Advanced Methods for Bayesian Optimization in Complex Scenarios Course

Presented by: Eduardo C. Garrido–Merchán.

Universidad Pontificia Comillas
June, 2023.

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- Fundamentals of Bayesian Optimization.

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- Advanced scenarios: Mixed, multi-fidelity, high-dim, topologies.

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- References.

First Session: Bayesian optimization fundamentals

Introduction.

Challenges in Machine Learning, Finance, Robotics, Engineering, Business...

Companies face complex scenarios dealing with lots of scenarios!




Challenges in Machine Learning, Finance, Robotics, Engineering, Business...

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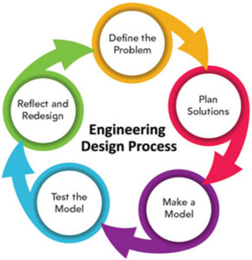

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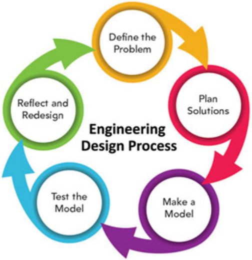

- Many choices at each step.

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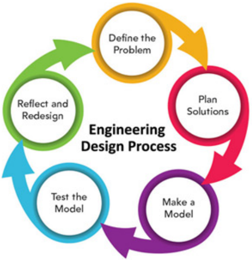

- Many choices at each step.
- Complicated and high dimensional.

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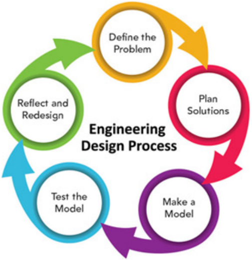

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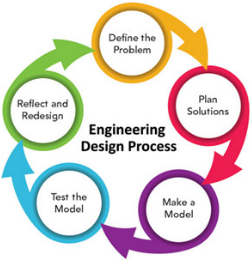

- Many choices at each step.
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- Difficult for individuals to reason about.
- Prone to human bias.

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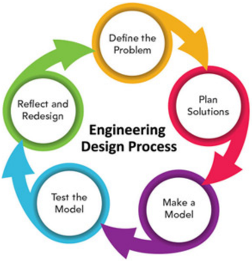

- Many choices at each step.
- Complicated and high dimensional.
- Difficult for individuals to reason about.
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- It may be possible to test various models in parallel.

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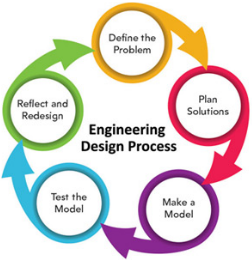

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- Complicated and high dimensional.
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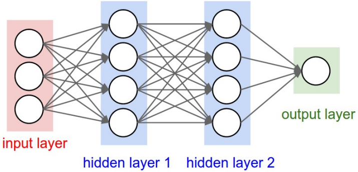
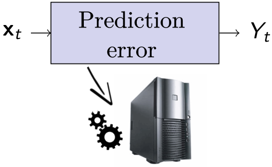
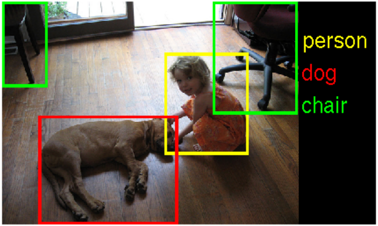
- It may be possible to test various models in parallel.

Optimization is a challenging task in real-life choices!

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







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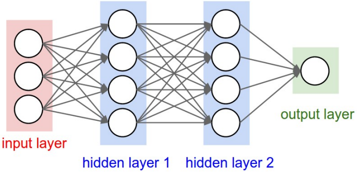

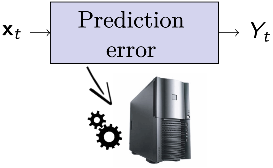

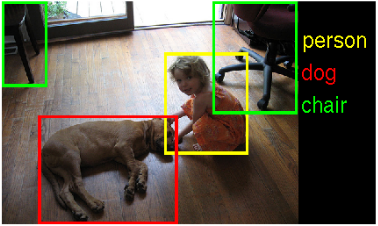

Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc.

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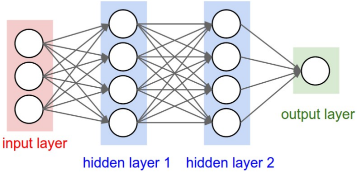
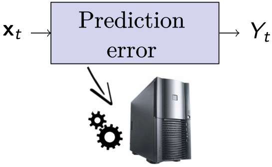
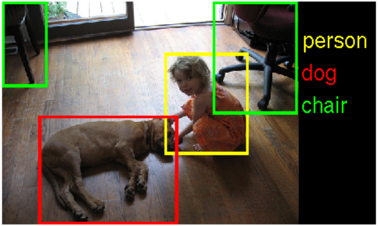
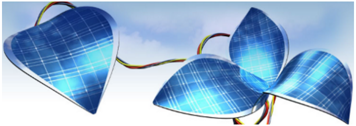


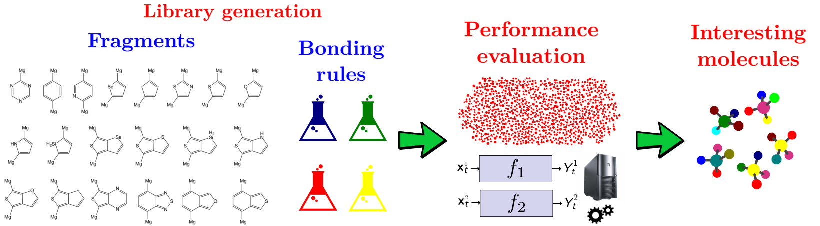




Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc. If **multiple processors** were available, we could test **various configurations in parallel**, in order to **gain more information**.

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





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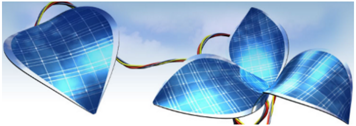
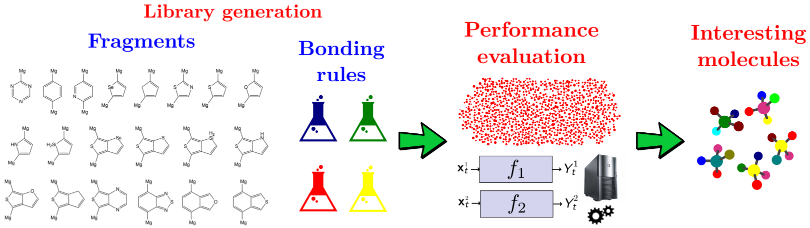
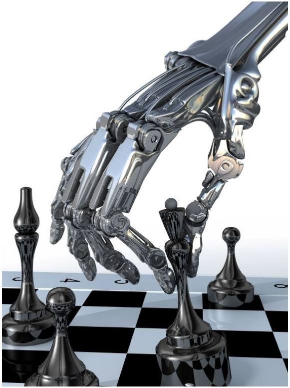




Explore **millions of candidate molecule structures** to identify the compounds with the best properties.

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



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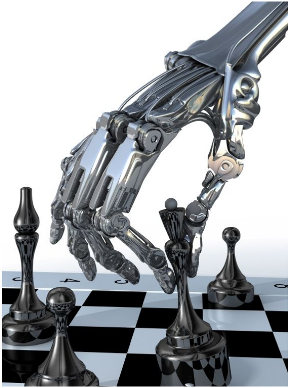
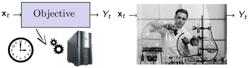


Parameters to tune: initial pose for the robot's hand and finger joint trajectories.

Optimization Problems: Common Features

- Very expensive evaluations.



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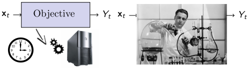

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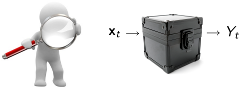

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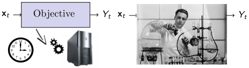

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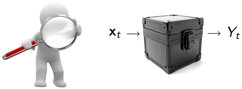
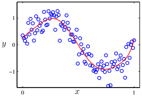


- The evaluation can be noisy.

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



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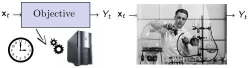

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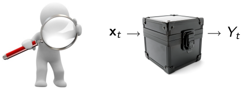

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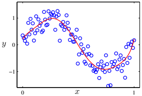
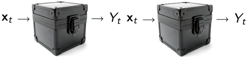
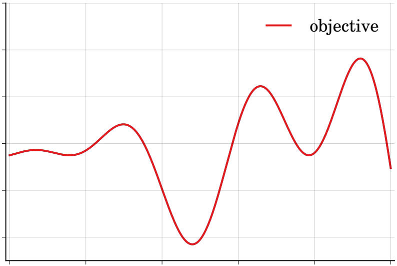


- Evaluations may be done in parallel.



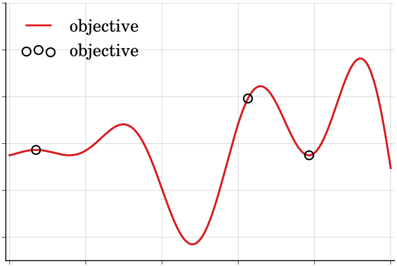
Bayesian optimization methods can be used to solve these problems!

Bayesian Optimization



1. Get initial sample.

Bayesian Optimization



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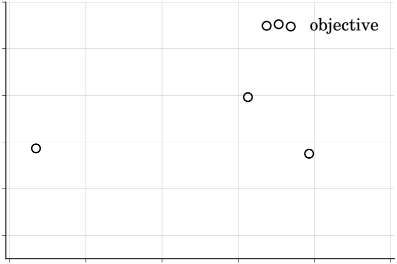
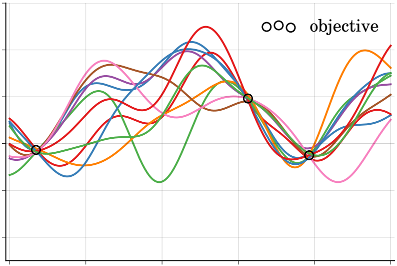


1. Get initial sample.
2. Fit a model to the data:

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

Bayesian Optimization



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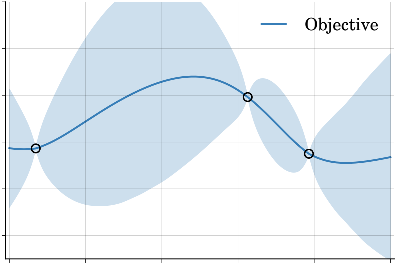

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3. Select data collection strategy:

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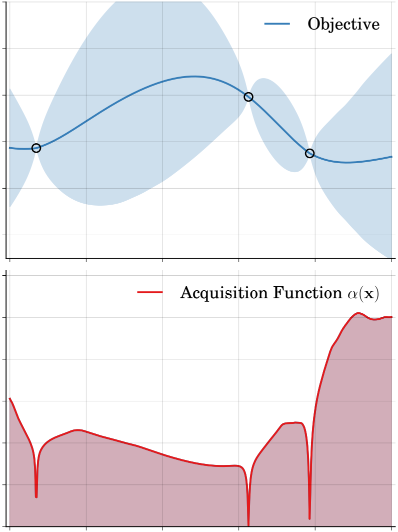
Bayesian Optimization



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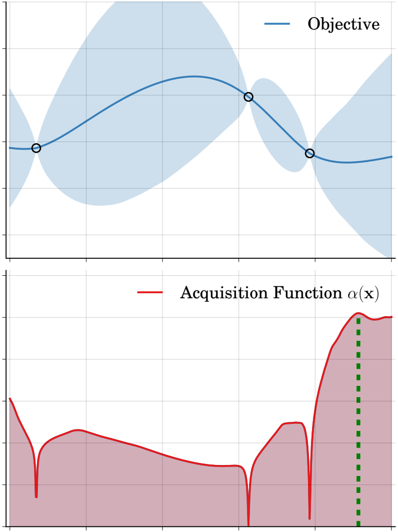

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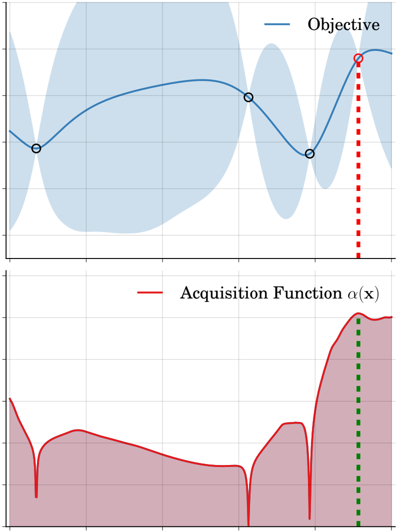

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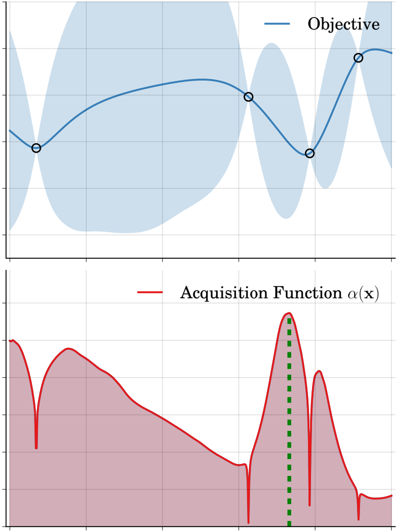

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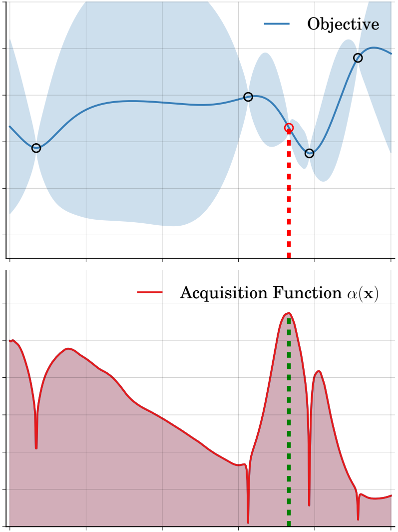

