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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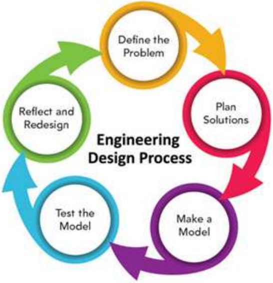

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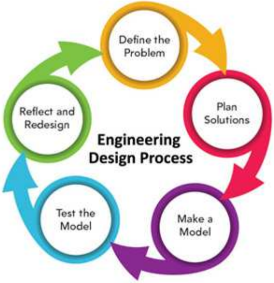

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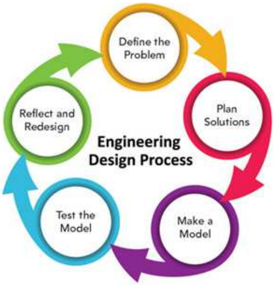

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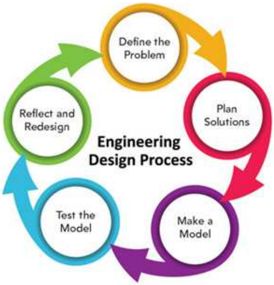

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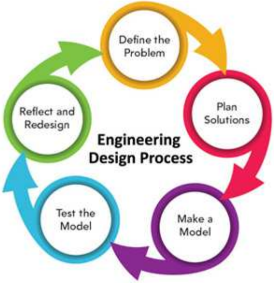

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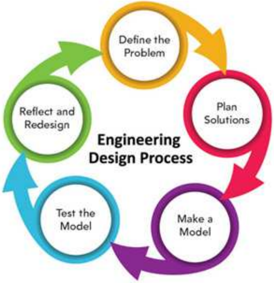

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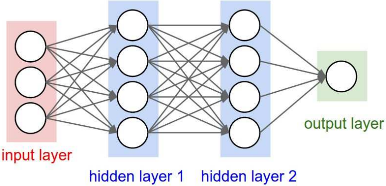
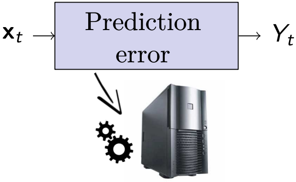
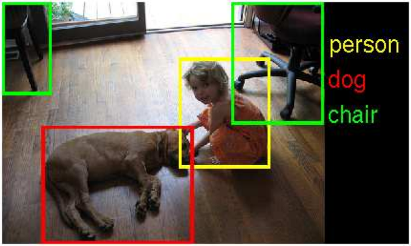
Optimization is a challenging task in new products design!

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







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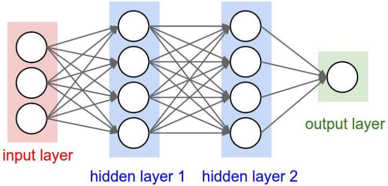
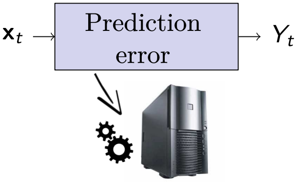
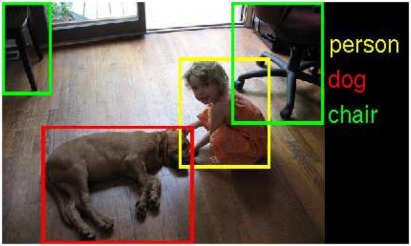
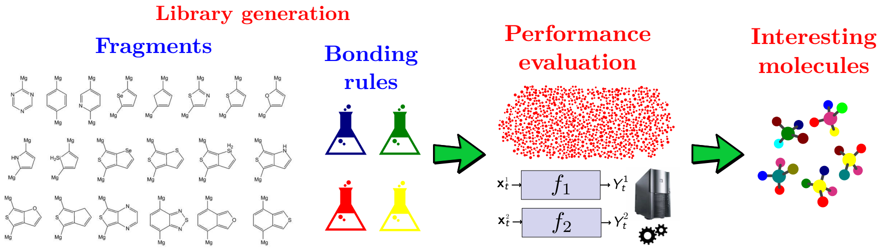






Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc.

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



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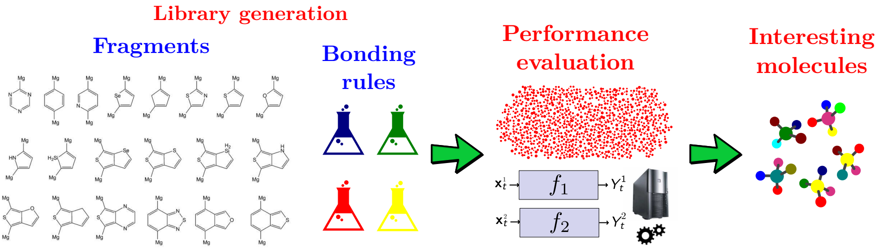
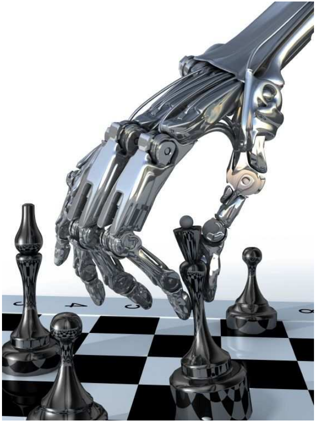


Explore **millions of candidate molecule structures** to identify the compounds with the best properties.

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



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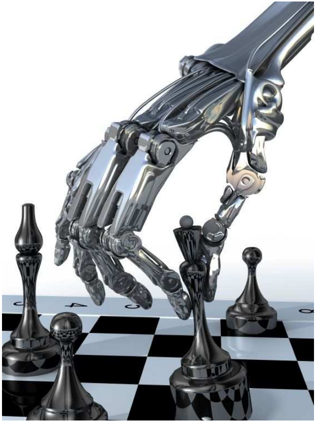
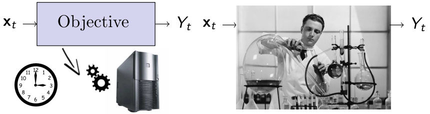


Parameters to tune: initial pose for the robot's hand and finger joint trajectories.

Optimization Problems: Common Features

- Very expensive evaluations.



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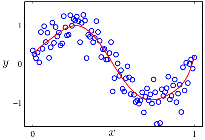
$$y = f(\mathbf{x}) + \epsilon$$



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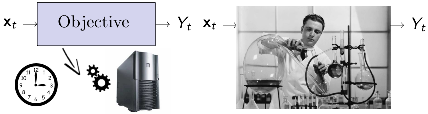

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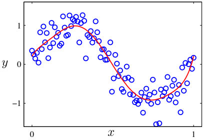
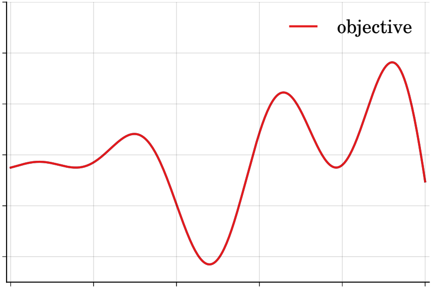


Bayesian optimization methods can be used to solve these problems!

Bayesian Optimization in Practice



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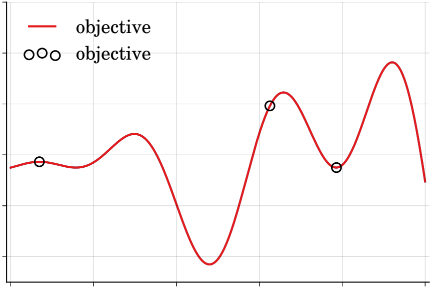

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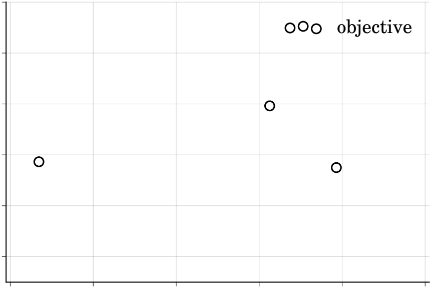

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❷ Fit a model to the data:

$$p(y|\mathbf{x}, \mathcal{D}_n) \,.$$

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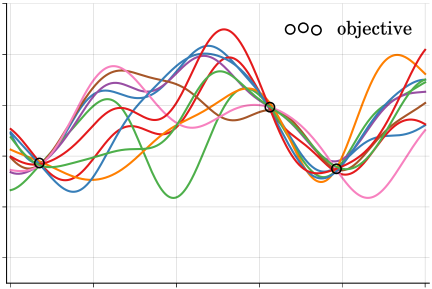

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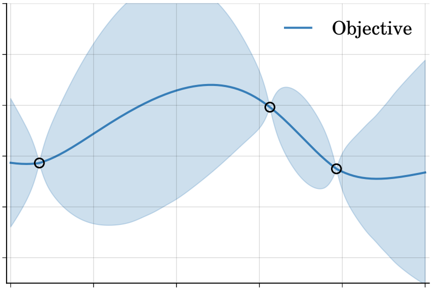

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3. Select data collection strategy:

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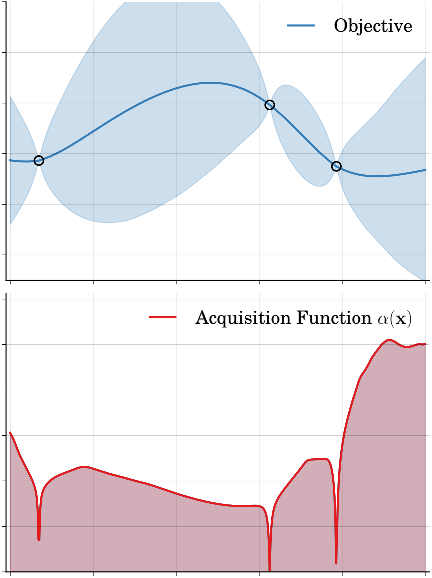

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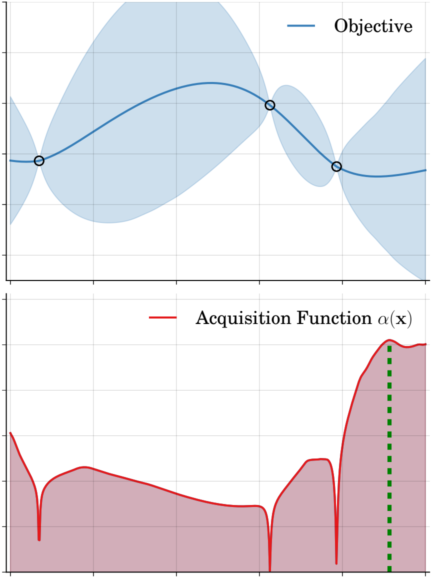

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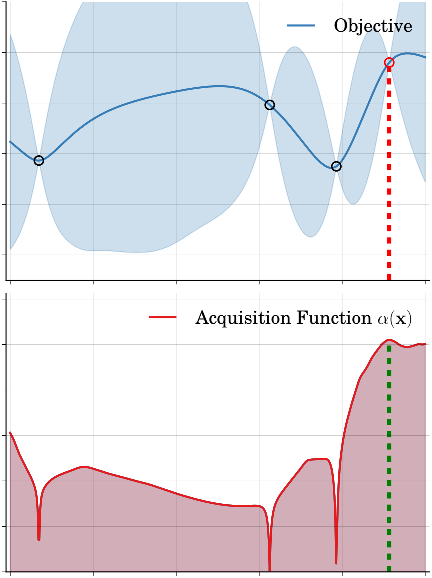

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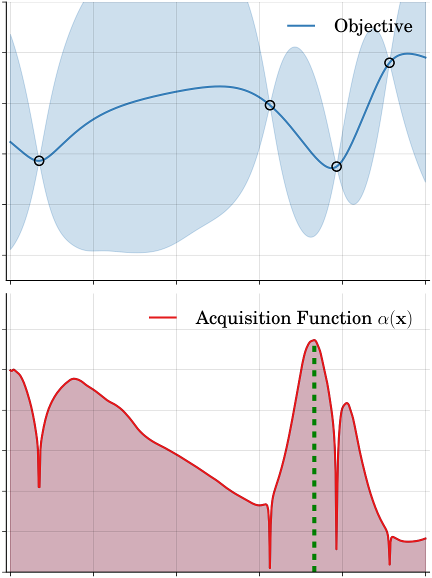

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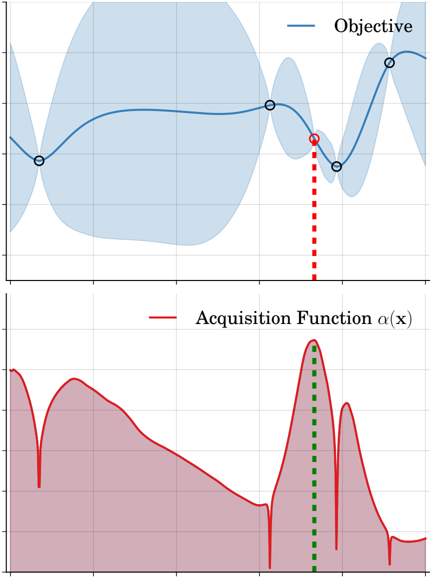

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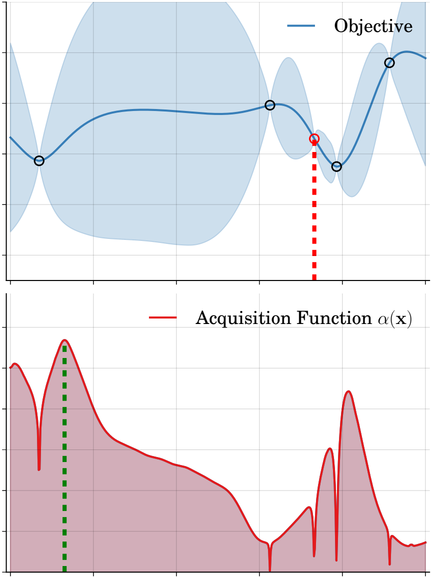

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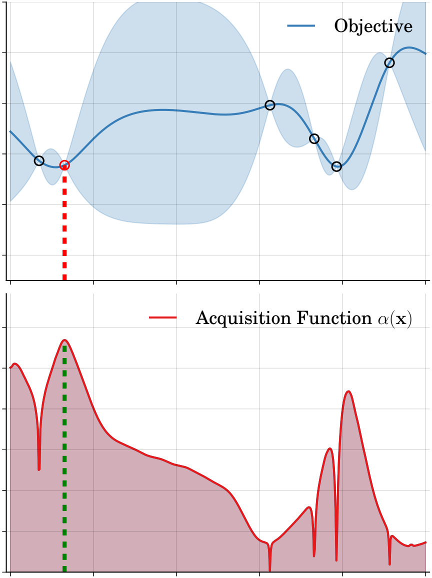

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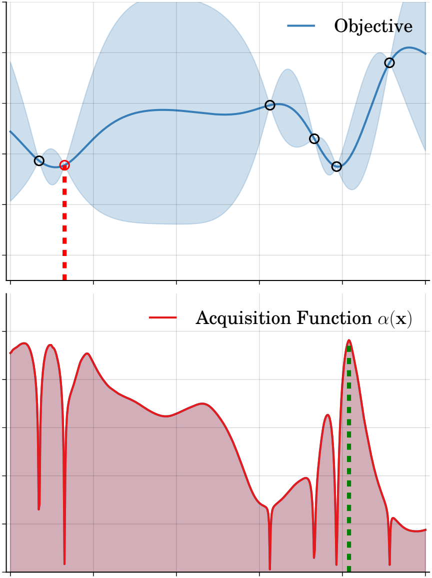

