Advanced Methods for Bayesian Optimization in Complex Scenarios Course

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Quantitative Methods Department

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June, 2024.

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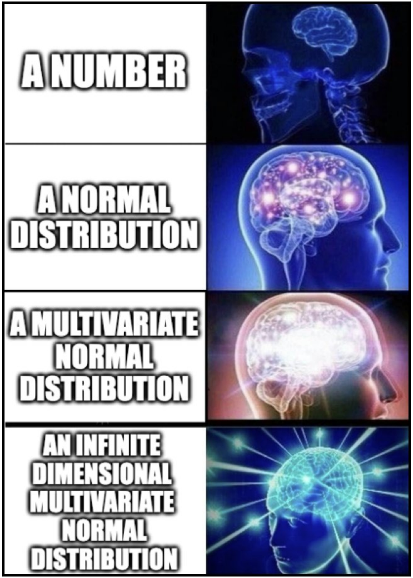
- References.

First Session: Bayesian optimization fundamentals

Introduction.

GPs are great... so now... how can they be used for optimization?



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

Companies face complex scenarios dealing with lots of scenarios!

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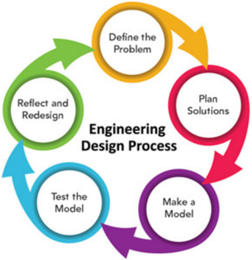

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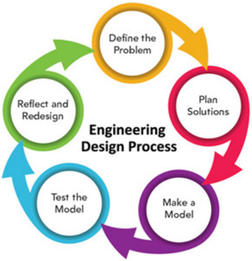

- Many choices at each step.

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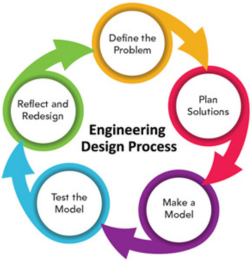

- Many choices at each step.
- Complicated and high dimensional.

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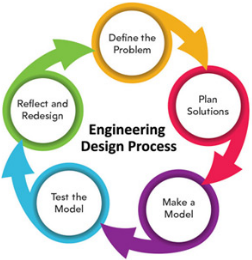

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- Complicated and high dimensional.
- Difficult for individuals to reason about.

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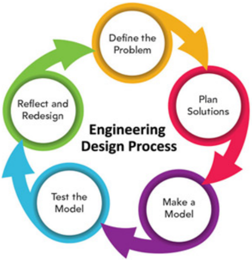

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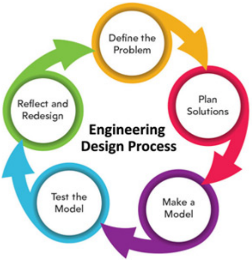

- Many choices at each step.
- Complicated and high dimensional.
- Difficult for individuals to reason about.
- Prone to human bias.
- It may be possible to test various models in parallel.

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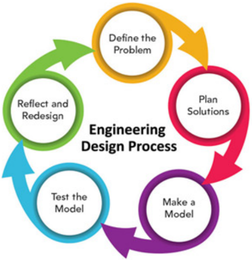

- Many choices at each step.
- Complicated and high dimensional.
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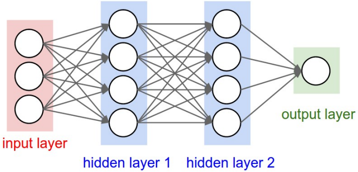
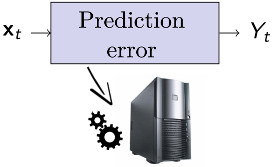
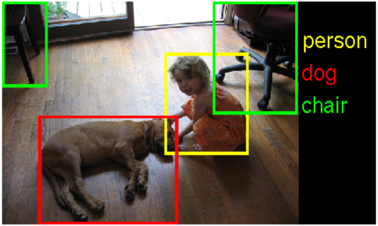
- It may be possible to test various models in parallel.

Optimization is a challenging task in real-life choices!

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







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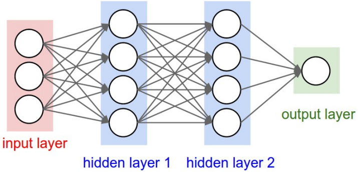

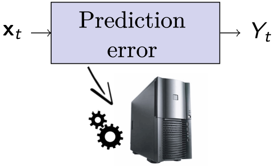

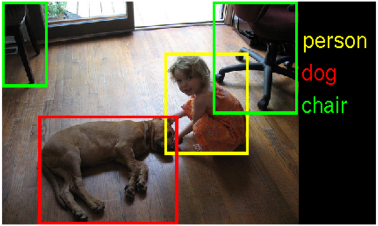

Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc.

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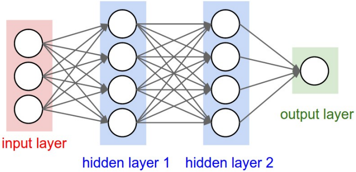
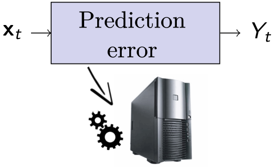
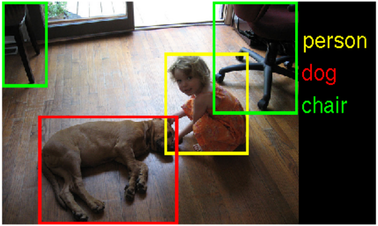
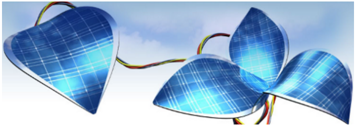


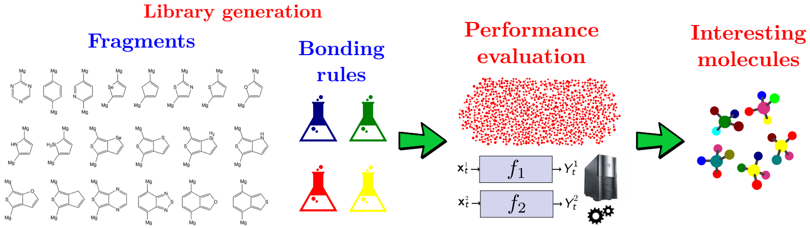




Parameters to tune: Number of neurons, number of layers, learning-rate, level of regularization, momentum, etc. If **multiple processors** were available, we could test **various configurations in parallel**, in order to **gain more information**.

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





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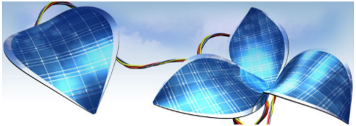
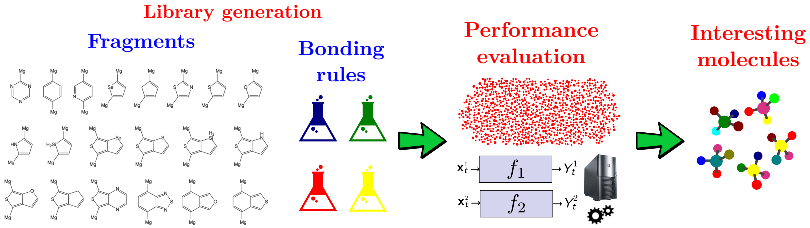
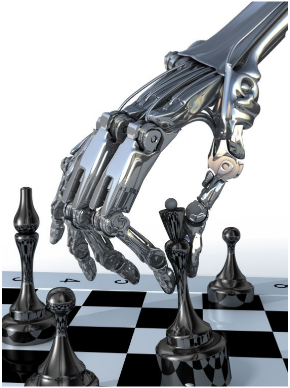




Explore **millions of candidate molecule structures** to identify the compounds with the best properties.

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



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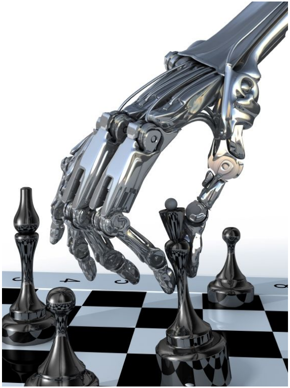
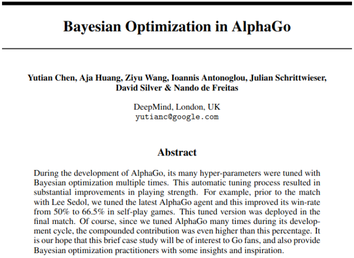


Finger Joint Trajectories

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

Bayesian optimization, the secret sauce of AlphaGo (and Alphazero)



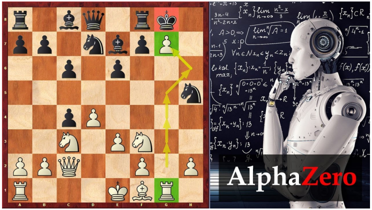
Bayesian Optimization in AlphaGo

Yutian Chen, Aja Huang, Ziyu Wang, Ioannis Antonoglou, Julian Schrittwieser, David Silver & Nando de Freitas

DeepMind, London, UK
yutianc@google.com

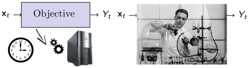
Abstract

During the development of AlphaGo, its many hyper-parameters were tuned with Bayesian optimization multiple times. This automatic tuning process resulted in substantial improvements in playing strength. For example, prior to the match with Lee Sedol, we tuned the latest AlphaGo agent and this improved its win-rate from 50% to 66.5% in self-play games. This tuned version was deployed in the final match. Of course, since we tuned AlphaGo many times during its development cycle, the compounded contribution was even higher than this percentage. It is our hope that this brief case study will be of interest to Go fans, and also provide Bayesian optimization practitioners with some insights and inspiration.



Optimization Problems: Common Features

- Very expensive evaluations.



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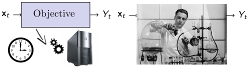
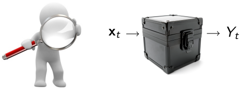


- The objective is a black-box.



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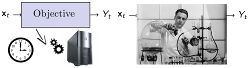

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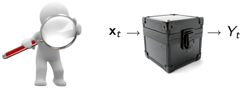
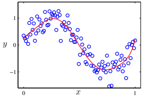


- The evaluation can be noisy.

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



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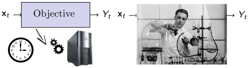

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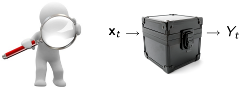

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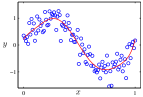
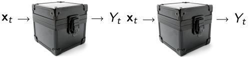


- Evaluations may be done in parallel.



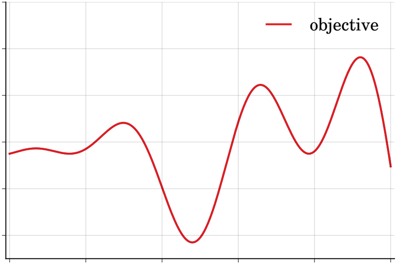
Bayesian optimization methods can be used to solve these problems!

Activity

Think about a real problem that can be solved with Bayesian optimization. 15 mins individual. 10 mins in groups. 3 presentations with slides.

- Which is the function to optimize?
- Does it satisfy the BO assumptions?
- Which are the independent variables that are taken into account?
- Which are the lower and upper bounds in the optimization?
- Is f(X) a sample of a Gaussian process?
- What is the prior mean of the Gaussian process?
- Which kernel would you use?

Bayesian Optimization



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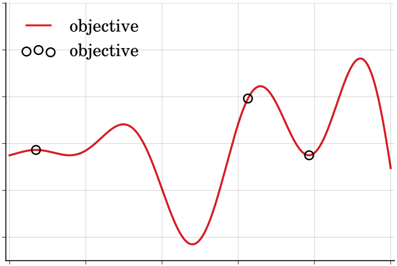
Bayesian Optimization



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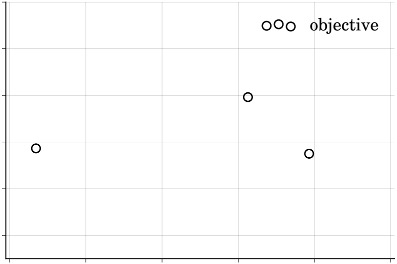

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2. Fit a model to the data:
$$p(y|\mathrm{x}, \mathcal{D}_n)\,.$$

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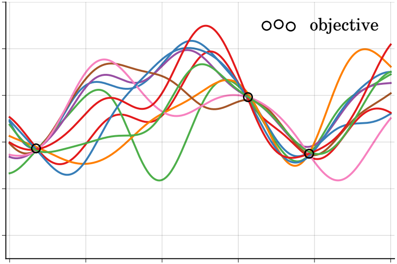

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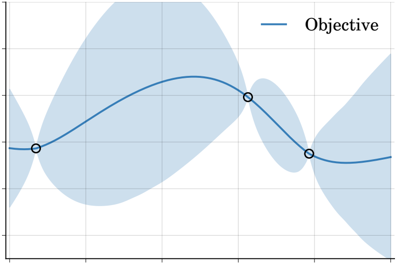

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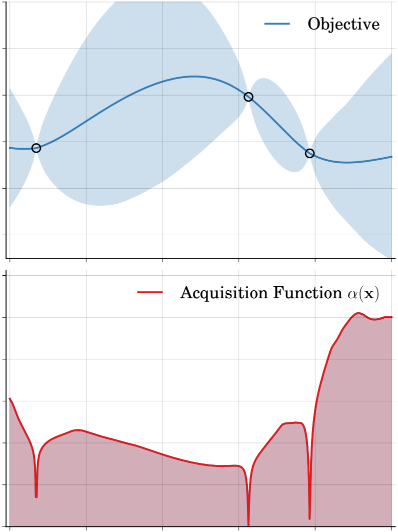

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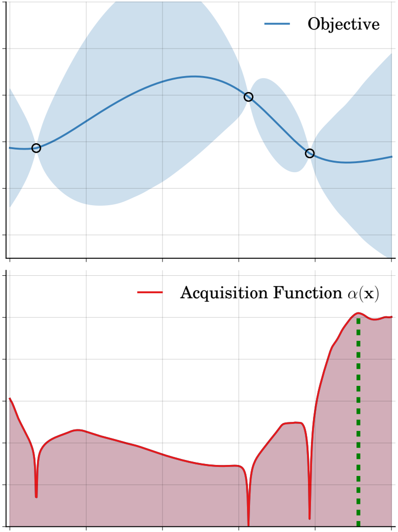

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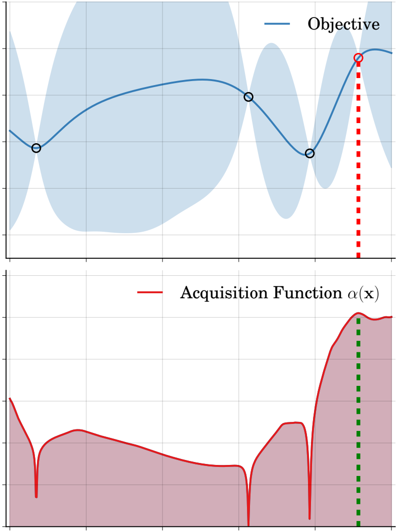

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6. Repeat!