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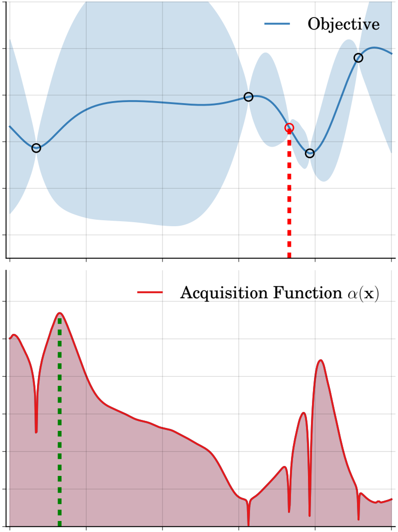

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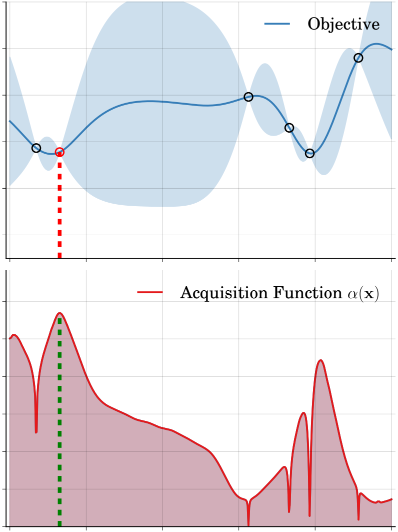

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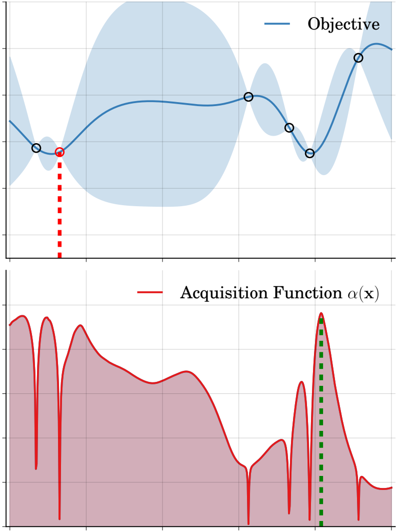

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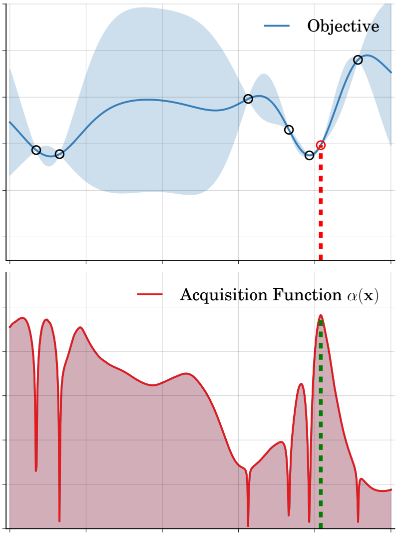

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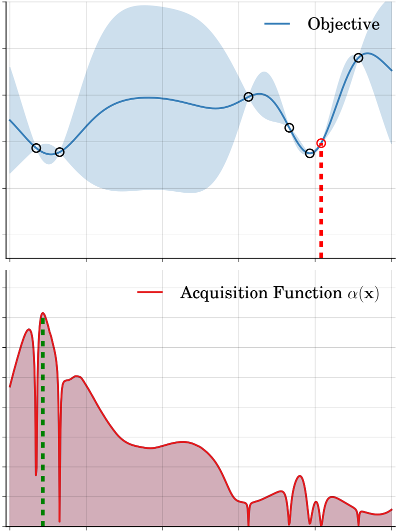

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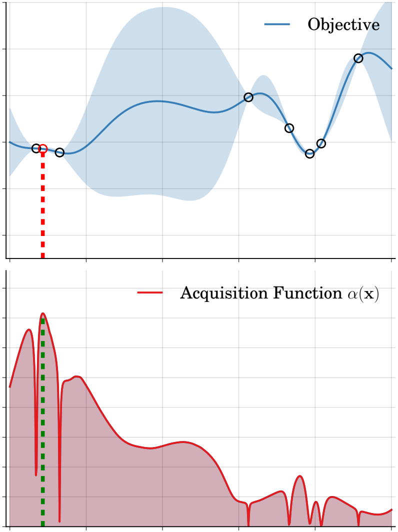

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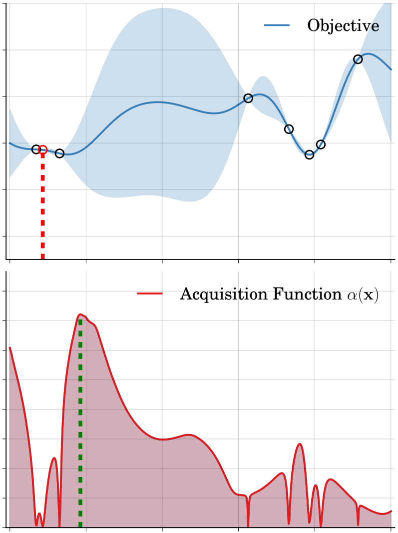

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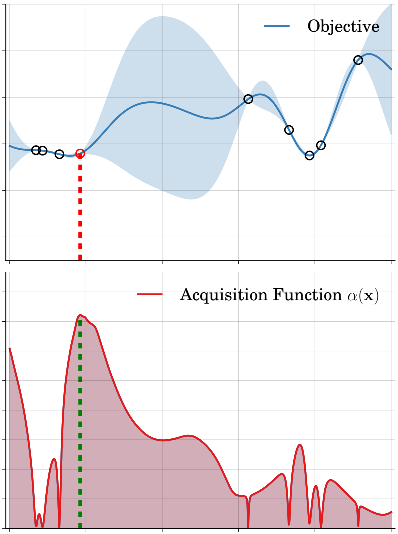

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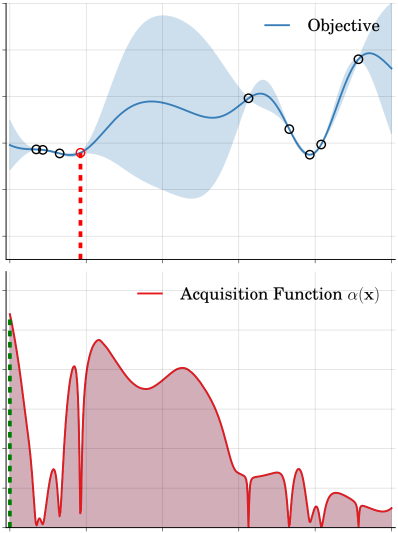

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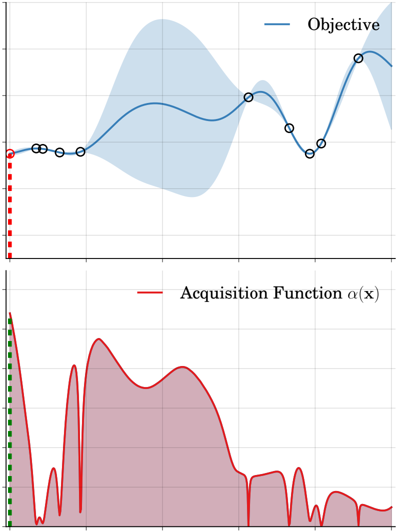

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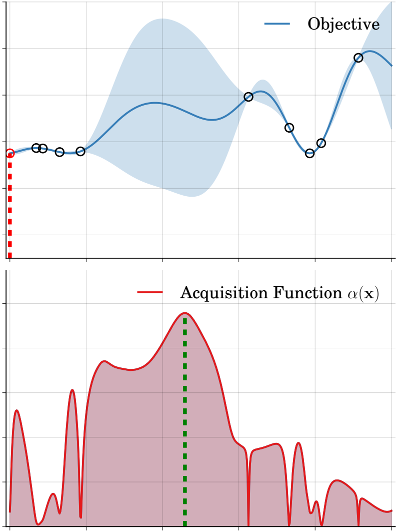

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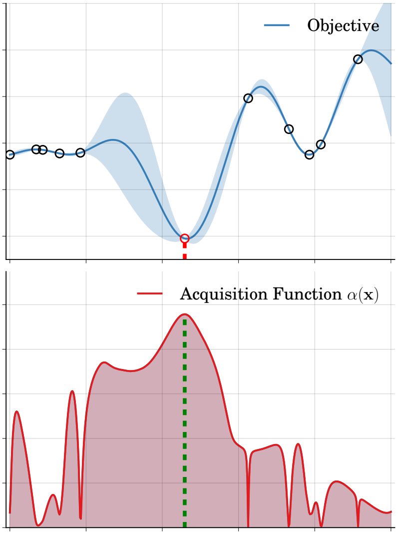

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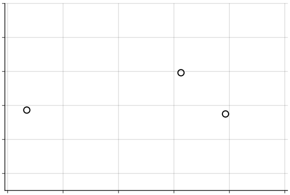

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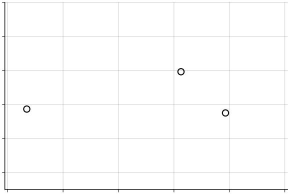

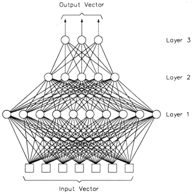

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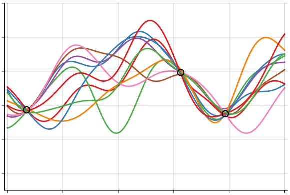

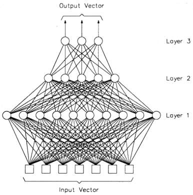

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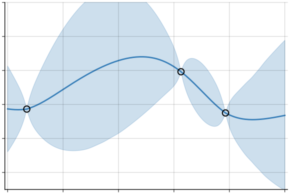

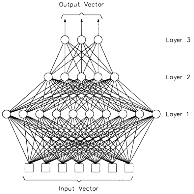

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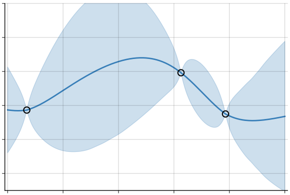

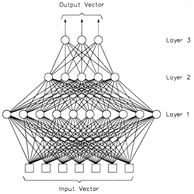

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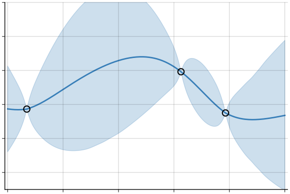

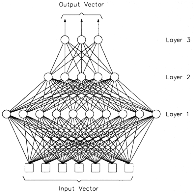

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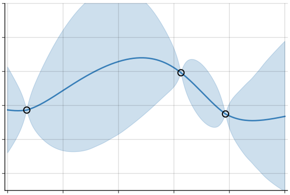

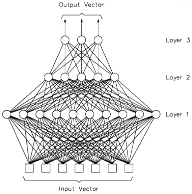

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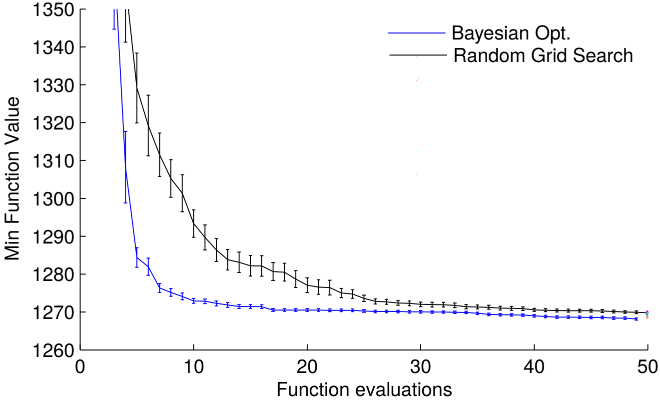
Solved by setting $p(\mathrm{W}) = \prod_{ij} \mathcal{N}(w_{ji}|0, \sigma^2 H^{-1})$ and letting $H \to \infty$!

Bayesian Optimization vs. Uniform Exploration



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

Using the GP Uncertainty in Optimization

Where to evaluate **next**?