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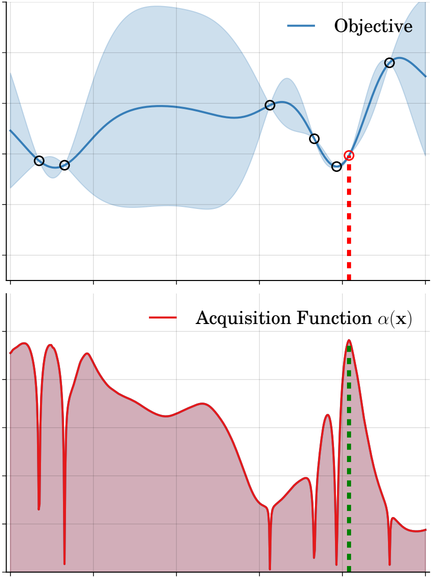

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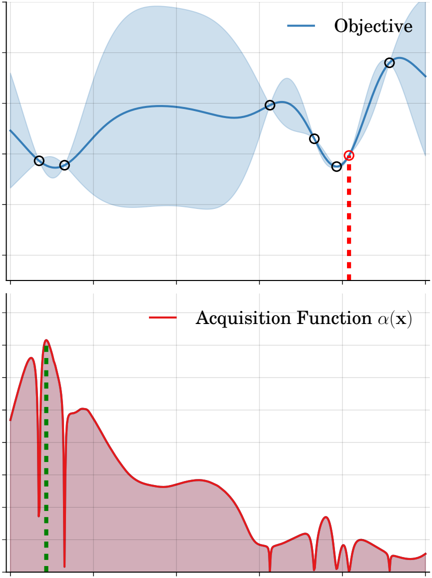

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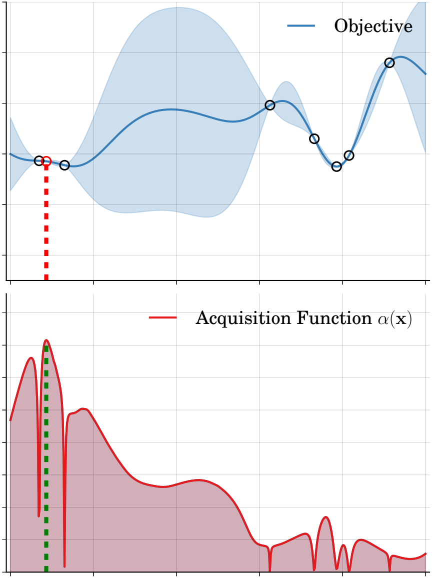

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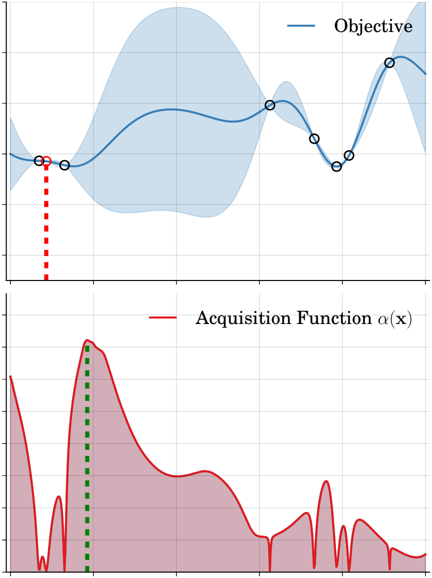

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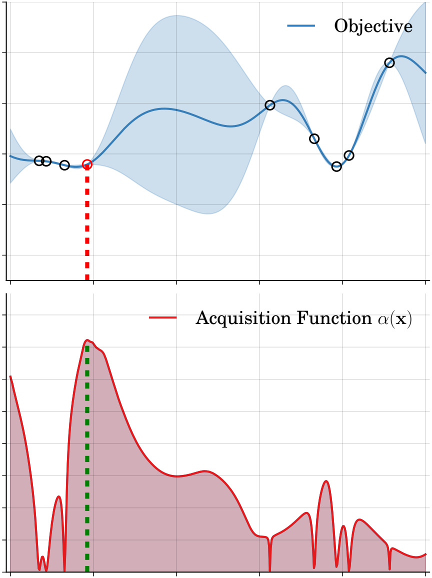

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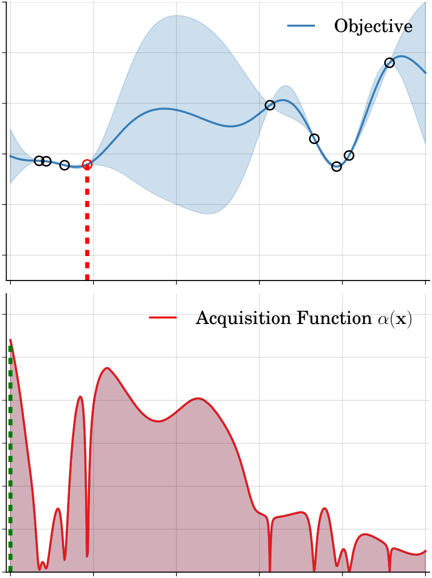

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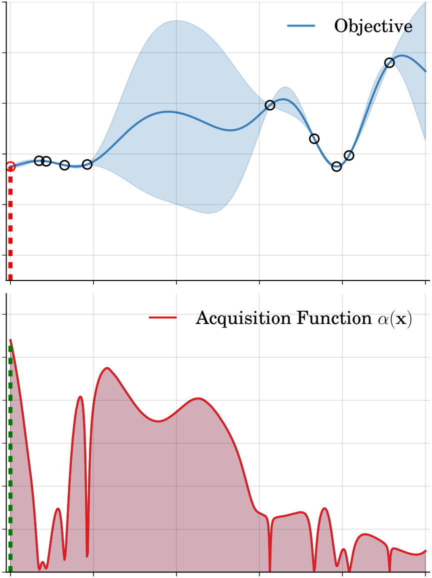

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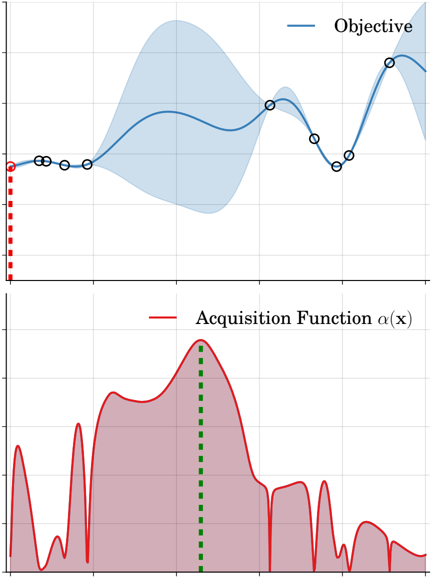

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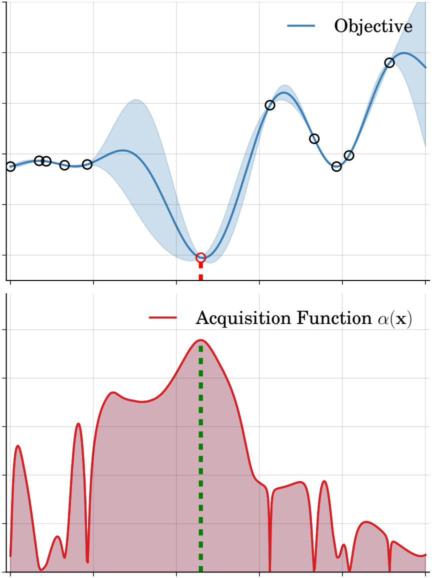

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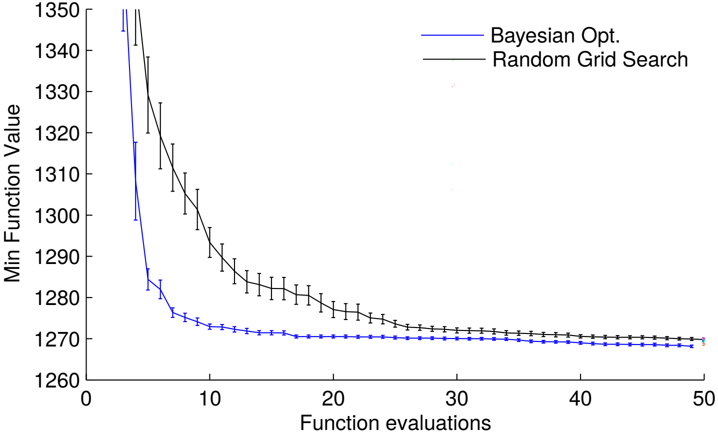
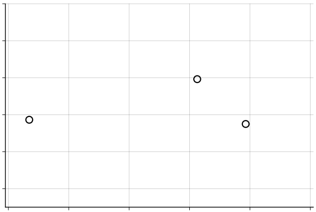
Bayesian Optimization vs. Uniform Exploration



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

Fitting a Model to the Data



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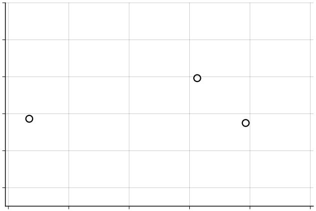
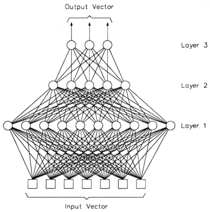
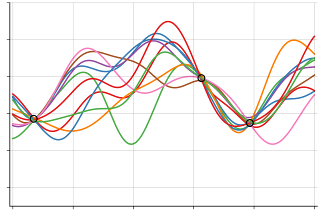


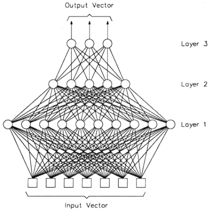


$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

$$f(\mathbf{x}) = \sum_{j=1}^{H} v_j h_j(\mathbf{x})$$

Fitting a Model to the Data





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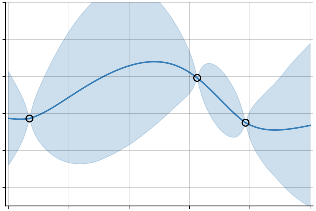

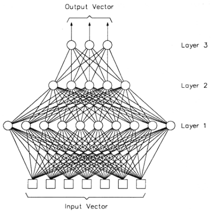

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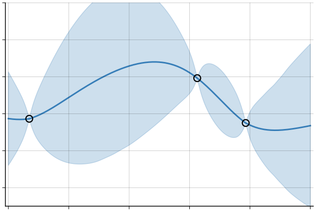

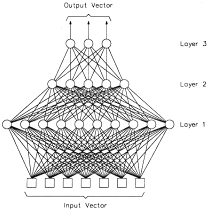

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Posterior Dist. $p(\mathbf{W}|\text{Data}) = p(\mathbf{W})p(\text{Data}|\mathbf{W})/p(\text{Data})$

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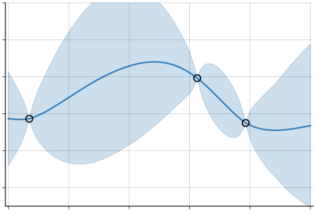

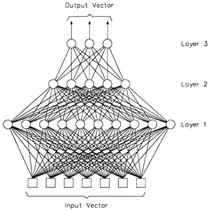

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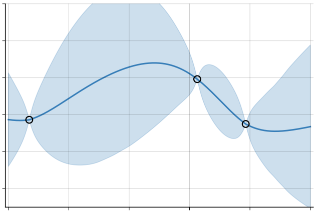

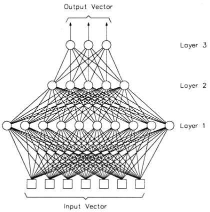

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Challenges: The model should be non-parametric (the world is complicated) and computing $p(\text{Data})$ is intractable!

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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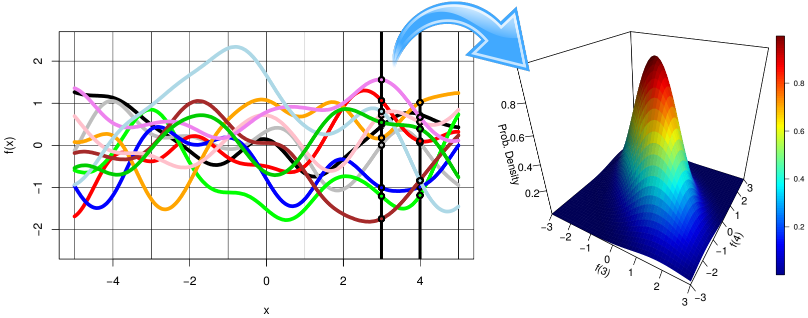

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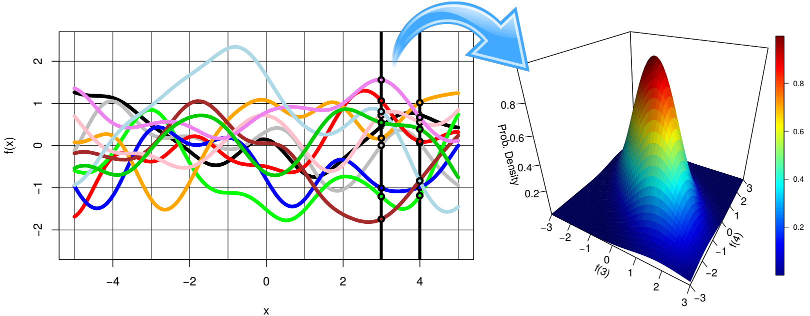

When $H \to \infty$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathrm{T}$ follows an N-dimensional Gaussian where $\mathbb{E}[f(\mathbf{x}_i)f(\mathbf{x}_k)] = \sigma^2 \mathbb{E}[h_j(\mathbf{x}_i)h_j(\mathbf{x}_k)]$ by the **central limit theorem**.

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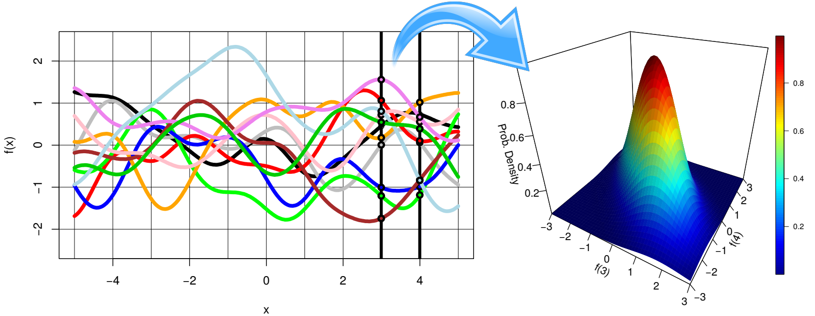

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Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.

