Lecture 6: Bayesian optimization and contextual bandits applications

Hrvoje Stojic

May 17, 2021

Bayesian optimization

Bayesian optimization with GP's

Source: Shahriari et al 2016

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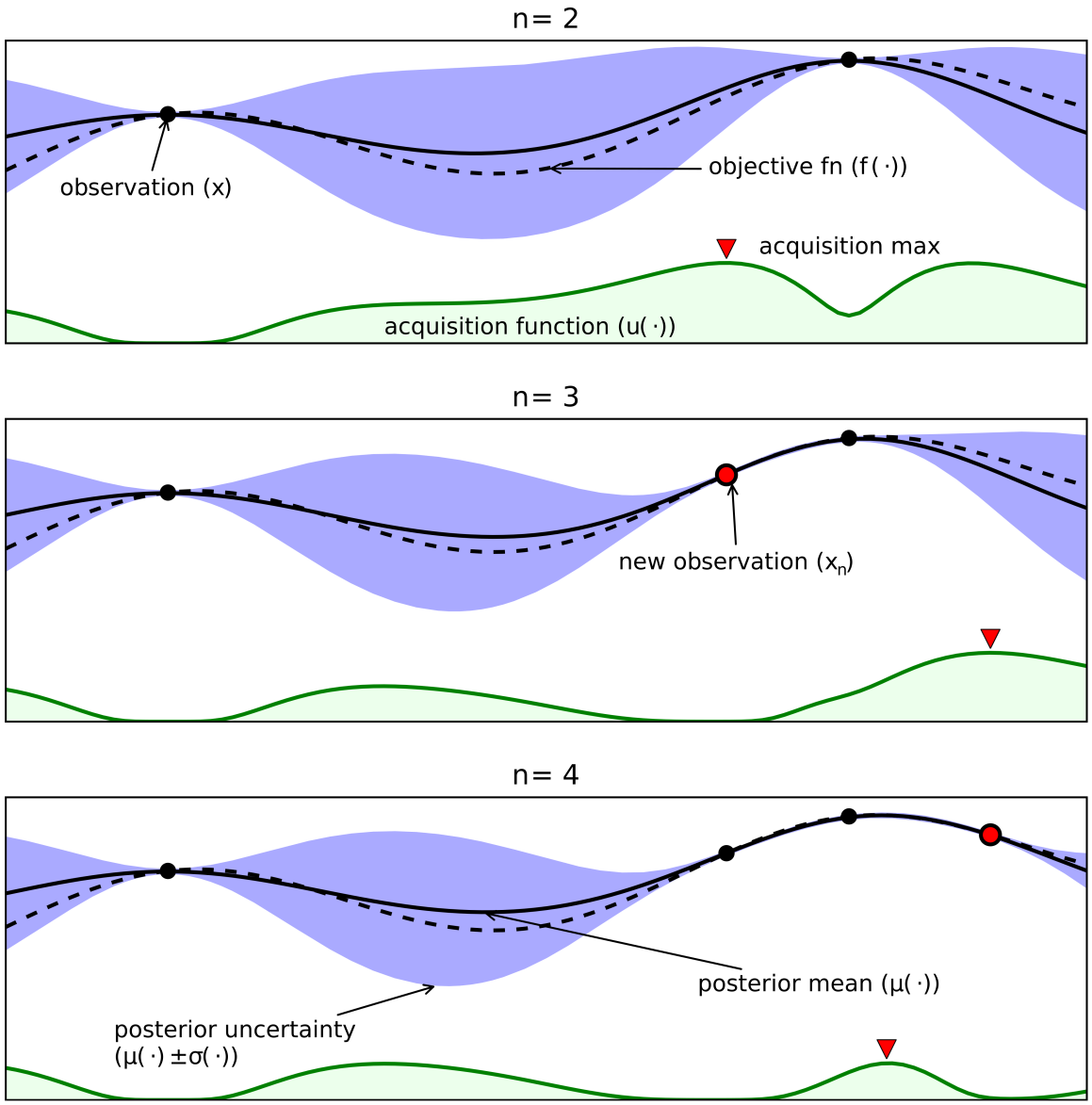

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Bayesian optimization algorithm

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1. **for** $t = 1, 2, \ldots$ do
2. Choose $\mathbf{x}_t$ by combining attributes of the posterior distribution in an acquisition function α and maximizing

$$\mathbf{x}_t = \text{argmax}_x \alpha(\mathbf{x}; \mathcal{D}_{1:t-1})$$

3. Obtain the reward (i.e. outcome of the objective function)

$$y_t = f(\mathbf{x}_t) + \epsilon_t$$

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- A bit of history: searching for gold with "kriging"

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- Recall the expressions for GP prediction

$$P(y_{t+1}|\mathcal{D}_{1:t}, \mathbf{x}_{t+1} = \mathcal{N}(\mu_t(\mathbf{x}_{t+1}), \sigma_t^2(\mathbf{x}_{t+1}) + \sigma_n^2)$$

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- Regret bound for RBF kernel: $\sqrt{T(\log T)^{d+1}}$ (Srinivas et al., 2010)

Probability of Improvement (PI)

Source: de Freitas lectures, 2013

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- Favours points that are likely to improve on best so far
- Defined as

$$\mathrm{PI}(\mathbf{x}) = P(f(\mathbf{x}) \geq \mu^+ + \epsilon) = \Phi\left(\frac{\mu_t(\mathbf{x}) - \mu^+ - \epsilon}{\sigma_t(\mathbf{x})}\right)$$

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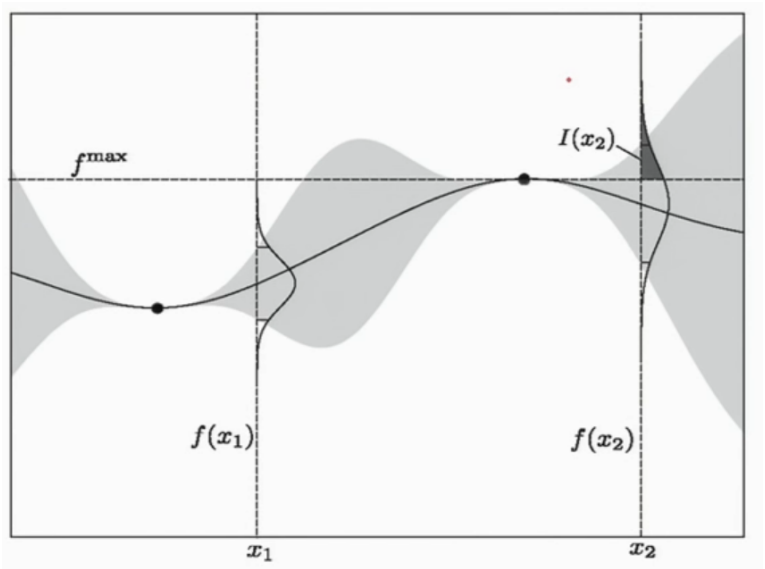

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$$\text{EI}(\mathbf{x}) = (\mu_t(\mathbf{x}) - \mu^+ - \epsilon)\Phi(Z) + \sigma_t(\mathbf{x})\phi(Z)$$

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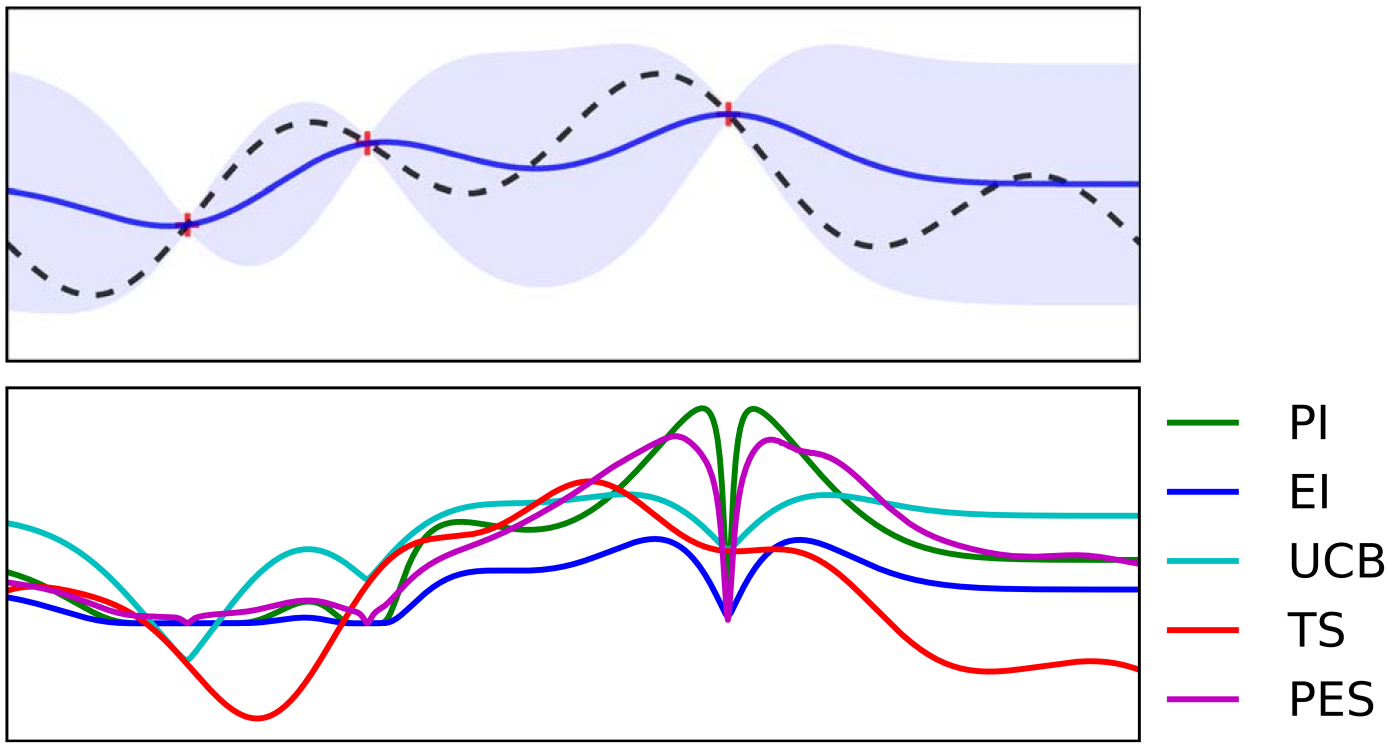
  - where $Z = \frac{\mu_t(\mathbf{x}) - \mu^+ - \epsilon}{\sigma_t(\mathbf{x})}$
- EI is high when the (posterior) expected value $\mu_t(\mathbf{x})$ is higher than the current best value μ^+; or when the uncertainty $\sigma_t(\mathbf{x})$ around the point $\mathbf{x}$ is high.