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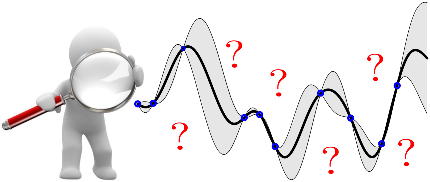

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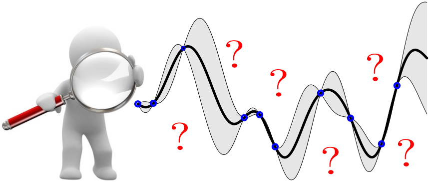

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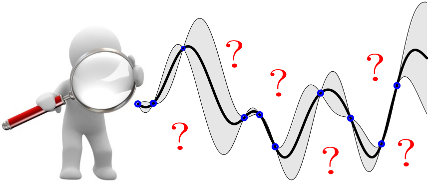

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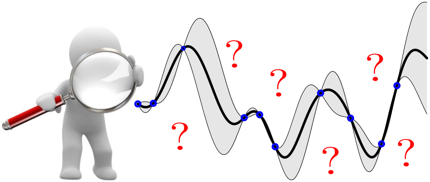

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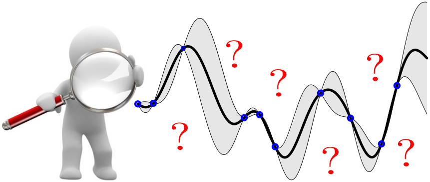

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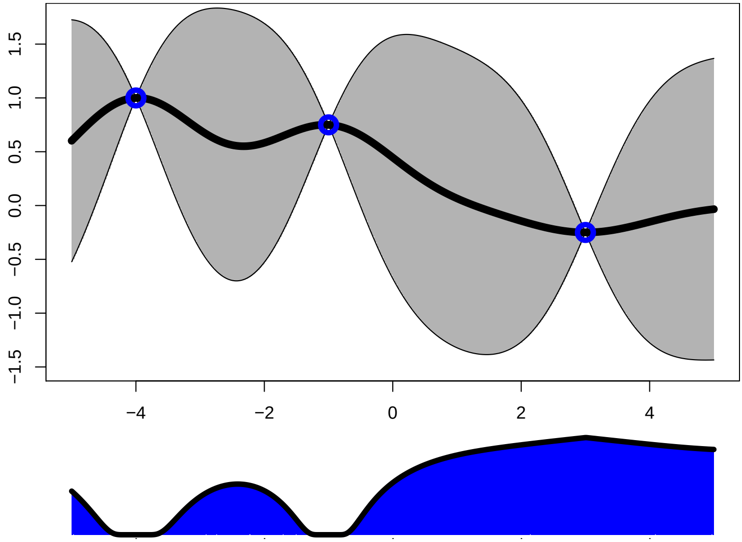
Some Acquisition Functions: Prob. Improvement



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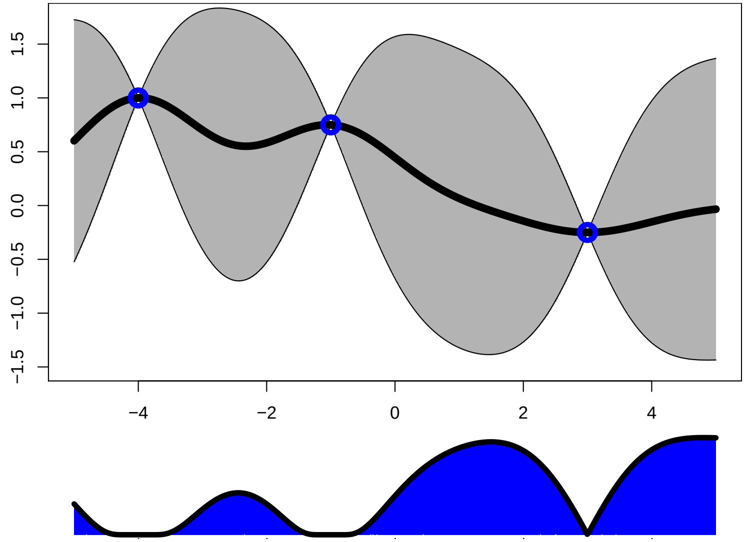

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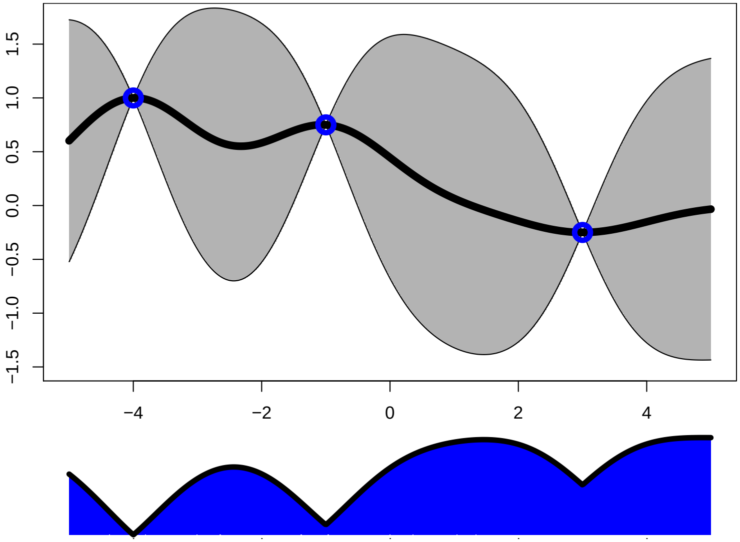

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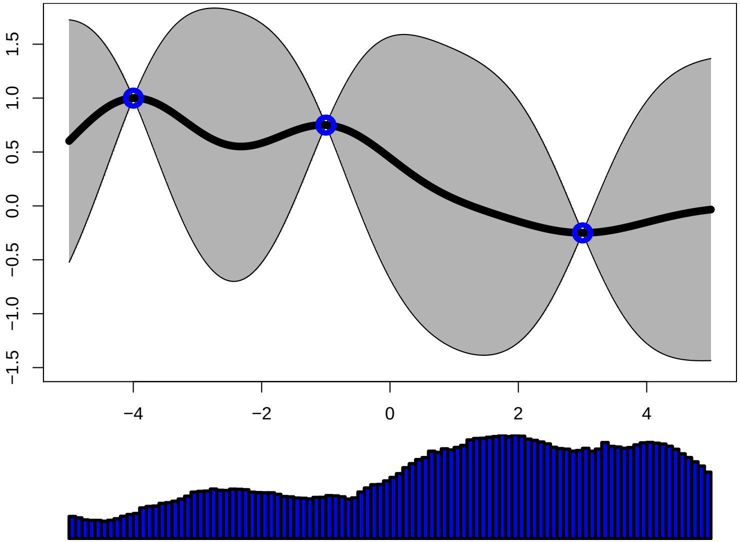

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Information is measured by the **entropy** of $p(\mathrm{x}^*|\mathcal{D})$.

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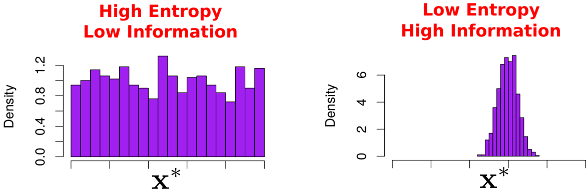

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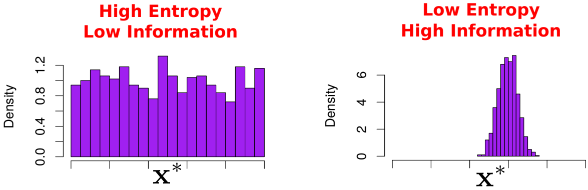

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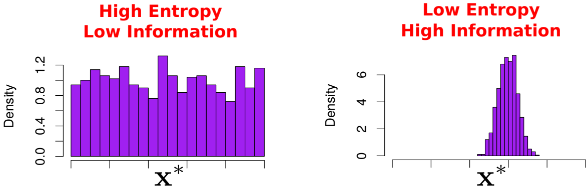

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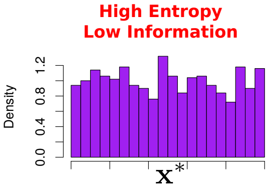

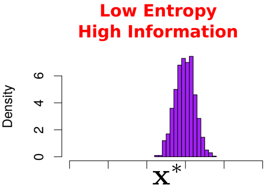

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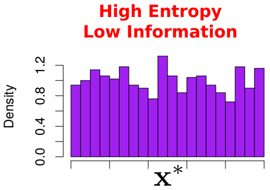

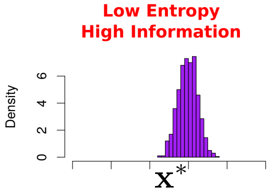

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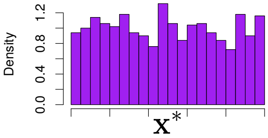

Low Entropy
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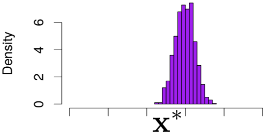

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Computing (1) is **very difficult in practice**!

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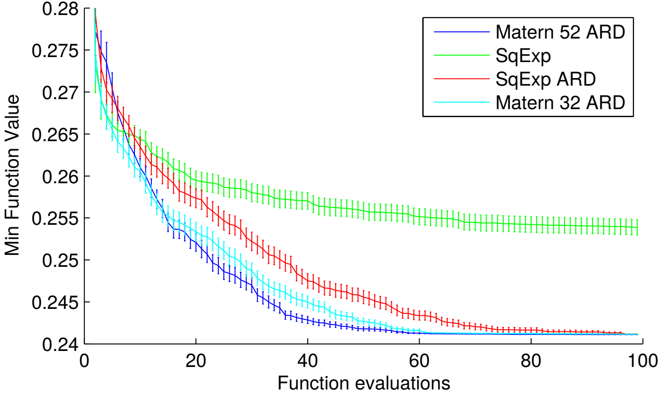

Structured SVM for protein motif finding (Snoek *et al.*, 2012).

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Slice sampling means no additional hyper-parameters!

(Neal, 2003)

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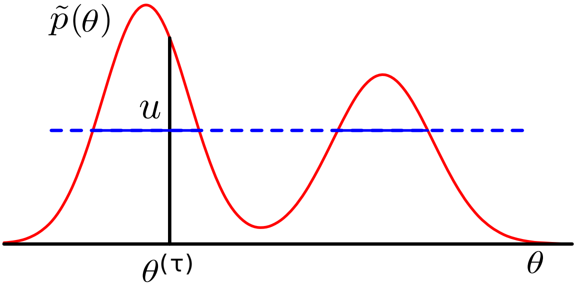
Slice sampling means no additional hyper-parameters!



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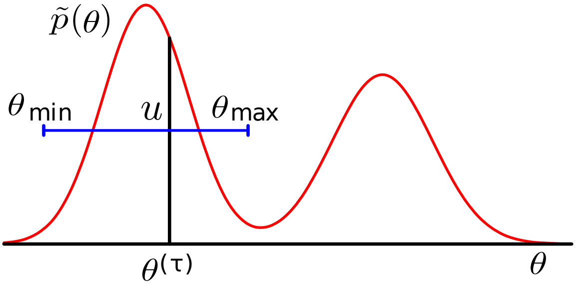

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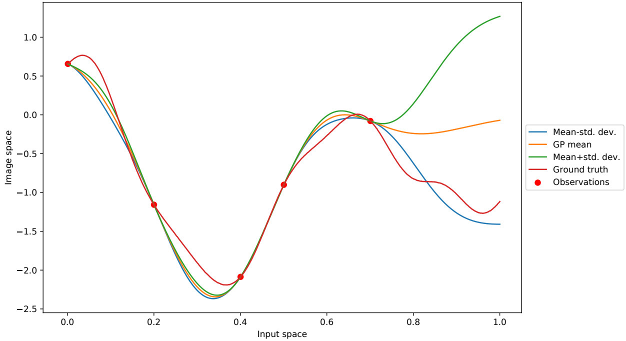
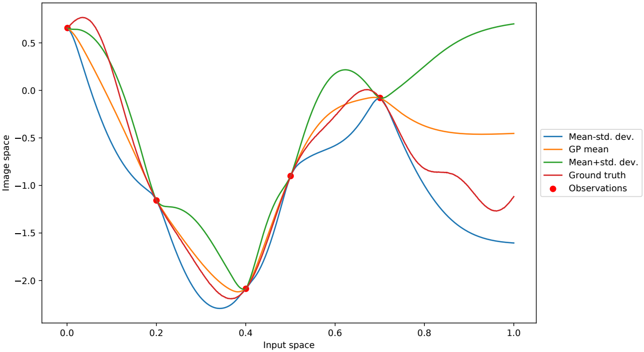
GP fitting an unknown function using Maximum Likelihood



GP fitting an unknown function sampling hyperparameters



Integrated Acquisition Function

$$\hat{\alpha}(\mathrm{x}) = \int \alpha(\mathrm{x};\theta)p(\theta|\mathrm{y})d\theta \approx \frac{1}{K}\sum_{k=1}^{K}\alpha(\mathrm{x};\theta^{(k)}) \quad \theta^{(k)} \sim p(\theta|\mathrm{y}),$$

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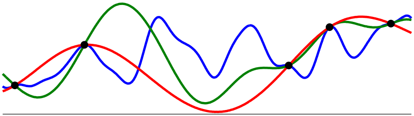
Posterior samples with three different length-scales



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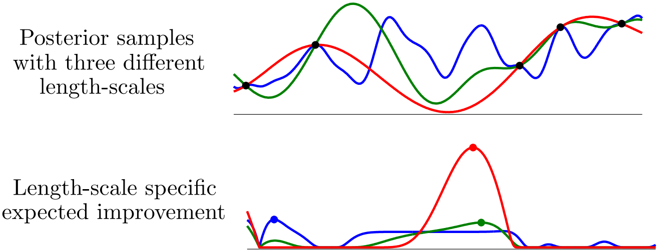

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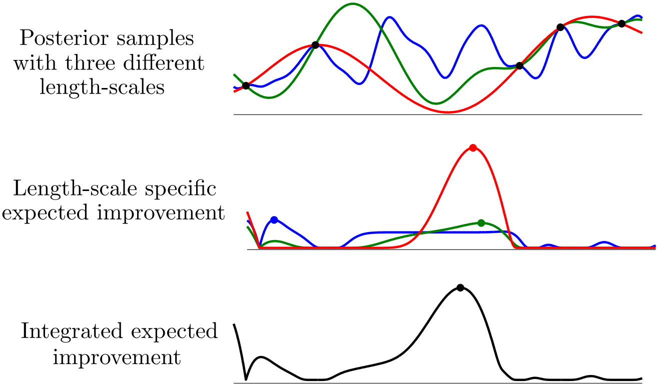

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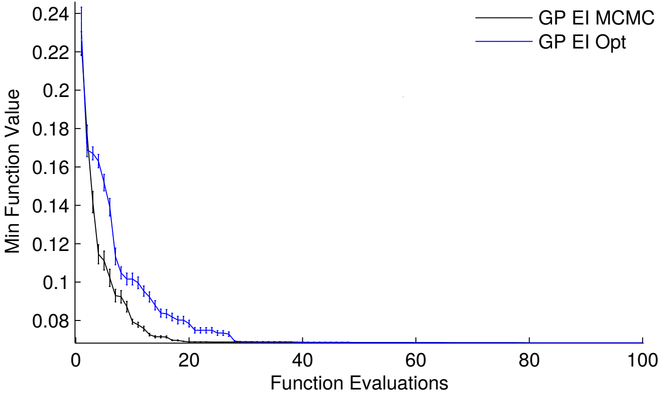
MCMC estimation vs. Maximization



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

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Expected Improvement per-second:

$$\alpha(\mathrm{x}) = \frac{\sigma(\mathrm{x})\left(\gamma(\mathrm{x})\Phi\left(\gamma(\mathrm{x})\right) + \phi(\gamma(\mathrm{x}))\right)}{\exp\left\{\mu_{\text{log-time}}(\mathrm{x})\right\}}$$

