AutoML: Bayesian Optimization for HPO

Overview of Bayesian Optimization

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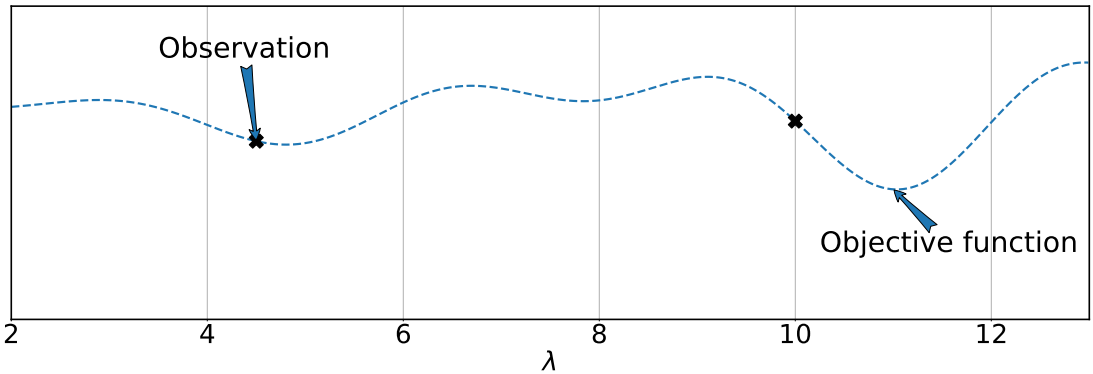
- Blackbox optimization can be used for hyperparameter optimization (HPO)
  - Define $f(\boldsymbol{\lambda}) := \mathcal{L}(\mathcal{A}_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$
  - Note: for formulations of HPO that go beyond blackbox optimization, see next lecture

Bayesian Optimization of a blackbox function in a nutshell



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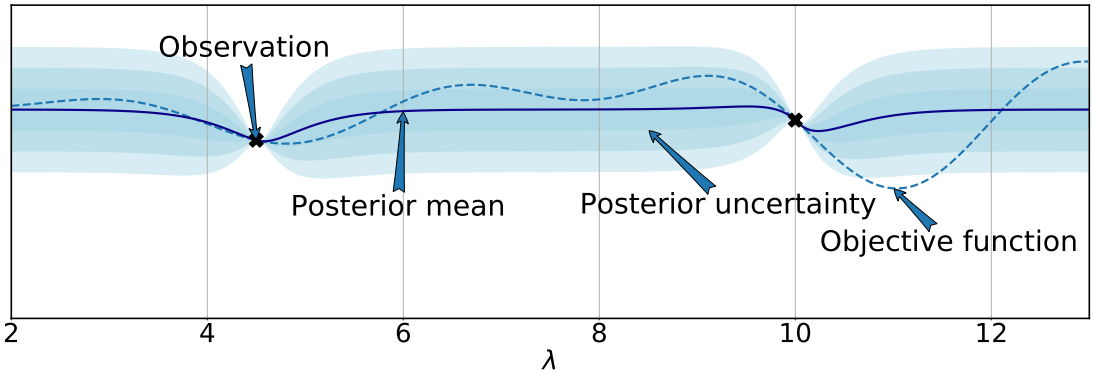

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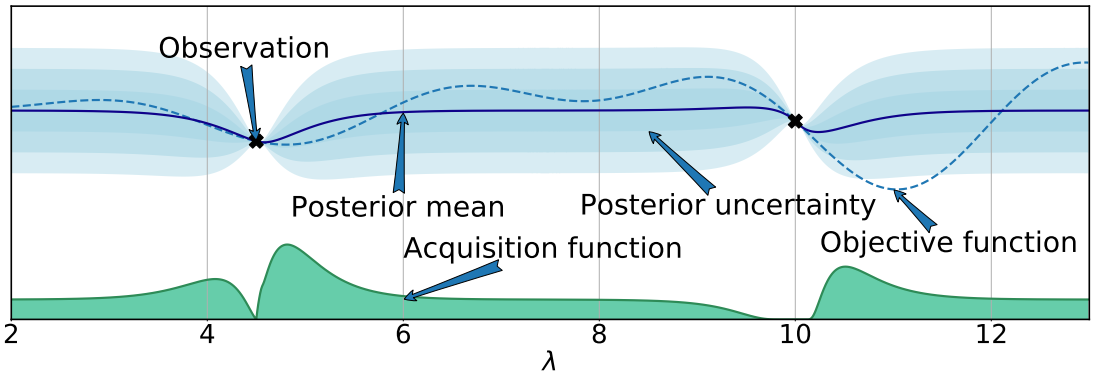