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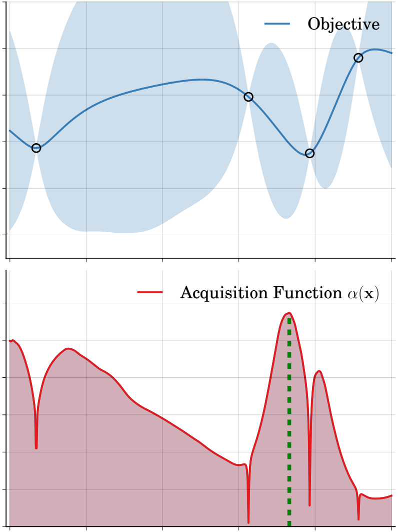

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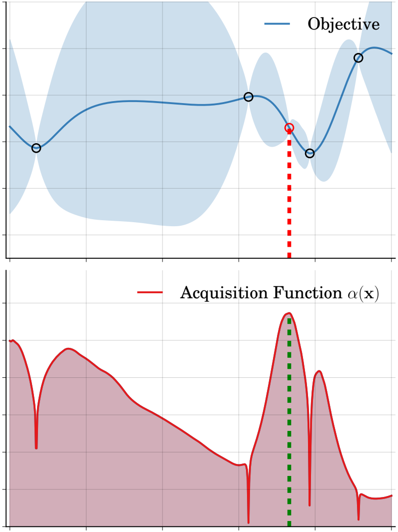

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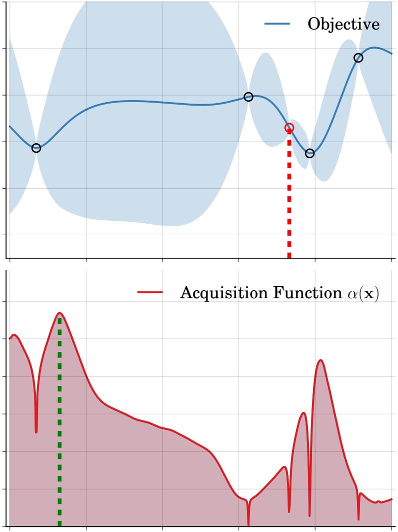

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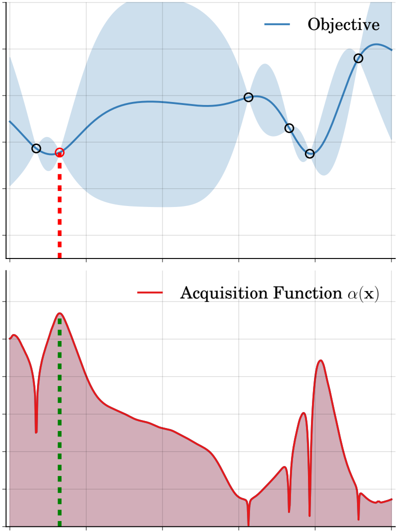

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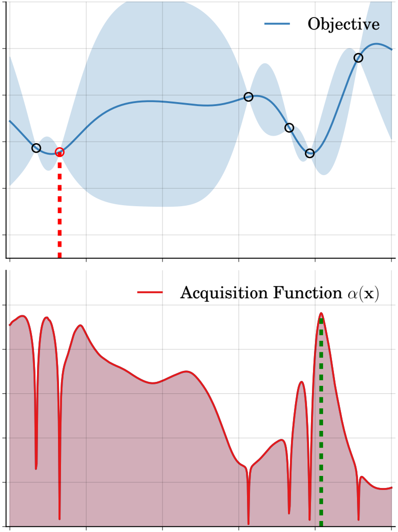

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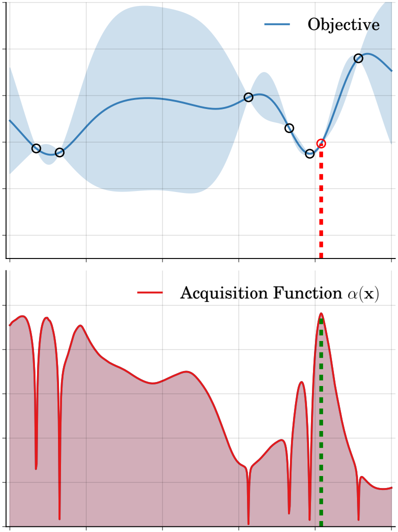

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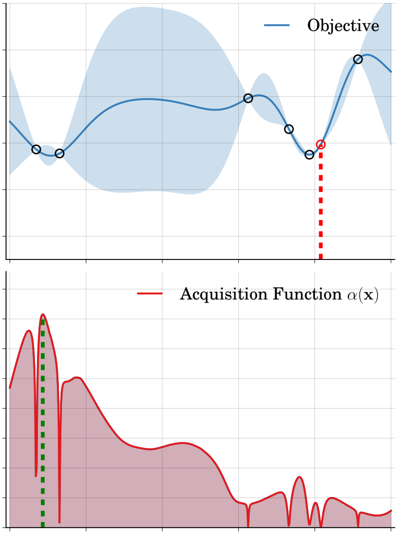

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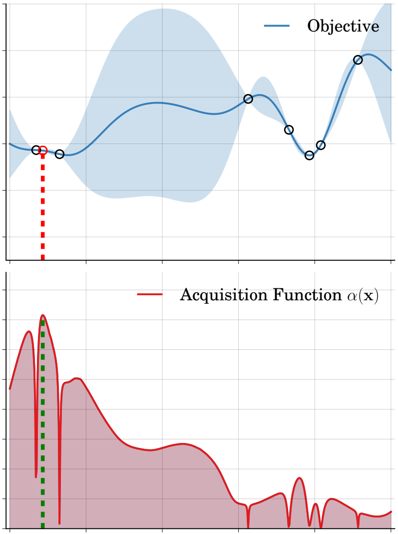

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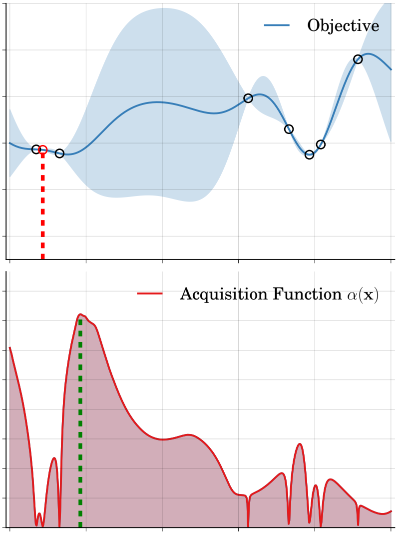

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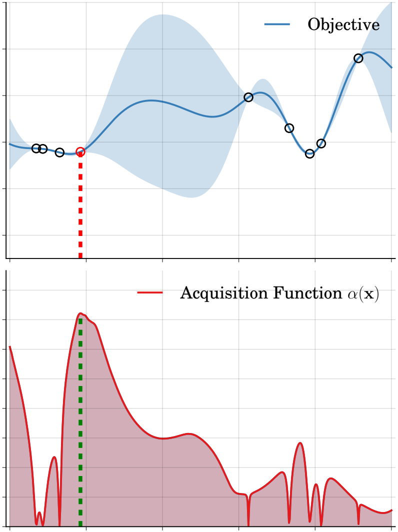

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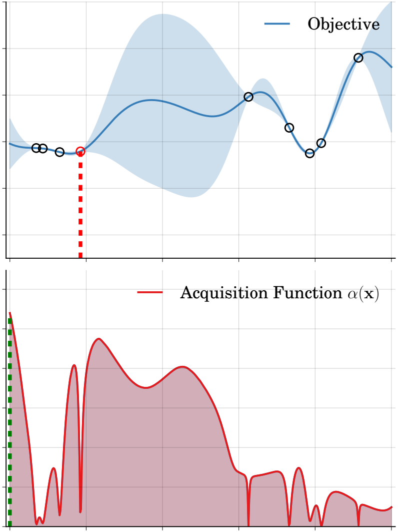

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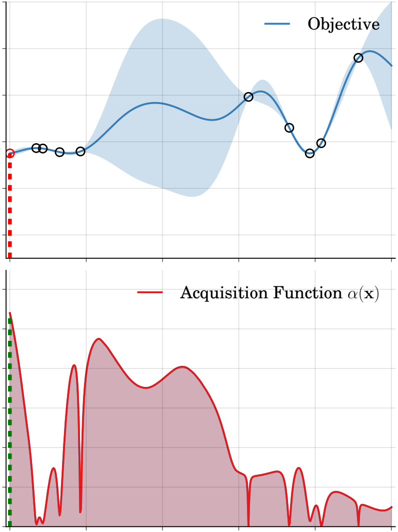

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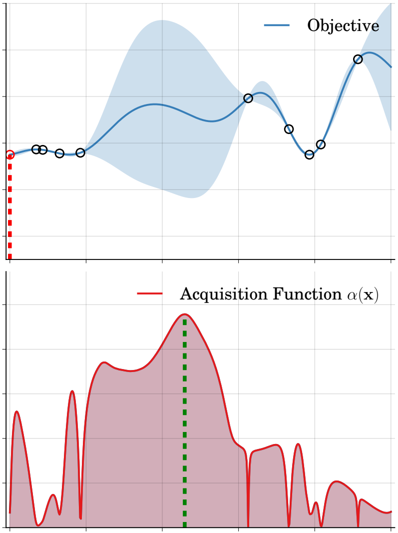

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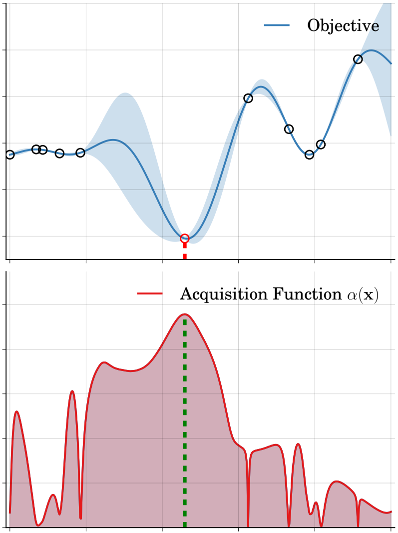

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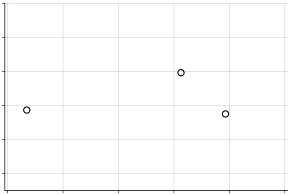

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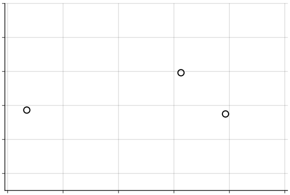

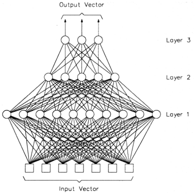

$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

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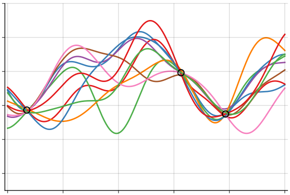

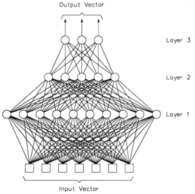

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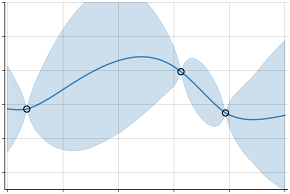

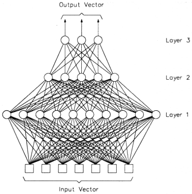

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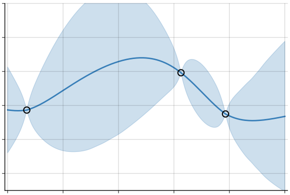

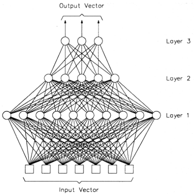

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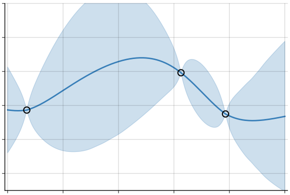

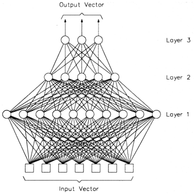

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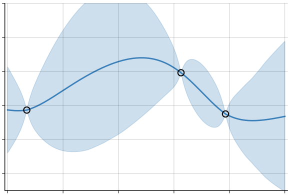

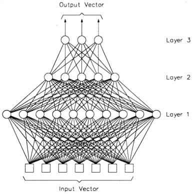

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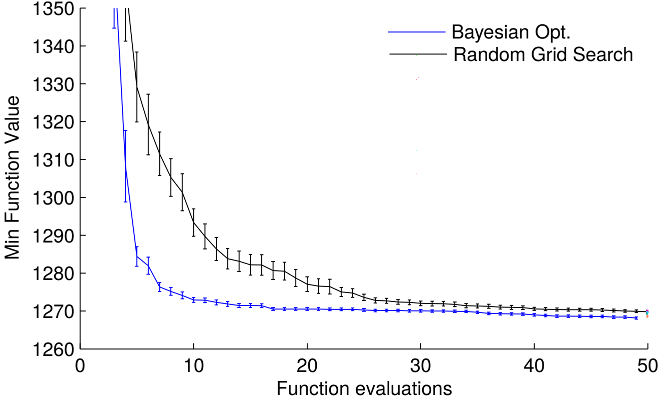
Solved by setting $p(\mathrm{W}) = \prod_{ij} \mathcal{N}(w_{ji}|0, \sigma^2 H^{-1})$ and letting $H \to \infty$!

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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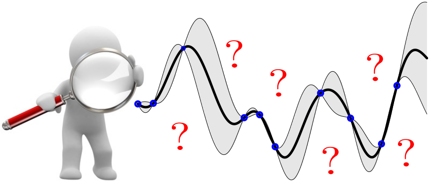

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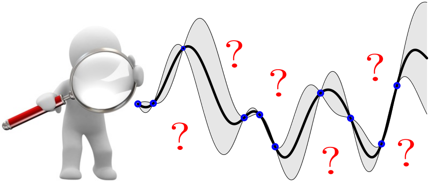

- **Exploration:** seek places with high variance.

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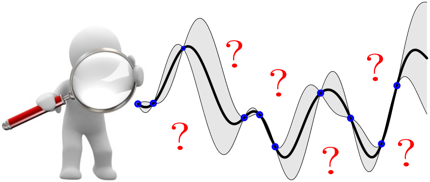

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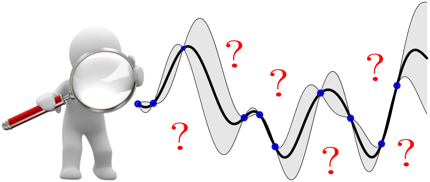

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The acquisition function balances these two, to choose in an intelligent way the next evaluation point!