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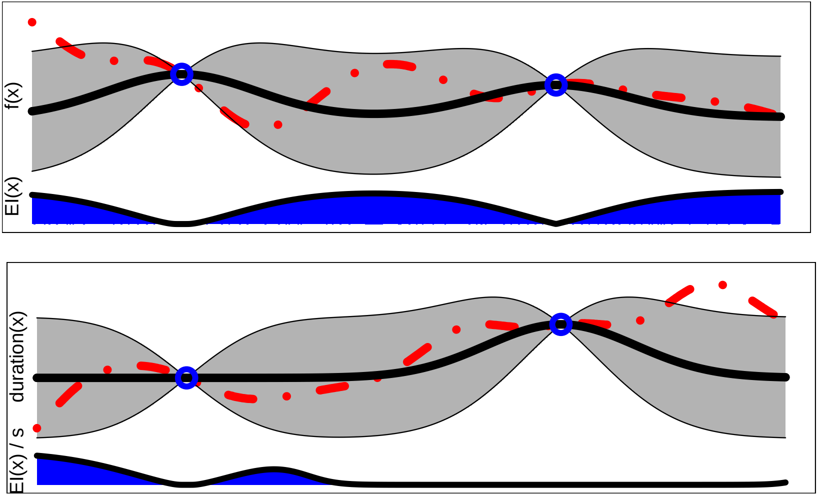

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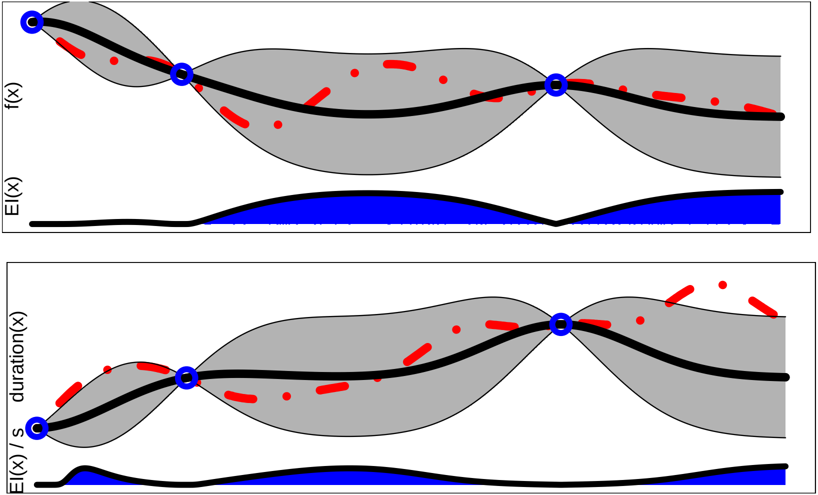

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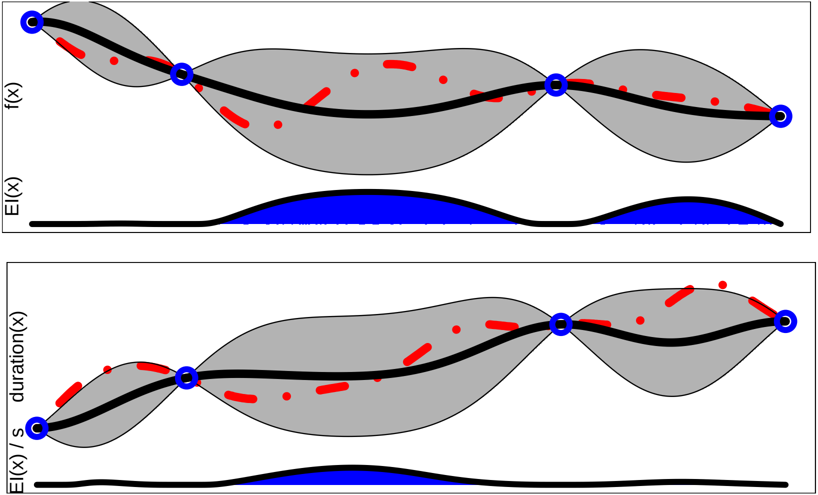

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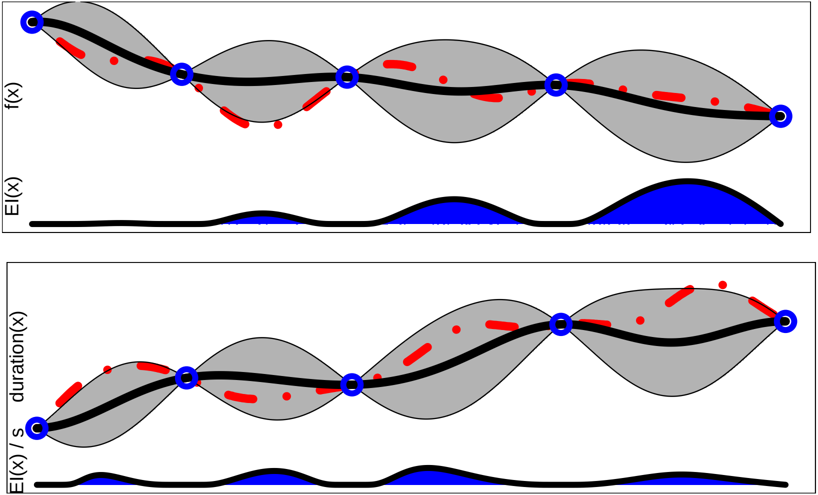

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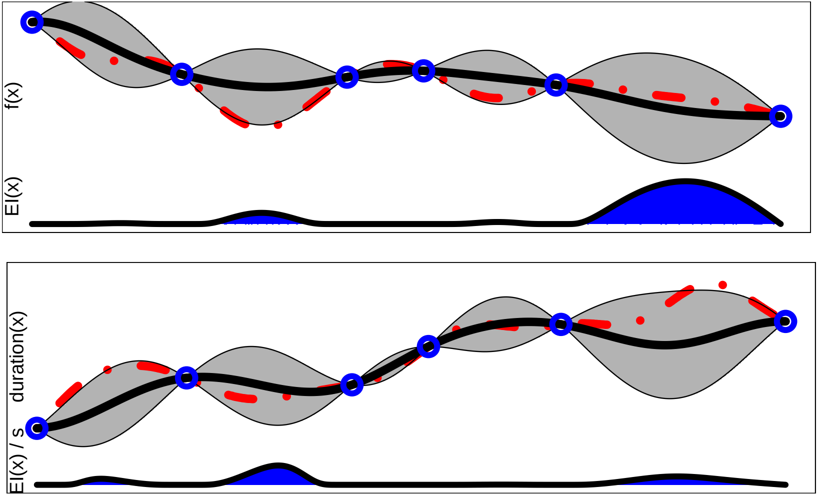

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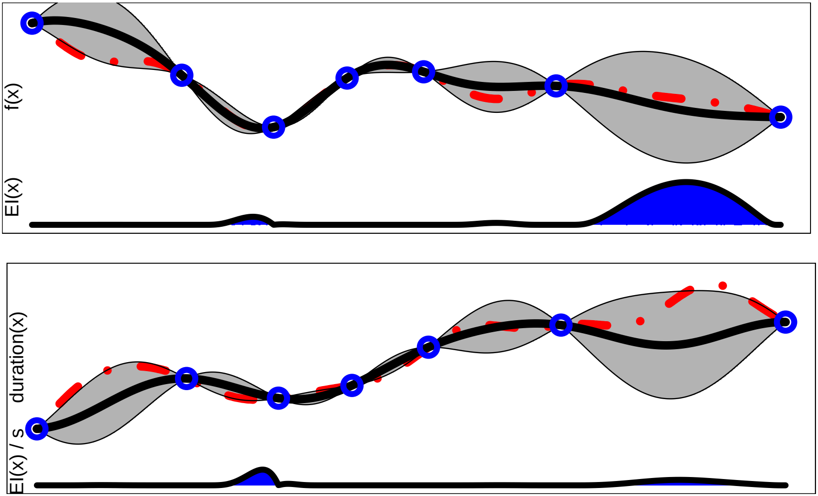

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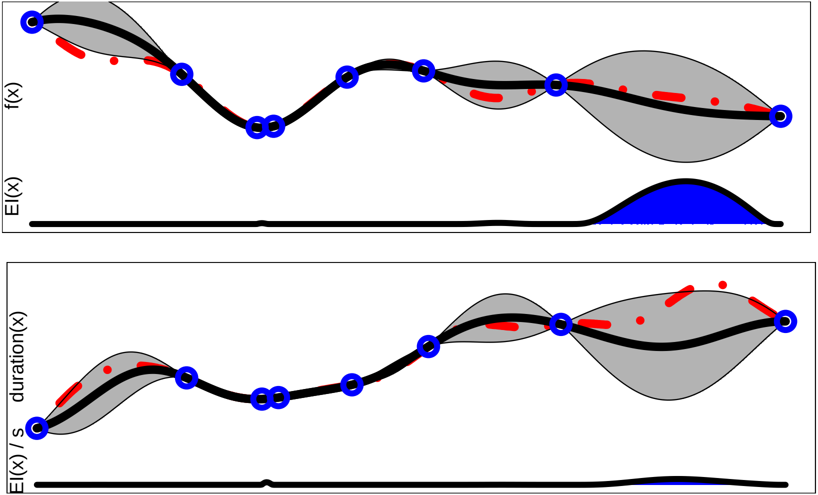

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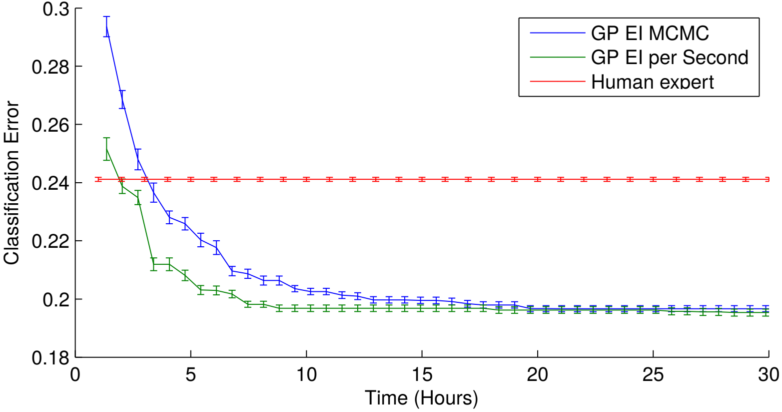

Deep neural network on the CIFAR dataset (Snoek *et al.*, 2012)

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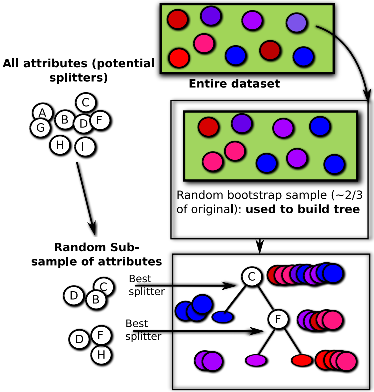

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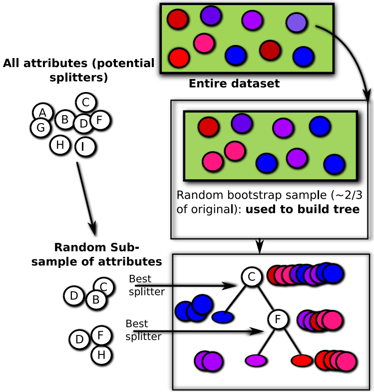

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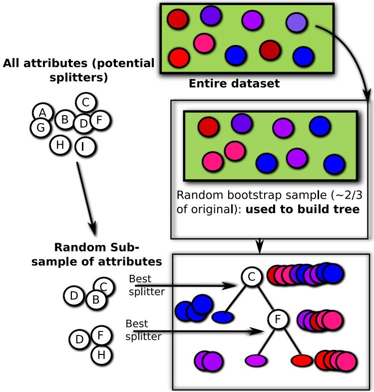

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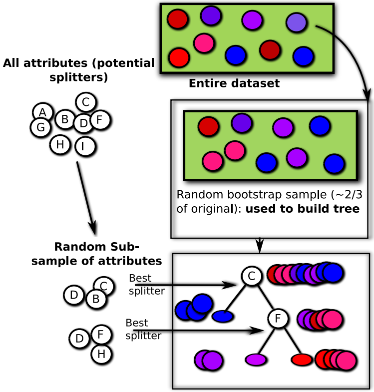

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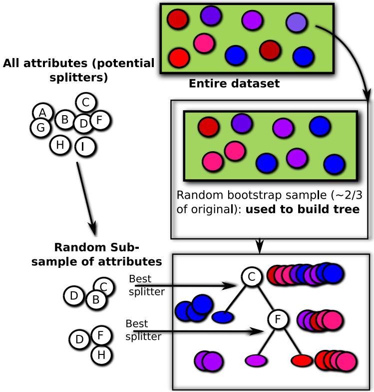

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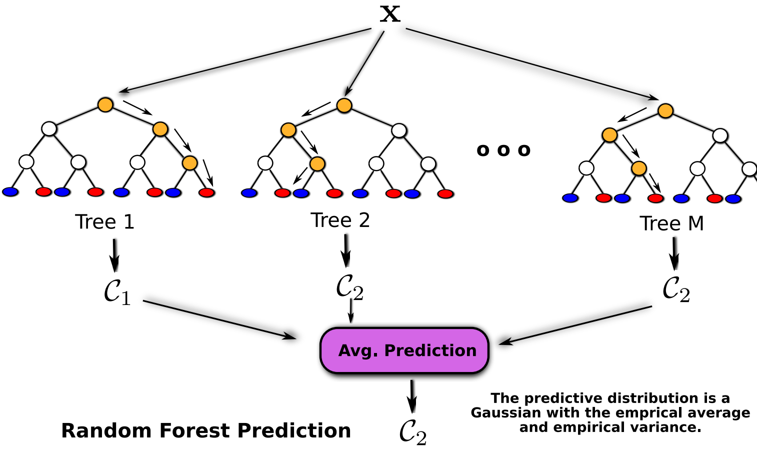
Very cheap to compute and massively paralelizable!