Acquisition function illustration



Source: Shahriari et al (2016) Figure 5

Portfolio of acquisition functions

Source: Hoffman, Brochu, de Freitas (2011); Shahriari et al (2014)

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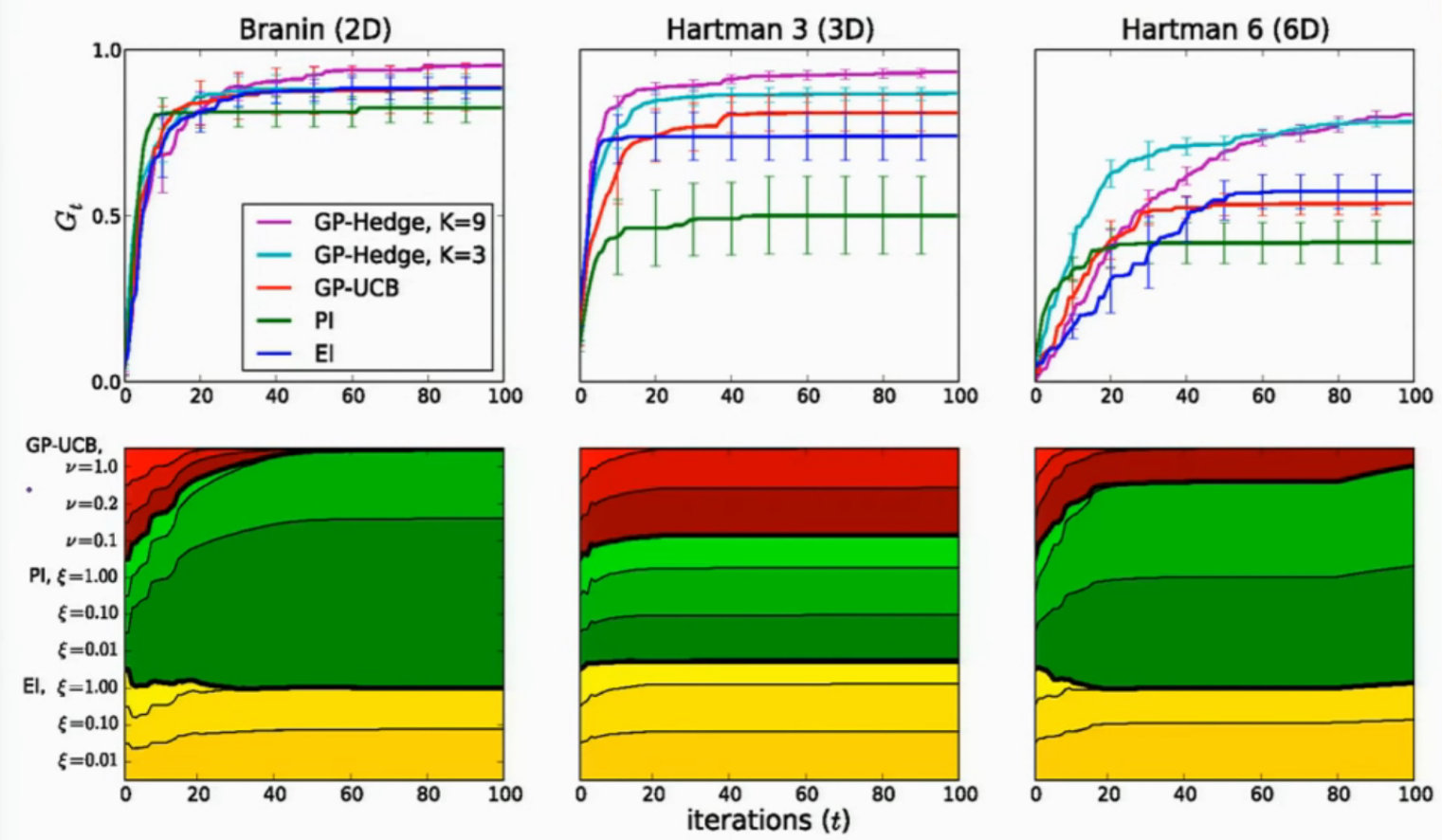

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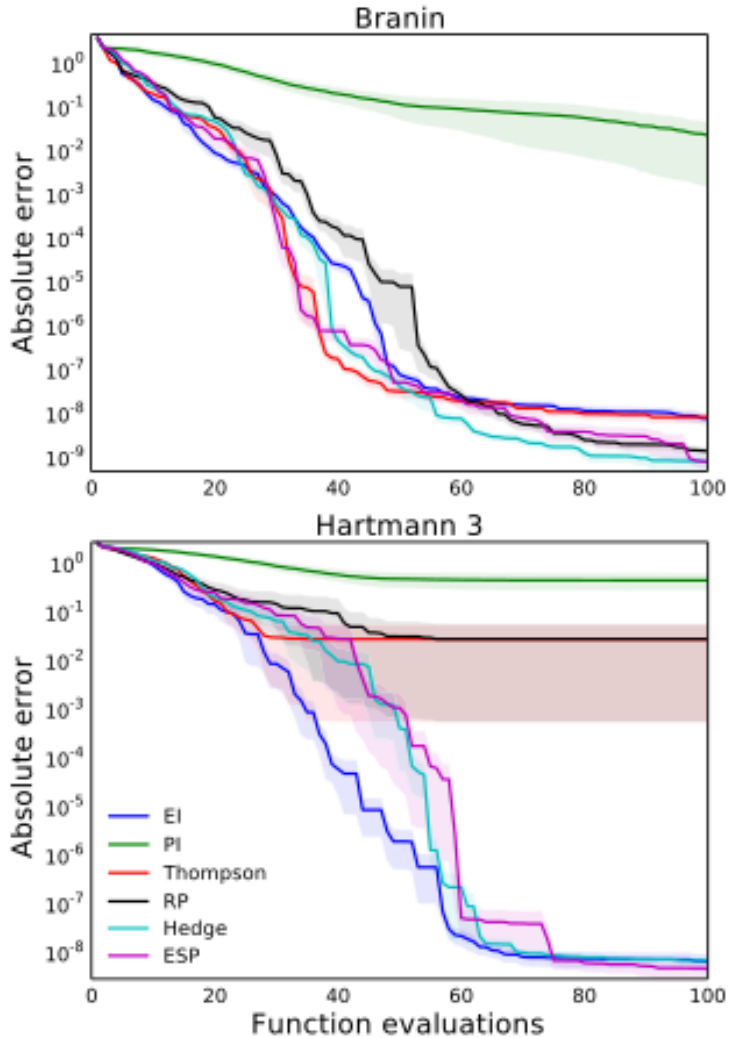
Portfolios might be the best approach



Source: Shahriari et al (2016) Figure 6

Optimization: handling GP hyperparameters

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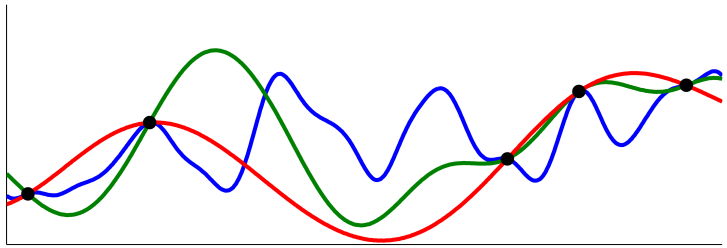
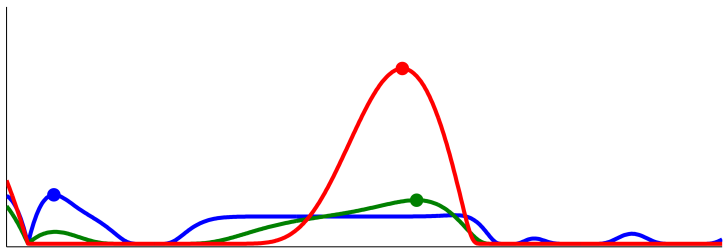
- Takes into account uncertainty about GP's hyperparameters and tends to improve uncertainty estimates of the function
- This can be done using either quadrature or Monte Carlo estimate (e.g. via slice sampling - Murray & Adams, 2010)