Gaussian Processes

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

$$p(\mathbf{y}^\star, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{k}_\theta & \mathbf{K}_\theta \\ \boldsymbol{\kappa}_\theta & \mathbf{k}_\theta^\top \end{bmatrix} \right)$$

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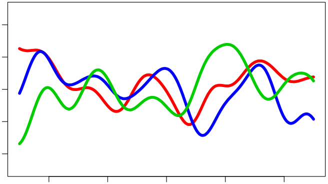
- The log of the **marginal likelihood**, $p(\mathbf{y}|\theta)$, is:

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

Some Covariance Functions

Squared Exponential



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

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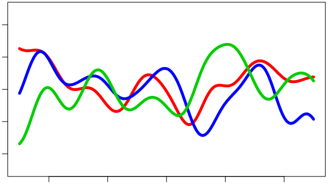

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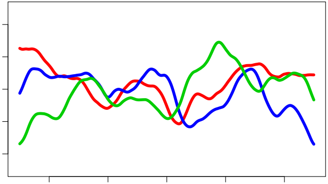
Matérn



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

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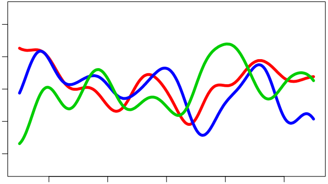

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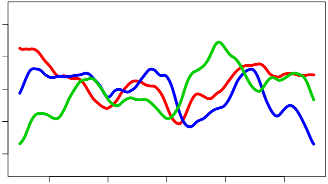

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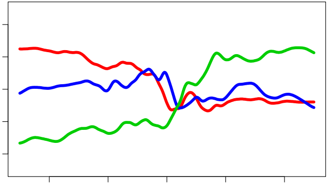
Neural Network



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

Some Covariance Functions

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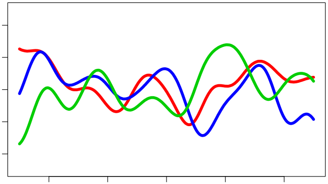

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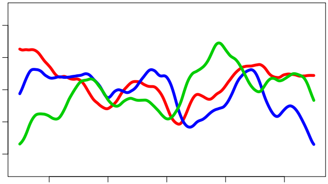

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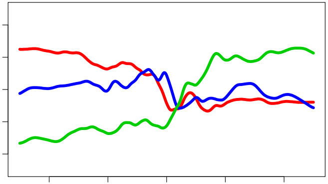

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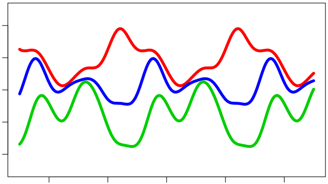
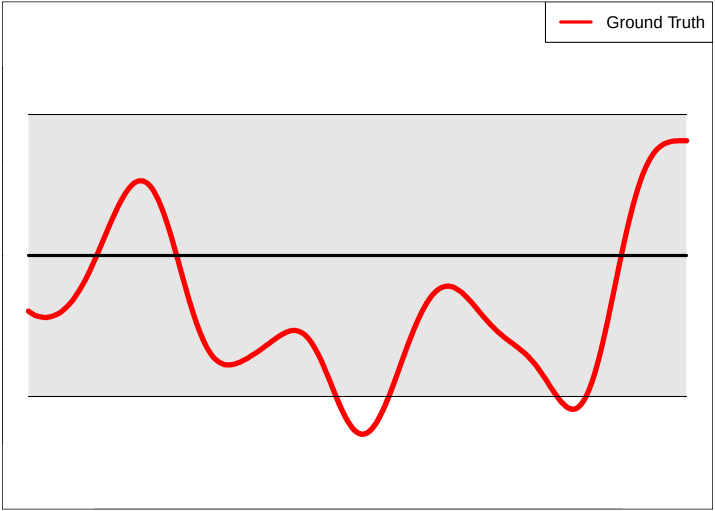
Periodic



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

From the Prior to the Posterior

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



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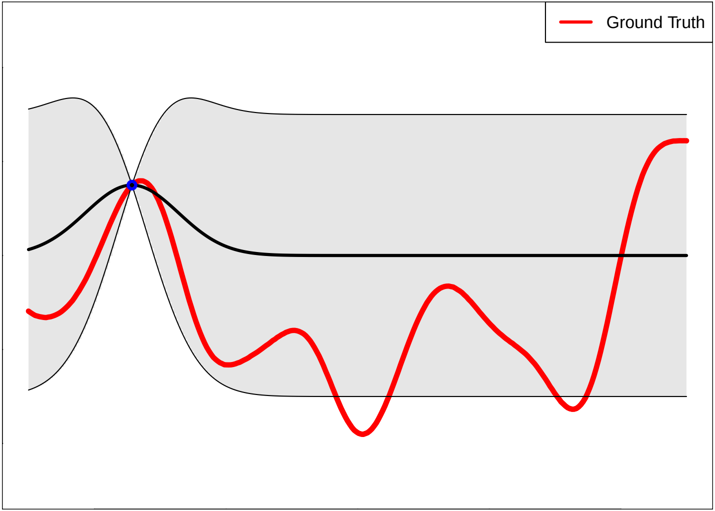

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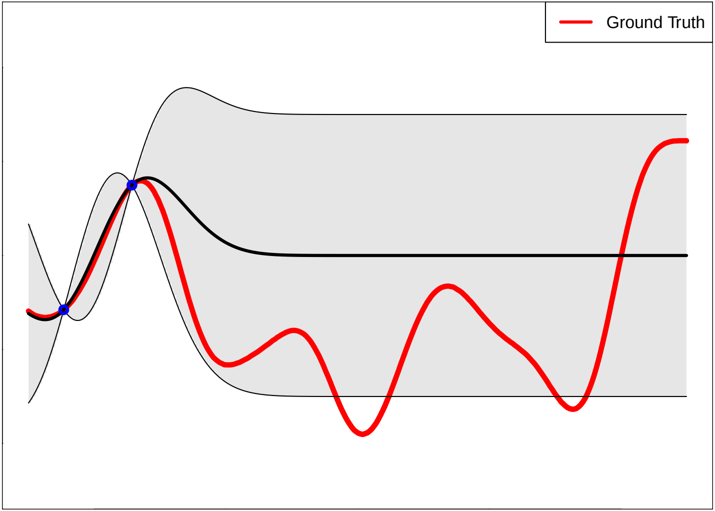

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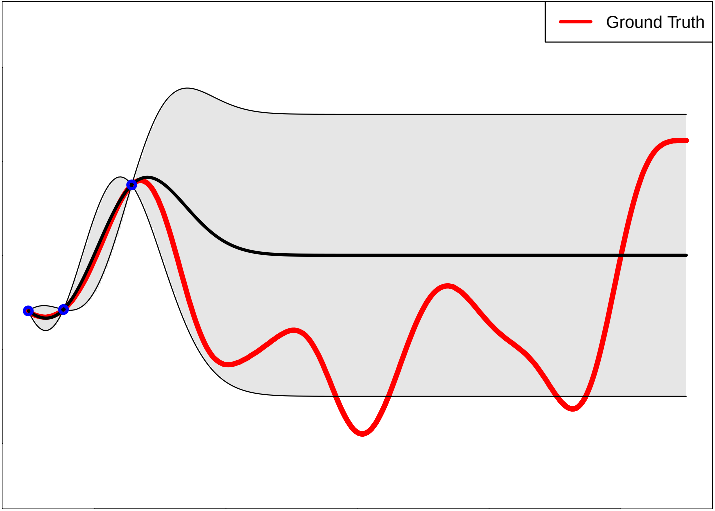

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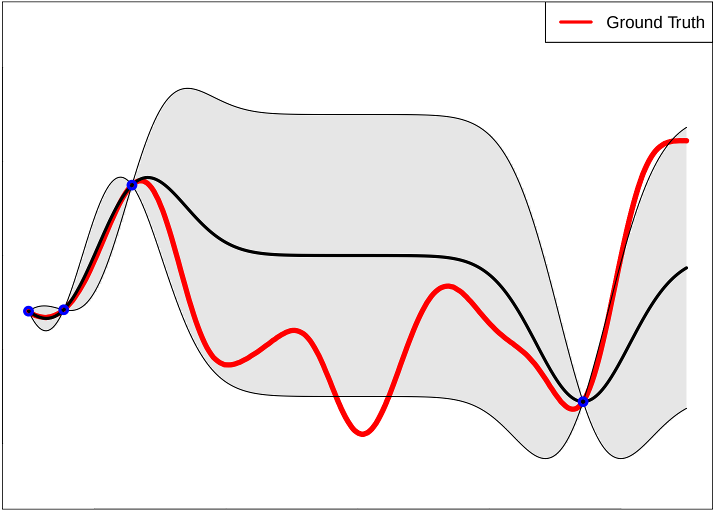

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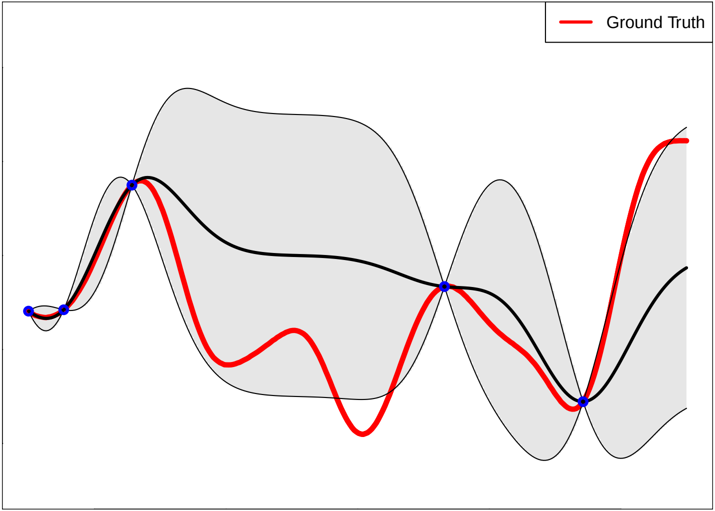

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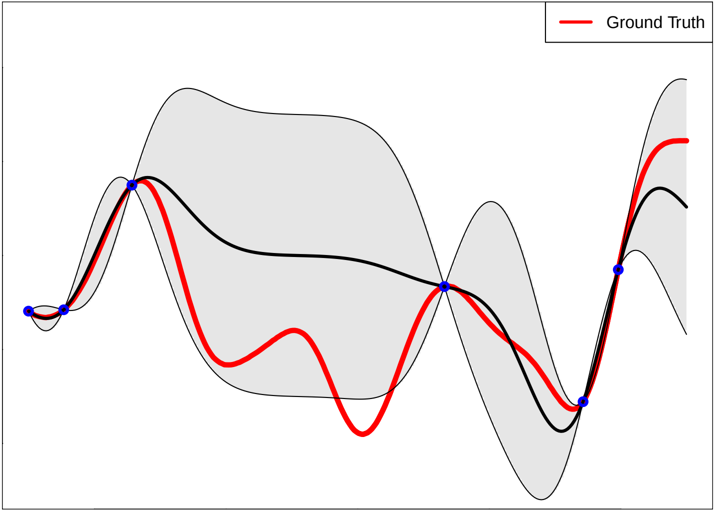

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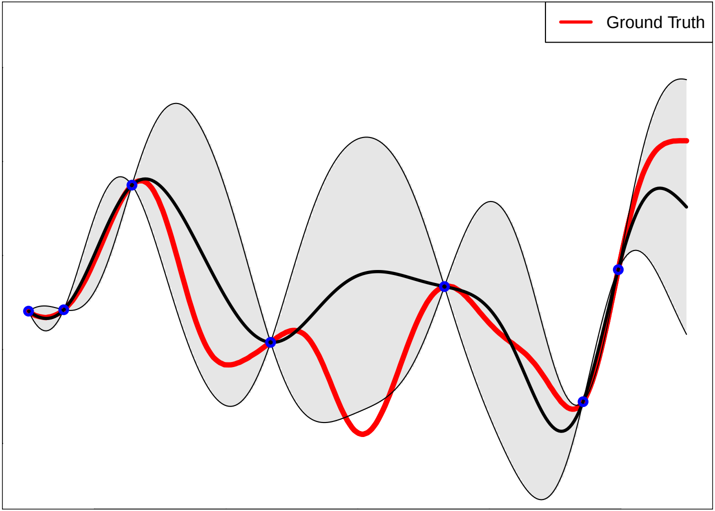

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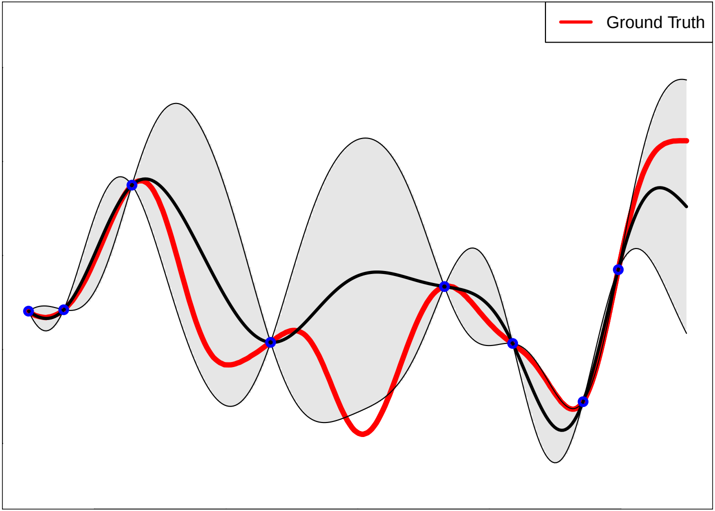

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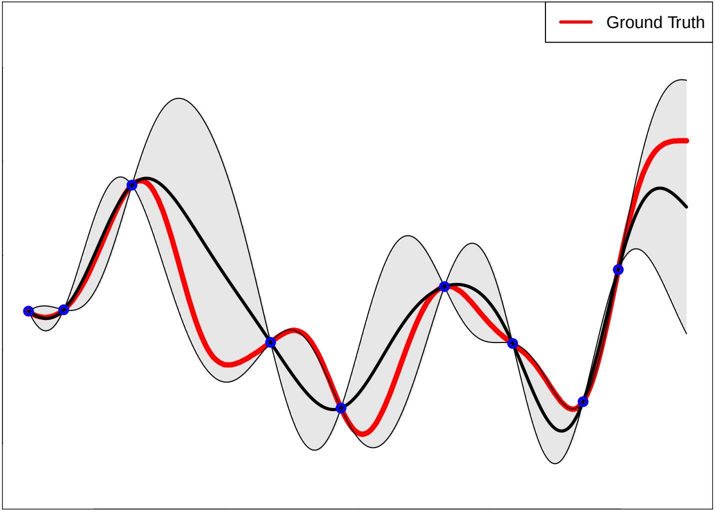

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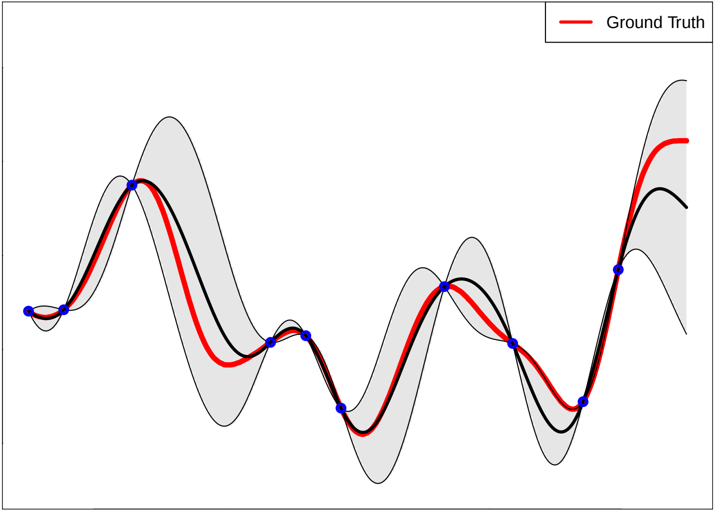