Random Forest: Predictive Distribution



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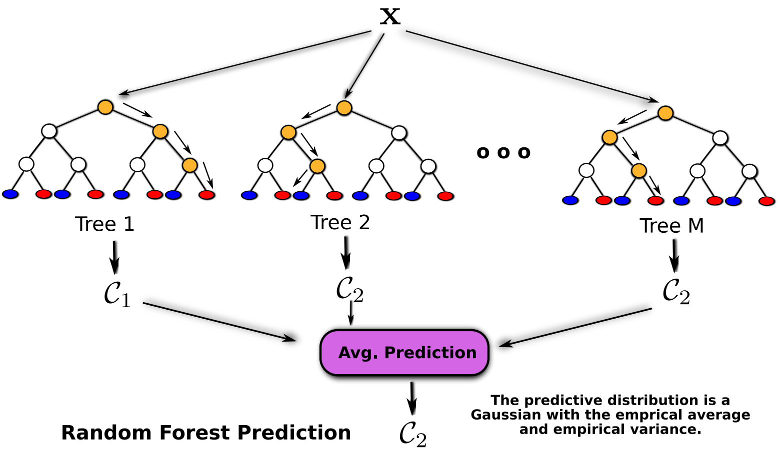
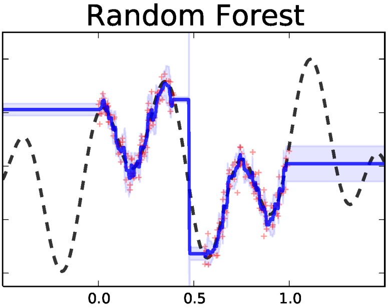


$$p(f^\star|\mathcal{D}_n) = \mathcal{N}(f^\star|\overline{\mu}, \overline{\nu}^2)$$

(Hutter et al., 2011)

Random Forest in Practice



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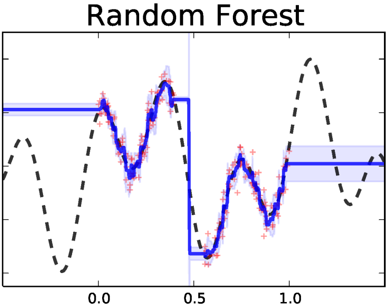

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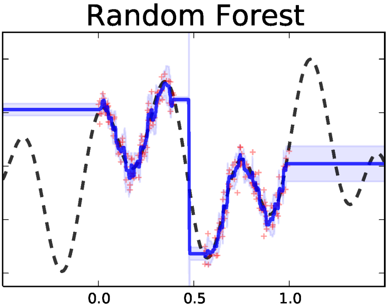

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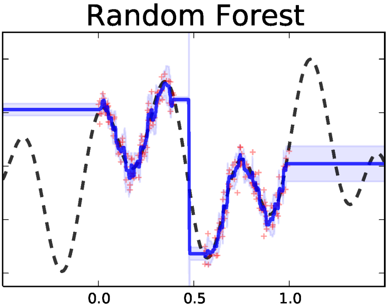

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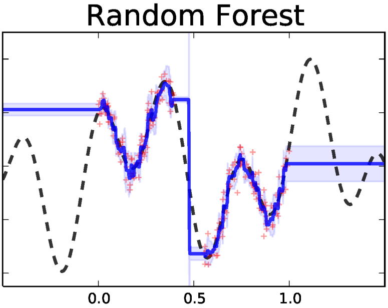

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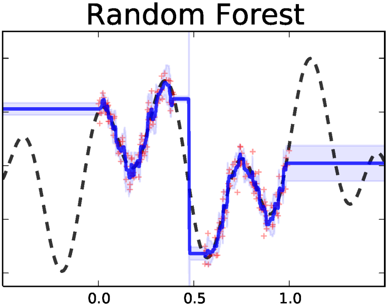

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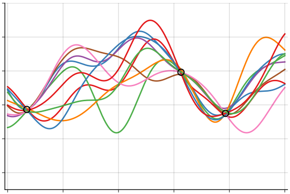

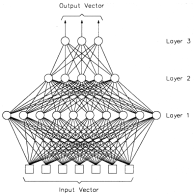

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- Neural networks scale well to the training data (linear cost).

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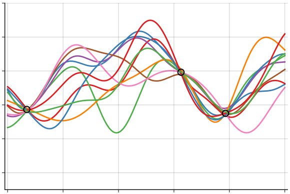

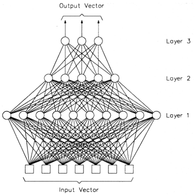

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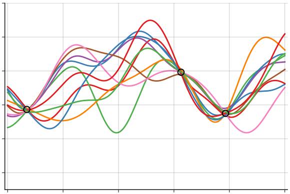

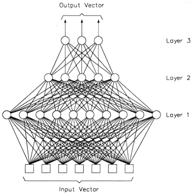

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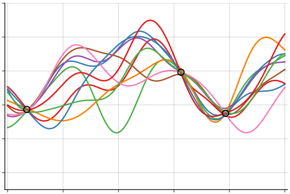

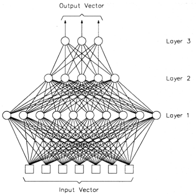

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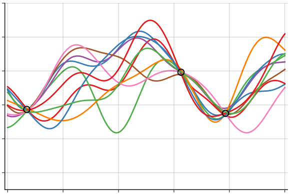

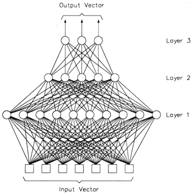

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Trade-off between accuracy of the predictive distribution and scalability! Still a lot of research going on!

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Other tools: SMAC3 (Python-RFs), GPyOpt (Python3), Spearmint (Python2.7-sampling), mlrMBO (R).

Time to practice!

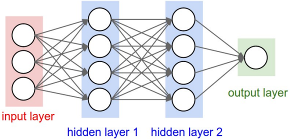
1. Bayesian optimization of a benchmark optimization function.
2. Bayesian optimization of the hyper-parameters of a machine learning model.
3. Bayesian optimization of the hyper-paramaters of a deep reinforcement learning algorithm.

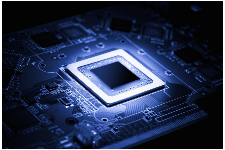
Second Session: Advanced Bayesian optimization.

(Parallel) Multi-objective Bayesian optimization with constraints.

Several Objectives and Constraints

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





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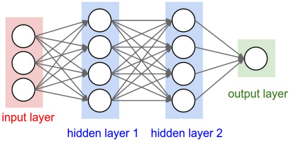

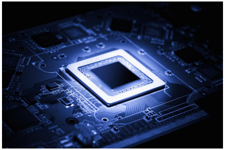

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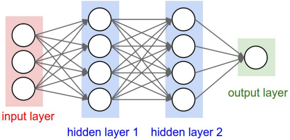

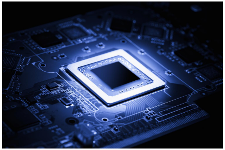

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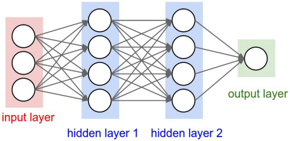

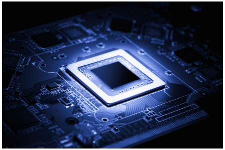

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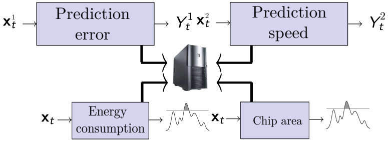

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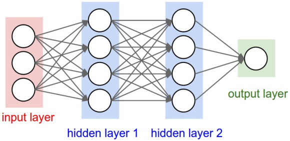

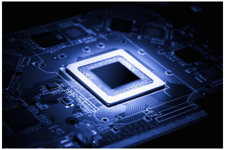

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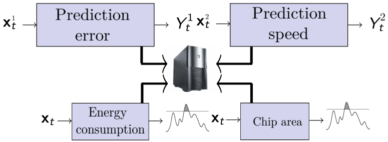
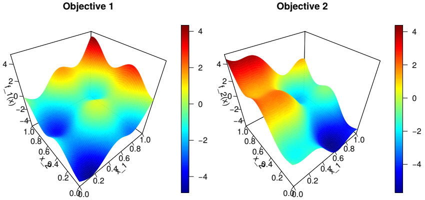


Challenges:

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

Constrained Multi-Objective Optimization



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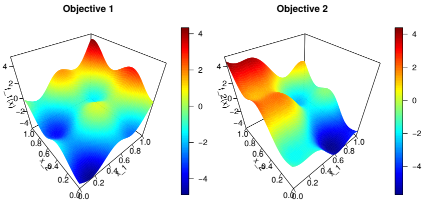

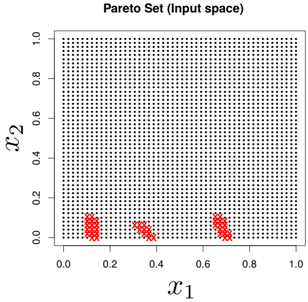

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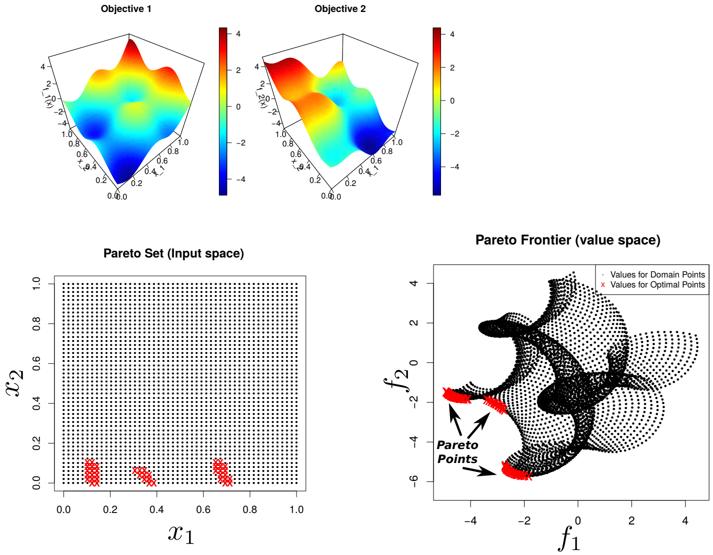

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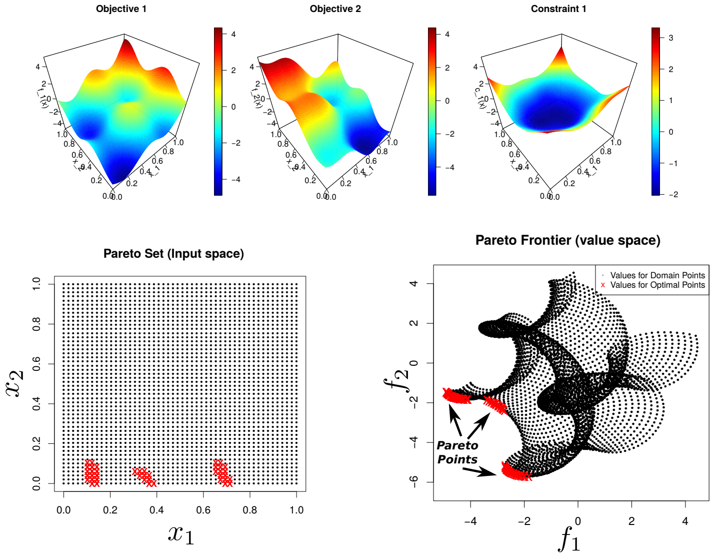

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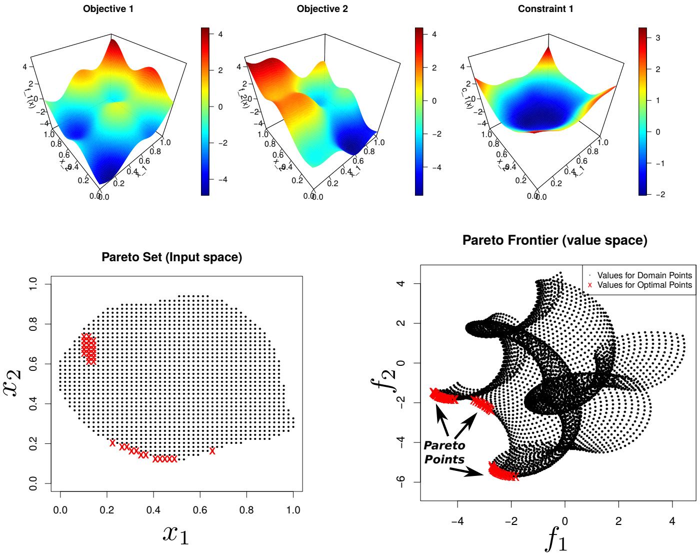

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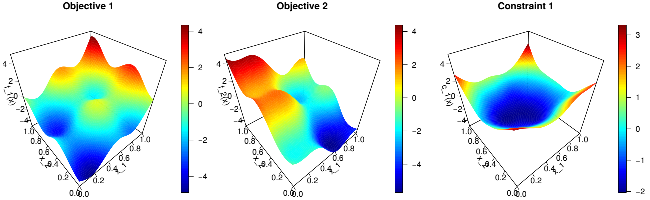

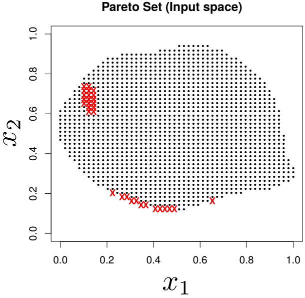

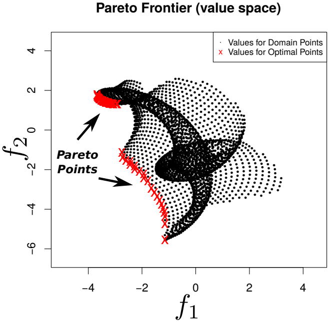

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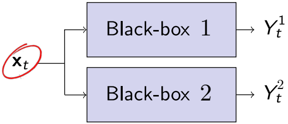