Optimization: handling GP hyperparameters

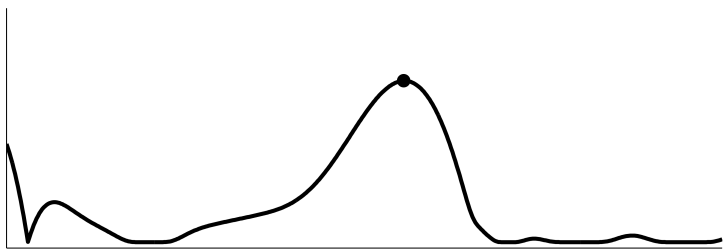
- Example of marginalizing out the hyperparameters with EI



(a) Posterior samples under varying hyperparameters



(b) Expected improvement under varying hyperparameters



(c) Integrated expected improvement

Source: Snoek et al (2012) Figure 1

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- In practice:
  - Discretization and grid search (e.g. Snoek et al 2012)
  - Adaptive grids (Badernet, Kegl, 2010)
  - If gradients available (or can be approximated cheaply), then multi-started quasi-Newton hill climbing approach or multi-started local search
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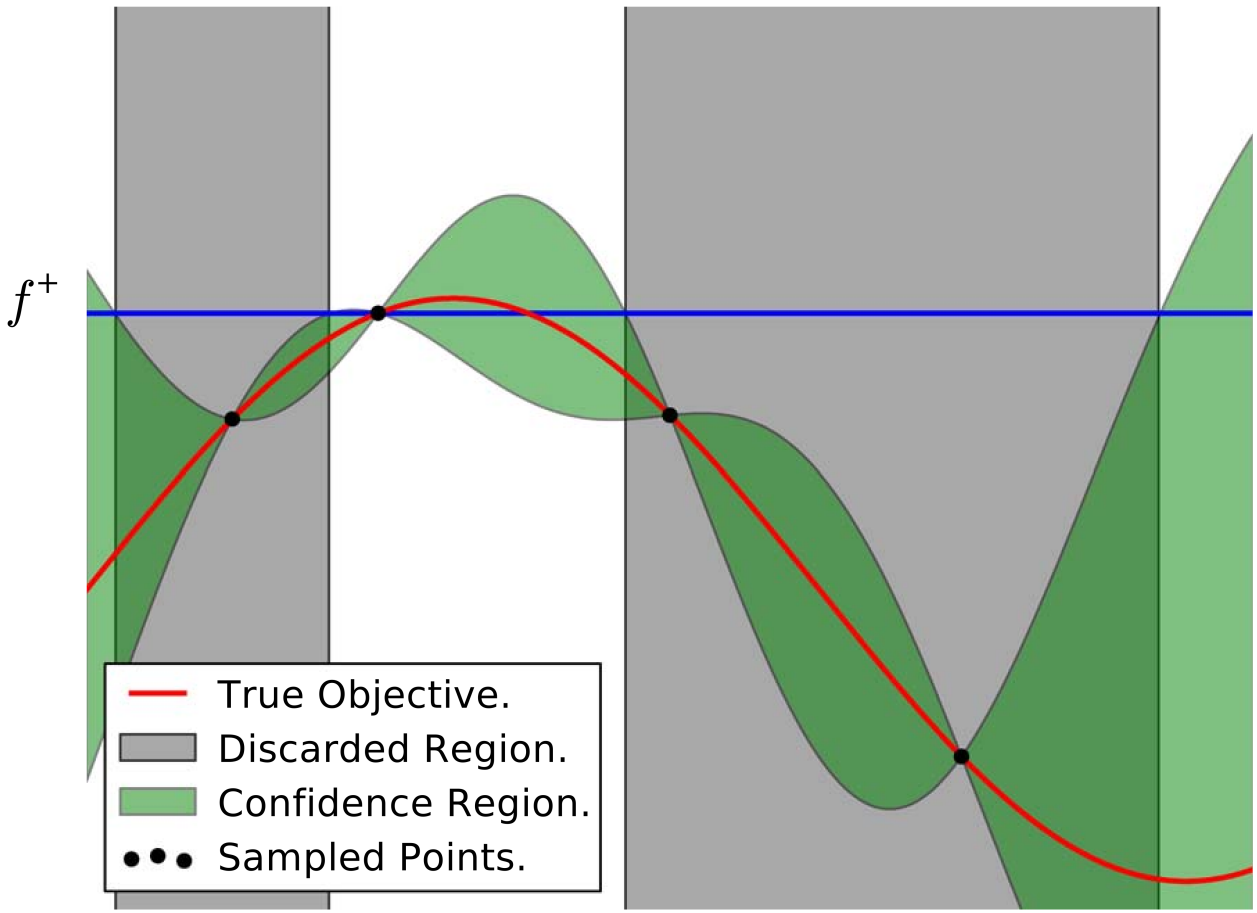
- Recent developments
  - Optimistic optimization: Use the same optimism in the face of uncertainty on acquisition function optimization level as well (de Freitas, Smola and Zoghi, 2012))
  - BamSOO: shrinks the region in every iteration to the most promising ones (Wang, Shakibi, Jin and de Freitas, 2014)

Optimizing acquisition functions with optimistic optimization



Source: de Freitas, Smola, Zoghi (2012)

Going further: Taking into account evaluation costs

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- In realistic settings, evaluating objective function might entail different costs for different $\mathbf{x}$ and you might have access to it
  - E.g. training a neural network with 100 vs. 10000 nodes requires much more memory and would take linger time - you could use training duration as a cost, or cost of renting a larger cloud instance for a longer time
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- If there is a limited budget, then the search should be biased toward low-cost areas
- Snoek et al (2012): *expected improvement per second*
  - Duration function is also not known
  - $c(\mathbf{x}) : \mathcal{X} \rightarrow R^{+}$
  - We can use another GP model to estimate $c()$
  - Combine the expected improvement with duration, $\mathrm{EI}(\mathbf{x}, \mathcal{D}_t)/c(\mathbf{x})$
  - Biases the search toward good models with fast training times

Expected improvement per second

Source: Snoek et al (2012) Figure 3

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- Optimizing hyperparameters for training logistic regression on MNIST dataset

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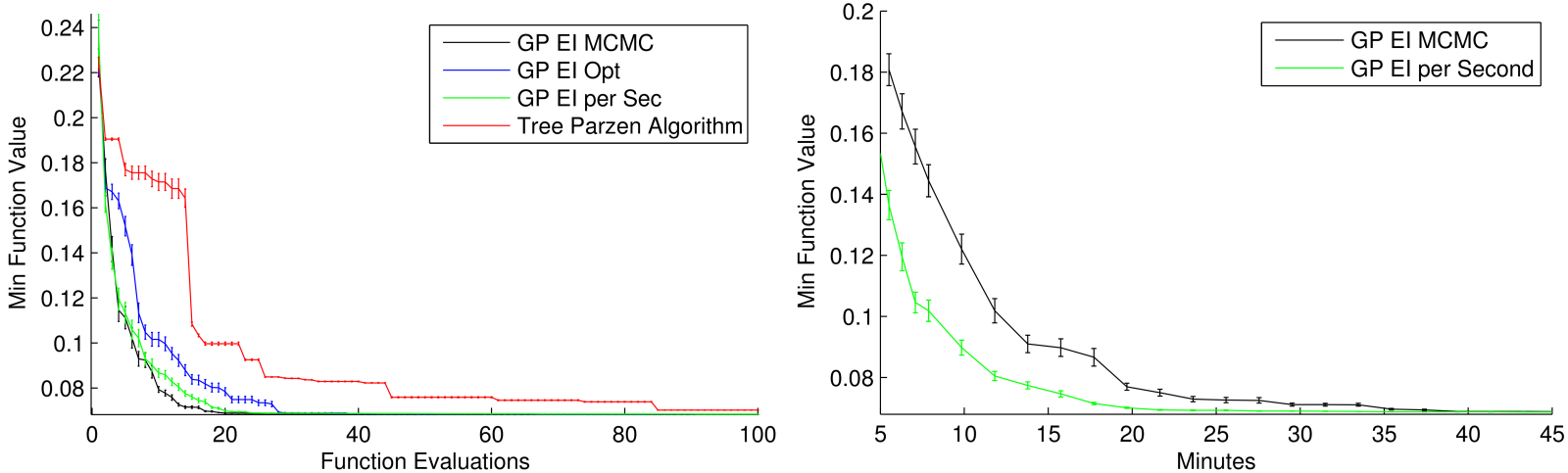