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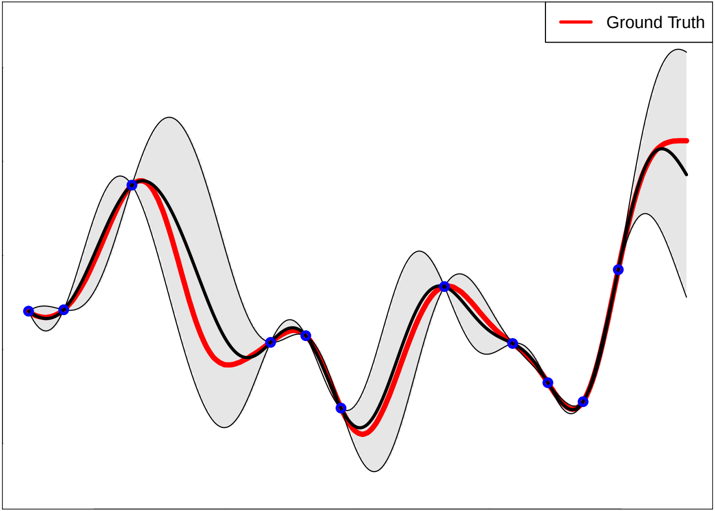

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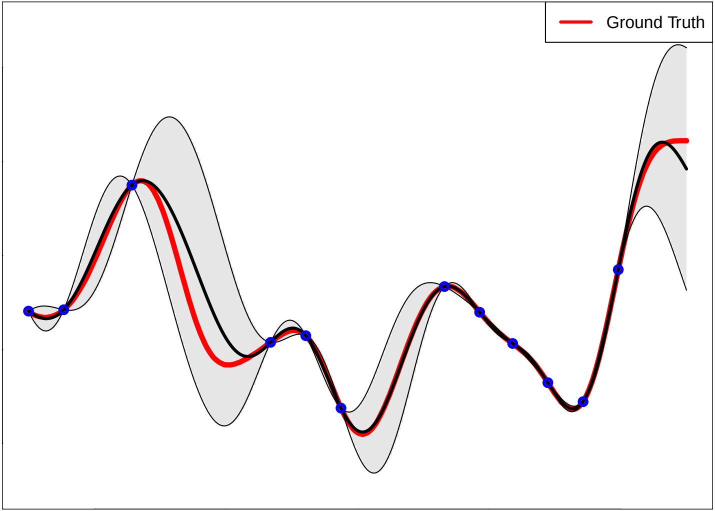

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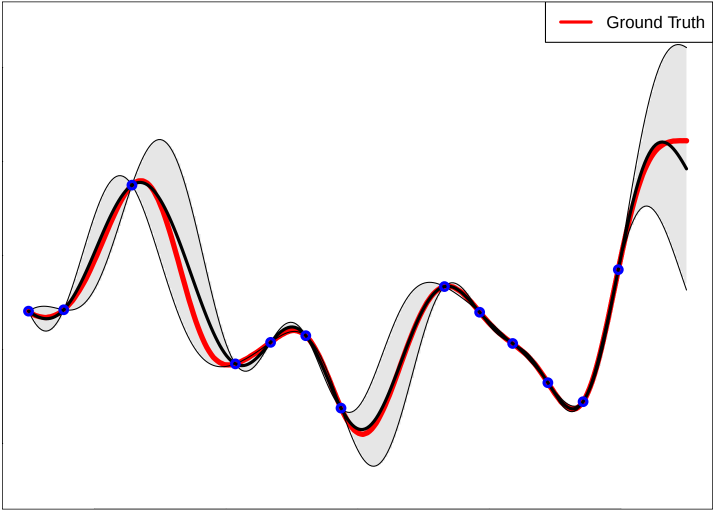

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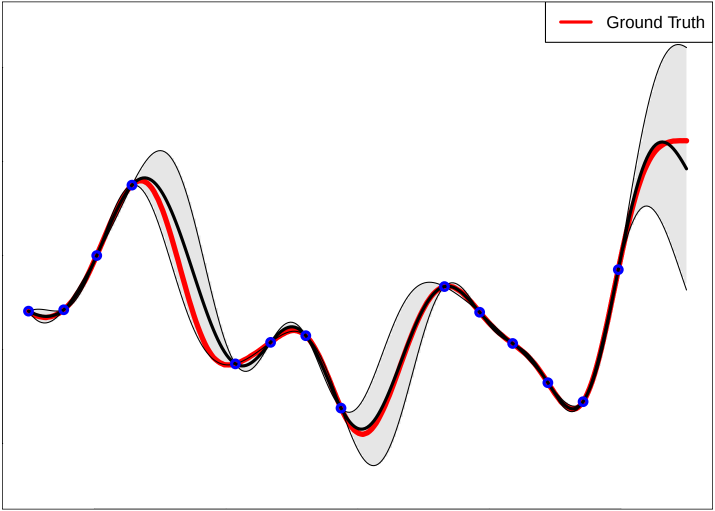

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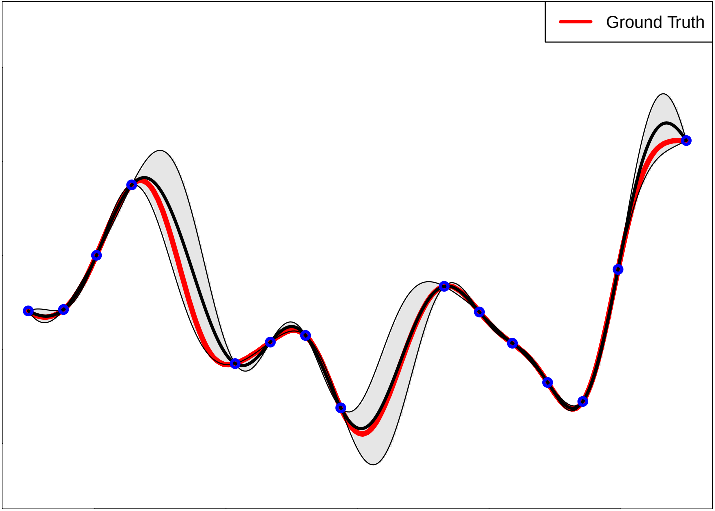

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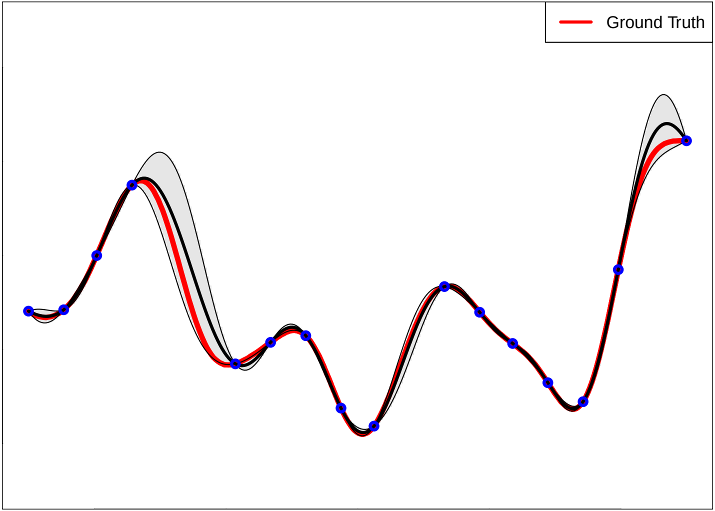

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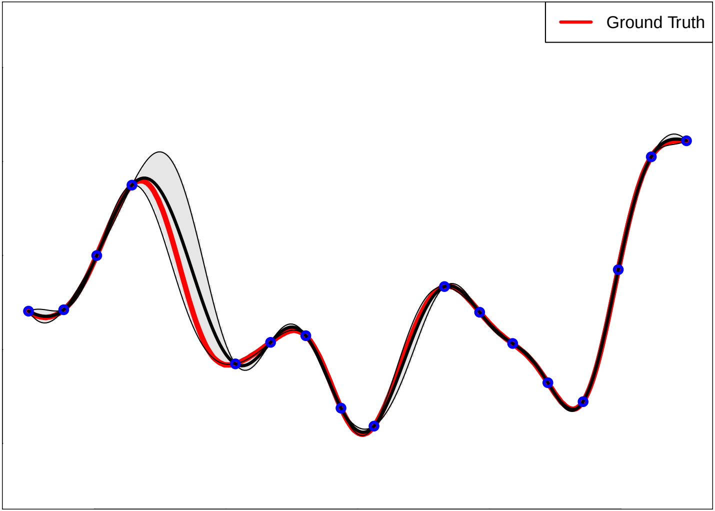

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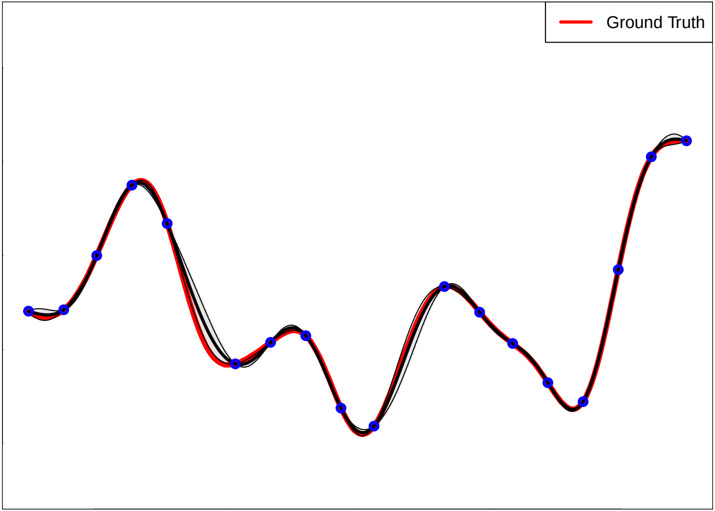

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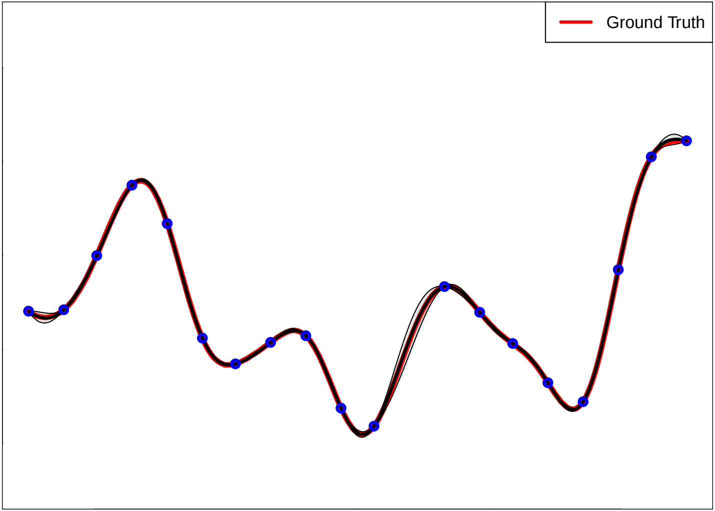

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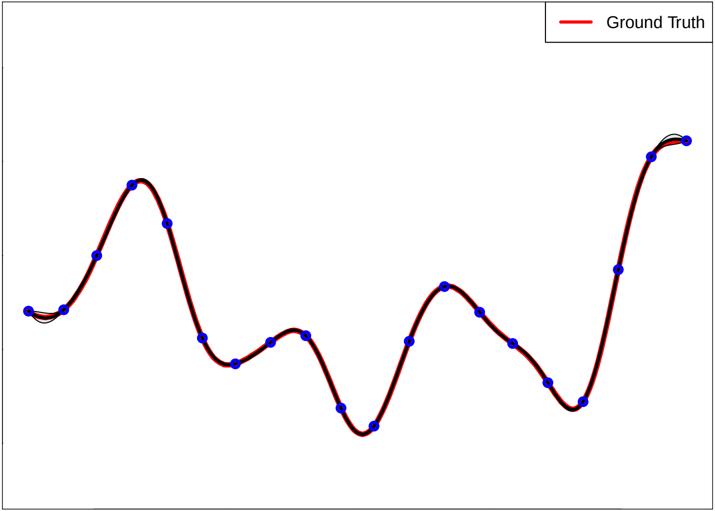

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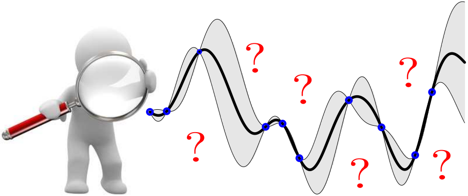

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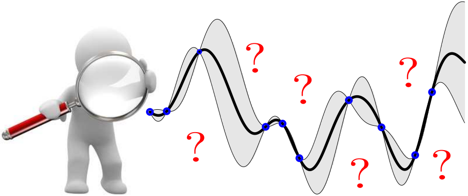

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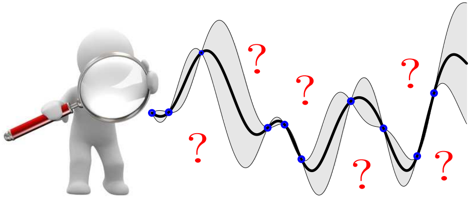

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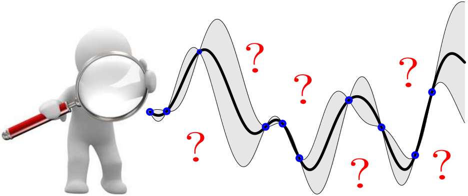

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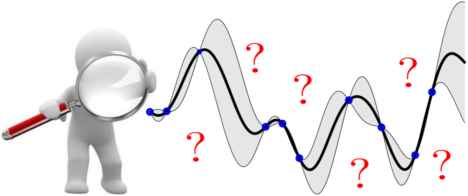

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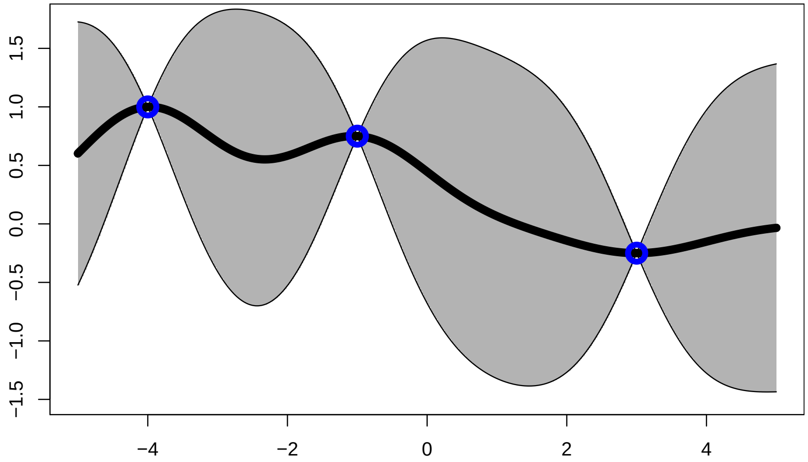

