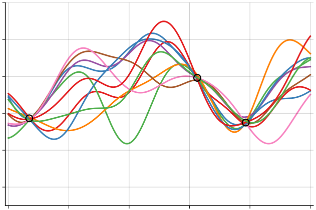

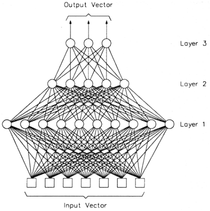

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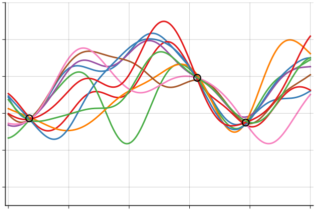

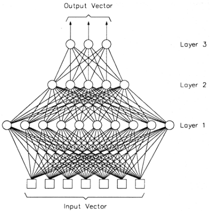

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The posterior distribution of the networks weights W is intractable!

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Trade-off between accuracy of the predictive distribution and scalability! Still a lot of research going on!

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Other tools: SMAC (Java), Hyperopt (Python), Bayesopt (C++), PyBO (Python), MOE (Python / C++).

Further Extensions and Open Issues

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4. **Safe Bayesian Optimization**: Sometimes we should avoid evaluating the objective at particular input locations (system failure) where it falls below some critical value (Berkenkamp *et al.*, 2016).

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Thank you very much!

References

- M. Bauer, M. van der Wilk & C. E. Rasmussen. Understanding probabilistic sparse Gaussian process approximations. In Advances in neural information processing systems (pp. 1533-1541), 2016.
- F. Berkenkamp, A. Krause, A. P. Schoellig. Bayesian Optimization with Safety Constraints: Safe and Automatic Parameter Tuning in Robotics, arXiv:1602.04450, 2016.
- E. Brochu, V. M. Cora and N. de Freitas. A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning. eprint arXiv:1012.2599, 2010.
- E. C. Garrido-Merchán, D. Hernández-Lobato. Predictive Entropy Search for Multi-objective Bayesian Optimization with Constraints. Neurocomputing, 2019. In press.
- J. González, M. Osborne, N. Lawrence. GLASSES: Relieving The Myopia Of Bayesian Optimisation. International Conference on Artificial Intelligence and Statistics, 2016.
- P. Henning, C. J. Schuler. Entropy Search for Information-Efficient Global Optimization. Journal of Machine Learning Research, 13, 1809-1837, 2012.
- D. Hernández-Lobato, J.M. Hernández-Lobato, A. Shah, R. P. Adams. Predictive Entropy Search for Multi-objective Optimization. International Conference on Machine Learning, 2016.
- J. M. Hernández Lobato, M. A. Gelbart, R. P. Adams, M. W. Hoffman, Z. Ghahramani. A General Framework for Constrained Bayesian Optimization using Information-based Search. Journal of Machine Learning Research, 17, 153, 2016.
- J. M. Hernández-Lobato, M. A. Gelbart, M. W. Hoffman, R. P. Adams, Z. Ghahramani. Predictive Entropy Search for Bayesian Optimization with Unknown Constraints, International Conference on Machine Learning, 2015.
- J. M. Hernández-Lobato, M. W. Hoffman, Z. Ghahramani. Predictive Entropy Search for Efficient Global Optimization of Black-box Functions. Neural Information Processing Systems, 2014.
- D. R. Jones, M. Schonlau, and W. J. Welch. Efficient global optimization of expensive black-box functions. Journal of Global Optimization, 13, 455492, 1998.
- J. H. Kushner. A new method of locating the maximum of an arbitrary multipeak curve in the presence of noise. Journal of Basic Engineering, 86, 97106, 1968.
- R. Neal. Slice Sampling. Annals of Statistics, 31, 705-767, 2003.

References

- A. Shah, Z. Ghahramani. Pareto Frontier Learning with Expensive Correlated Objectives. International Conference on Machine Learning, 2016.
- A. Shah, Z. Ghahramani. Parallel Predictive Entropy Search for Batch Global Optimization of Expensive Functions. Neural Information Processing Systems, 2015.
- Minka, T. Expectation Propagation for approximate Bayesian inference. Uncertainty in Artificial Intelligence, 2001.
- J. Močkus. On Bayesian methods for seeking the extremum. IFIP Technical Conference on Optimization Techniques, 1978.
- C. E. Rasmussen, C. K. I. Williams. Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning). The MIT Press, 2006.
- J. Snoek, H. Larochelle, R. P. Adams. Practical Bayesian Optimization of Machine Learning Algorithms. Advances in Neural Information Processing Systems, 2012.
- J. Snoek, O. Rippel, K. Swersky, R. Kiros, N. Satish, ..., R. Adams, Scalable bayesian optimization using deep neural networks. In International conference on machine learning, 2171-2180, 2015.
- K. Swersky, J. Snoek, R. P. Adams. Multi-task Bayesian optimization. Advances in neural information Processing Systems, 2013.
- K. Swersky, J. Snoek, & R. P. Adams. Freeze-thaw Bayesian optimization. arXiv preprint arXiv:1406.3896, 2014.
- B. Shahriari, K. Swersky, Z. Wang, R. P. Adams and N. de Freitas Taking the Human Out of the Loop: A Review of Bayesian Optimization. Proceedings of the IEEE, 104, 148–175, 2016.
- J. T. Springenberg, A. Klein, S. Falkner, F. Hutter. Bayesian optimization with robust Bayesian neural networks. Advances in Neural Information Processing Systems, 4134-4142, 2016.
- N. Srinivas, A. Krause, S. Kakade, M. Seeger. Gaussian Process Optimization in the Bandit Setting: No Regret and Experimental Design International Conference on Machine Learning, 2010.
- F. Hutter, H. H. Hoos, and K. Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In LION, pages 507-523, 2011.
- Z. Wang M. Zoghi F. Hutter D. Matheson, N. de Freitas Bayesian Optimization in High Dimensions via Random Embeddings. International Joint Conferences on Artificial Intelligence, 2013.