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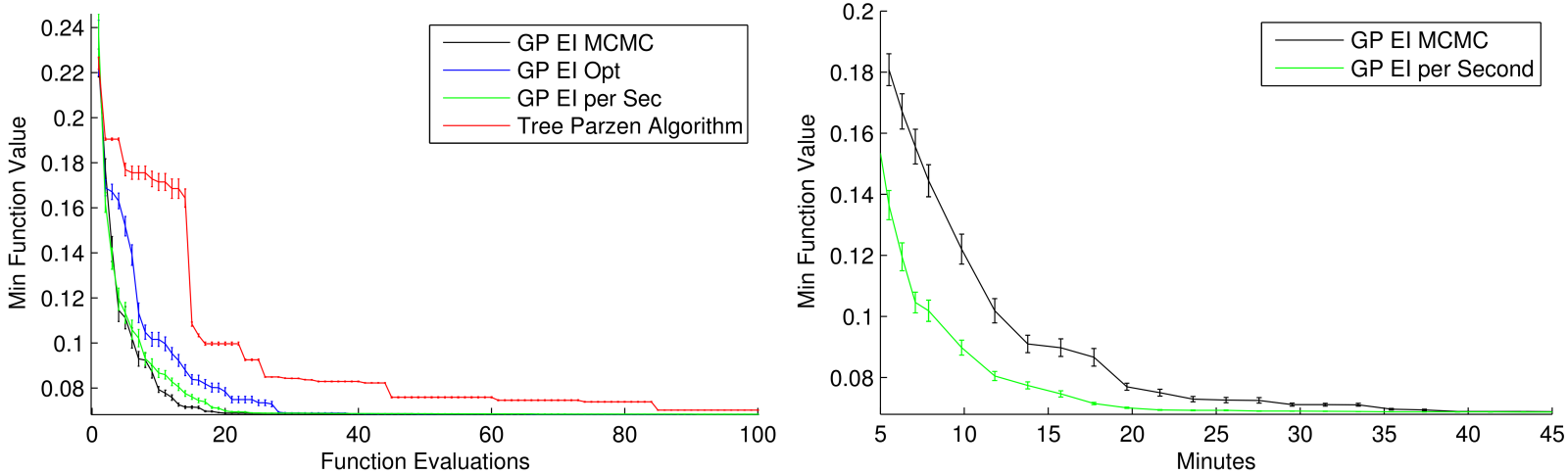

- Little difference in performance (approaching min) between EI MCMC and EI per second, but there is a large difference in amount of time it takes

Source: Snoek et al (2012) Figure 3

Going further: Safe exploration and risk-averse BO

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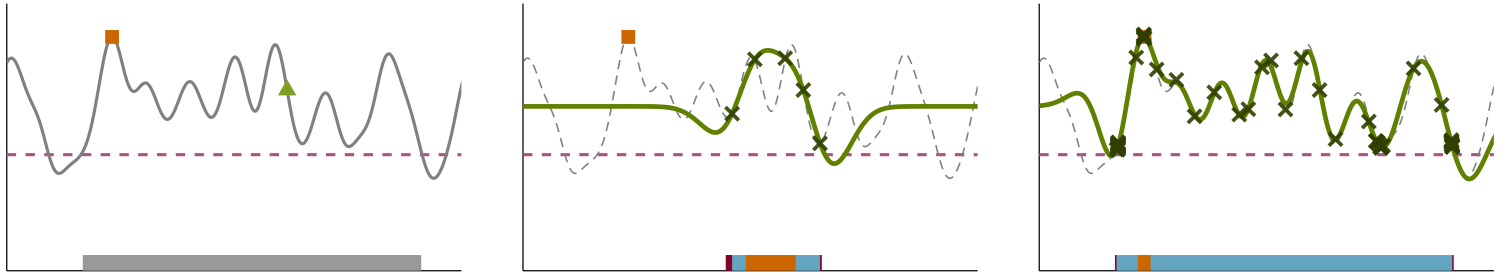

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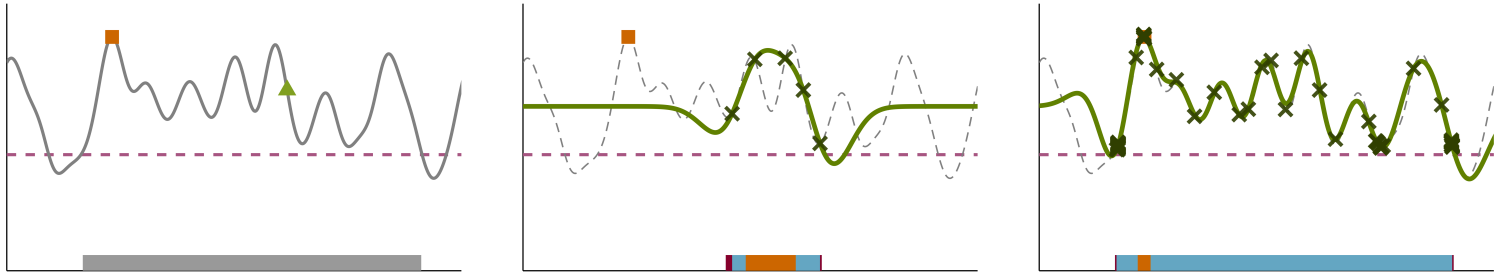

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- Related to this is risk-averse BO - accounting for the distribution tails (see Torossian, Picheny and Durrande, 2020)

Going further: Beyond low-dimensional problems with REMBO

Source: Shahriari et al (2016) Figure 10

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- In continuous action space, Bayesian optimization is restricted to problems of moderate dimension (approx 20)
- In practice, some dimension reduction can be done first
- Random forests scale more easily (SMAC algorithm)

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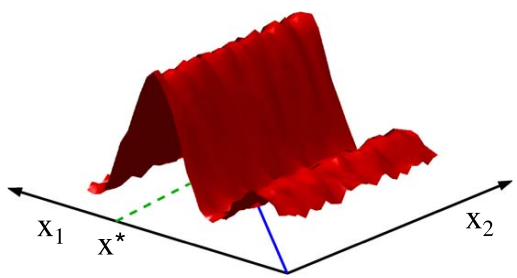
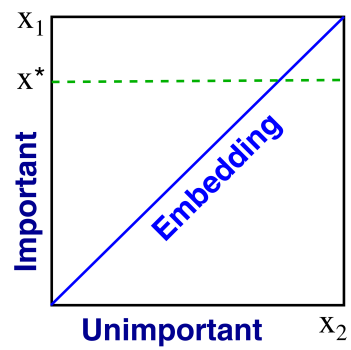
- In practice, some dimension reduction can be done first
- Random forests scale more easily (SMAC algorithm)

- New approaches combining BO with random search
  - Many problems have low effective dimensionality
  - Rationale why random search sometimes performs well (Bergstra, Bengio, 2012)
  - Bayesian optimization with random embedding (REMBO; Wang et al. 2013)





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- If we are concerned with wallclock time, there are several ways to speed up evaluation

1. At decision time
   - When using portfolios
   - We could optimize in parallel many acquisition functions (or a single one with multiple exploration values)
2. While waiting for evaluation of the objective function
   - We could consider what $\mathbf{x}$ should be evaluated next
   - Snoek et al (2012) propose to compute MC estimates of the acquisition function under different possible results from pending function evaluations
   - With function like EI we can leverage Gaussian integration property

Addendum: Random forests as an alternative to GP

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- Scale much better and can deal with categorical data
- Variance in predictions can be used as uncertainty estimate

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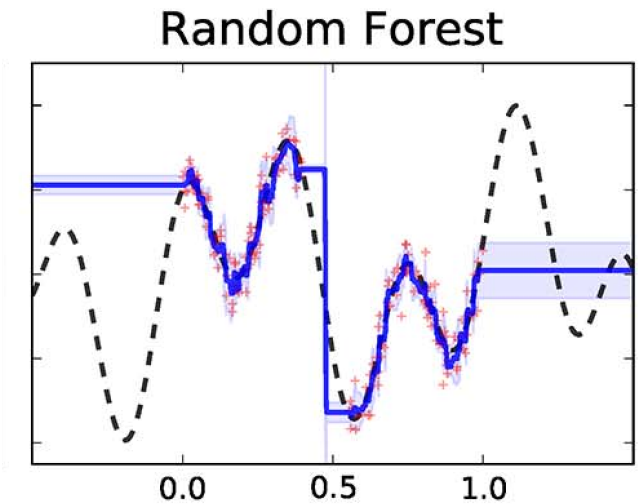

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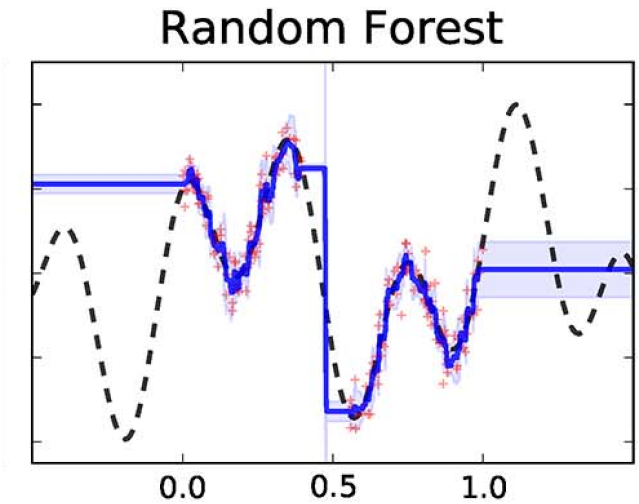