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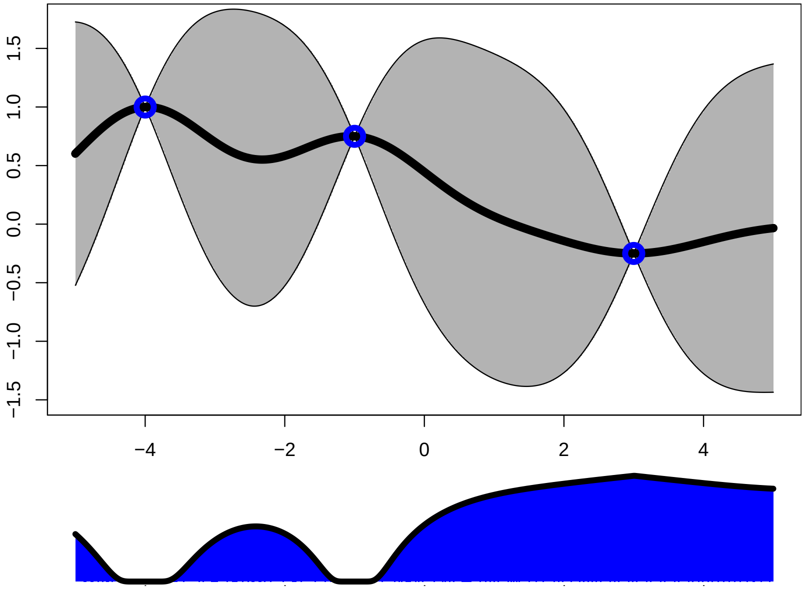

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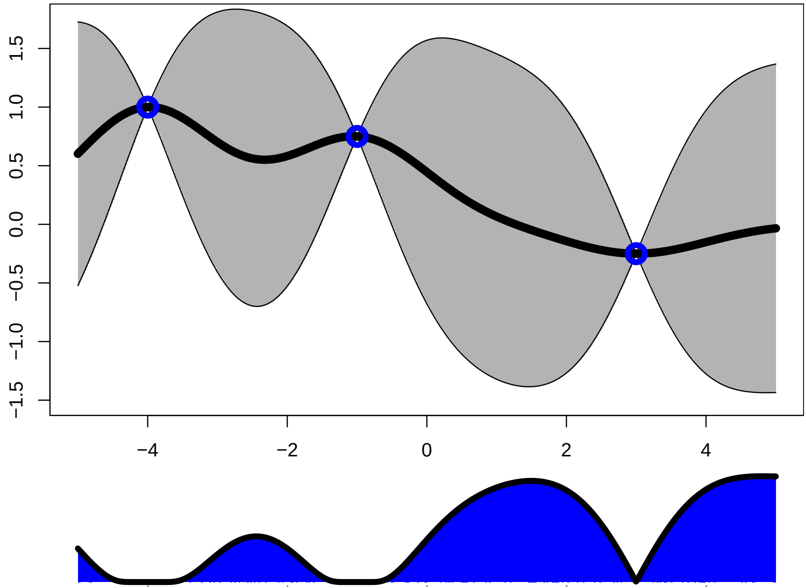

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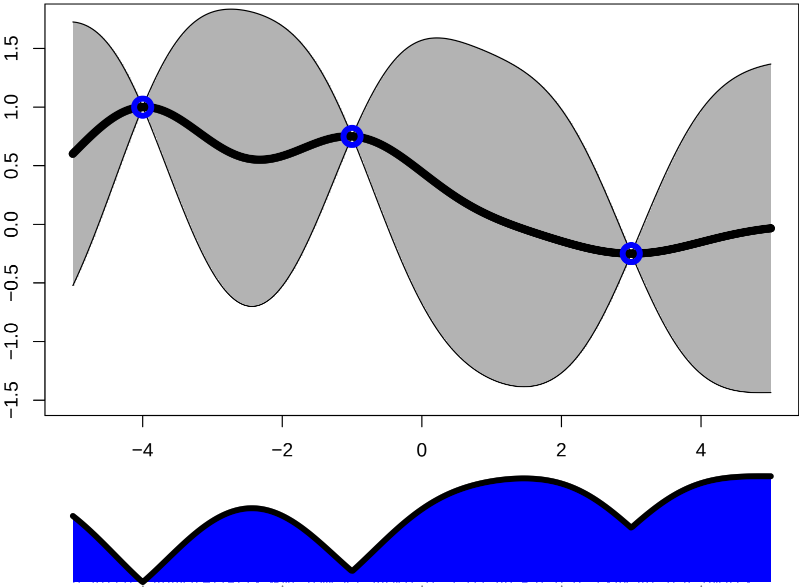

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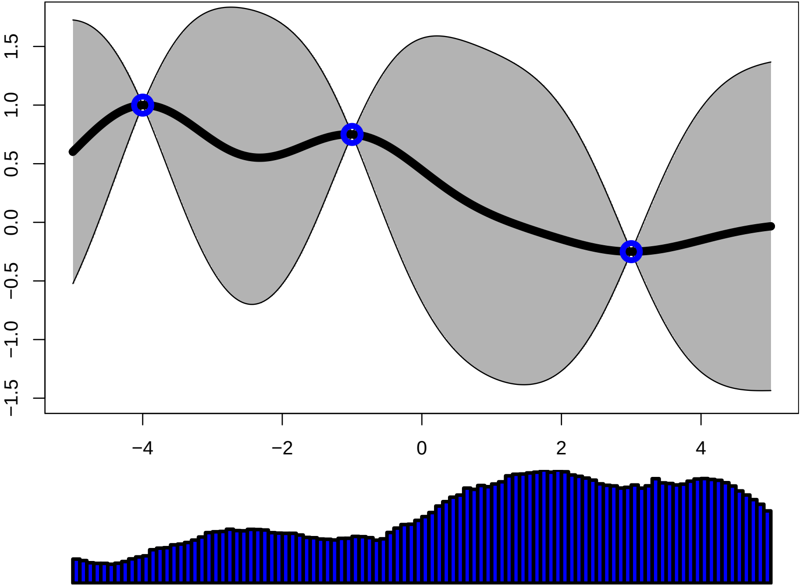

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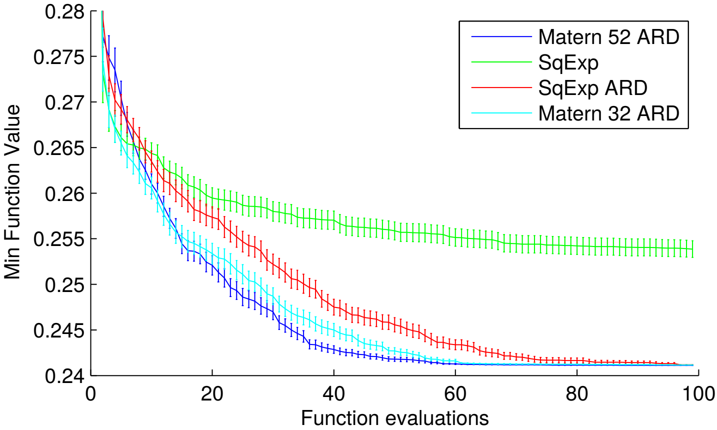

Structured SVM for protein motif finding (Snoek *et al.*, 2012).

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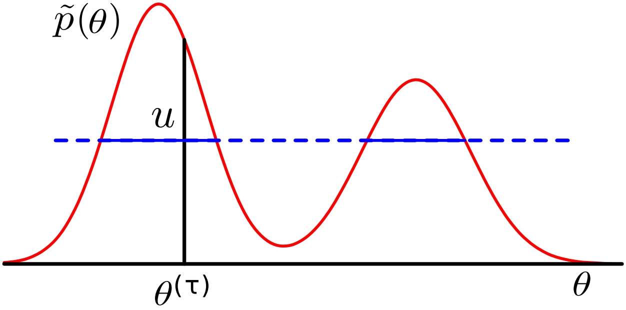

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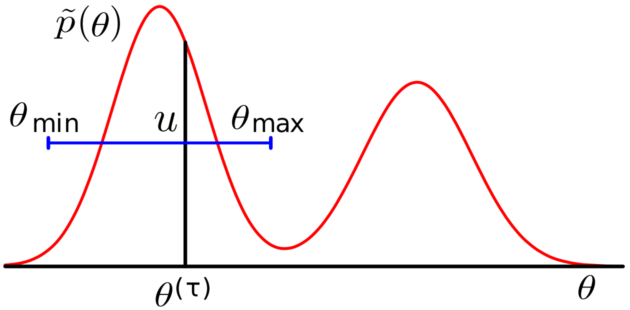

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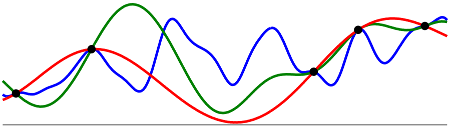
Posterior samples with three different length-scales



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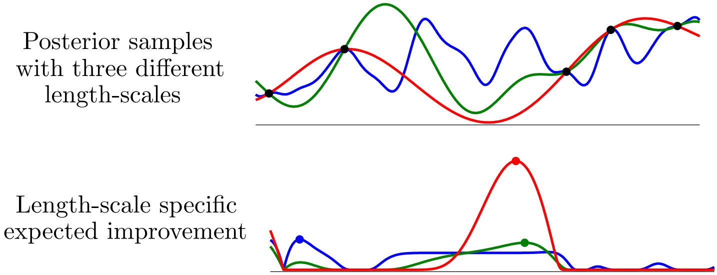

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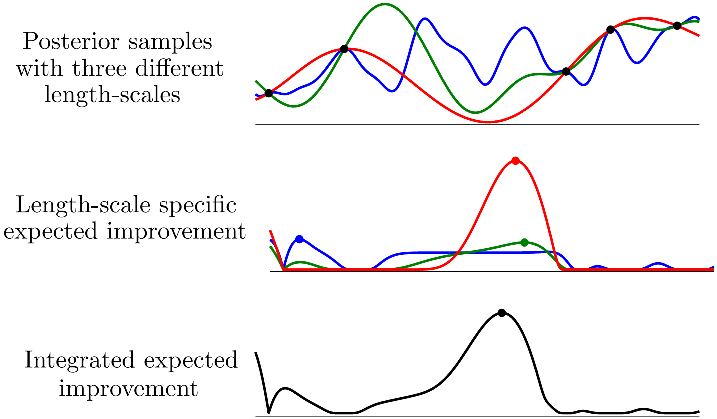

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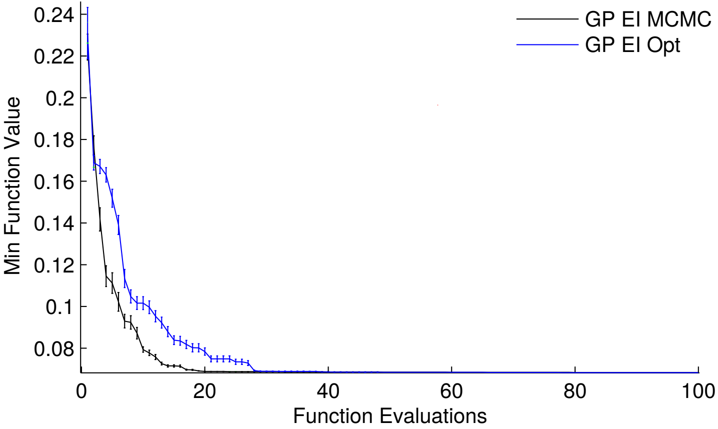
MCMC estimation vs. Maximization



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

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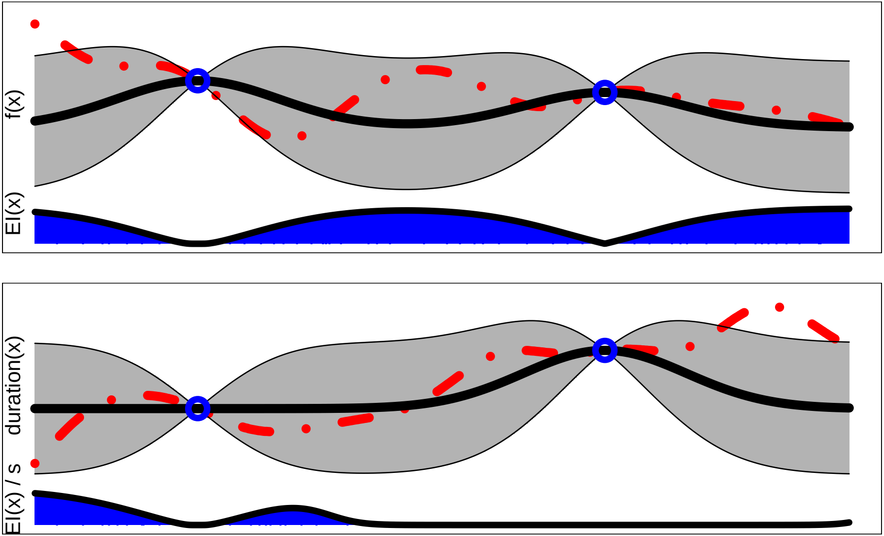

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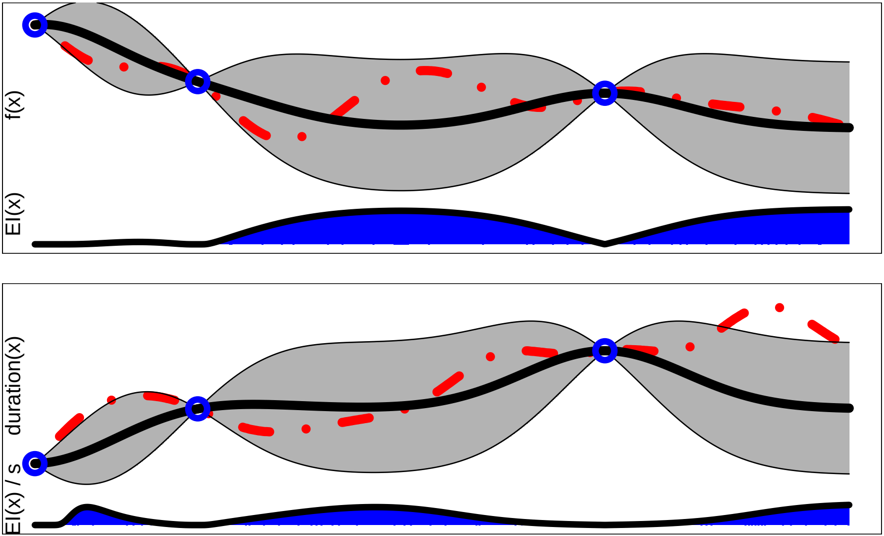

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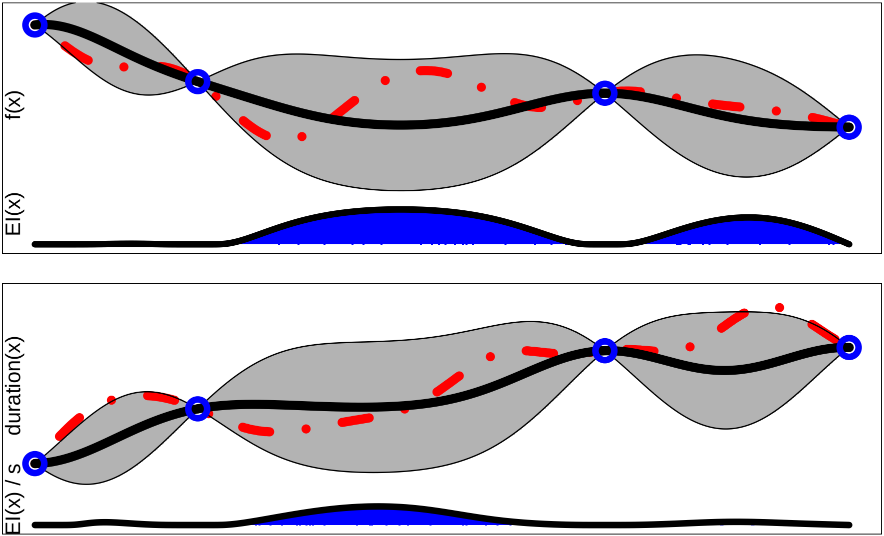