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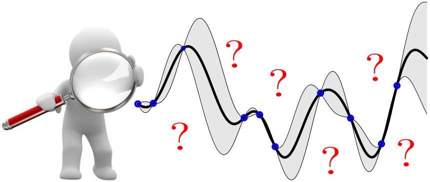

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Let $\nu = \min\{y_1, \ldots, y_N\}$ and $\gamma(\mathsf{x}) = \frac{\nu - \mu(\mathsf{x})}{\sigma(\mathsf{x})}$.

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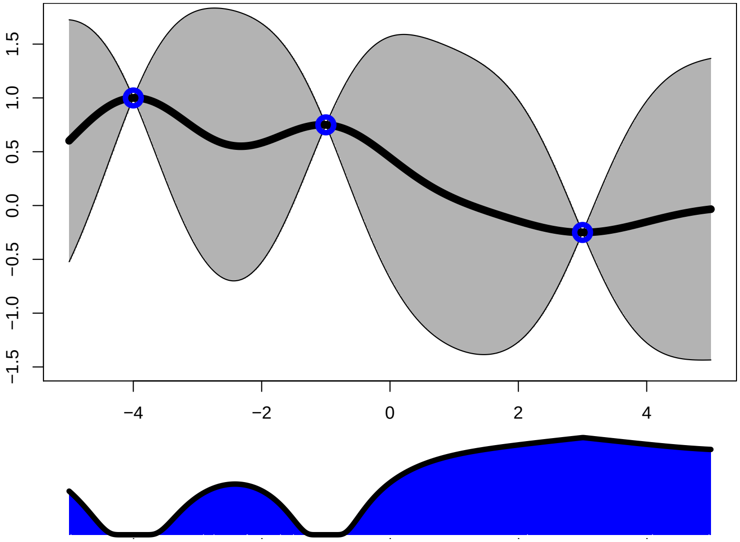
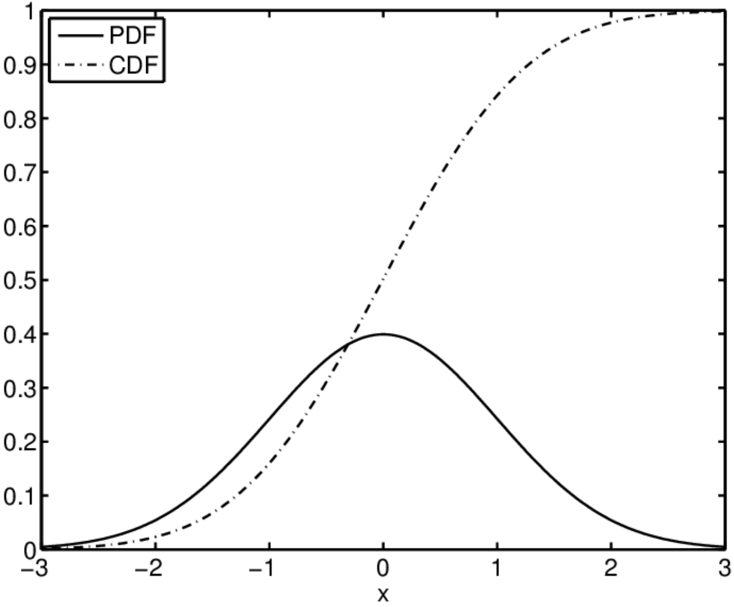
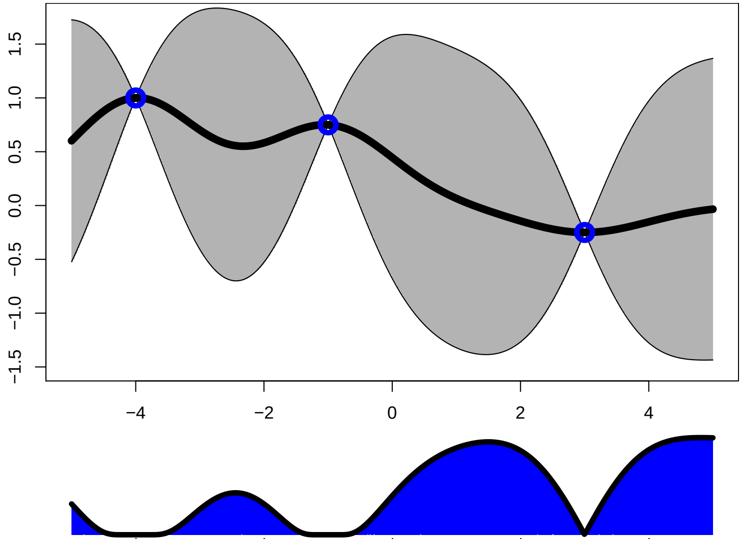
Some Acquisition Functions: Prob. Improvement



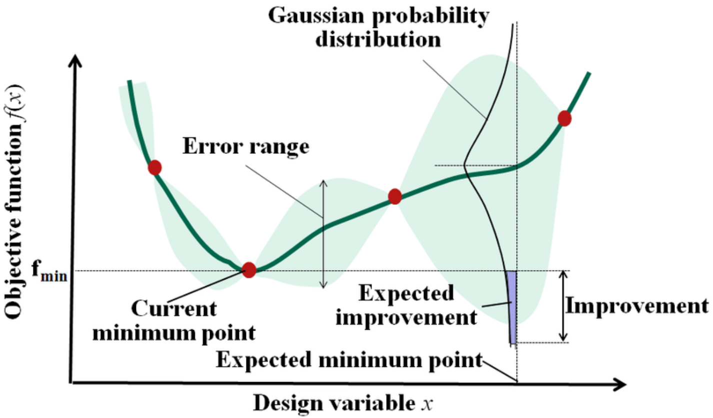
Prob. Improvement: CDF



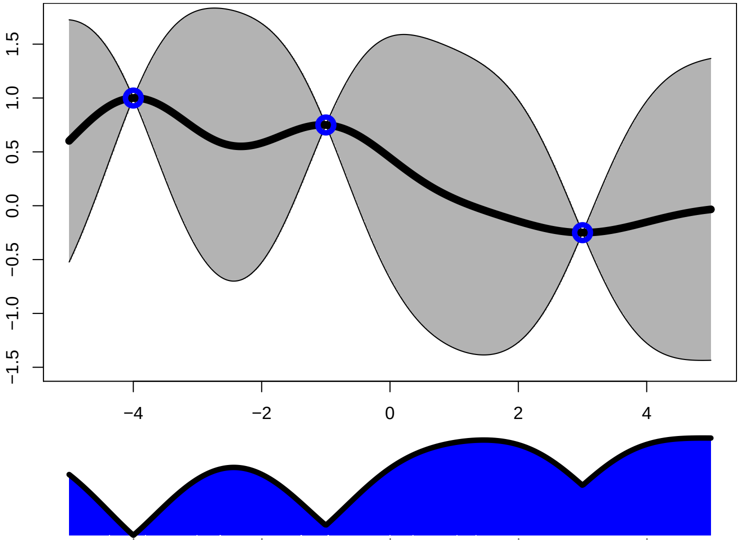
Some Acquisition Functions: Exp. Improvement



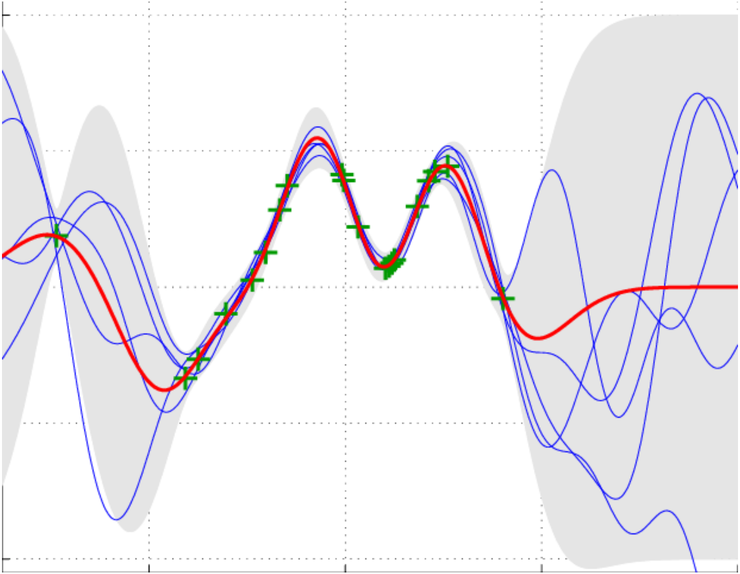
Expected Improvement: intuition



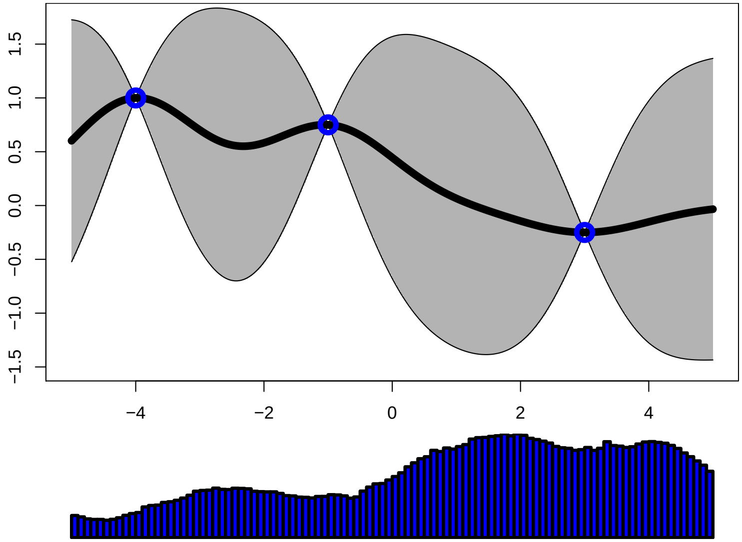
Some Acquisition Functions: Lower Conf. Bound

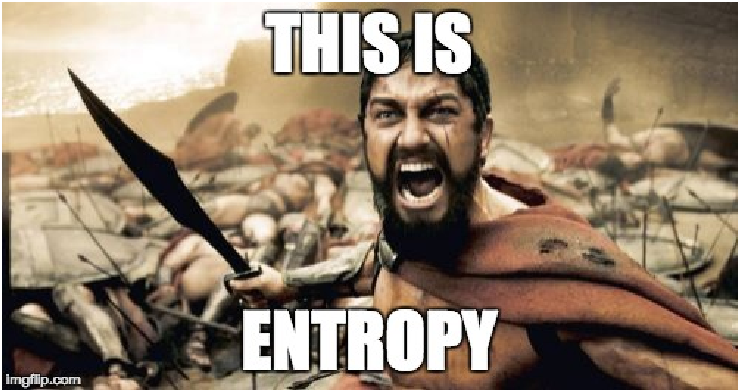


kappa=0. Use only GP samples and optimize to suggest!



Some Acquisition Functions: Entropy Search

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ENTROPY
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Information-based Approach

The minimizer, x^*, can be modelled as a **random variable**!

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

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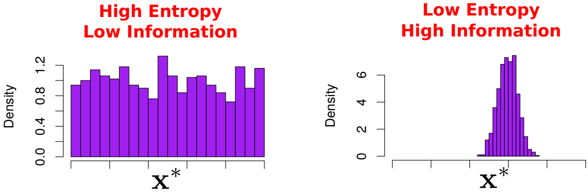

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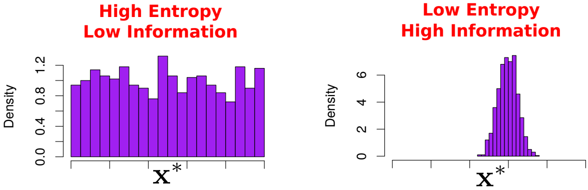

The acquisition function is

$$\alpha(\mathbf{x}) = \mathsf{H}\left[\mathbf{x}^*\middle|\mathcal{D}_t\right] - \mathbb{E}_{\mathbf{y}}\left[\mathsf{H}\left[\mathbf{x}^*\middle|\mathcal{D}_t \cup \{\mathbf{x}, \mathbf{y}\}\right]\middle|\mathcal{D}_t, \mathbf{x}\right] \quad (1)$$

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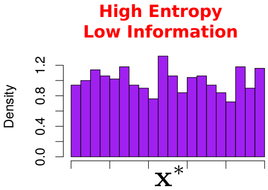

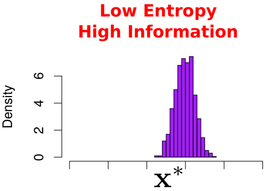

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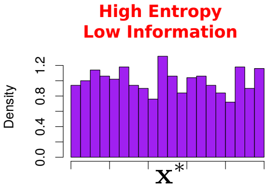

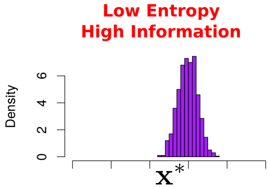

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How much we know about $\mathbf{x}^*$ now.

How much we will know about $\mathbf{x}^*$ after collecting y at $\mathbf{x}$.

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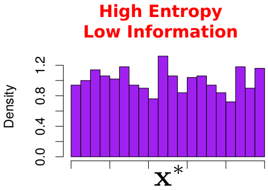
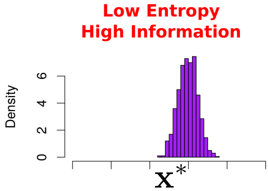
Information is measured by the **entropy** of $p(\mathrm{x}^*|\mathcal{D})$.





The acquisition function is

$$\alpha(\mathbf{x}) = \mathrm{H}\left[\mathbf{x}^* \middle| \mathcal{D}_t\right] - \mathbb{E}_{\mathbf{y}}\left[\mathrm{H}\left[\mathbf{x}^* \middle| \mathcal{D}_t \cup \{\mathbf{x}, \mathbf{y}\}\right] \middle| \mathcal{D}_t, \mathbf{x}\right] \quad (1)$$

How much we know about $\mathbf{x}^*$ now.

How much we will know about $\mathbf{x}^*$ after collecting y at $\mathbf{x}$.

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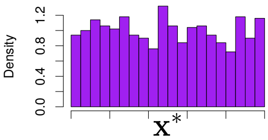

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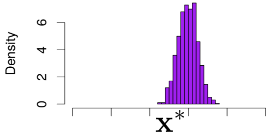

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Computing (1) is **very difficult in practice**!

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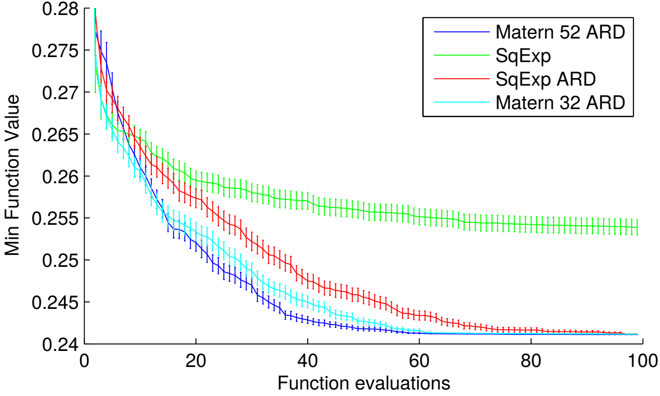

Structured SVM for protein motif finding (Snoek *et al.*, 2012).