- Poor extrapolation behaviour, but in practice seems to work well (Hutter, Hoos, Leyton-Brown, 2011 - SMAC algorithm)

Source: Shahriari et al (2016) Figure 4

Addendum: Ensemble of neural networks

Source: Pearce et al (2019)

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- A collection of a finite number of neural networks is trained for the same task (Hansen & Salamon, 1990)
- Variance in predictions can again be used as uncertainty estimate
- Recent work shows ensembles can represent uncertainty well, approaching GP's (Lakshminarayanan, Pritzel, Blundell, 2017; Pearce et al, 2019)

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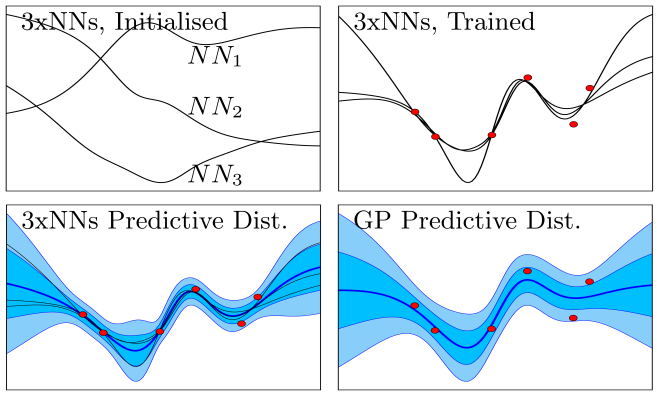

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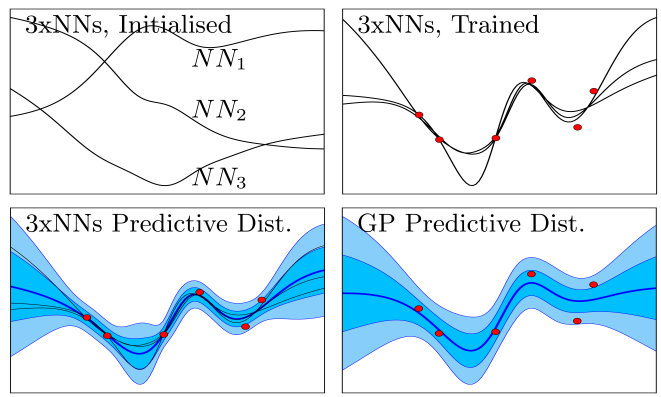

- Can be a costly method and not there yet in terms of representing uncertainty, but very promising

Source: Pearce et al (2019)

Application: Optimizing hyperparameters

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- Bayesian optimization as an alternative

Example 1: Tuning the SVM hyperparameters

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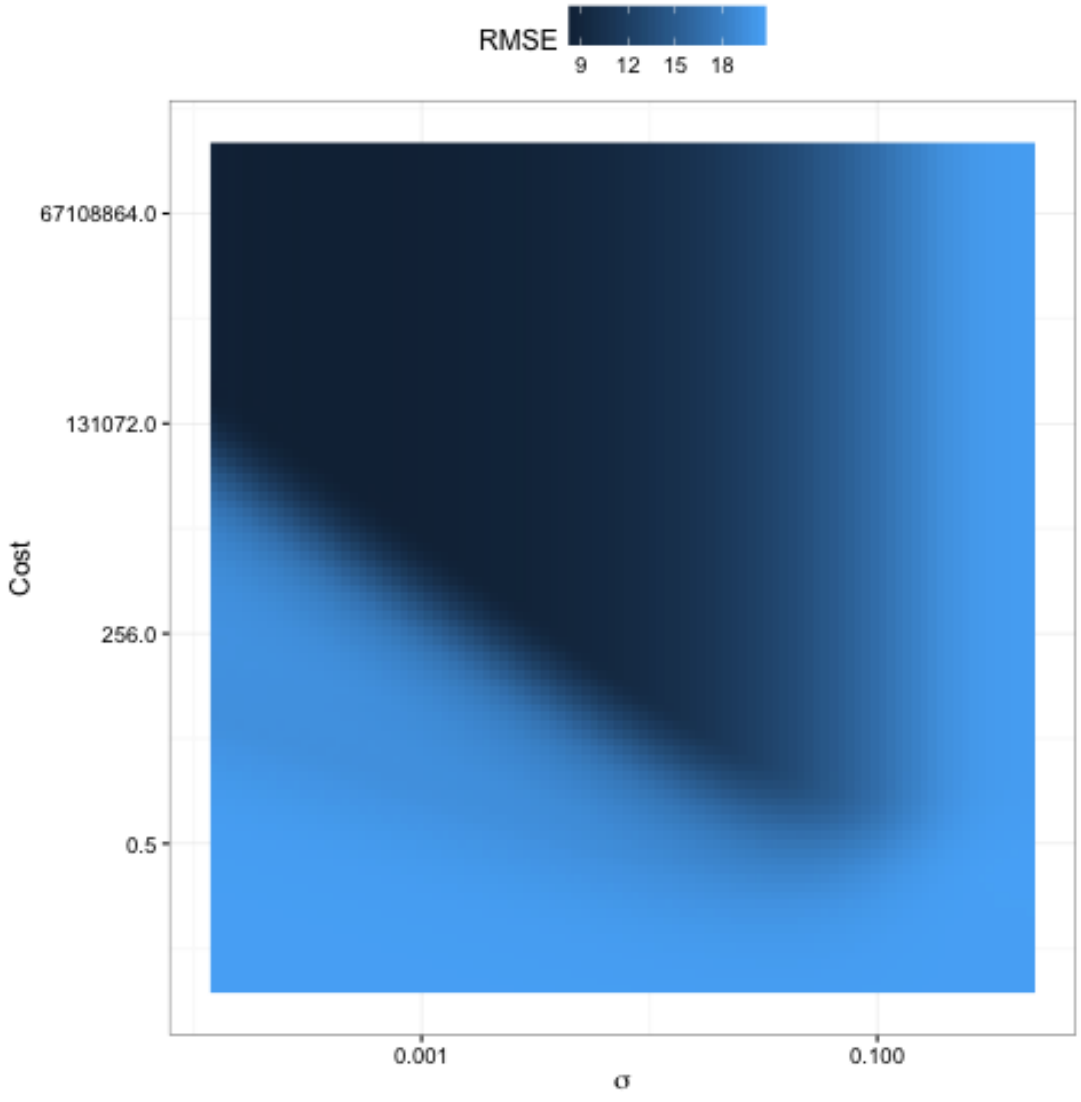
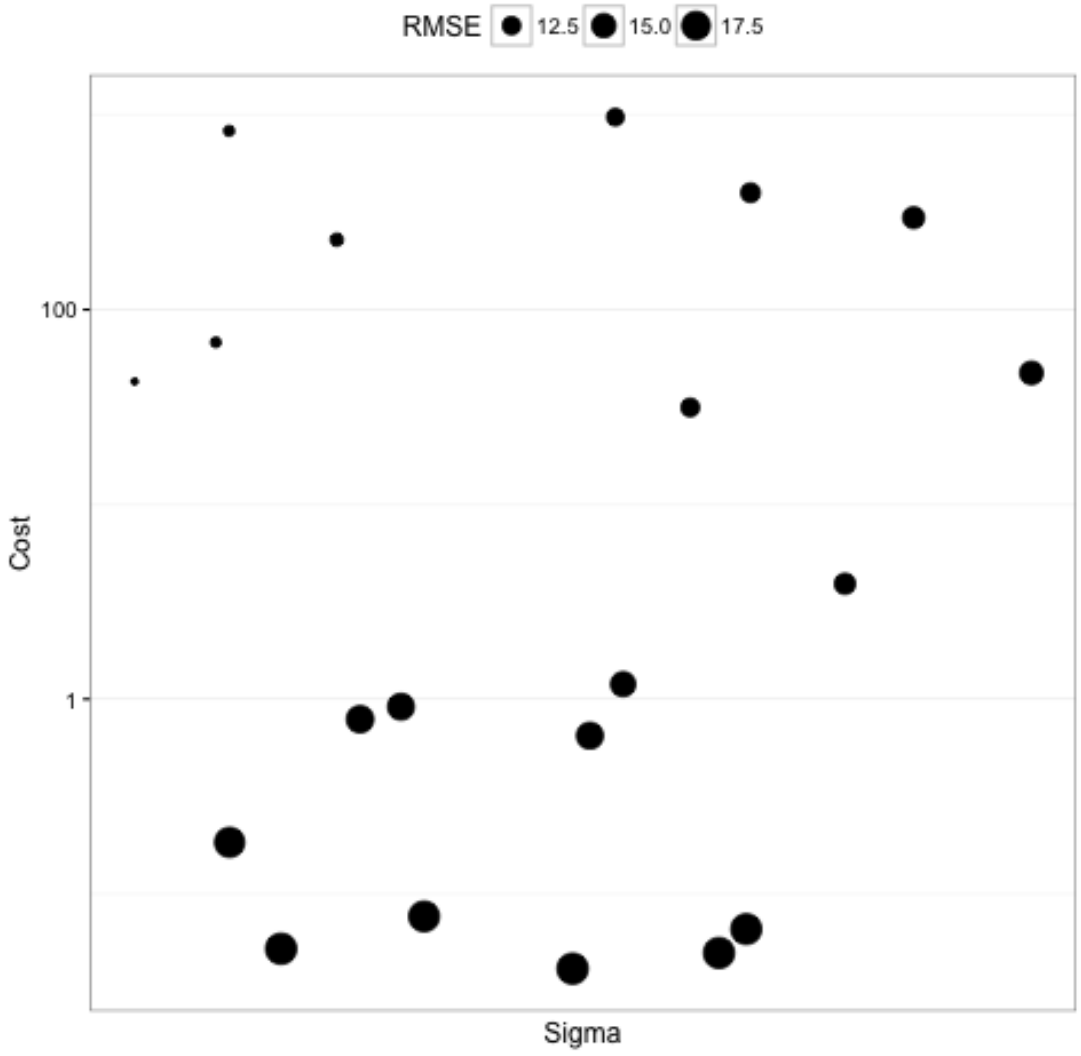
  - using kernlab and rBayesianOptimization