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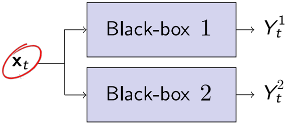

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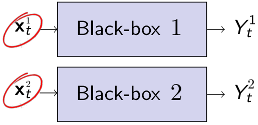

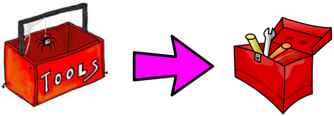

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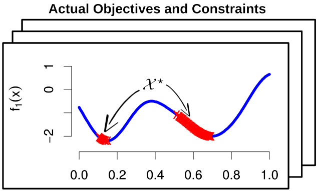

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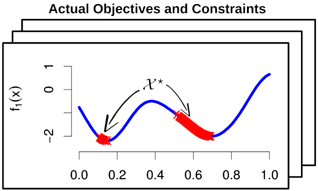

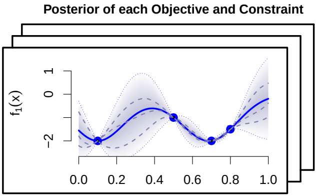

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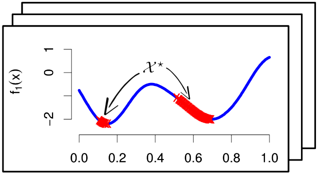
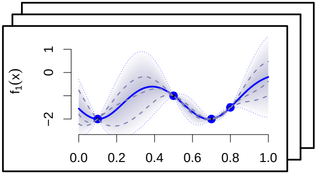
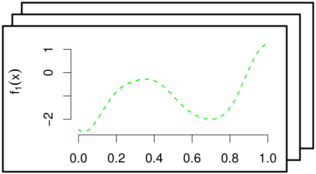


Posterior of each Objective and Constraint



Optimized Samples Drawn from the Posterior



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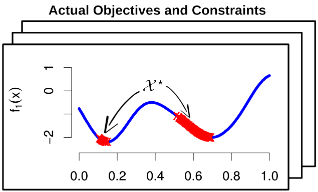

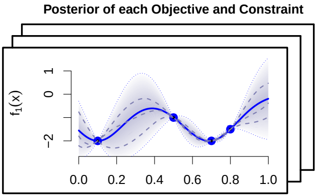

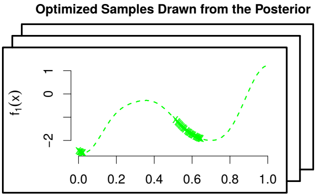

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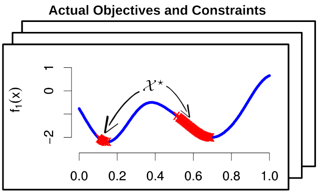

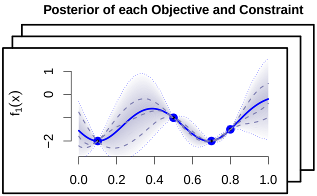

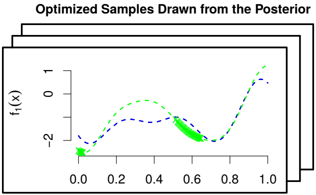

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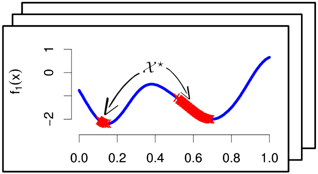

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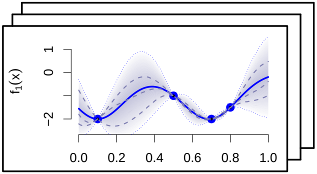

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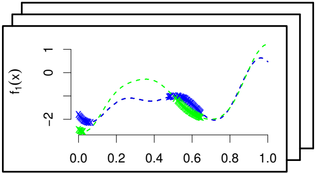

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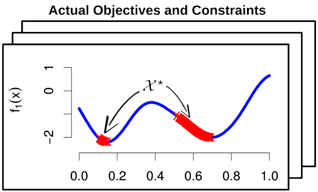

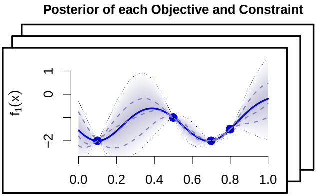

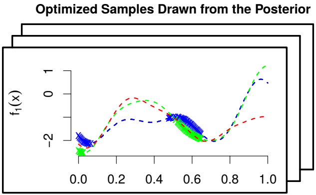

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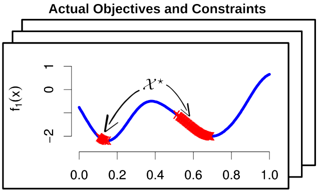

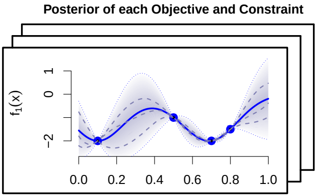

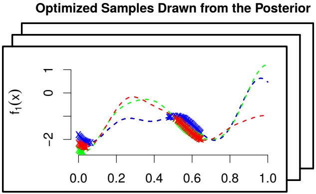

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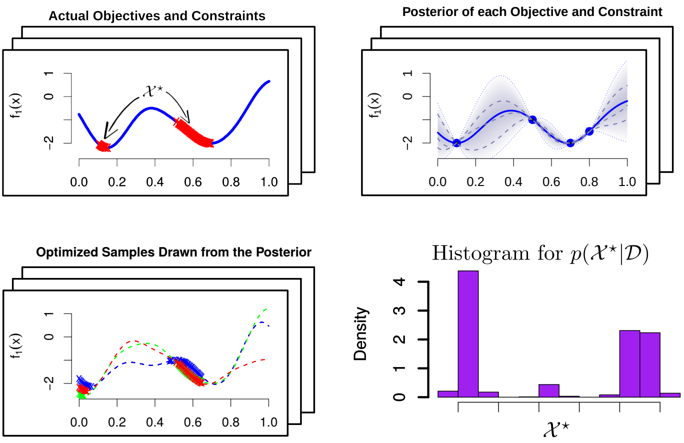

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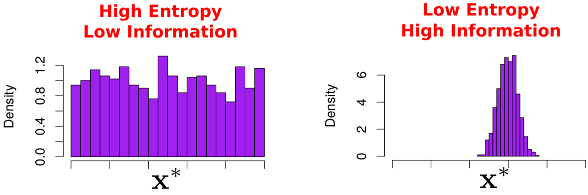

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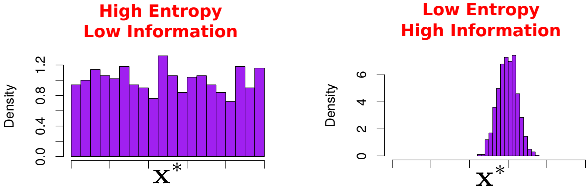

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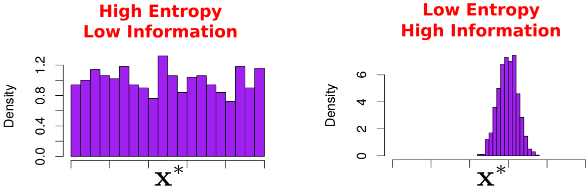

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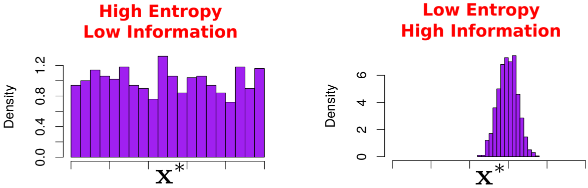

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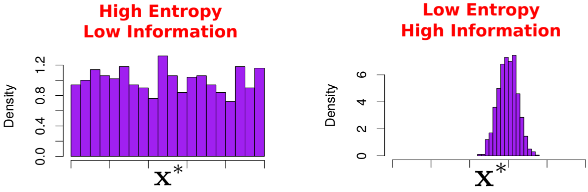

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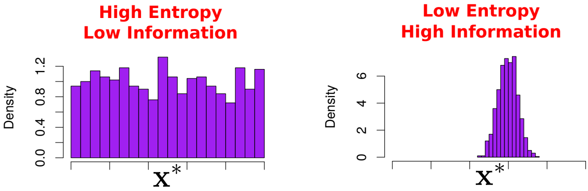

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Computing (1) is **very difficult in practice**!

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Factorized Gaussian approximation with **expectation propagation**. $\mathcal{X}^\star$ dominates any other point in $\mathcal{X}$.

(Minka, 2001)

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Factorized Gaussian approximation with **expectation**
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One acquisition per black-box

$$\alpha(\mathbf{x}) \approx \sum_{c=1}^{C} \log v_c^{PD}(\mathbf{x}) - \frac{1}{M}\sum_{m=1}^{M}\left(\sum_{c=1}^{C} \log v_c^{CPD}(\mathbf{x}|\mathcal{X}^\star_{(m)})\right) + \sum_{k=1}^{K} \log v_k^{PD}(\mathbf{x}) - \frac{1}{M}\sum_{m=1}^{M}\left(\sum_{k=1}^{K} \log v_k^{CPD}(\mathbf{x}|\mathcal{X}^\star_{(m)})\right) = \sum_{i=1}^{C+K} \alpha_i(\mathbf{x})$$

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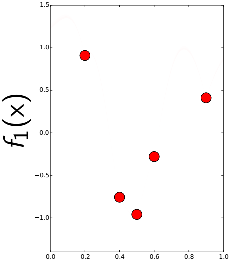
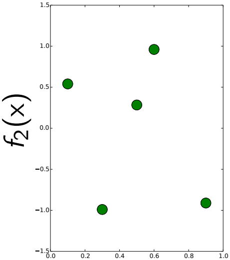
Example of PES' acquisition





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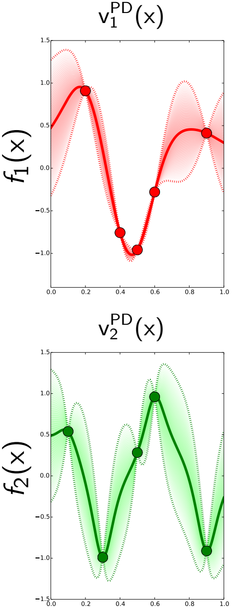

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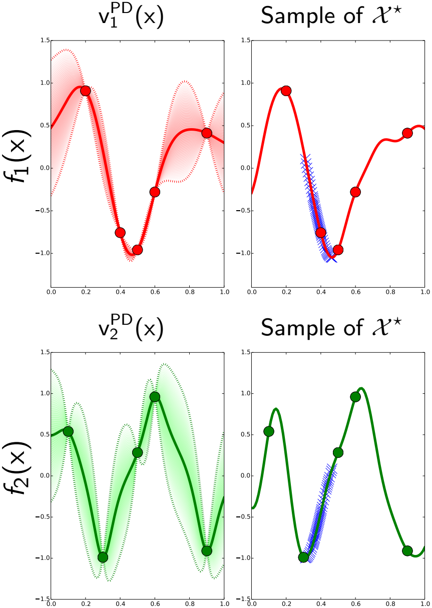

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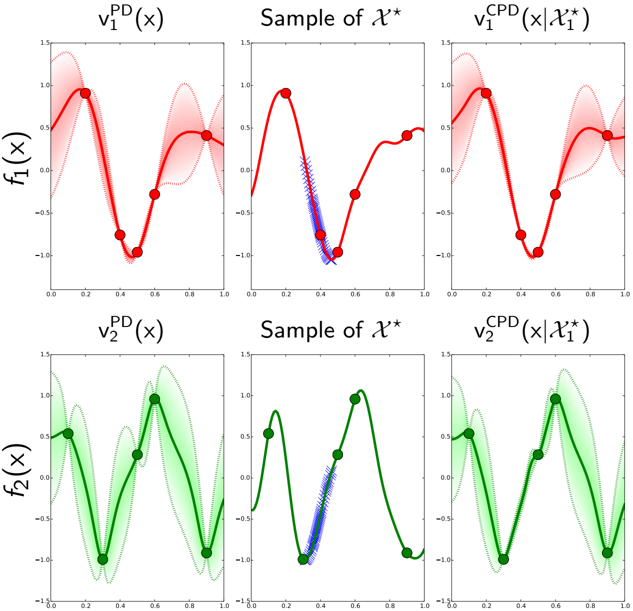

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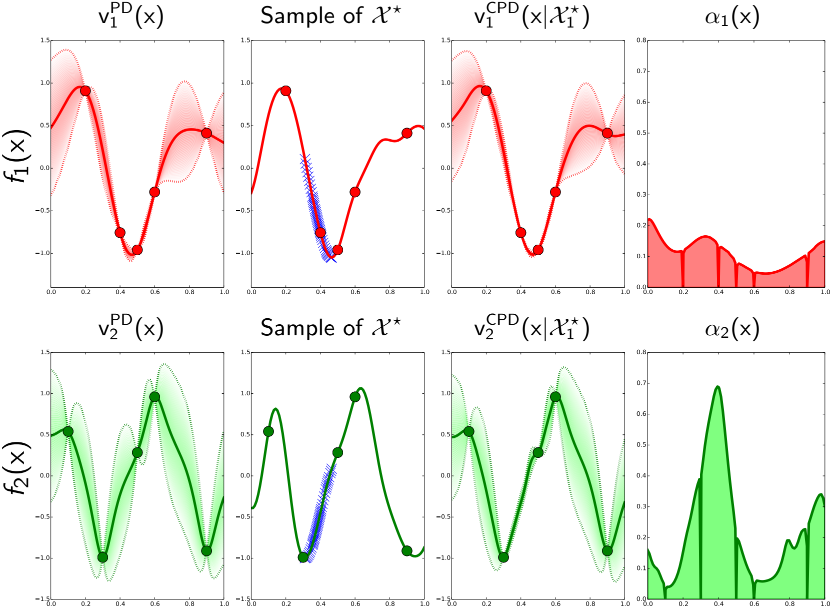