Bayesian Optimization and Model Selection

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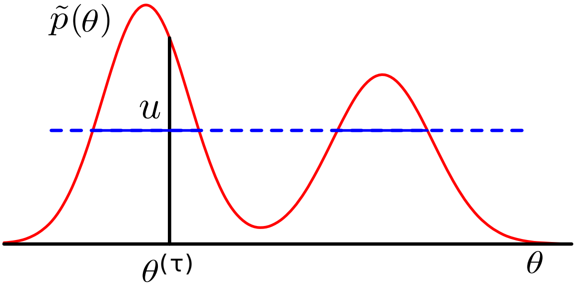

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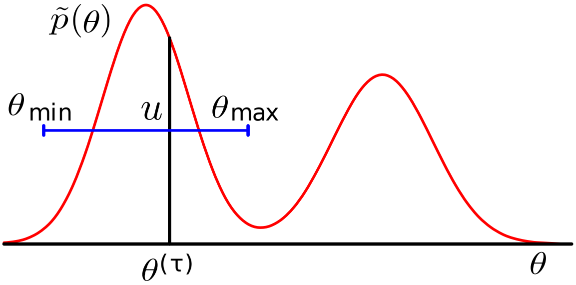

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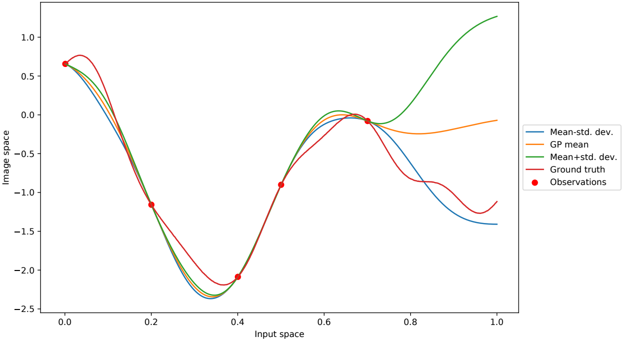
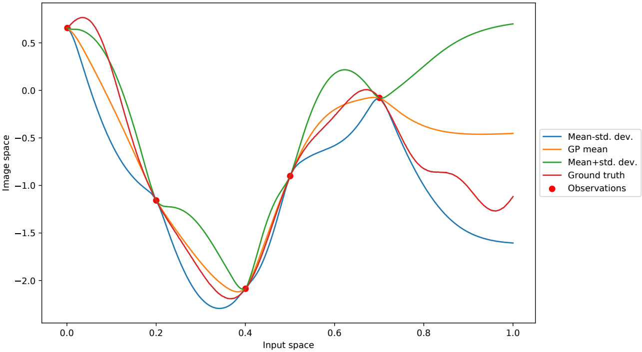
GP fitting an unknown function using Maximum Likelihood



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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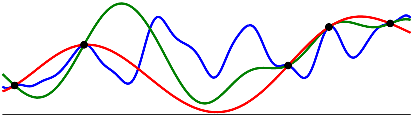
Posterior samples
with three different
length-scales



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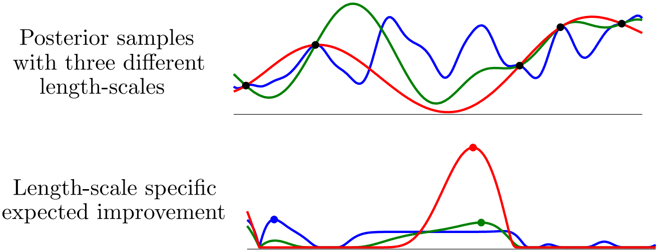

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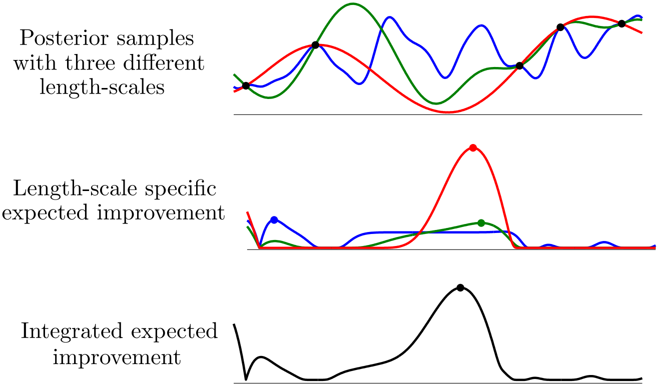

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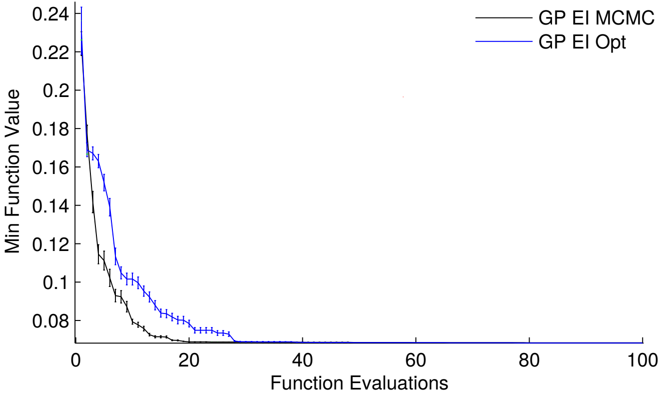
MCMC estimation vs. Maximization



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

Cost-sensitive Bayesian Optimization

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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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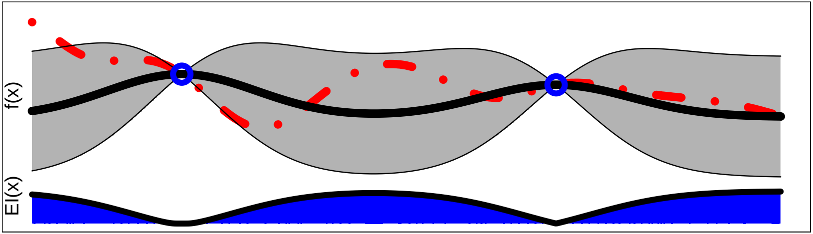

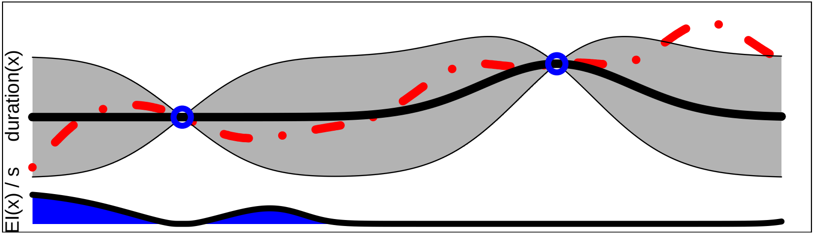

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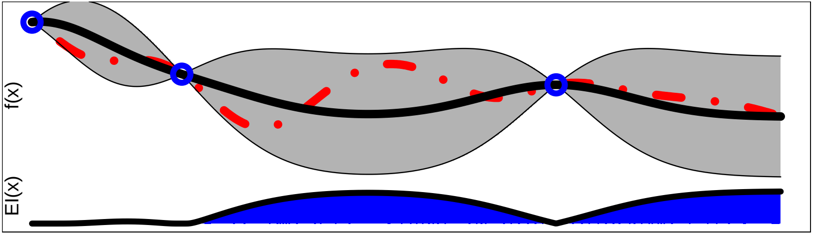

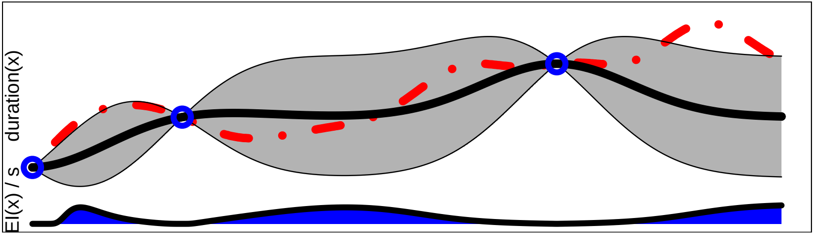

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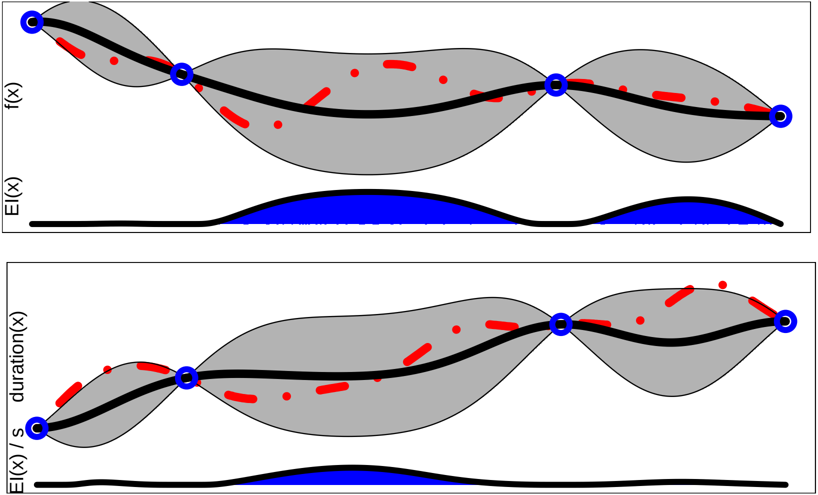

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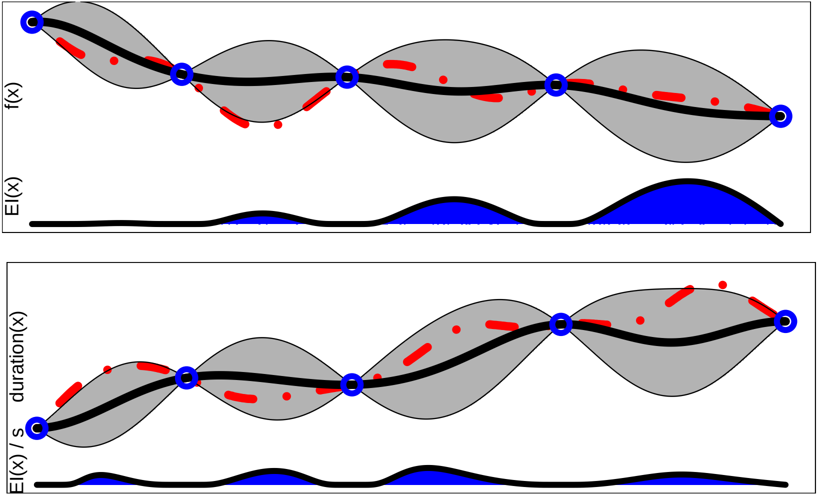

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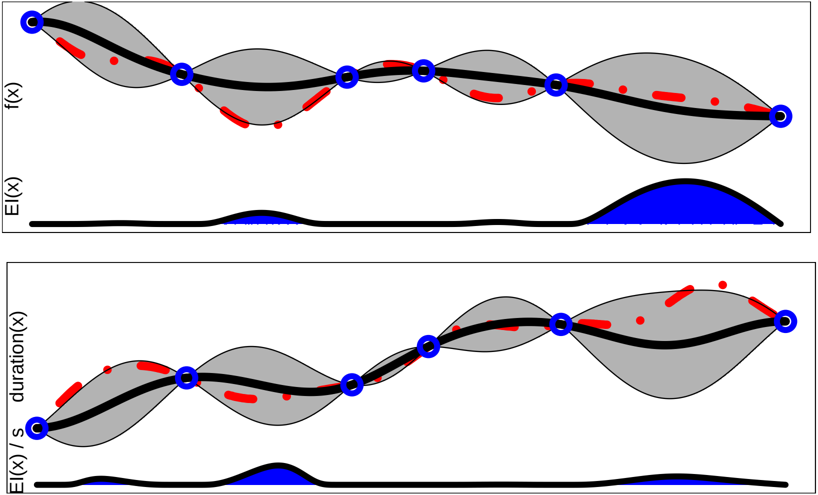

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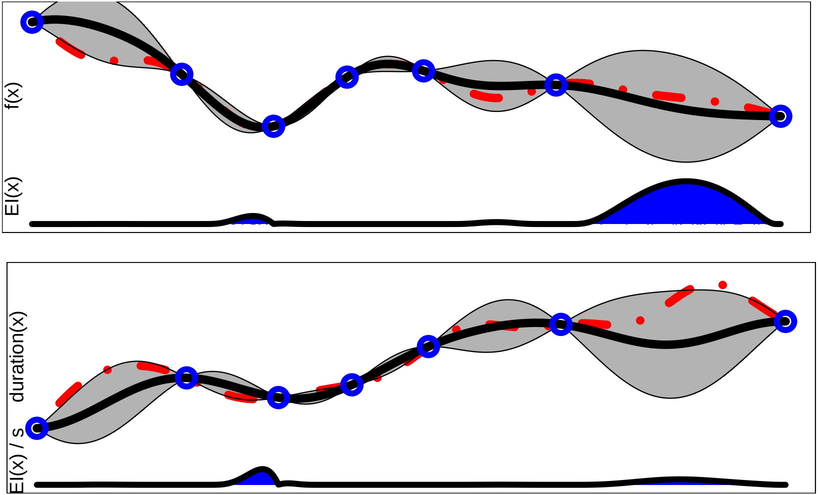

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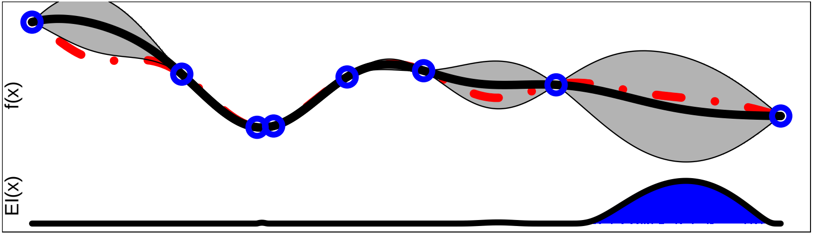

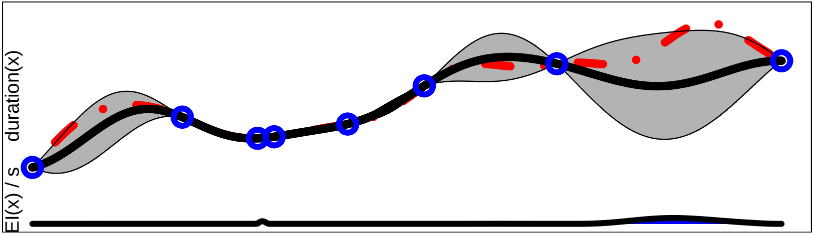

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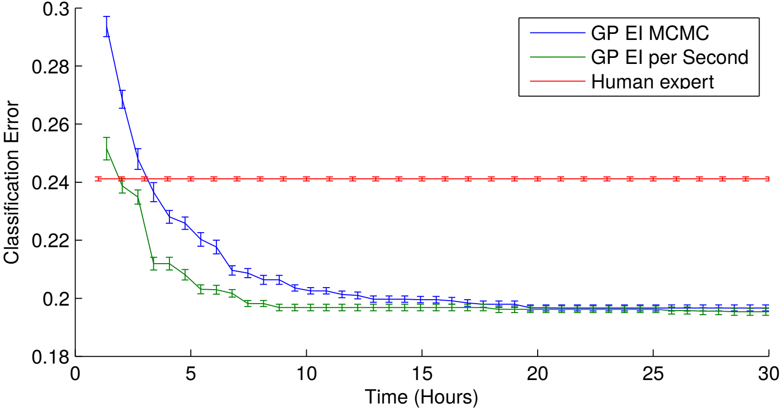

Deep neural network on the CIFAR dataset (Snoek *et al.*, 2012)

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6. **Deep Gaussian Process**: Increased expressivity, advantages of GPs.