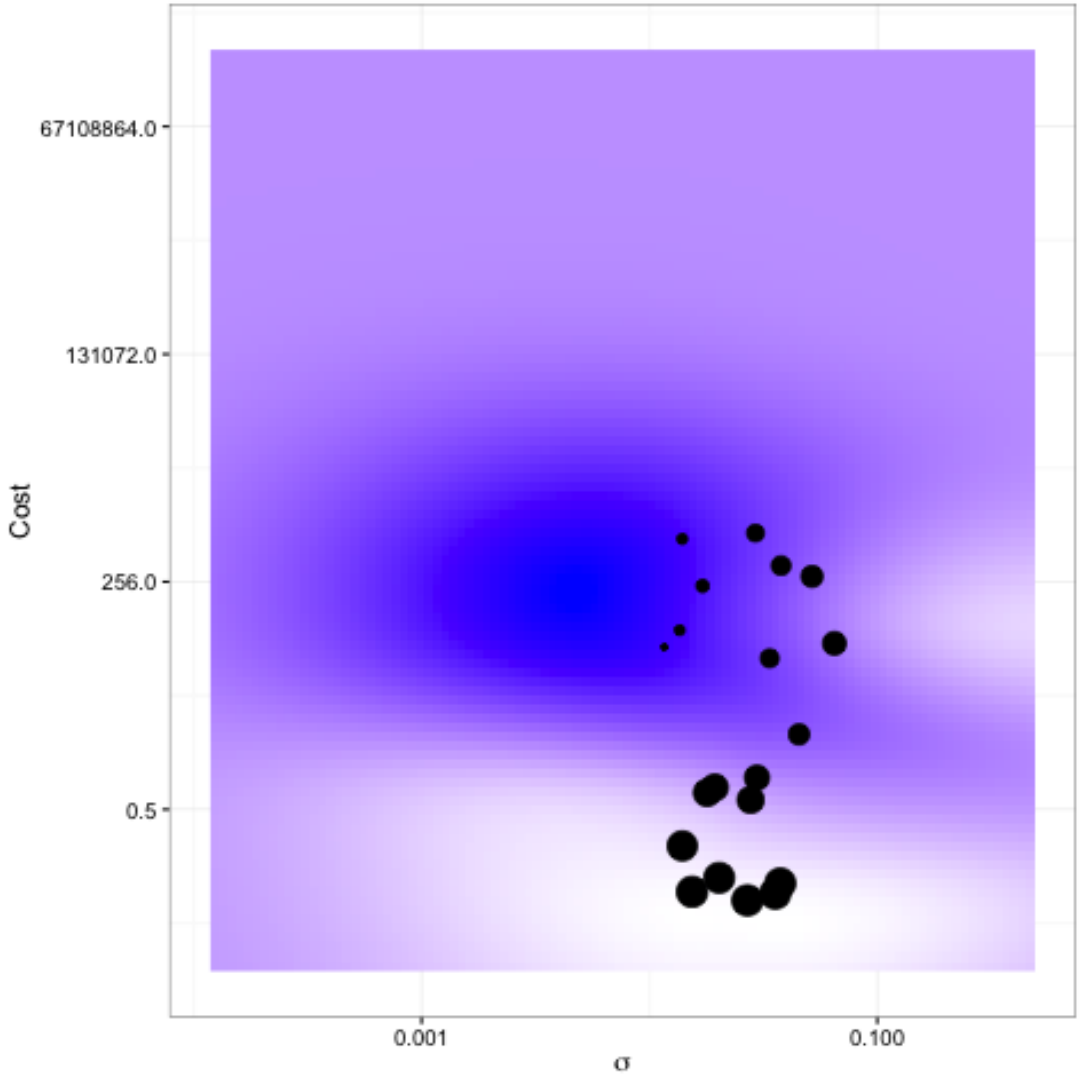
Example 1: RMSE surface



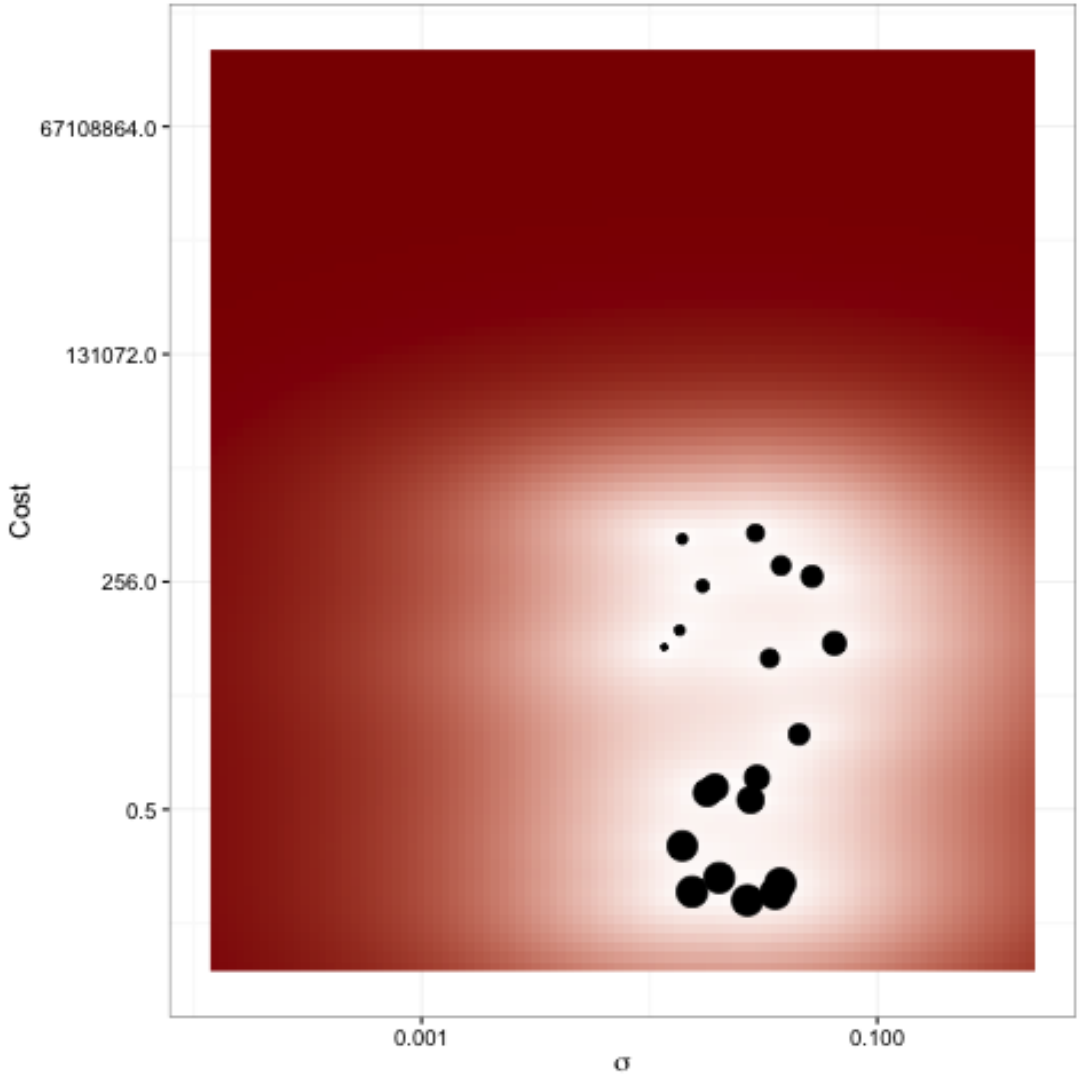
Example 1: Random search



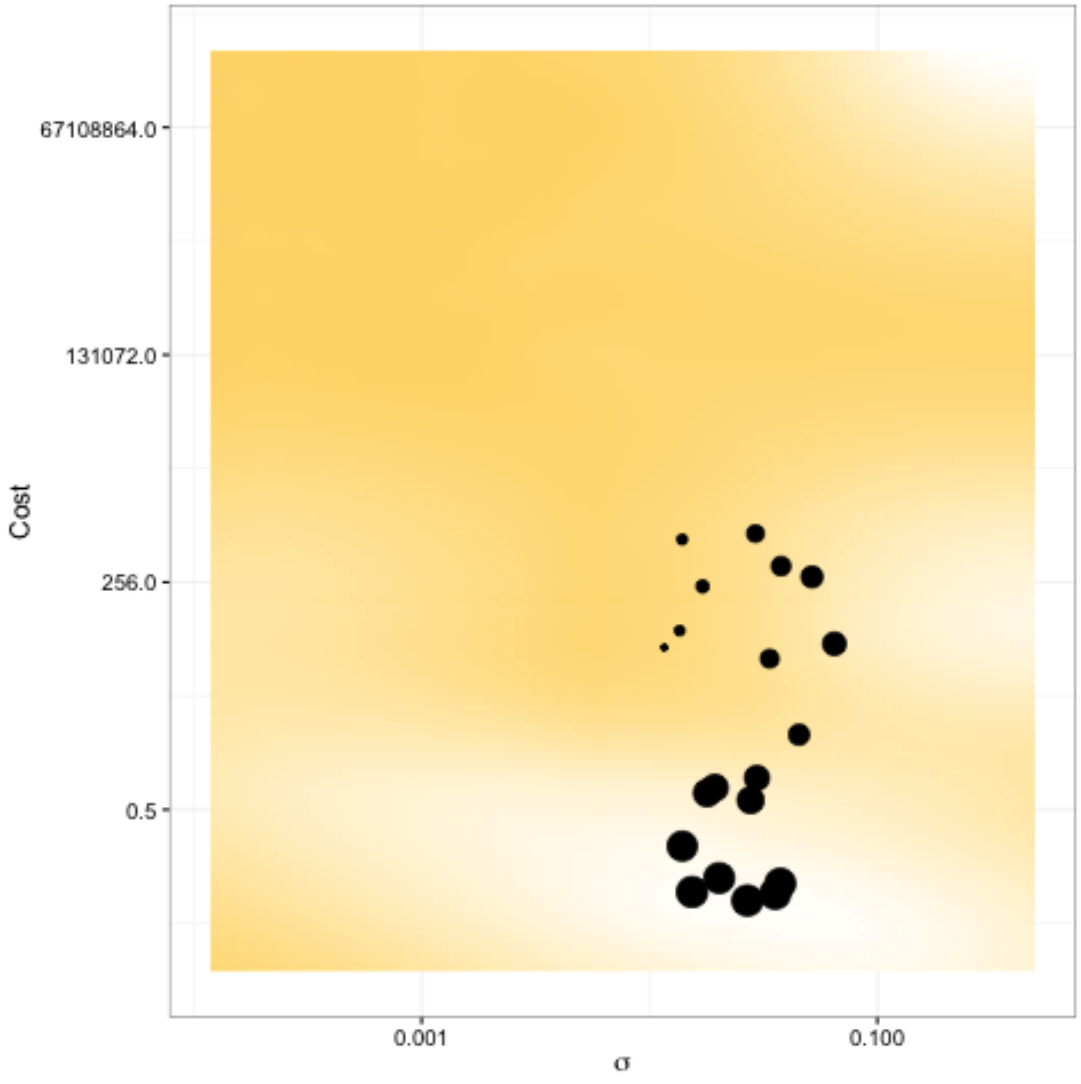