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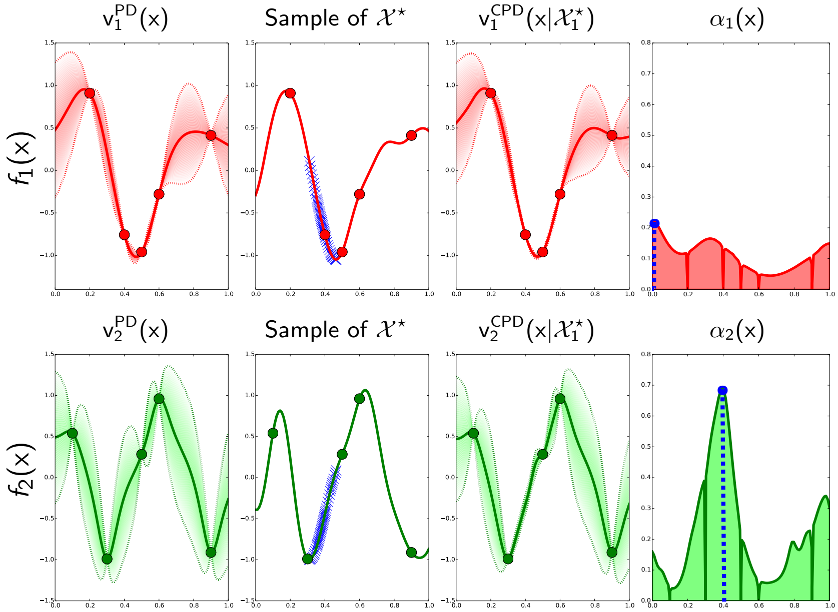
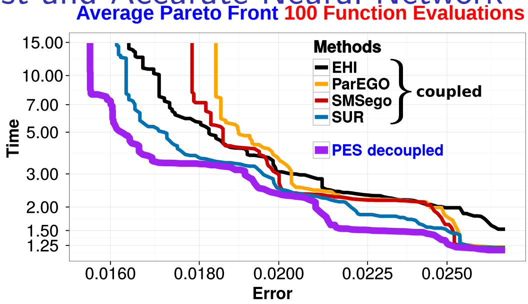


Finding a Fast and Accurate Neural Network



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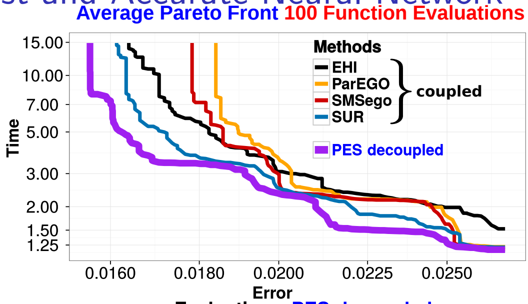

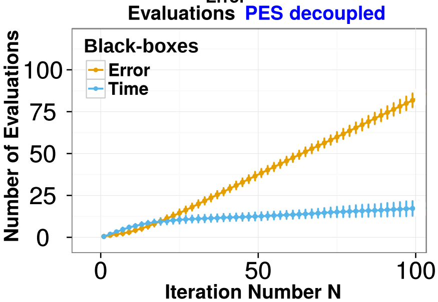

(Hernández-Lobato *et al.*, 2016)

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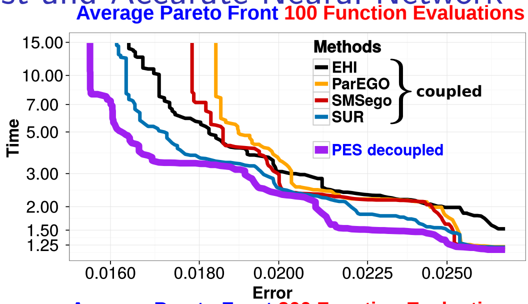

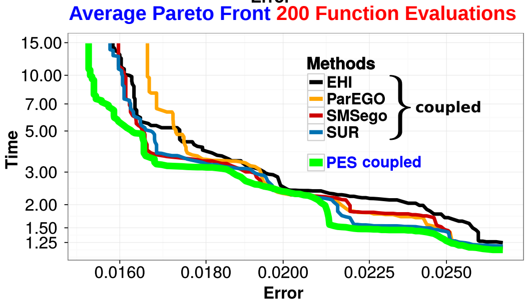

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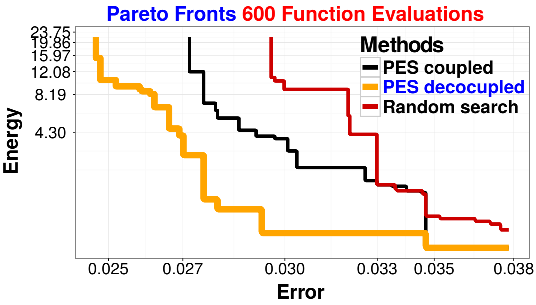
Low energy hardware accelerator



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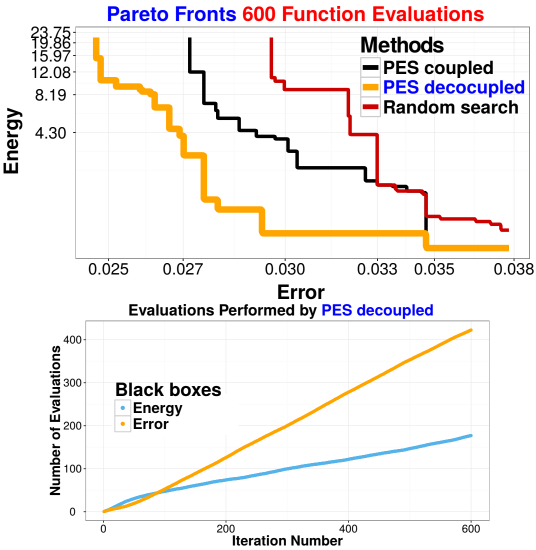

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Parallel Bayesian Optimization

Traditional Bayesian optimization is **sequential**!

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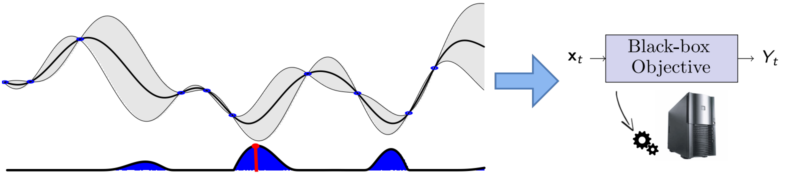

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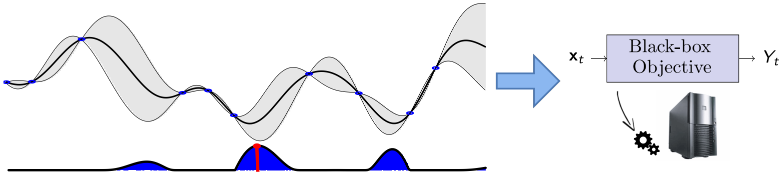

Computing clusters let us do **many things** at once!

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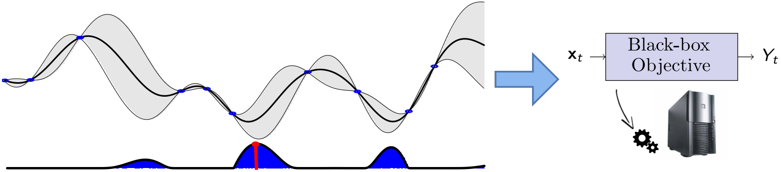

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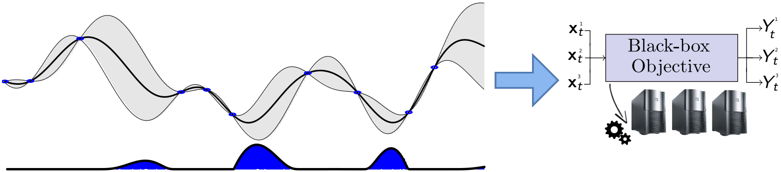

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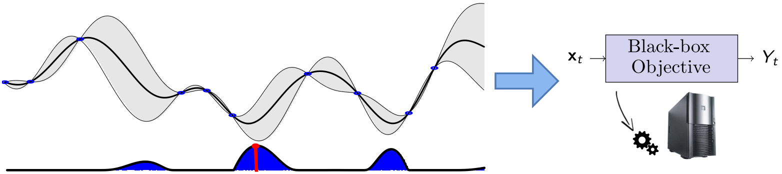

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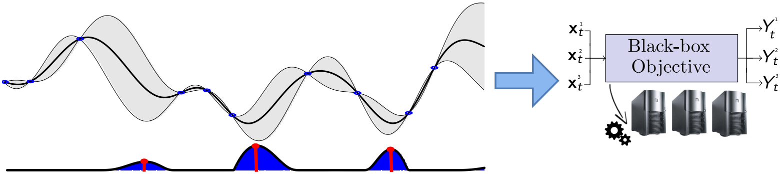

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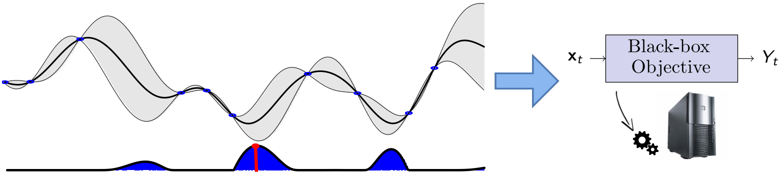

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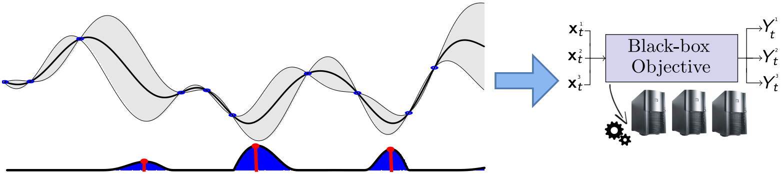

Parallel experiments should be highly informative but different!

Parallel Predictive Entropy Search

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

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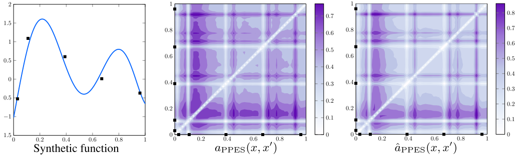
It is possible to compute the gradient of $\alpha(\cdot)$ w.r.t. each $\mathrm{x}_q \in \mathcal{S}_t$!

(Shah and Ghahramani, 2015)

Parallel Predictive Entropy Search: Level Curves



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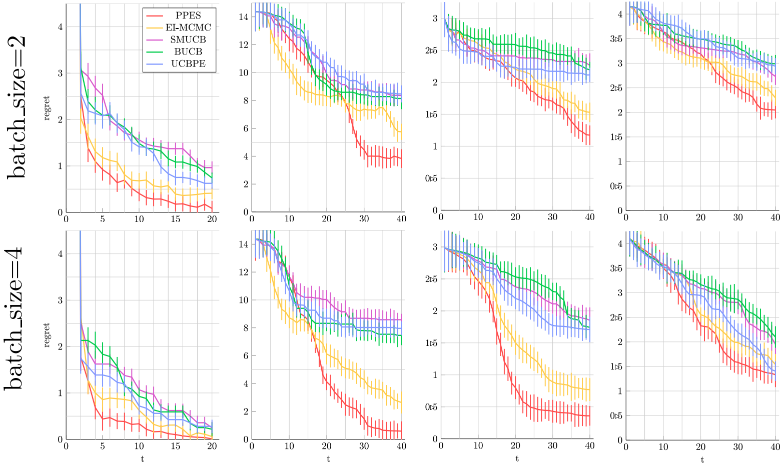
Parallel Predictive Entropy Search: Results



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

(Shah and Ghahramani, 2015)

BO with Integer-valued and Categorical Variables

Standard GPs assume continuous input variables which makes BO with integer-valued or categorical challenging.

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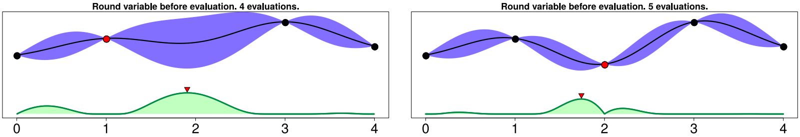

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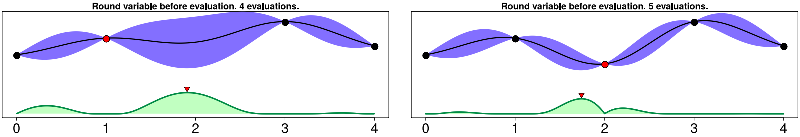
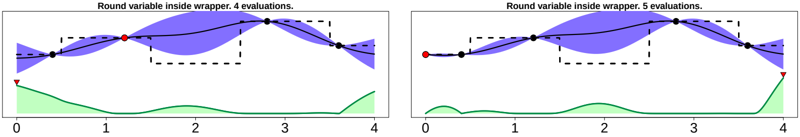


The BO algorithm may get stuck and may always perform the next evaluation at the same input location!