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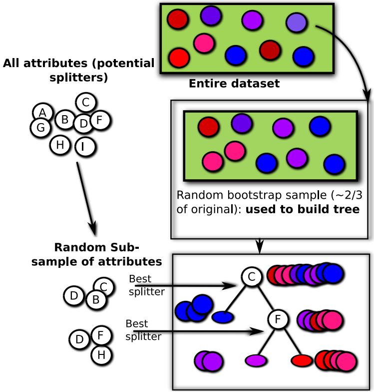

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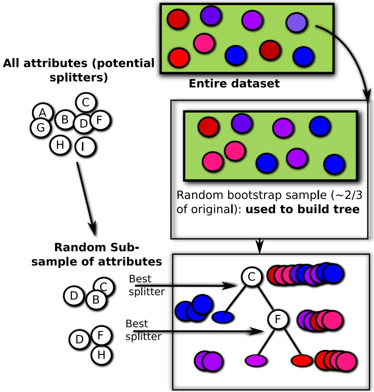

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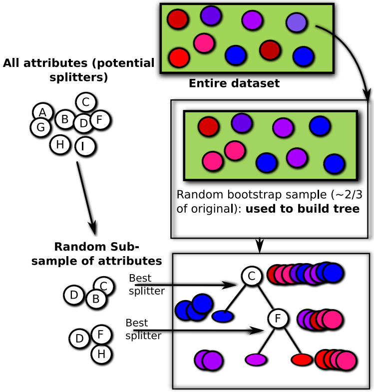

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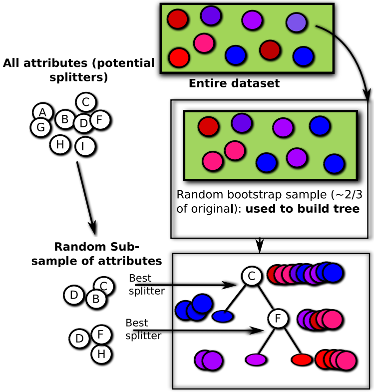

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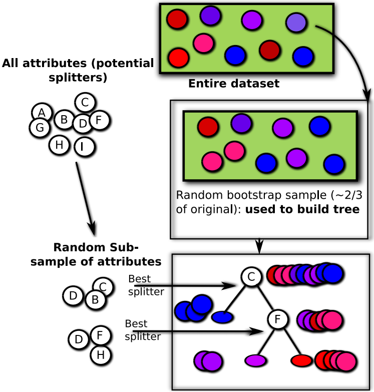

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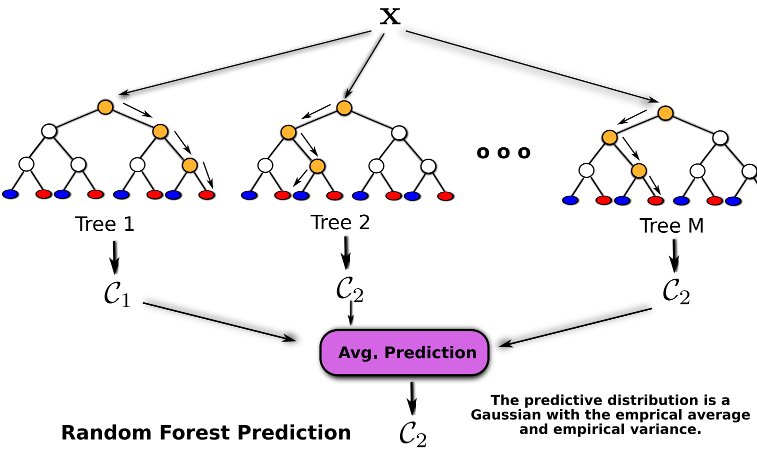
Very cheap to compute and massively paralelizable!

Random Forest: Predictive Distribution



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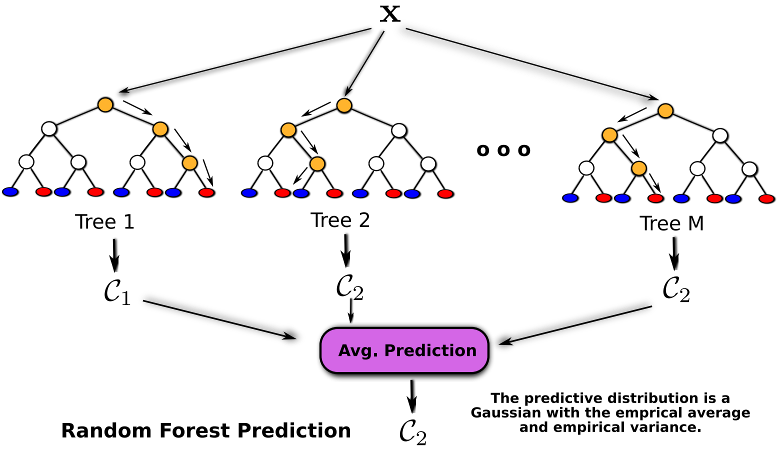
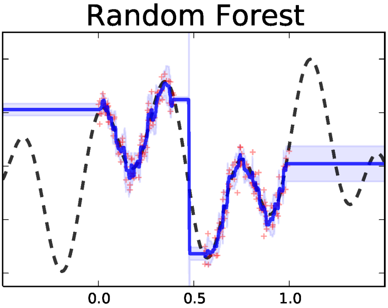


$$p(f^\star|\mathcal{D}_n) = \mathcal{N}(f^\star|\overline{\mu}, \overline{\nu}^2)$$

(Hutter et al., 2011)

Random Forest in Practice



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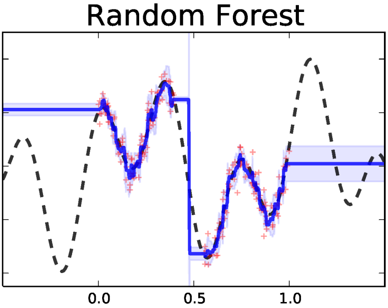

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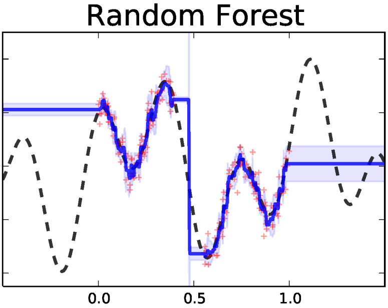

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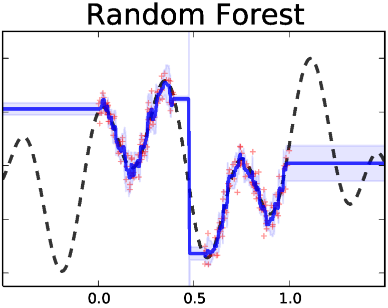

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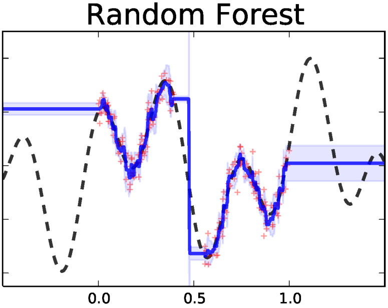

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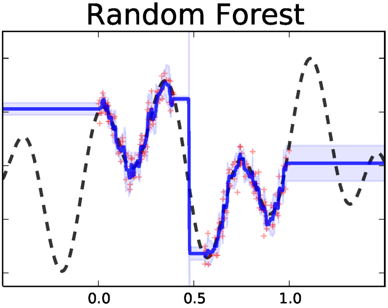

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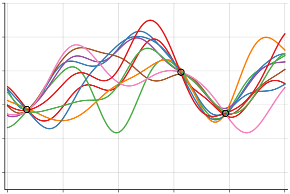

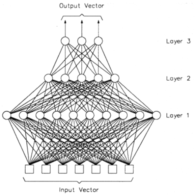

$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

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

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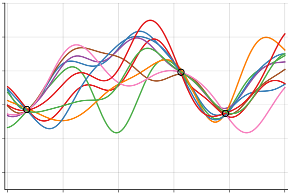

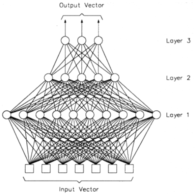

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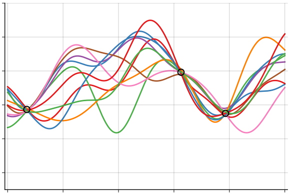

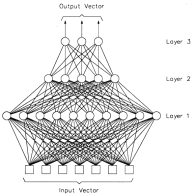

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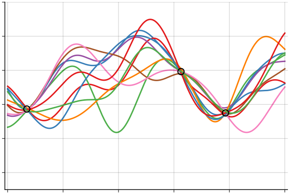

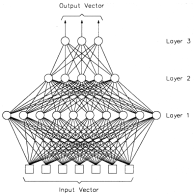

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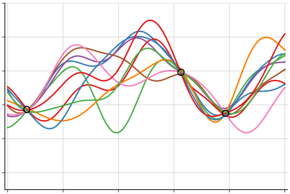

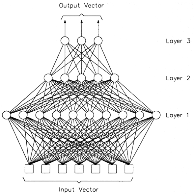

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The posterior distribution of the networks weights W **is intractable!**

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

Activity: Bayesian optimization of a ML algorithm

Use a generative AI to generate a BO code of a ML hyperparameter problem.

- Try to execute the code in your machine and fix it.
- Try to interpret everything.
- Tune it and improve the quality of the error estimator.
- Try to improve it with additional acquisition functions.
- Try to obtain the best score in the titanic problem with BO-ML!

Software for Bayesian Optimization

Many of the methods described are implemented into **BOTorch** using Python.
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Other tools: SMAC3 (Python-RFs), GPyOpt (Python3), Spearmint (Python2.7-sampling), mlrMBO (R).

Time to practice!

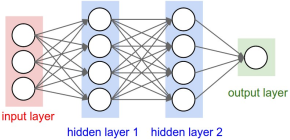
1. Bayesian optimization of a benchmark optimization function.
2. Bayesian optimization of the hyper-parameters of a machine learning model.
3. Bayesian optimization of the hyper-paramaters of a deep reinforcement learning algorithm.

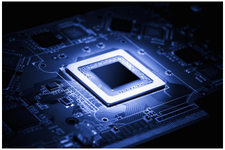
Second Session: Advanced Bayesian optimization.

(Parallel) Multi-objective Bayesian optimization with constraints.

Several Objectives and Constraints

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





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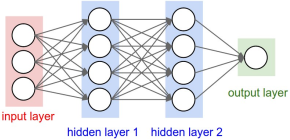

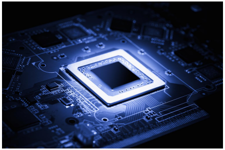

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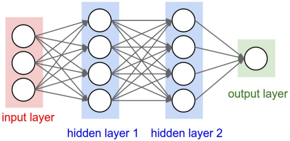

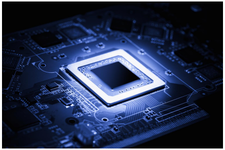

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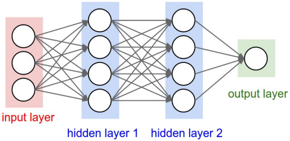

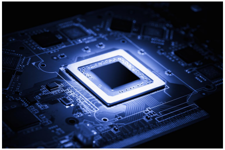

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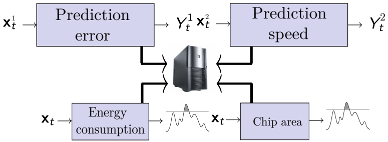

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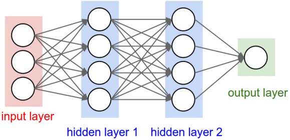

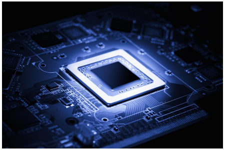

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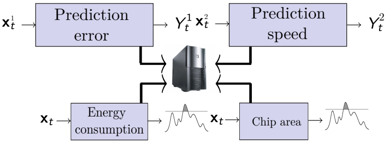
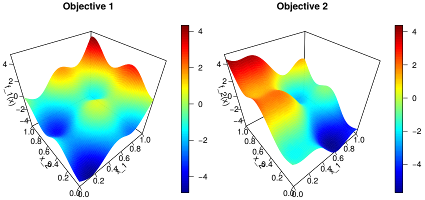


Challenges:

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

Constrained Multi-Objective Optimization



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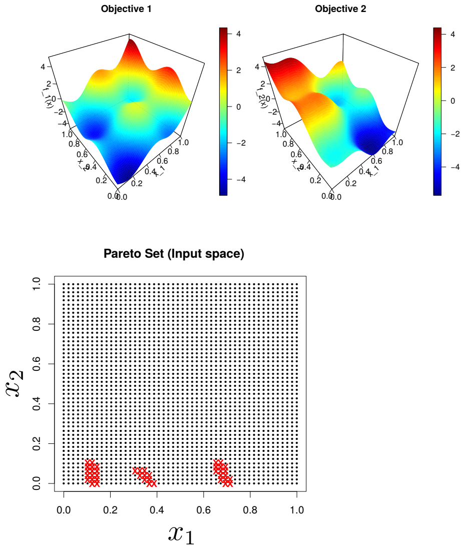

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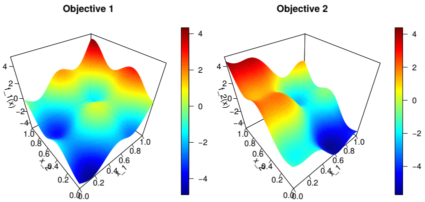