Example 1: GP predictive mean (based on initial random search)



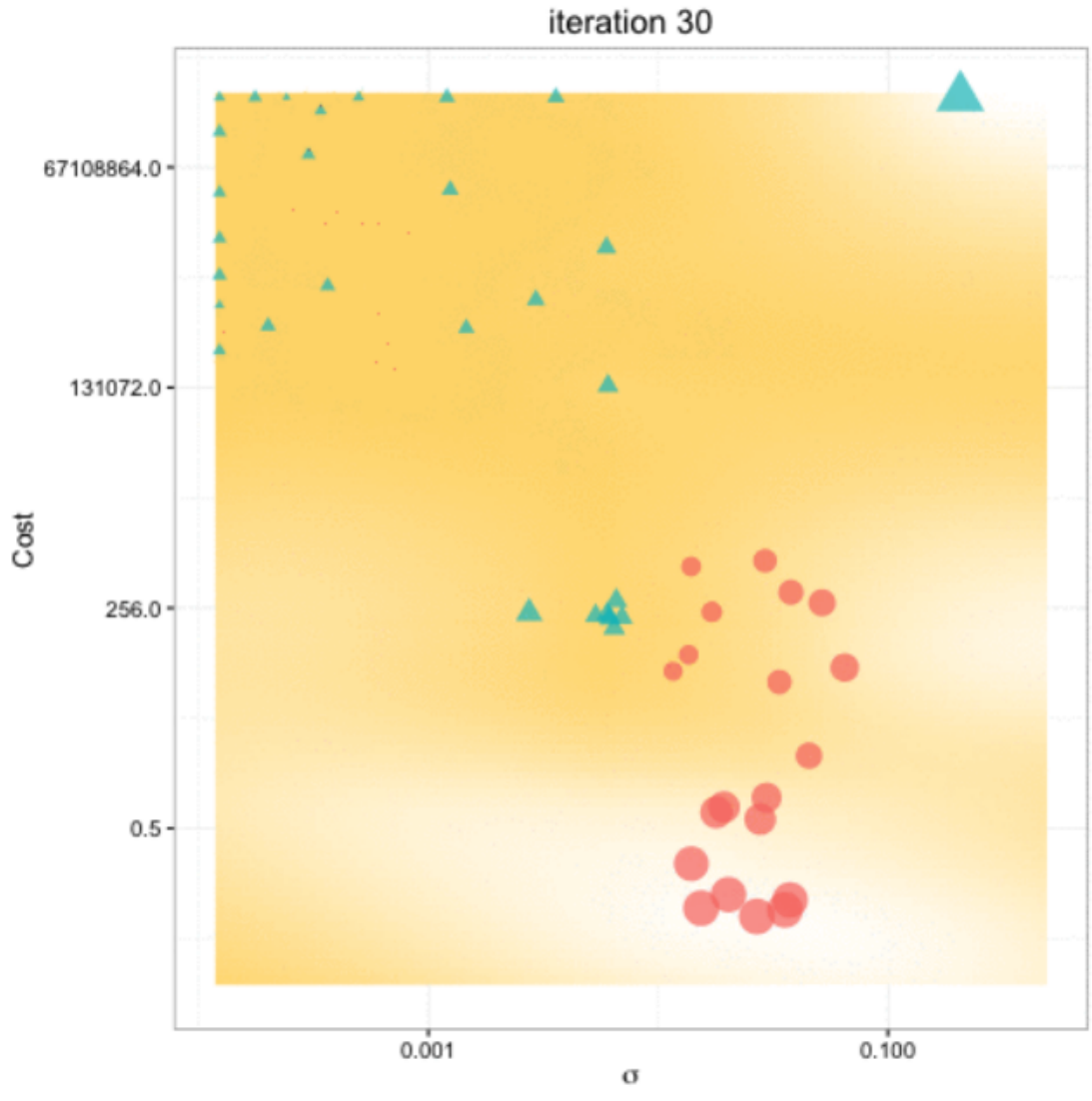
Example 1: GP predictive variance (based on initial random search)



Example 1: GP-UCB (based on initial random search)