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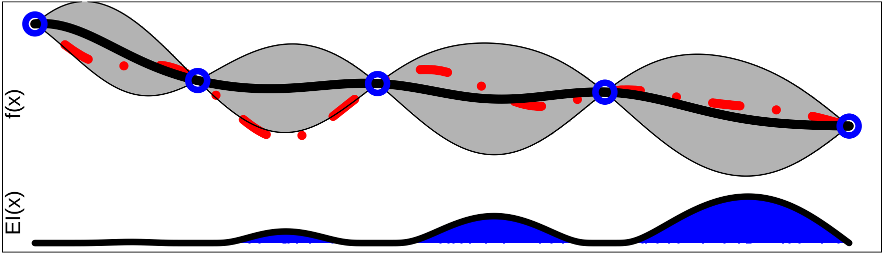

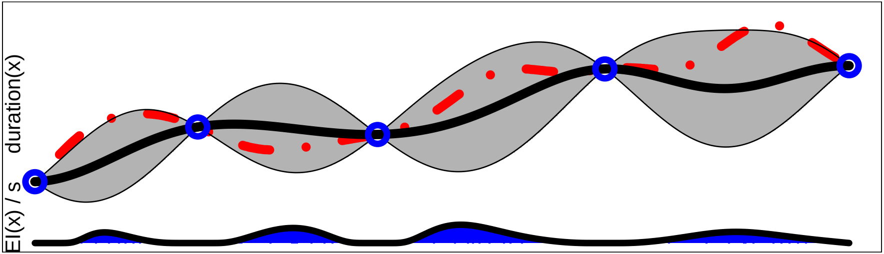

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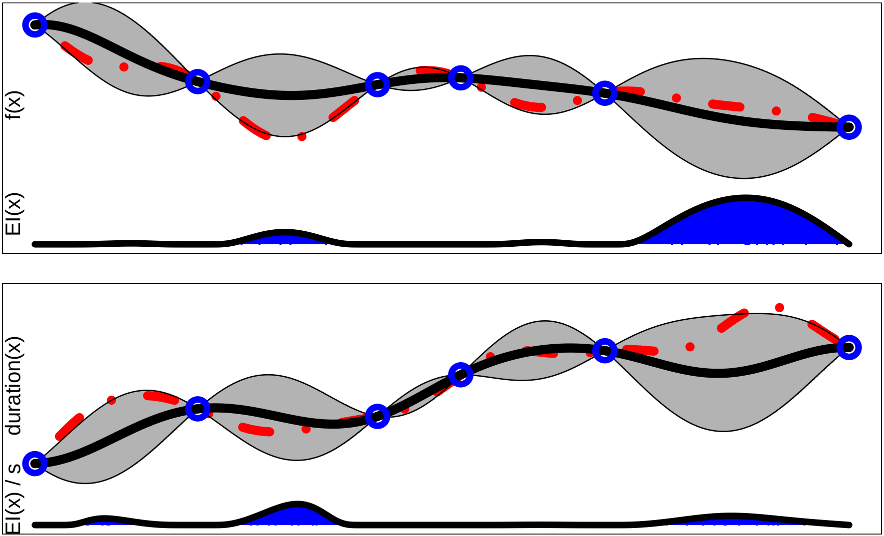

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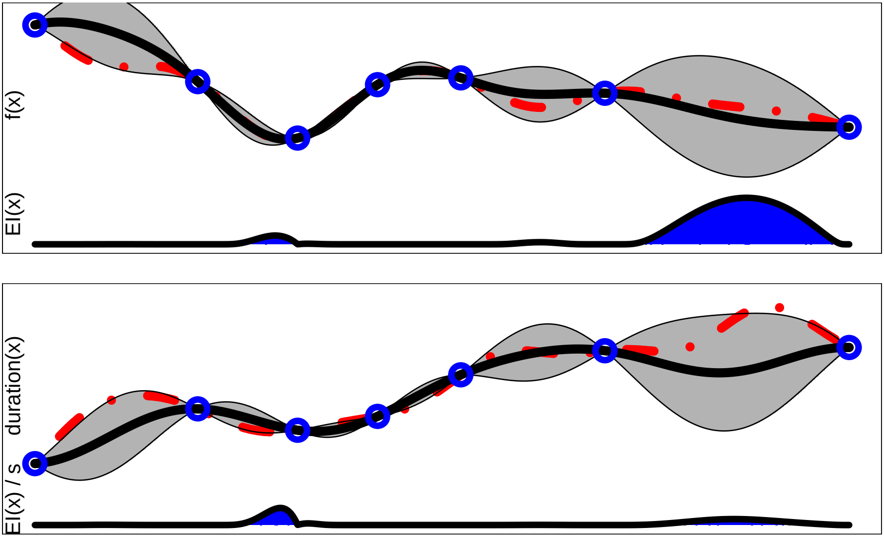

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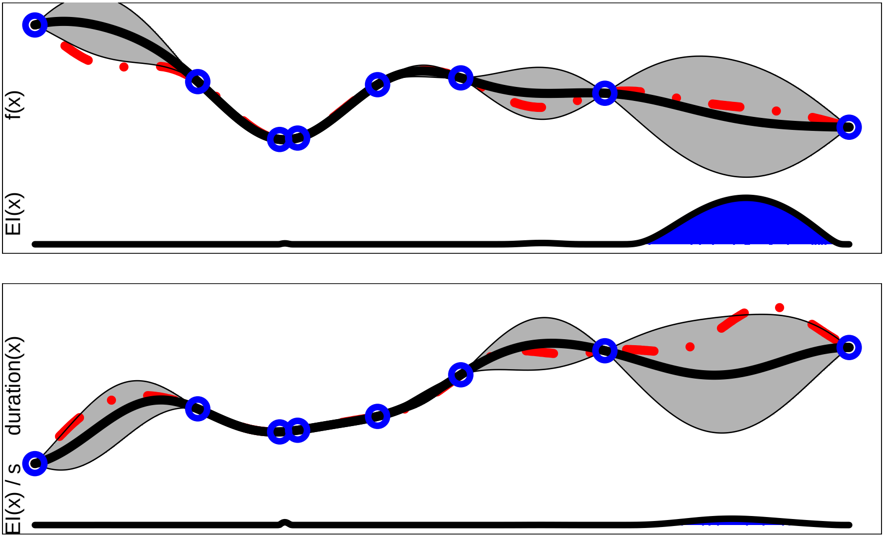

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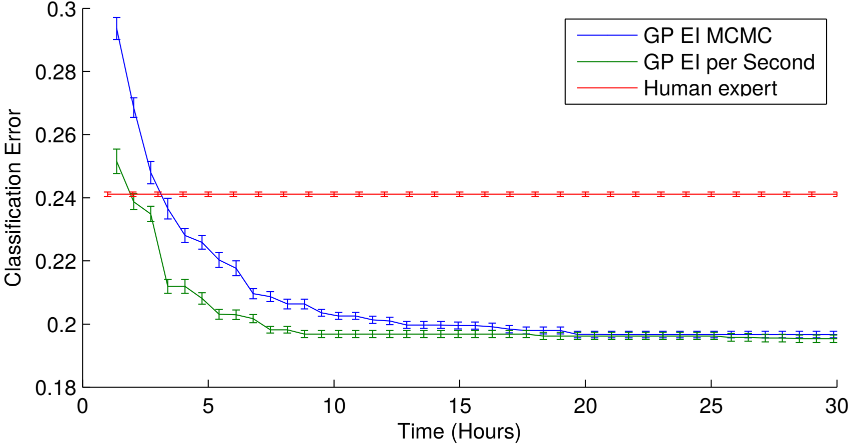
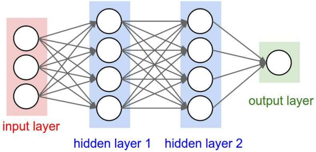
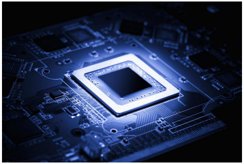


Deep neural network on the CIFAR dataset (Snoek *et al.*, 2012)

Several Objectives and Constraints

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





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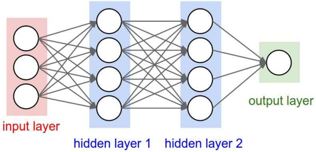

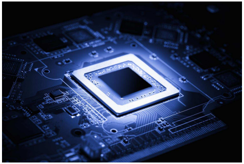

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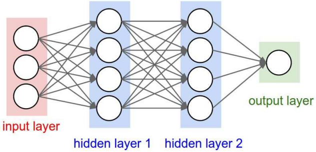

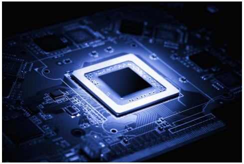

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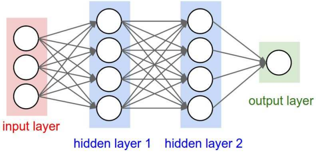

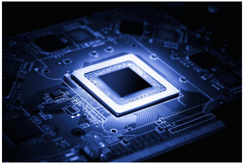

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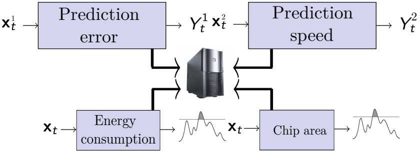

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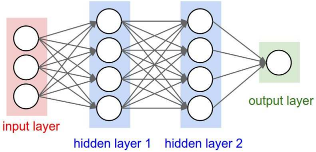

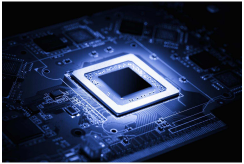

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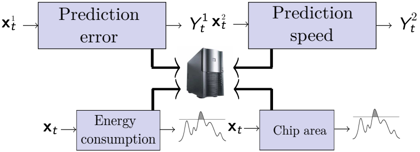
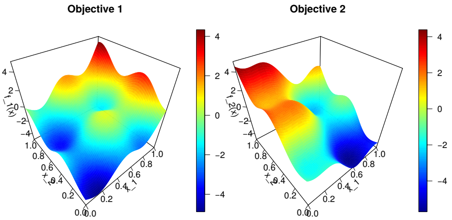


Challenges:

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

Constrained Multi-Objective Optimization



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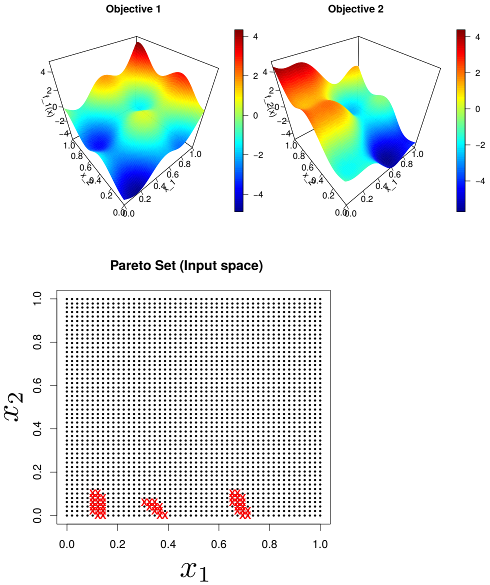

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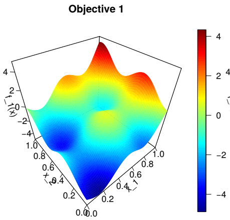

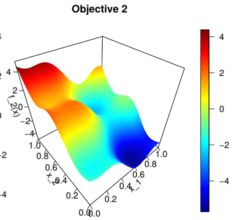

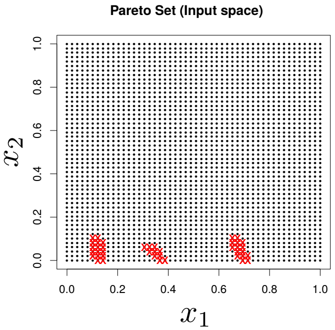

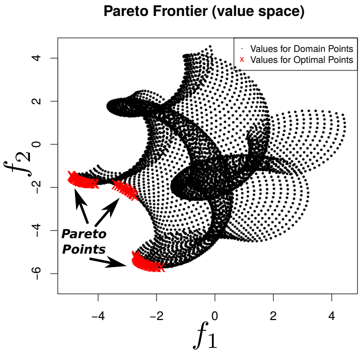

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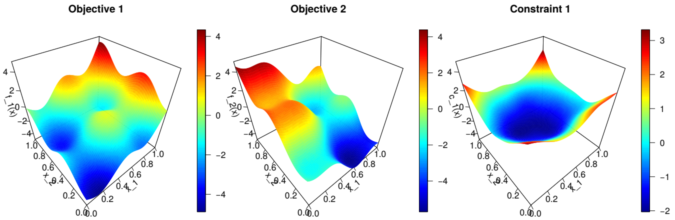

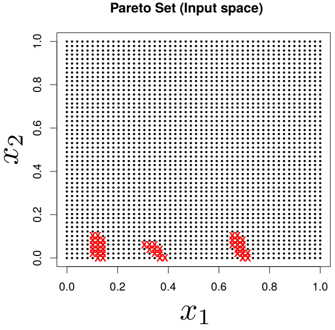

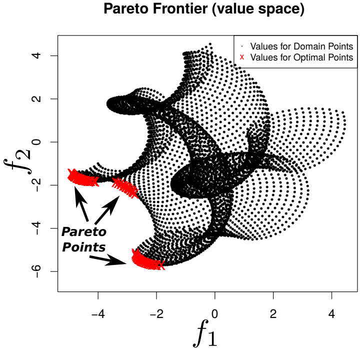

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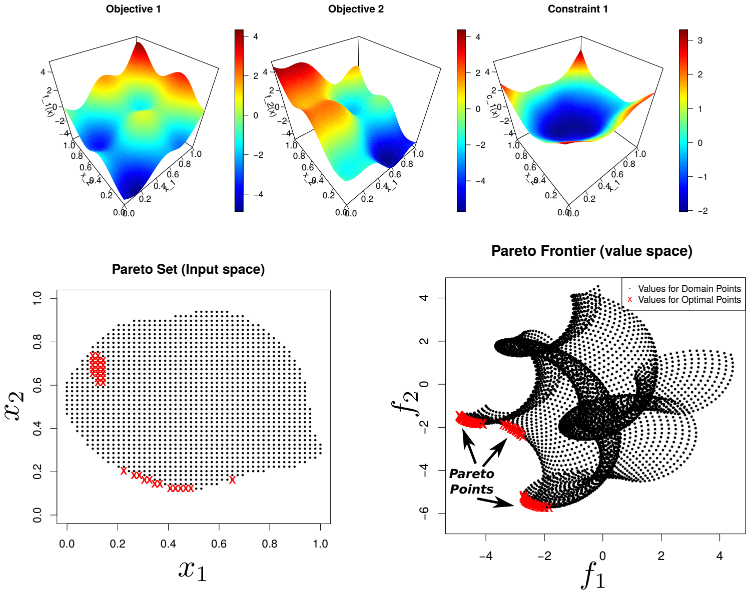