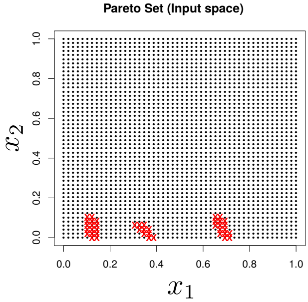

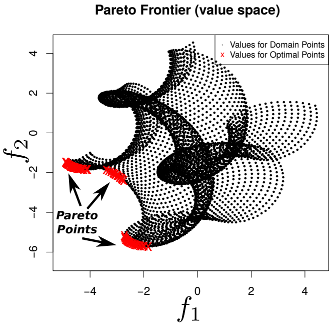

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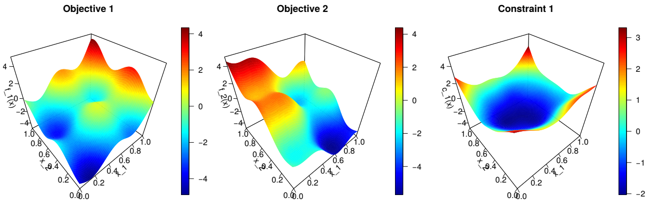

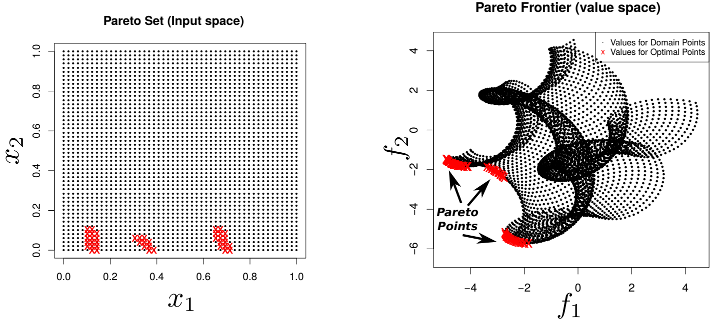

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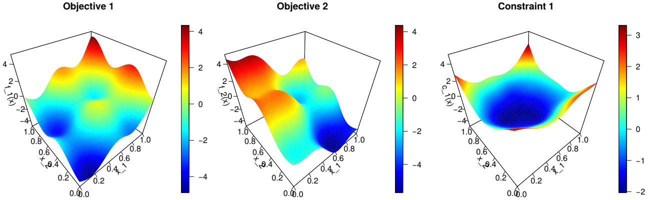

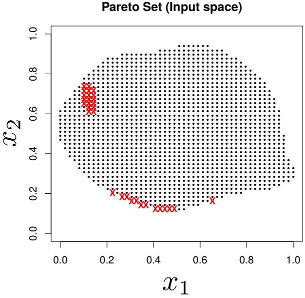

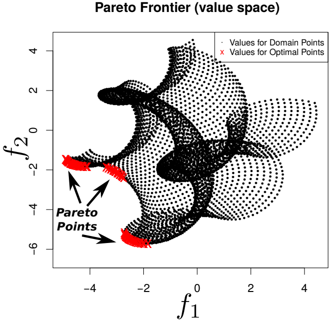

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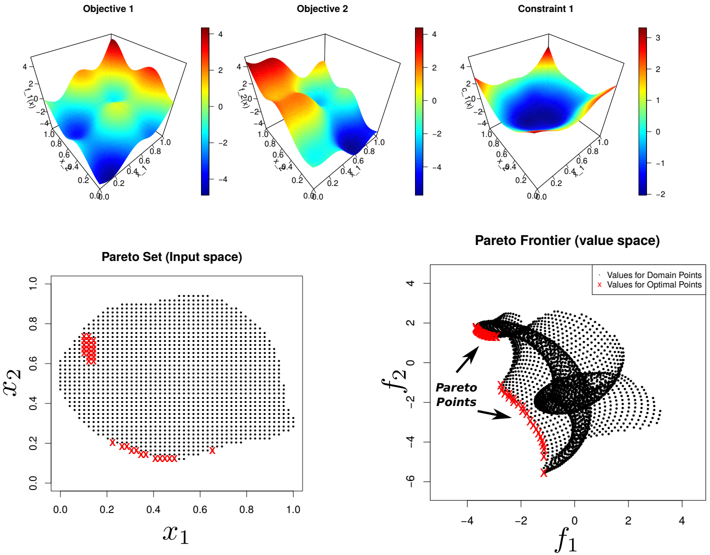

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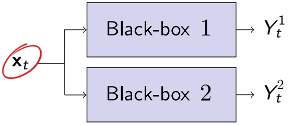

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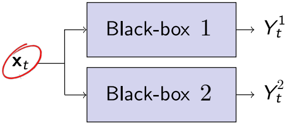

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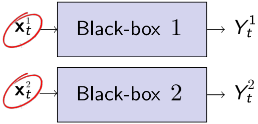

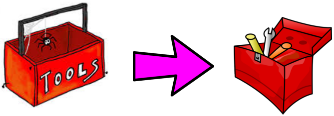

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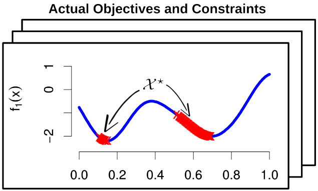

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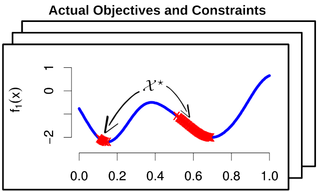

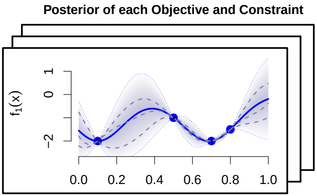

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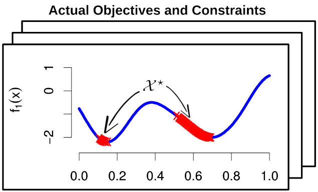

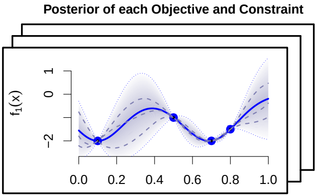

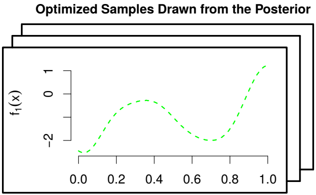

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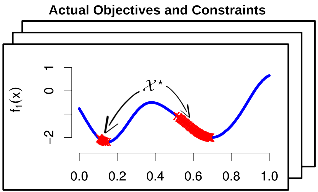

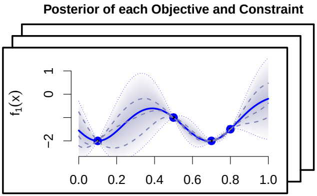

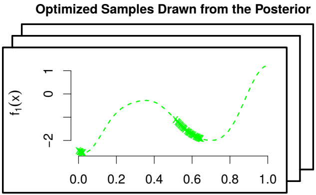

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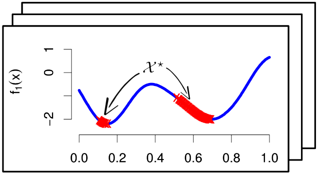
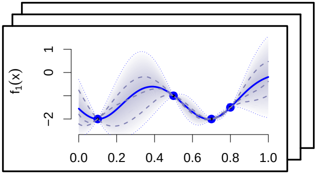
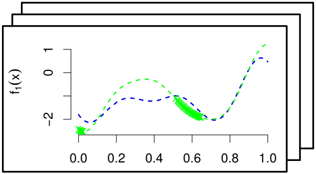


Posterior of each Objective and Constraint



Optimized Samples Drawn from the Posterior



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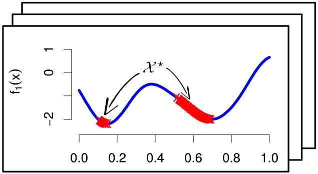

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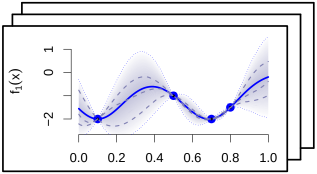

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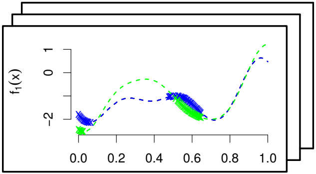

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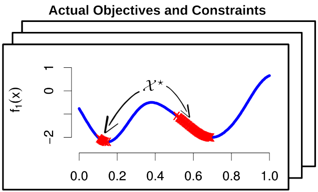

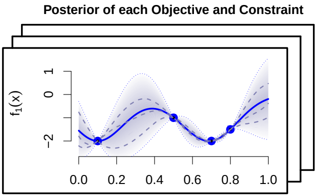

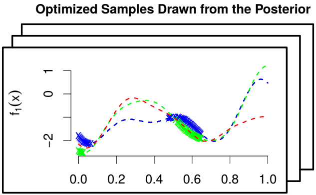

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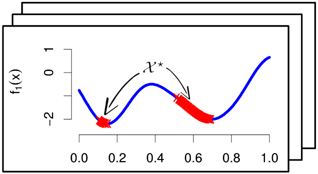

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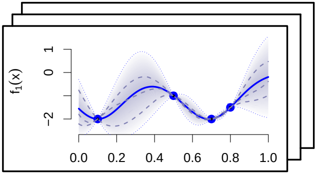
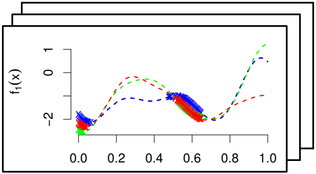


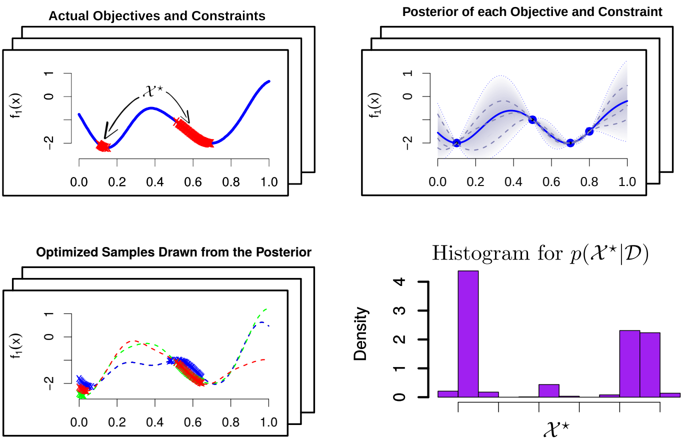
Optimized Samples Drawn from the Posterior



Information-based Approach

The Pareto set $\mathcal{X}^\star$ in the feasible space is a **random variable**!

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



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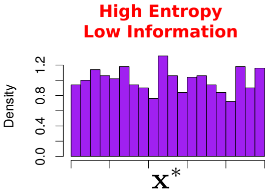

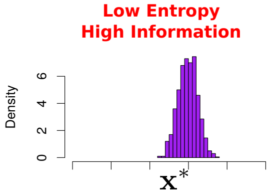

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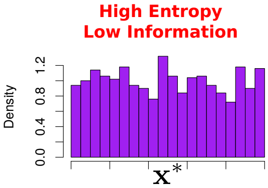

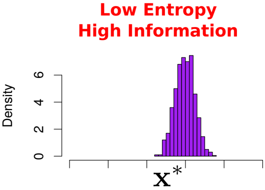

The acquisition function is

$$\alpha(\mathbf{x}) = \mathsf{H}\left[\mathbf{x}^* \middle| \mathcal{D}_t\right] - \mathbb{E}_{\mathbf{y}}\left[\mathsf{H}\left[\mathbf{x}^* \middle| \mathcal{D}_t \cup \{\mathbf{x}, \mathbf{y}\}\right] \middle| \mathcal{D}_t, \mathbf{x}\right] \quad (1)$$

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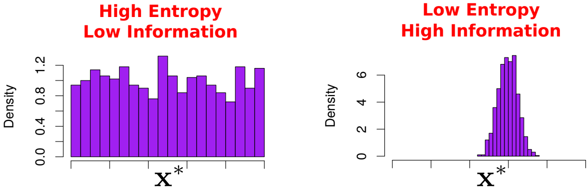

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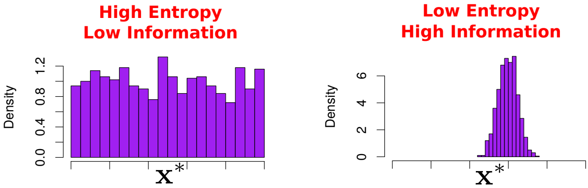

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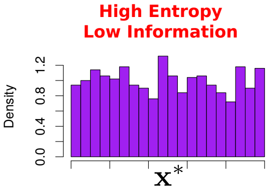

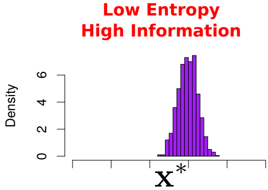

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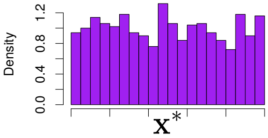
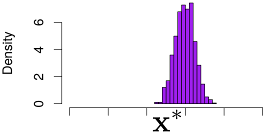
High Entropy
Low Information



Low Entropy
High Information



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

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We **swap** y **and** $\mathcal{X}^\star$ to obtain a reformulation of the acquisition function.