BO with Integer-valued and Categorical Variables

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



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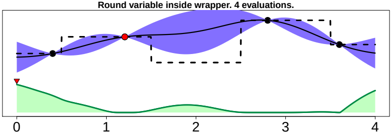

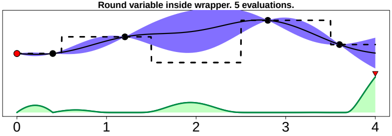

A modified GP covariance function accounts for this:

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

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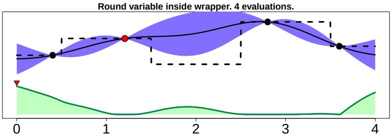

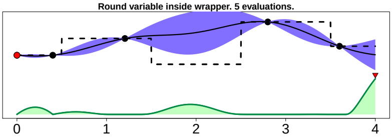

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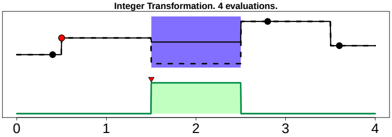

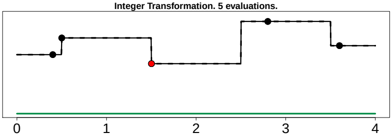

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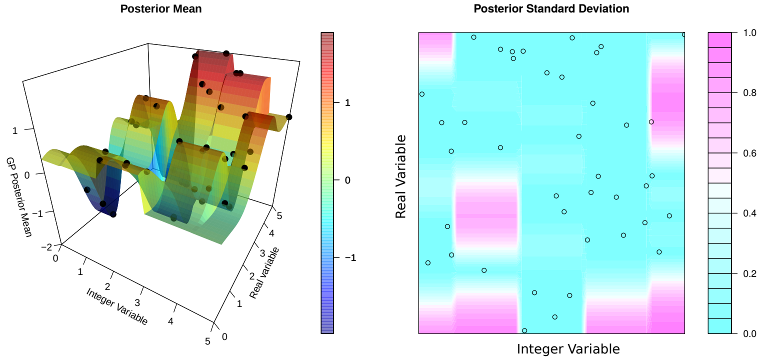

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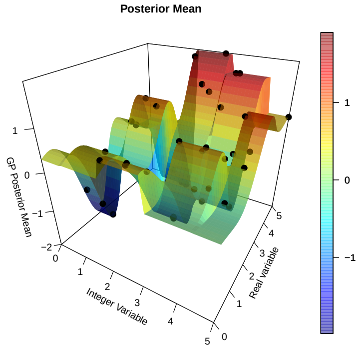
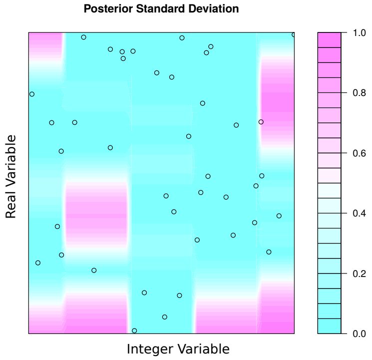
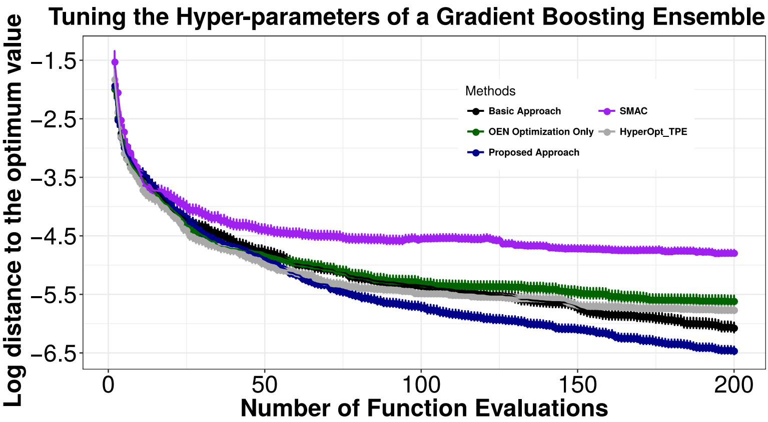




Similar results for categorical variables!

BO with Integer-valued and Categorical Variables



One continuous variable and two integer-valued variables.

Freeze-Thaw Bayesian Optimization

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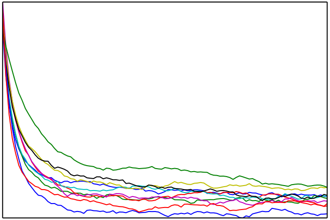

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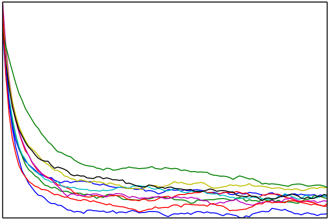

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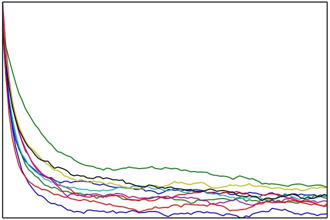

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Yes, that is precisely what Freeze-Thaw BO does!

(Swersky et al., 2014)

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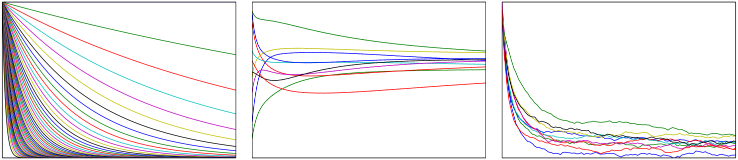

(a) Exponential Decay Basis (b) Samples (c) Training Curve Samples

Inference on Asymptotic Values

A standard GP is used as the prior for the asymptotic values of each training curve.

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$$\mathrm{x}_n \equiv n \text{ configuration}, \quad \mathrm{y}_n \equiv n \text{ observed curve},$$
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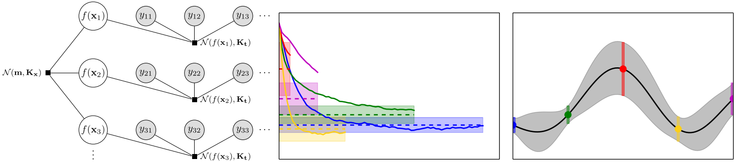
The joint distribution of $\{\mathrm{y}\}_{n=1}^N$ and f is Gaussian and hence so it is the predictive distribution $p(\mathrm{f} | \{\mathrm{y}\}_{n=1}^N)$!

Inference on Asymptotic Values and BO



(a) Graphical Model (b) Training curve predictions (c) Asymptotic GP

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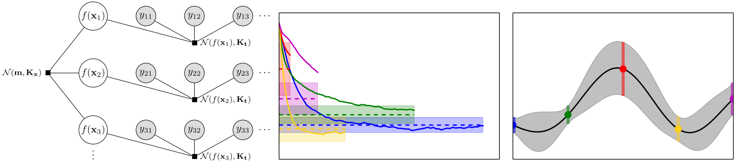

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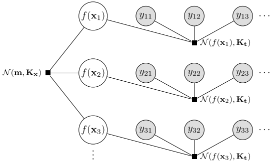

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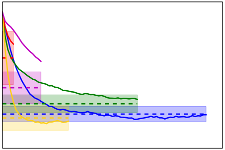

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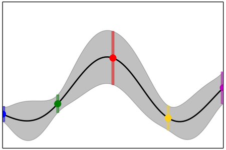

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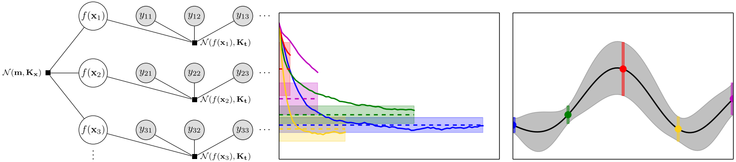

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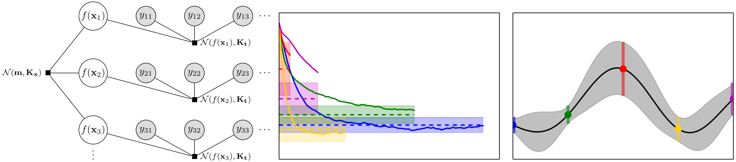

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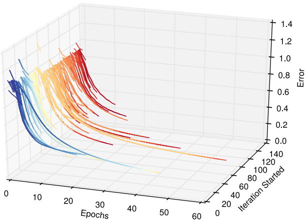
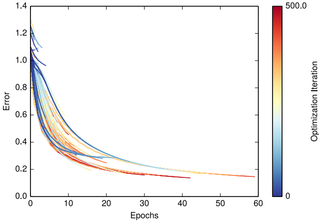
- A combination of EI and ES is used as the acquisition function.

(Swersky et al., 2014)

Freeze-Thaw BO in practice





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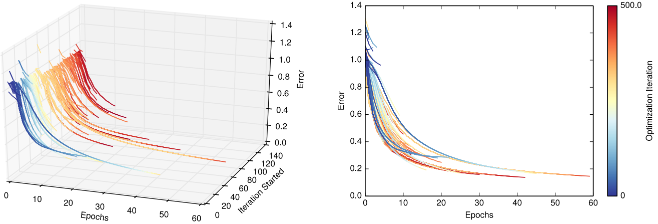
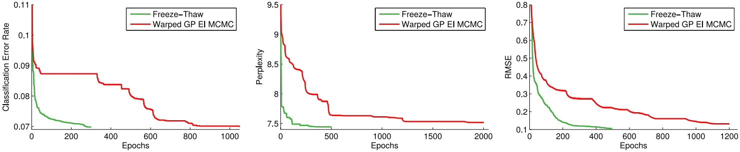
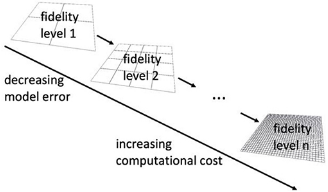


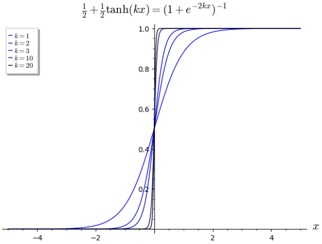


(a) Logistic Regression (b) Online LDA (c) PMF

(Swersky et al., 2014)

Multi-fidelity Bayesian optimization





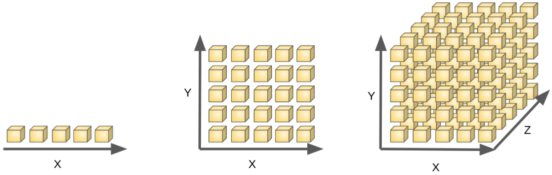
- **Concept of Fidelity:** Fidelity refers to the accuracy or reliability of the information, we use different levels of accuracy.
- **Example:** # layers in NNs, # of timesteps for DRL.
- *We assume that lower fidelities are correlated with higher.*
- **Cost-Efficiency:** Leveraging computationally cheaper versions of the functions to guide the search process.
- **The trick:** The acquisition function should balance exploration at cheaper fidelities with exploitation at the highest fidelity level.

Multi-fidelity Bayesian optimization example

- Trace-aware knowledge-gradient acquisition function.
- It values observations of a point (x) and a set of fidelities ($\mathcal{S}$) according to the ratio of the reduction in expected loss that it induces, to its computational cost.
- It measures the value of information per unit cost of sampling.
- It uses a function $L()$ to measure the extent to which observing trace information improves the quality of the solution. $L(0)$ will be the minimum.
- Its analytical expression basically penalizes the cost wrt the information obtained:

$$takg(x, \mathcal{S}) = \frac{L(0) - L(x, \mathcal{S})}{cost(x, max(\mathcal{S}))}$$

High-dimensional Bayesian optimization



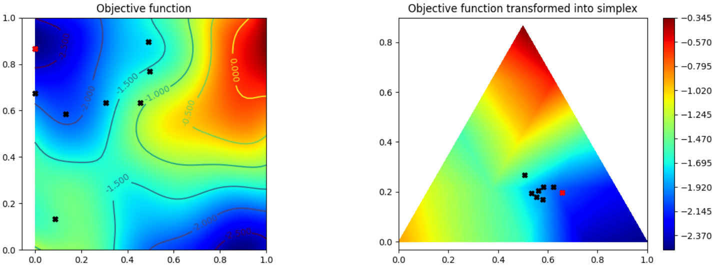
- GPs empirical performance tends to be lower if $d > 7$.
- **The problem:** The search space grows exponentially with the number of dimensions.
- **The trick:** We can project the high-dimensional problem into a lower-dimensional subspace that explains it well using embeddings.
- *Find the hidden most explicative manifold for the data, then optimize there!*
- Approaches differ in the type of embeddings (e.g. random), assumptions about the function (e.g. being a sum of functions), or use of models (Deep GP, GP-LVM.)

High-dimensional Bayesian optimization example

- Sparse Axis-Aligned Subspace Bayesian Optimization (SAASBO)
- **Goal:** Identify sparse subspaces relevant to modeling the unknown objective function.
- **Assumption:** High function variability being captured by axis-aligned blocks of input features.
- **Method:** Use complex GP prior to consider a smaller class of functions.
- **Effect:** Turn most non-explicative dims off,
- **Integration:** Perform hyper-parameter sampling with NUTS and EI.

[kernel variance]	$\sigma_k^2 \sim \mathcal{LN}(0, 10^2)$
[global shrinkage]	$\tau \sim \mathcal{HC}(\alpha)$
[length scales]	$\rho_i \sim \mathcal{HC}(\tau)$
[function values]	$\mathbf{f} \sim \mathcal{N}(\mathbf{0}, K^{\psi}_{\mathbf{XX}})$
[observations]	$\mathbf{y} \sim \mathcal{N}(\mathbf{f}, \sigma^2 \mathbb{1}_N)$

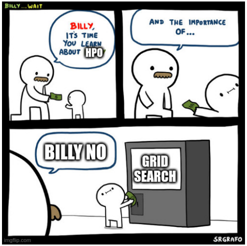
Bayesian optimization in a simplex (Portfolio optimization)



- Common financial metrics as Sharpe or Sortino ratio can be configured for a specific portfolio.
- For example using real-time ESG values of the assets.
- Garrido-Merchán, E. C., Piris, G. G., & Vaca, M. C. (2023). Bayesian optimization of ESG (Environmental Social Governance) financial investments. Environmental Research Communications, 5(5), 055003.

Conclusions and Further Work

- BO is a state-of-the-art class of methods used to optimize expensive and noisy black-box functions.
- We can generalize BO to tackle advanced scenarios: parallel constrained multi-obj, high-dim, multi-fidelity...
- BO can be applied in a wide array of applications: ML, DRL, finance, robotics, materials, business operations...
- Further work topics: causality, meta-BO, transfer learning, adaptation to specific domains.



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Thank you for your attention.