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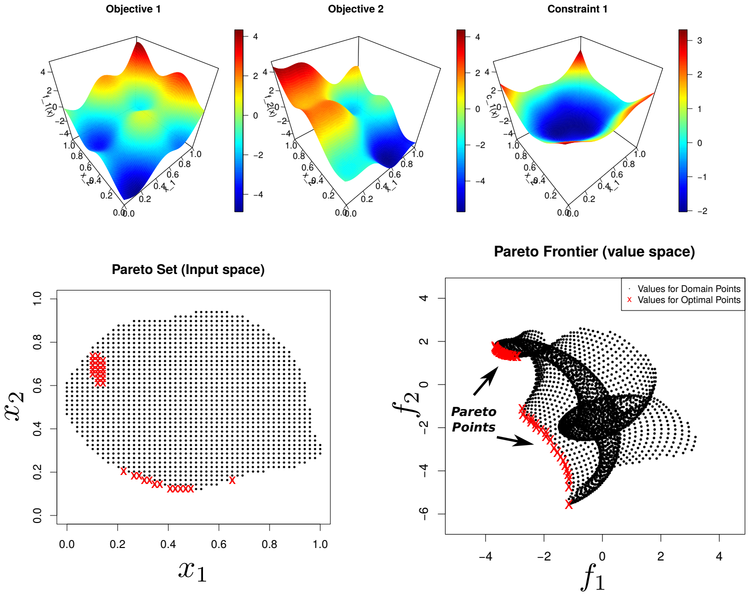

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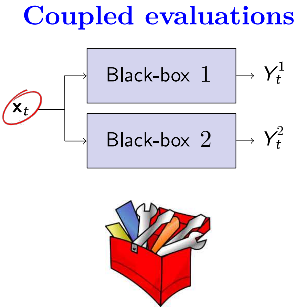

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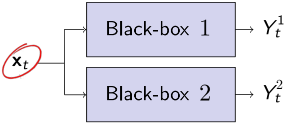

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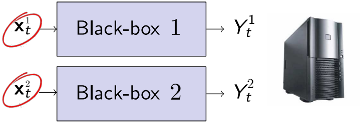

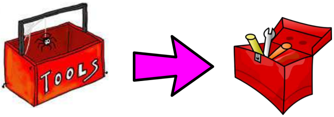

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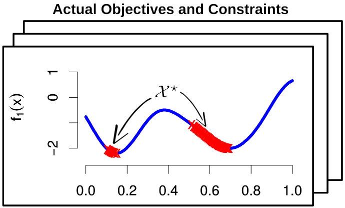

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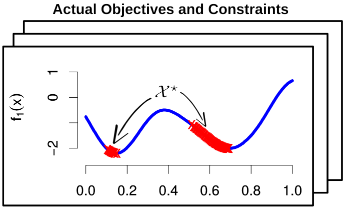

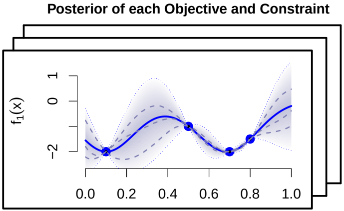

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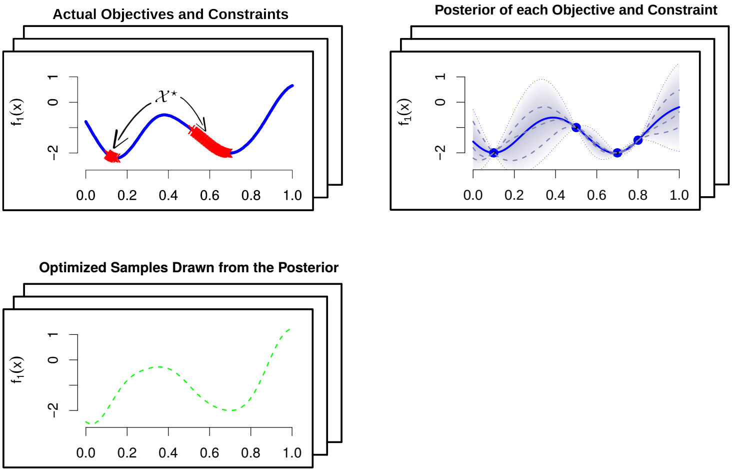

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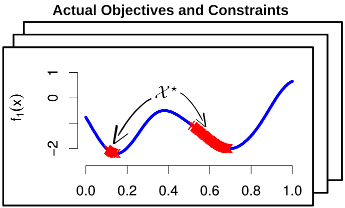

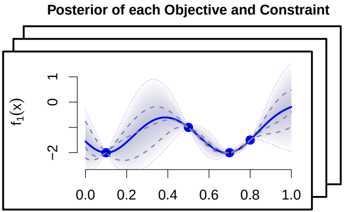

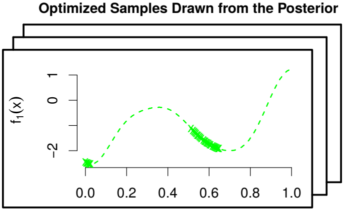

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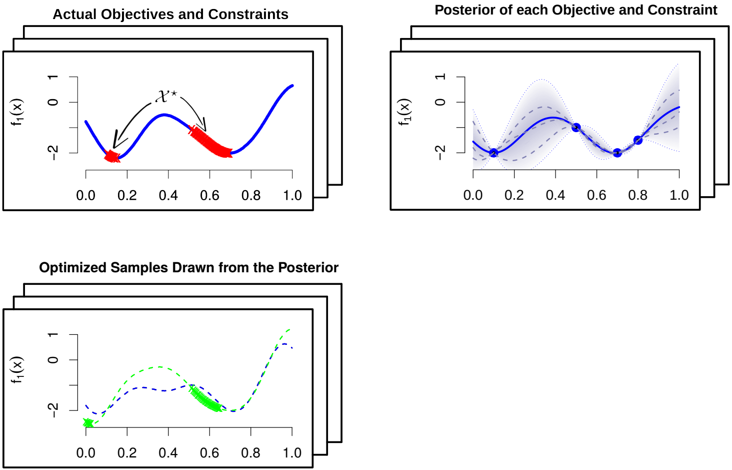

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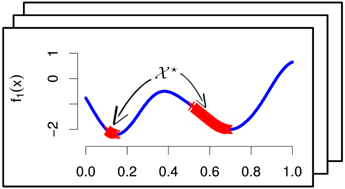
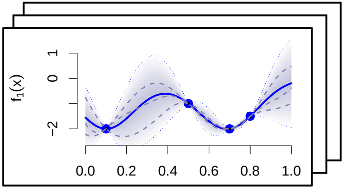
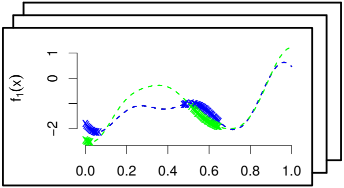


Posterior of each Objective and Constraint



Optimized Samples Drawn from the Posterior



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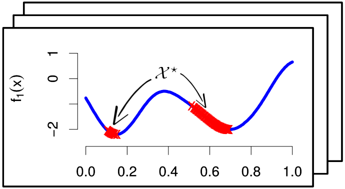

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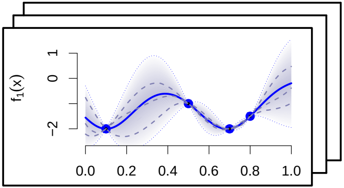

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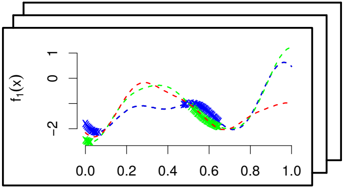

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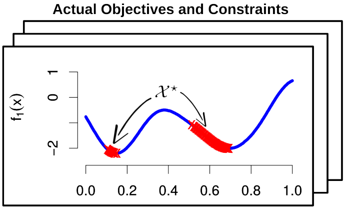

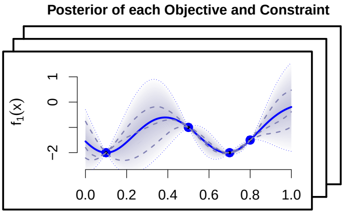

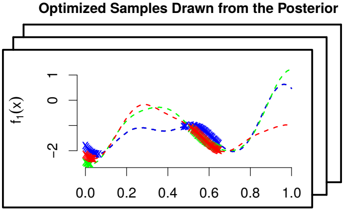

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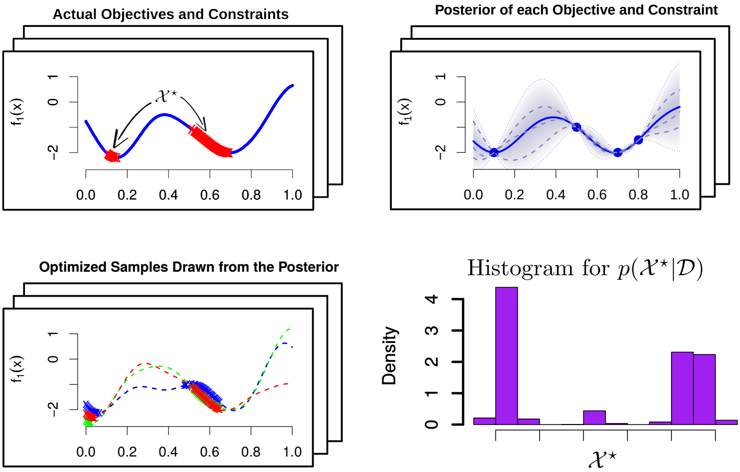

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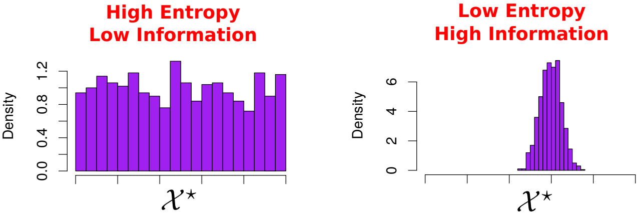

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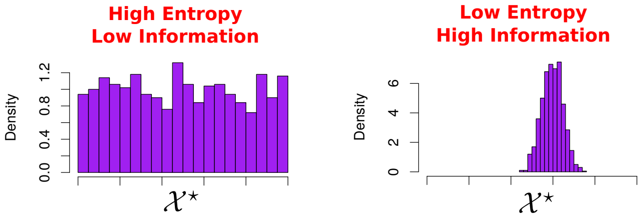

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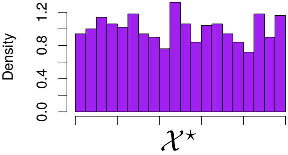
Low Information



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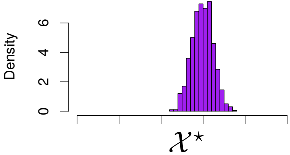

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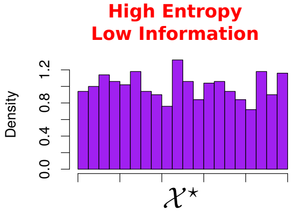

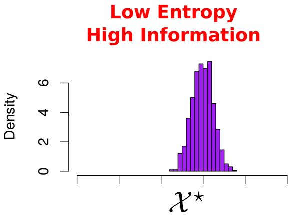

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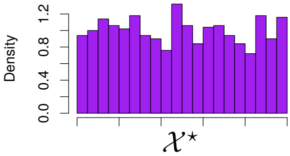

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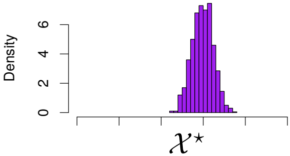

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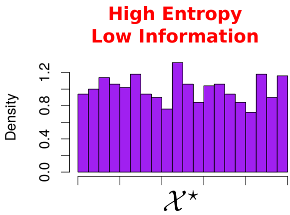

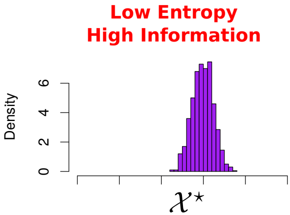

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Computing (1) is **very difficult in practice**!

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One acquisition per black-box

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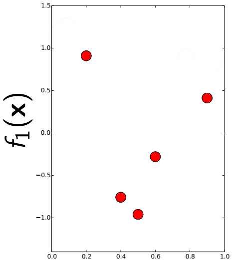
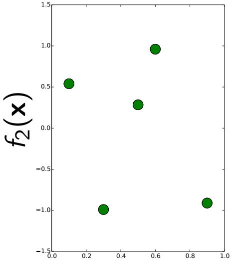
Example of PES' acquisition





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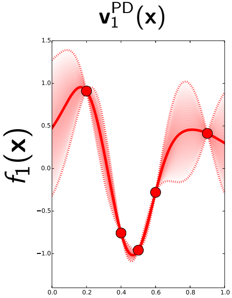

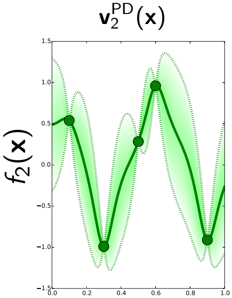

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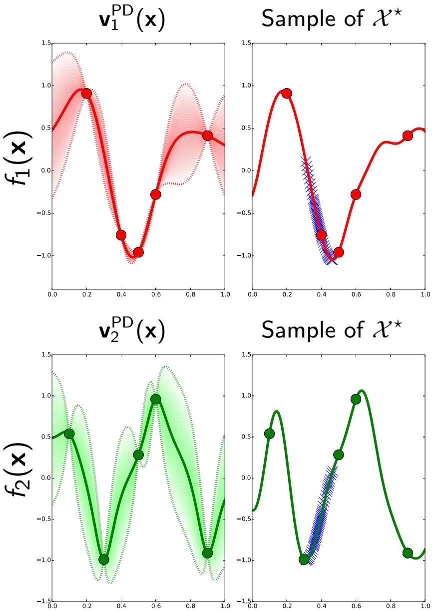

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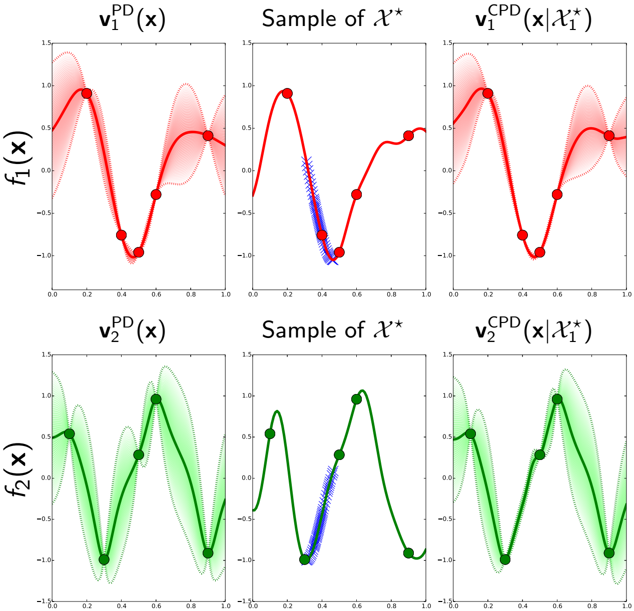