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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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One acquisition per black-box

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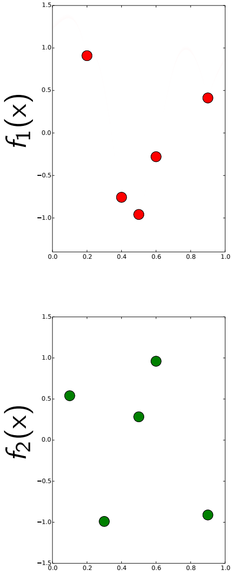

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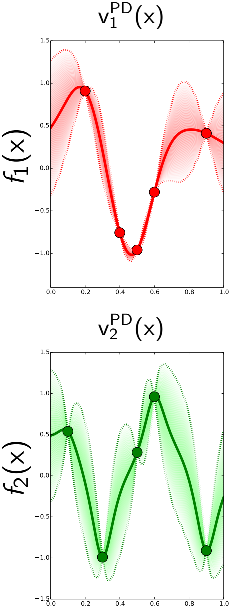

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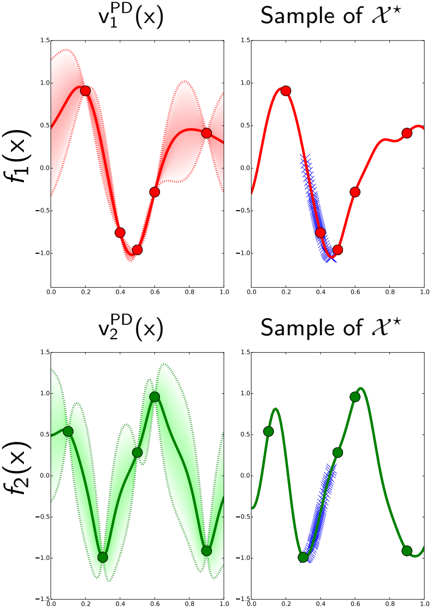

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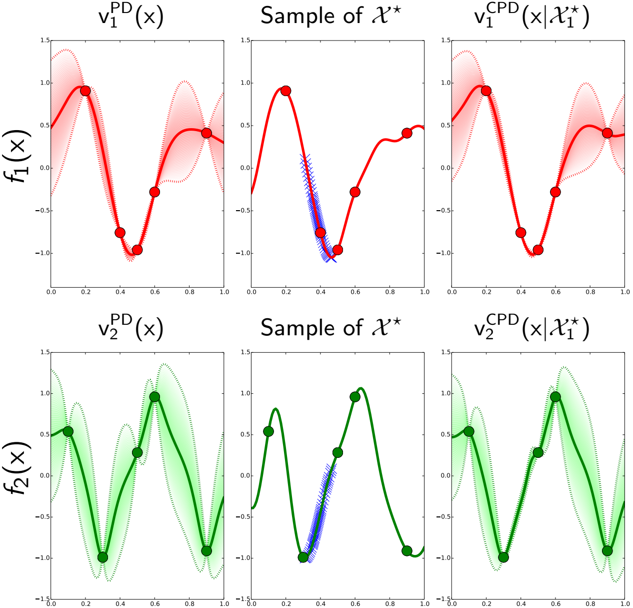

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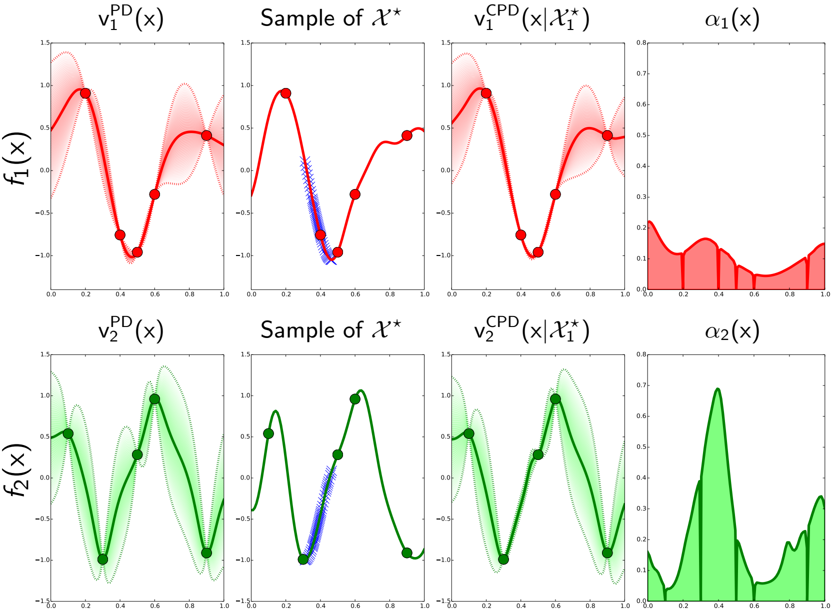

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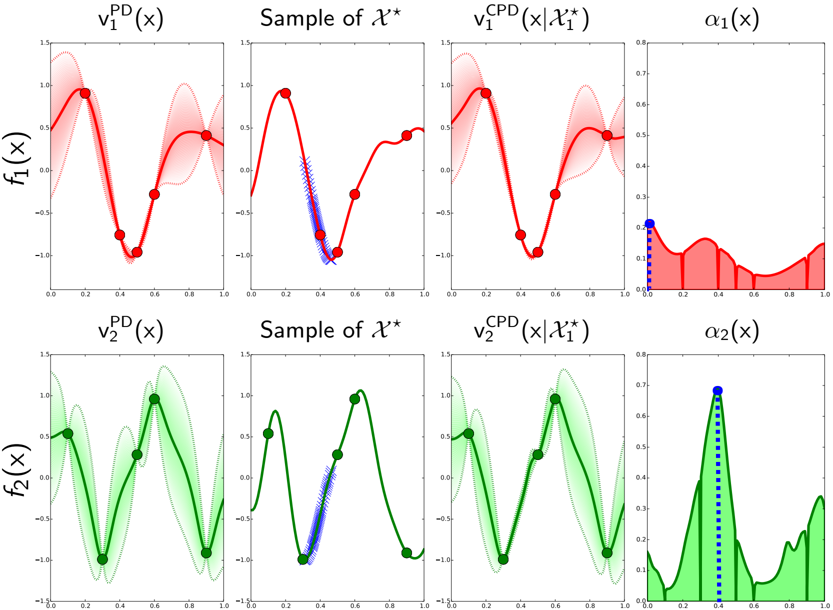
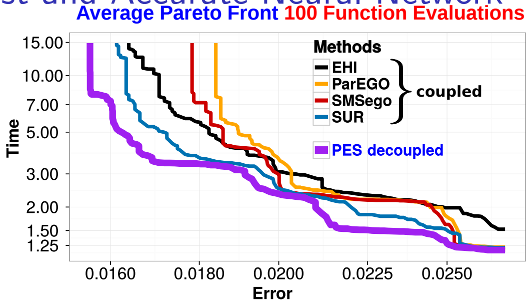


Finding a Fast and Accurate Neural Network



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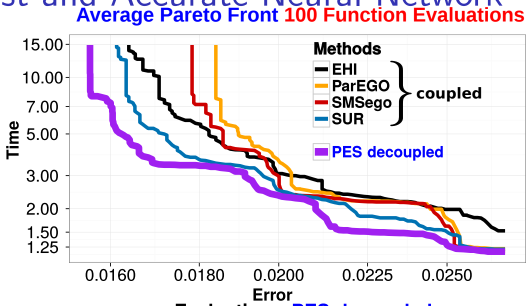

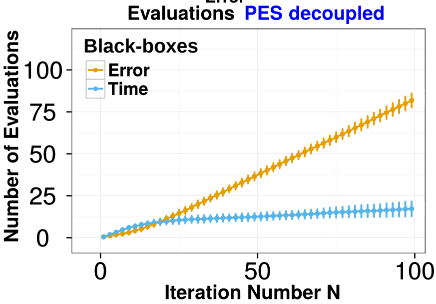

(Hernández-Lobato *et al.*, 2016)

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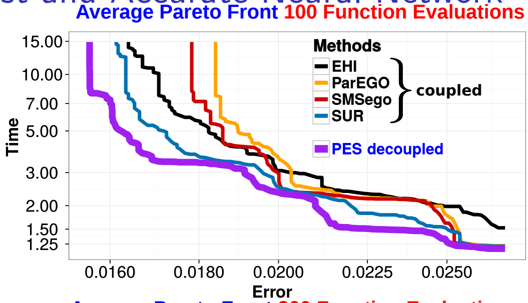

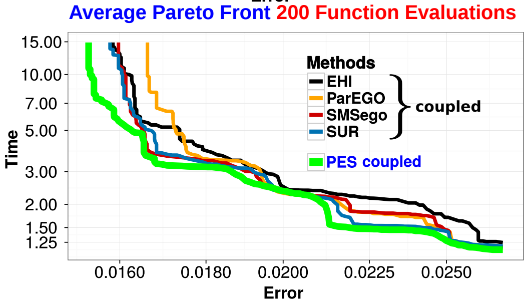

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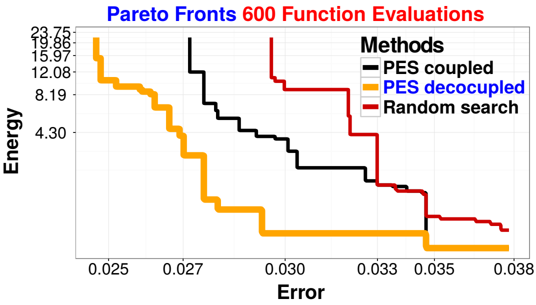
Low energy hardware accelerator



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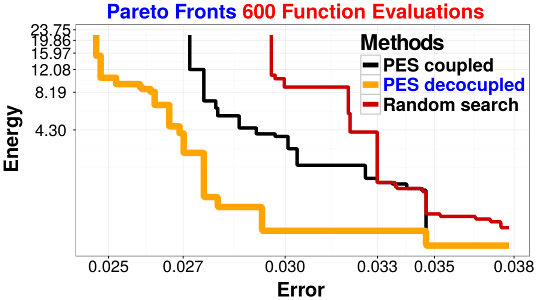

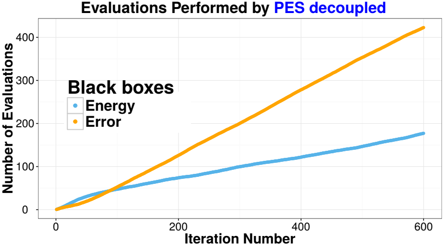

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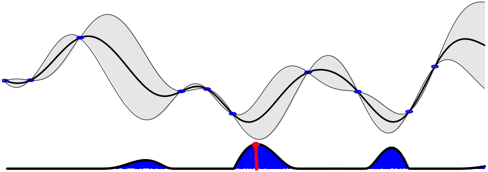

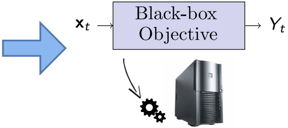

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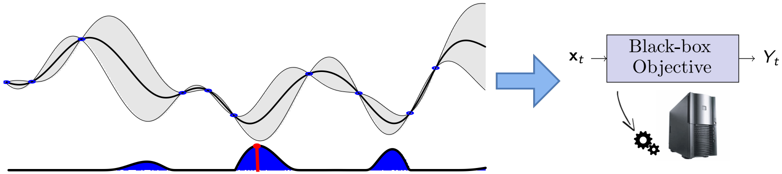

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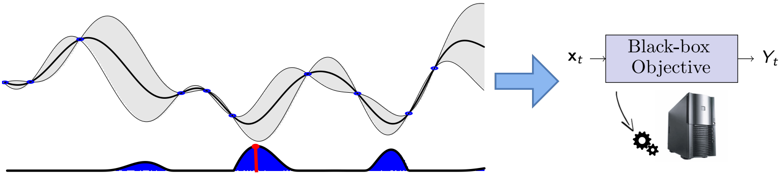

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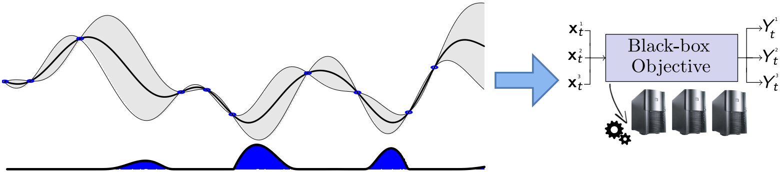

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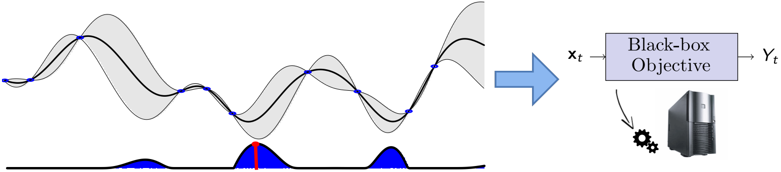

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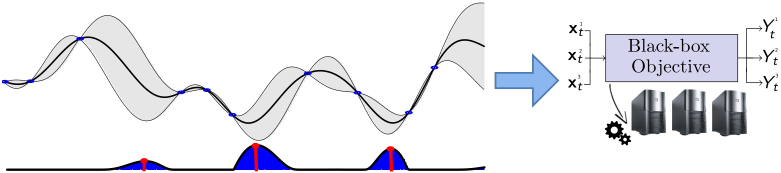

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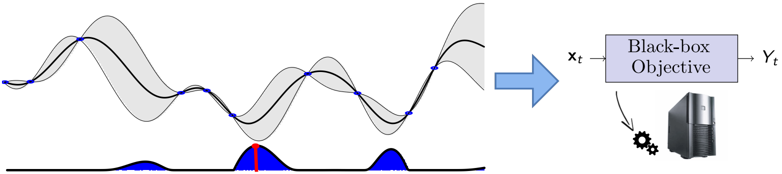

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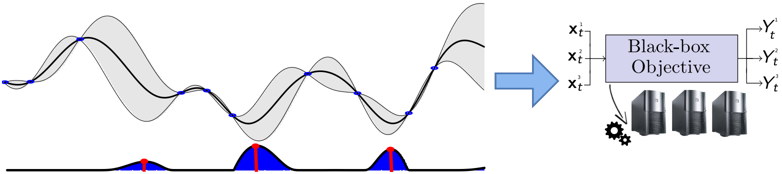

Parallel experiments should be highly informative but different!

Parallel Predictive Entropy Search

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

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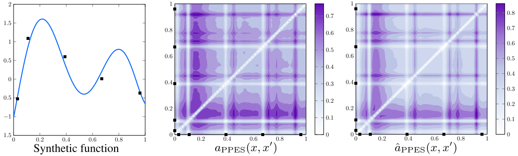
It is possible to compute the gradient of $\alpha(\cdot)$ w.r.t. each $\mathrm{x}_q \in \mathcal{S}_t$!

(Shah and Ghahramani, 2015)

Parallel Predictive Entropy Search: Level Curves



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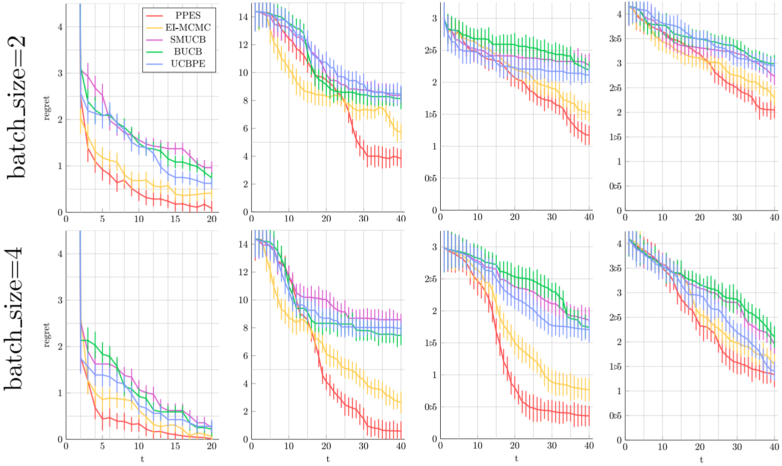
Parallel Predictive Entropy Search: Results



(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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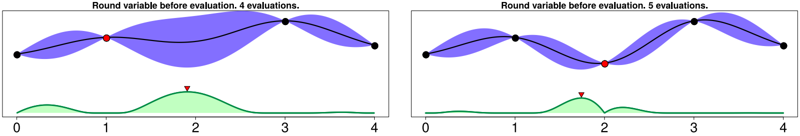

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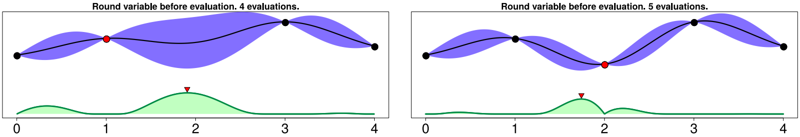
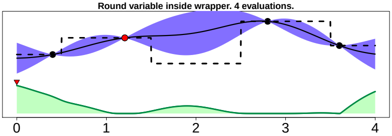
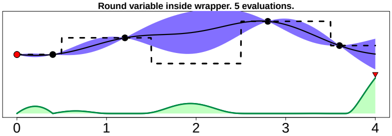


The BO algorithm may get stuck and may always perform the next evaluation at the same input location!