Example 1: GP-UCB solution after 30 evaluations



Example 2: Tuning the Random forest hyperparameters

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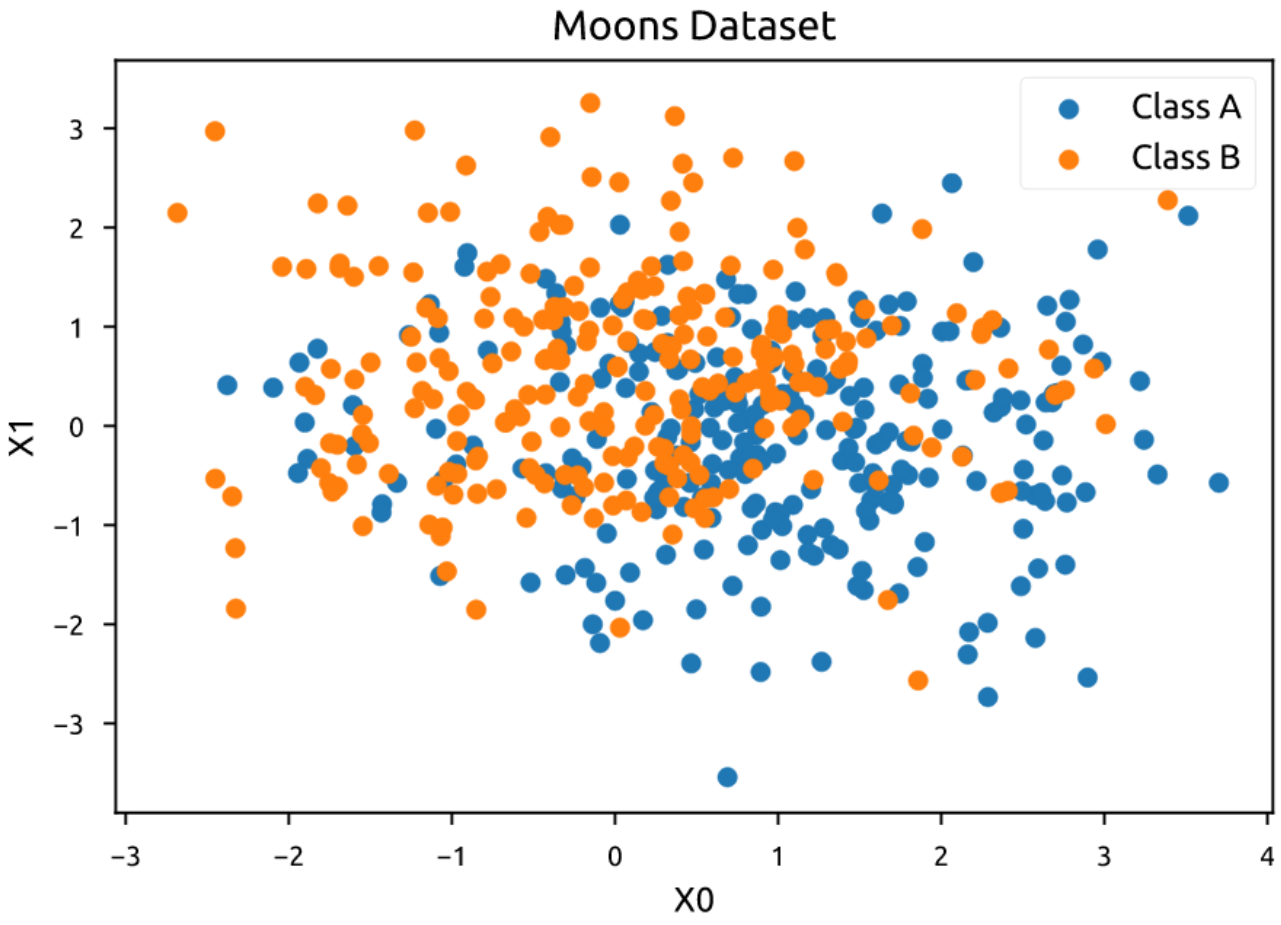
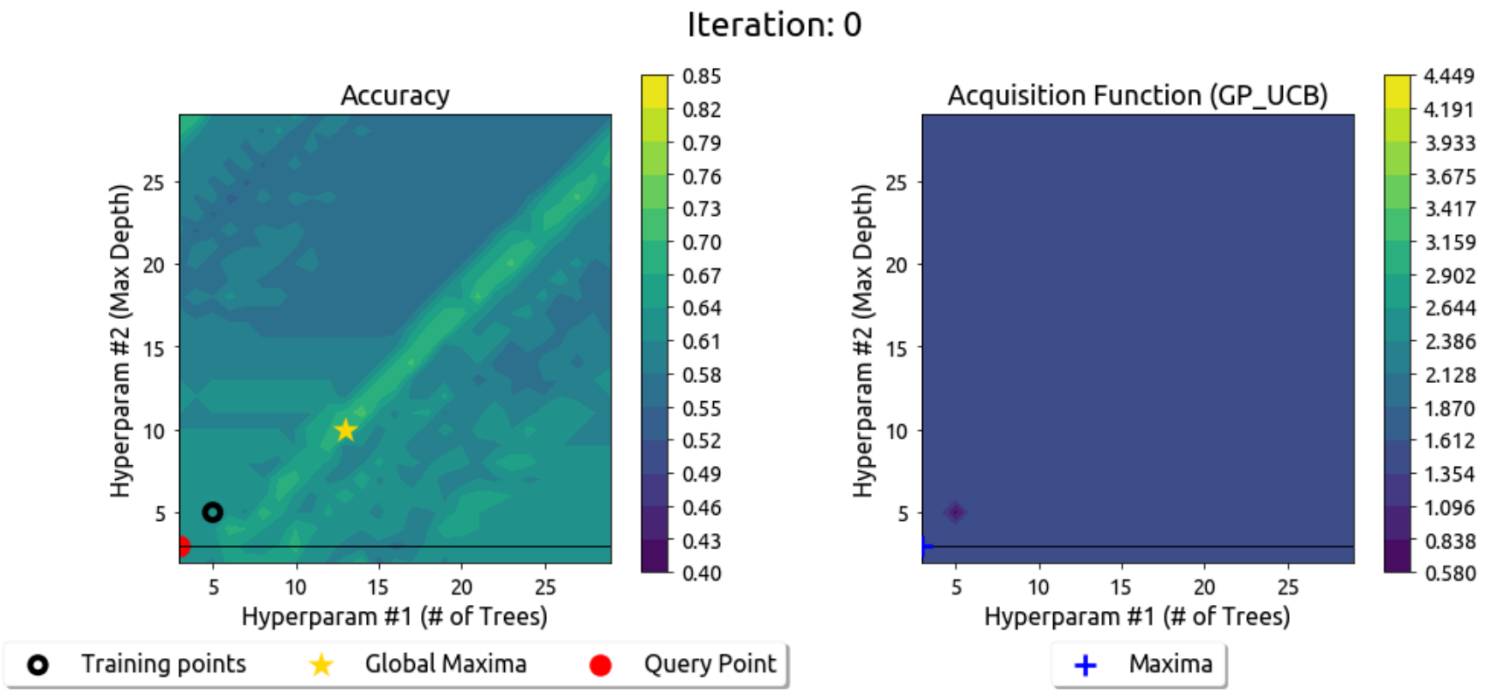
- example: Distill

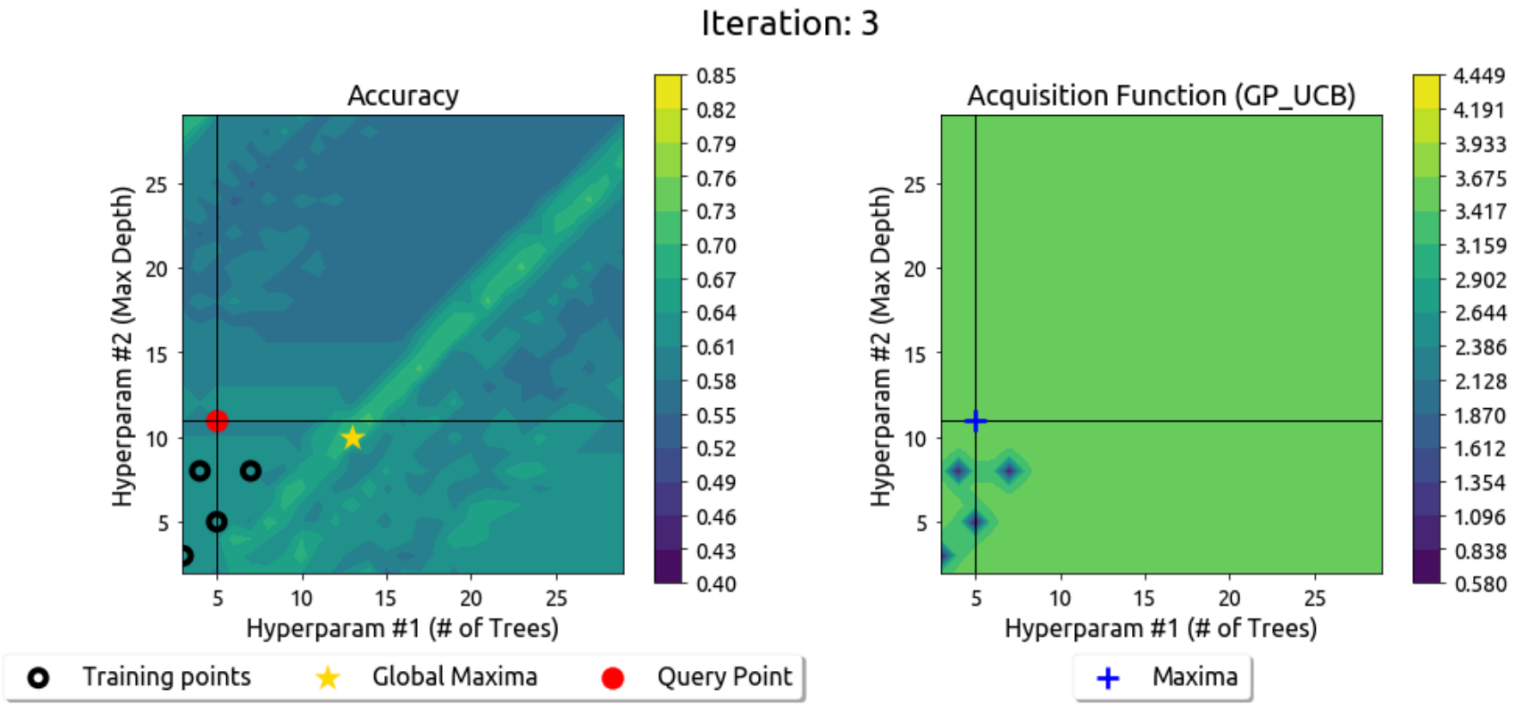
Example 2: Dataset



Example 2: GP-UCB solution after 0 evaluations



Example 2: GP-UCB solution after 3 evaluations



Example 2: GP-UCB solution after 9 evaluations