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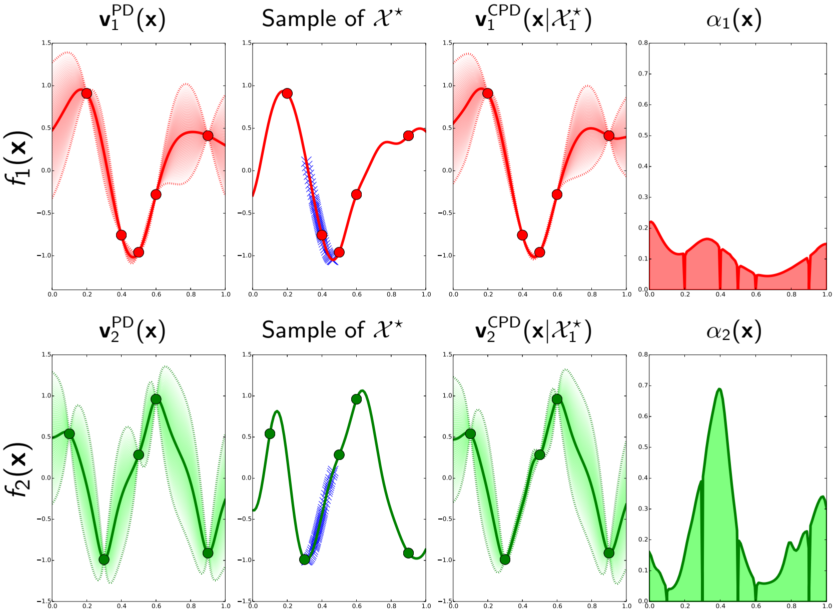

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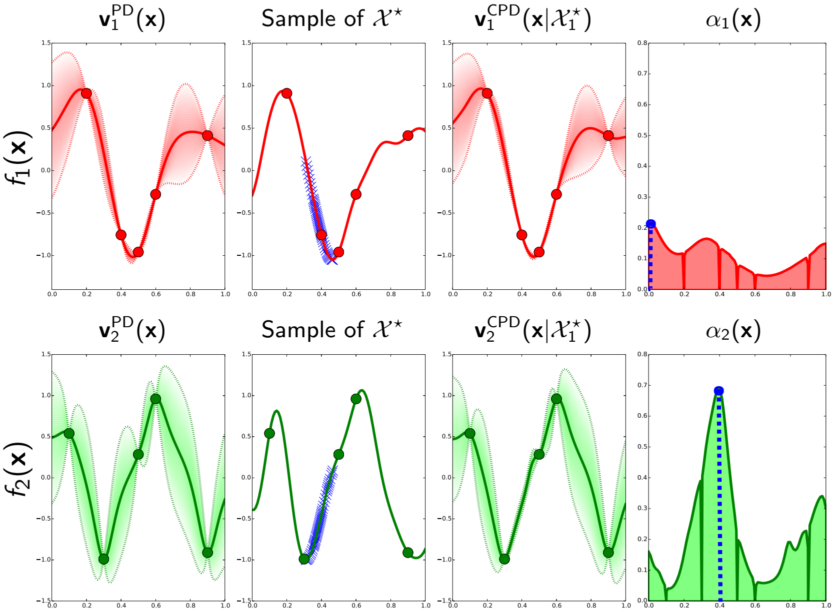
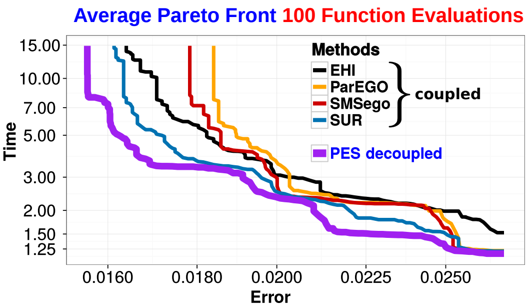


Finding a Fast and Accurate Neural Network



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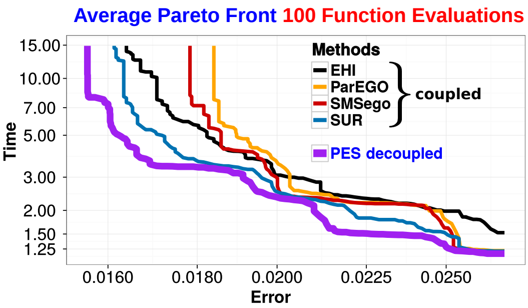

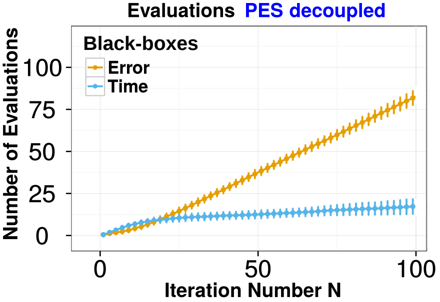

(Hernández-Lobato *et al.*, 2016)

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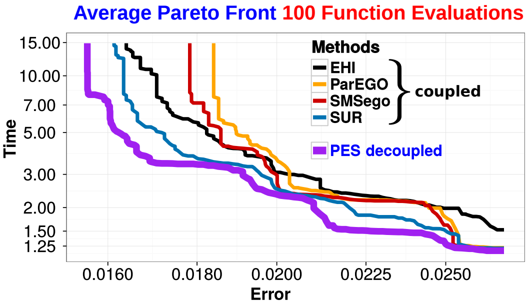

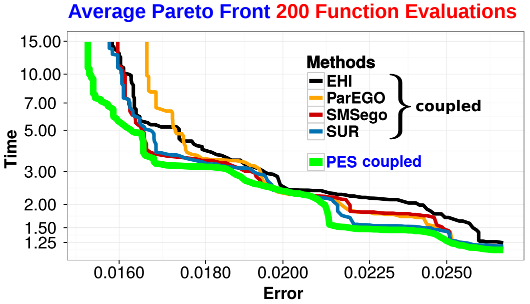

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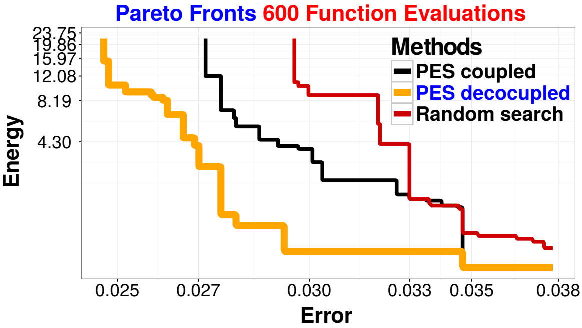
Low energy hardware accelerator



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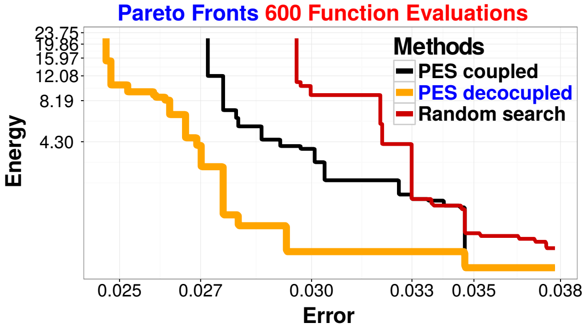

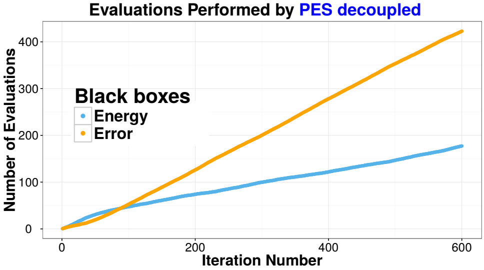

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Traditional Bayesian optimization is **sequential**!

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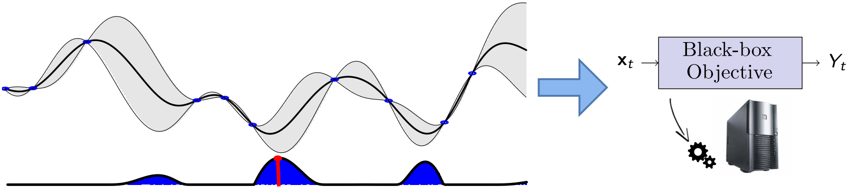

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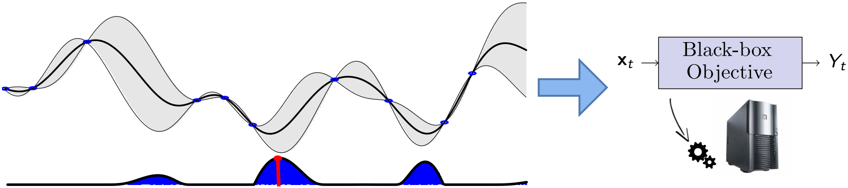

Computing clusters let us do **many things** at once!

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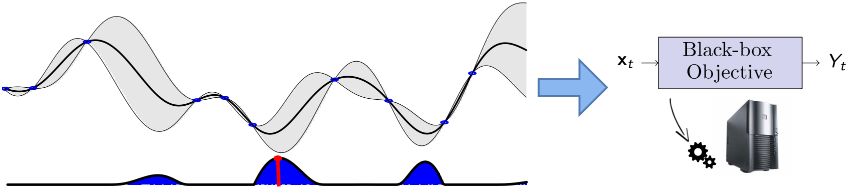

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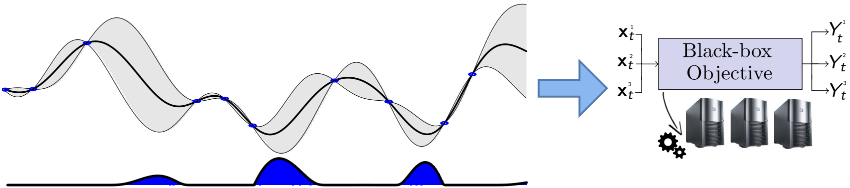

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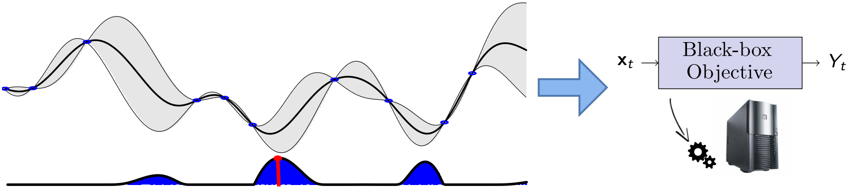

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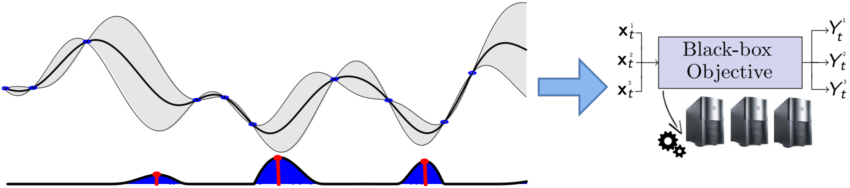

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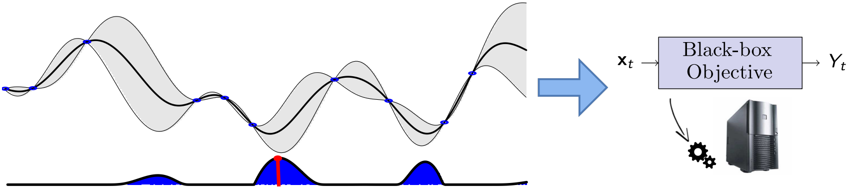

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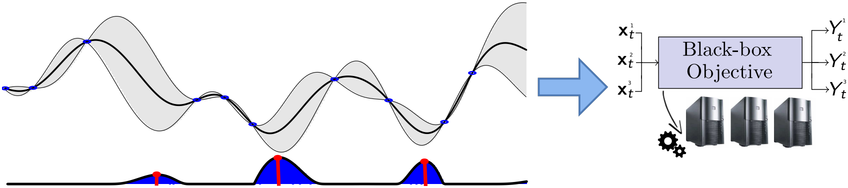

Parallel experiments should be highly informative but different!

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$$\mathrm{H}\left[\mathbf{x}^\star \middle| \mathcal{D}_t\right] - \mathbb{E}_{\mathbf{y}}\left[\mathrm{H}\left[\mathbf{x}^\star \middle| \mathcal{D}_t \cup \{\mathbf{x}_q, y_q\}_{q=1}^{Q}\right] \middle| \mathcal{D}_t, \mathbf{x}\right] \equiv \mathrm{MI}(\mathbf{y}, \mathbf{x}^\star) \quad \text{(Parallel ES)}$$

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Multi-variate Gaussian distribution

Approximated by sampling from $p(\mathbf{x}^\star|\mathcal{D}_t)$

Multivariate Gaussian approximation with **expectation propagation**
$\mathbf{x}^\star$ is better than any other point in $\mathcal{X}$

$$\alpha(\mathcal{S}_t) = \log|\mathbf{V}^{\mathrm{PD}}(\mathcal{S}_t)| - \frac{1}{M}\sum_{m=1}^{M} \log|\mathbf{V}^{\mathrm{CPD}}(\mathcal{S}_t|\mathbf{x}^\star_{(m)})|$$

(Shah and Ghahramani, 2015)

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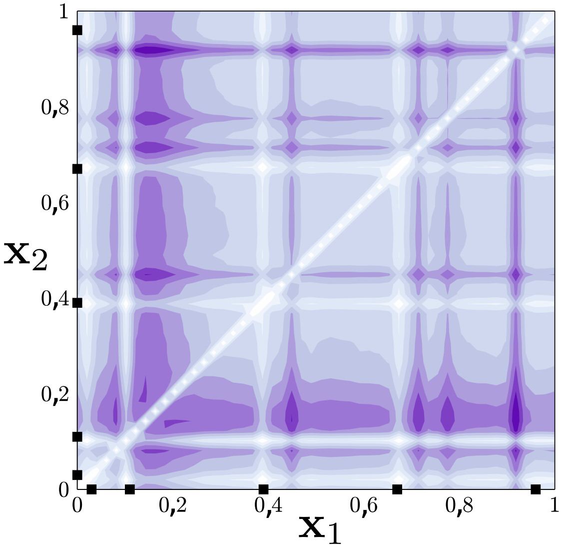
It is possible to compute the gradient of $\alpha(\cdot)$ w.r.t. each $\mathbf{x}_q \in \mathcal{S}_t$!

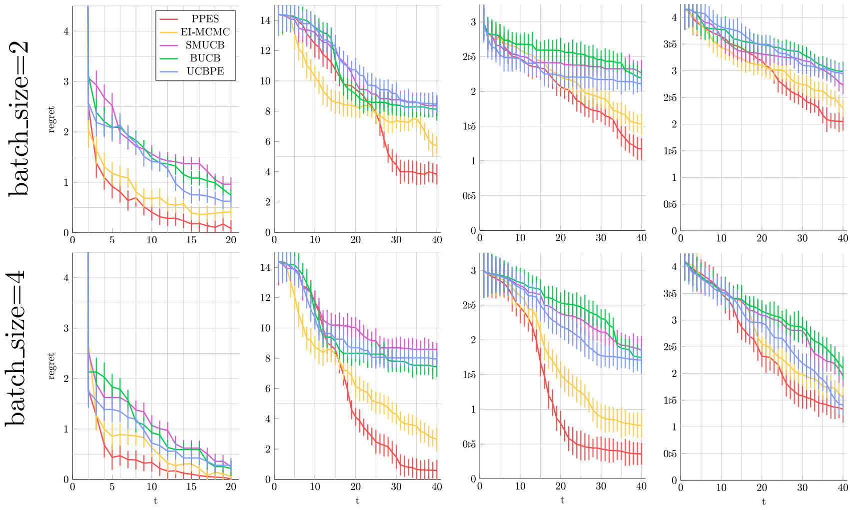
(Shah and Ghahramani, 2015)

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)

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

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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!

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