BO with Integer-valued and Categorical Variables

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





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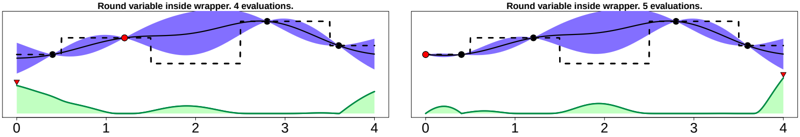

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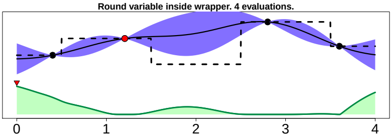

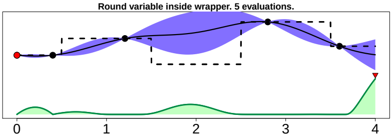

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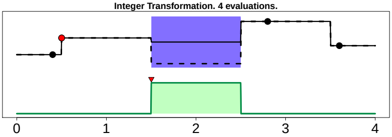

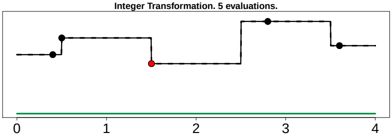

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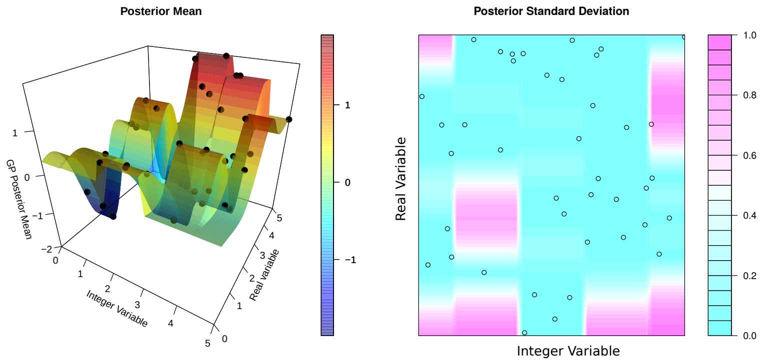

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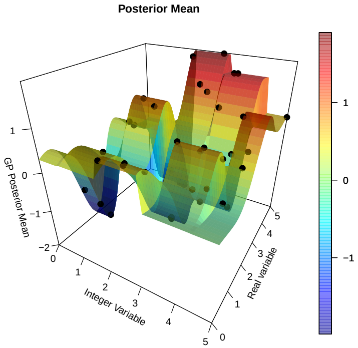
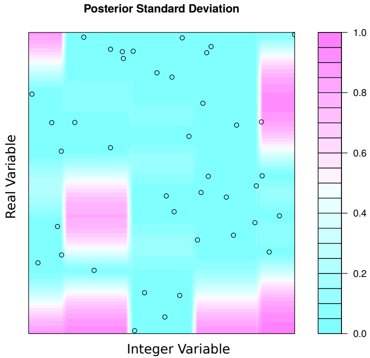
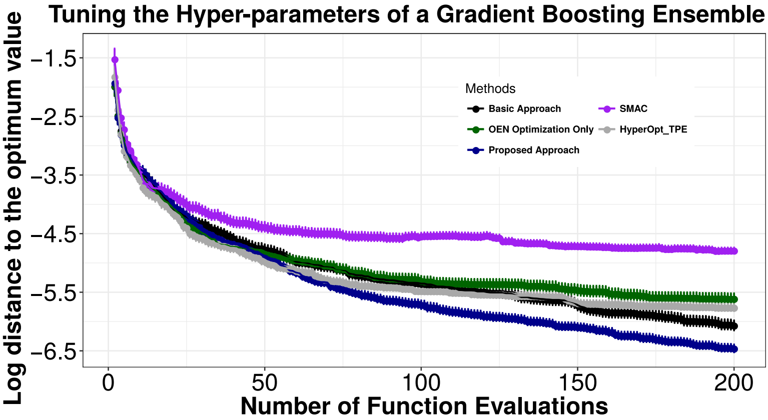




Similar results for categorical variables!

BO with Integer-valued and Categorical Variables



One continuous variable and two integer-valued variables.

Freeze-Thaw Bayesian Optimization

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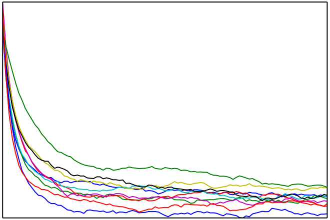

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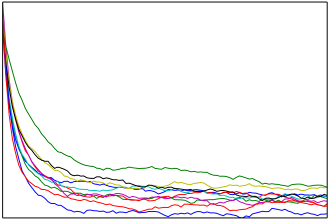

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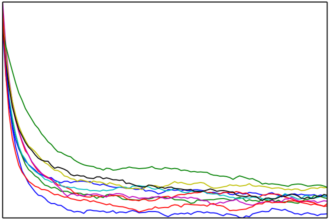

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Yes, that is precisely what Freeze-Thaw BO does!

(Swersky et al., 2014)

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The covariance between inputs t and t' is:

$$C(t, t') = \int_0^\infty e^{-\lambda t} e^{-\lambda t'} \psi(\lambda; \alpha, \beta) d\lambda = \frac{\beta^\alpha}{(t + t' + \beta)^\alpha}$$

where $\psi(\lambda; \alpha, \beta)$ is a gamma distribution with parameters α and β.

A GP Kernel for Training Curves

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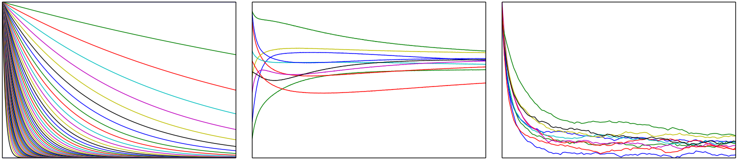

(a) Exponential Decay Basis (b) Samples (c) Training Curve Samples

Inference on Asymptotic Values

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

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Hierarchical generative model:

$$p(\{\mathrm{y}_n\}_{n=1}^N | \{\mathrm{x}_n\}_{n=1}^N) = \int \left[\prod_{n=1}^N \mathcal{N}(\mathrm{y}_n | f_n \mathrm{1}, \mathrm{K}_{t_n}) \right] \mathcal{N}(\mathrm{f}|\mathrm{m}, \mathrm{K}_\mathrm{x}) d\mathrm{f}$$

where

$$\mathrm{x}_n \equiv n \text{ configuration}\,, \qquad \mathrm{y}_n \equiv n \text{ observed curve}\,,$$

$$f_n \equiv n \text{ asymptotic value}\,, \qquad \mathrm{m} \equiv \text{prior asymptotic mean values}\,,$$

$$\mathrm{K}_{t_n} \equiv \text{covariances for curve values}\,, \quad \mathrm{K}_\mathrm{x} \equiv \text{cov. for asymptotic values}$$

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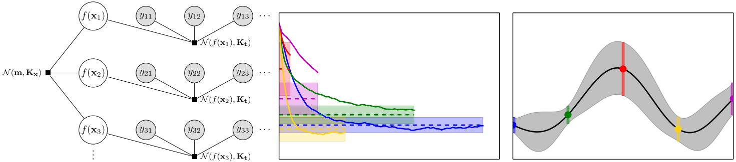
The joint distribution of $\{\mathrm{y}\}_{n=1}^N$ and f is Gaussian and hence so it is the predictive distribution $p(\mathrm{f}|\{\mathrm{y}\}_{n=1}^N)$!

Inference on Asymptotic Values and BO

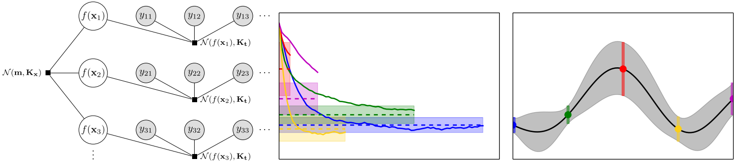


(a) Graphical Model

(b) Training curve predictions

(c) Asymptotic GP

Inference on Asymptotic Values and BO



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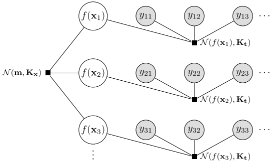
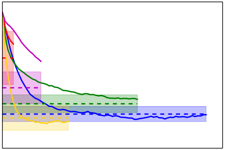
Bayesian Optimization:

- $p(\mathrm{f} | \{\mathrm{y}_n\}_{n=1}^N, \{\mathrm{x}_n\}_{n=1}^N)$ determines asymptotic values.

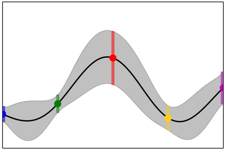
Inference on Asymptotic Values and BO



(a) Graphical Model



(b) Training curve predictions

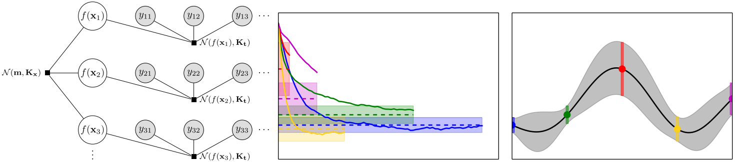


(c) Asymptotic GP

Bayesian Optimization:

- $p(\mathrm{f} | \{\mathrm{y}_n\}_{n=1}^N, \{\mathrm{x}_n\}_{n=1}^N)$ determines asymptotic values.
- This distribution can be used to make intelligent decisions!

Inference on Asymptotic Values and BO



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

Bayesian Optimization:

- $p(\mathrm{f}|\{\mathrm{y}_n\}_{n=1}^N, \{\mathrm{x}_n\}_{n=1}^N)$ determines asymptotic values.
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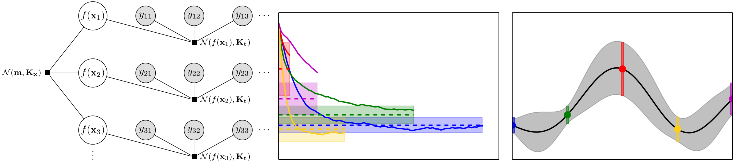
Inference on Asymptotic Values and BO



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Bayesian Optimization:

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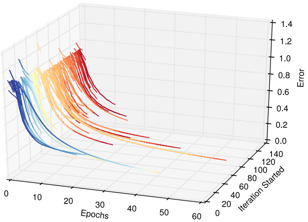
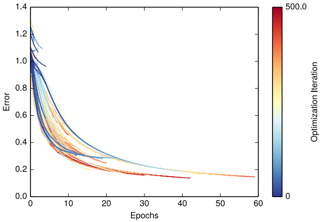
- This distribution can be used to make intelligent decisions!
- Shall we train more one configuration or shall we start a new one?
- A combination of EI and ES is used as the acquisition function.

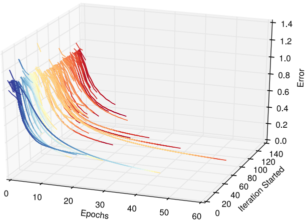
(Swersky et al., 2014)

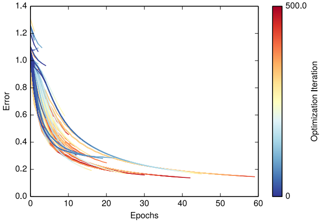
Freeze-Thaw BO in practice

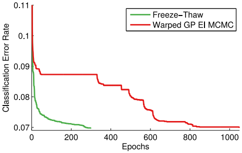




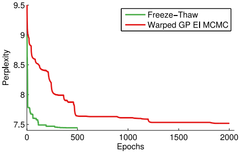
Freeze-Thaw BO in practice



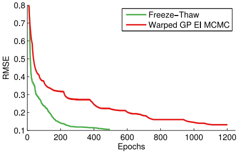




(a) Logistic Regression



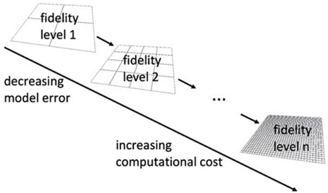
(b) Online LDA

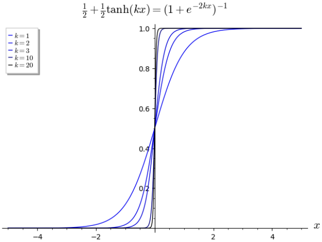


(c) PMF

(Swersky et al., 2014)

Multi-fidelity Bayesian optimization





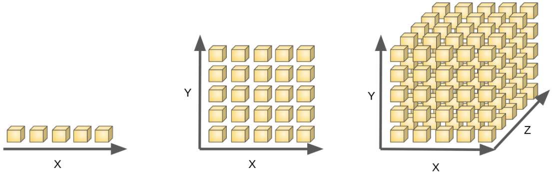
- **Concept of Fidelity:** Fidelity refers to the accuracy or reliability of the information, we use different levels of accuracy.
- **Example:** # layers in NNs, # of timesteps for DRL.
- *We assume that lower fidelities are correlated with higher.*
- **Cost-Efficiency:** Leveraging computationally 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



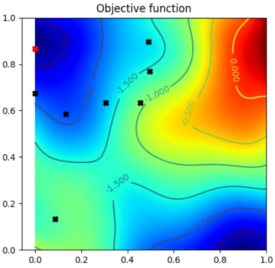
- GPs empirical performance tends to be lower if $d > 7$.
- **The problem:** The search space grows exponentially with the number of dimensions.
- **The trick:** We can project the high-dimensional problem into a lower-dimensional subspace that explains it well using embeddings.
- *Find the hidden most 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.)

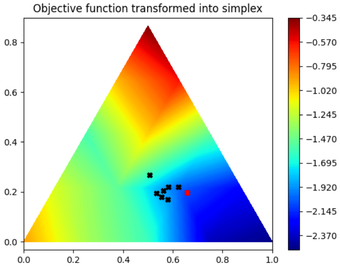
High-dimensional Bayesian optimization example

- 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)

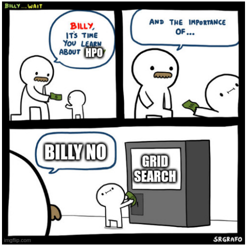




- Common financial metrics as Sharpe or Sortino ratio can be configured for a specific portfolio.
- For example using real-time ESG values of the assets.
- Garrido-Merchán, E. C., Piris, G. G., & Vaca, M. C. (2023). Bayesian optimization of ESG (Environmental Social Governance) financial investments.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