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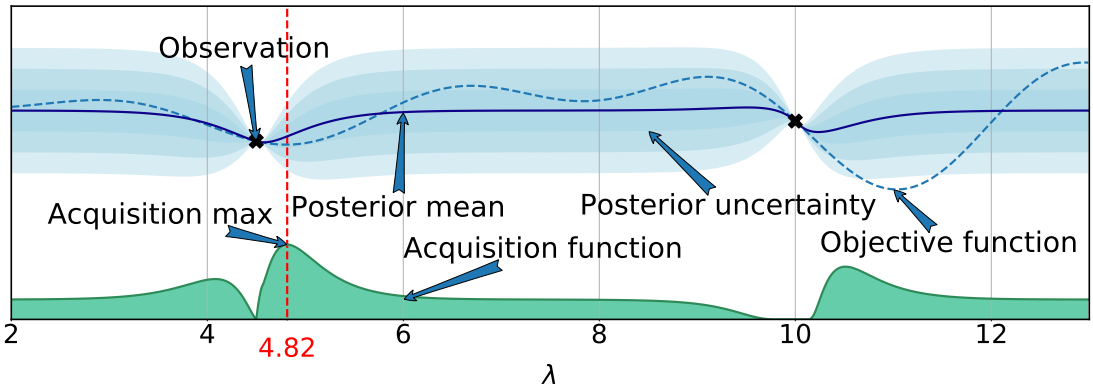
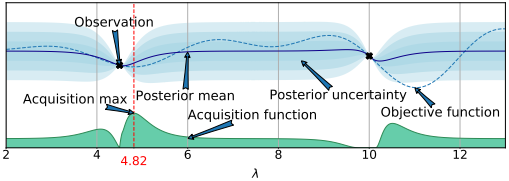


Bayesian Optimization of a blackbox function in a nutshell

General approach

- Fit a probabilistic model to the collected function samples $\langle \boldsymbol{\lambda}, c(\boldsymbol{\lambda}) \rangle$
- Use the model to guide optimization, trading off exploration *vs* exploitation



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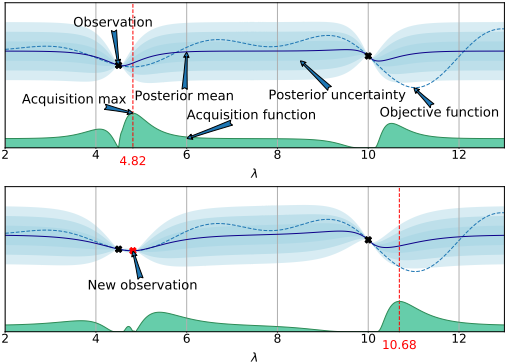

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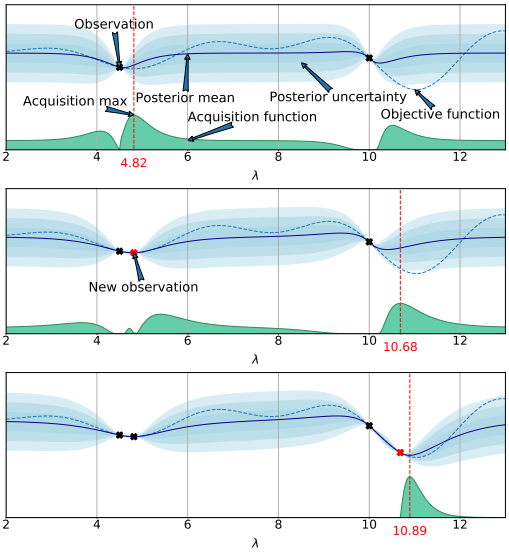

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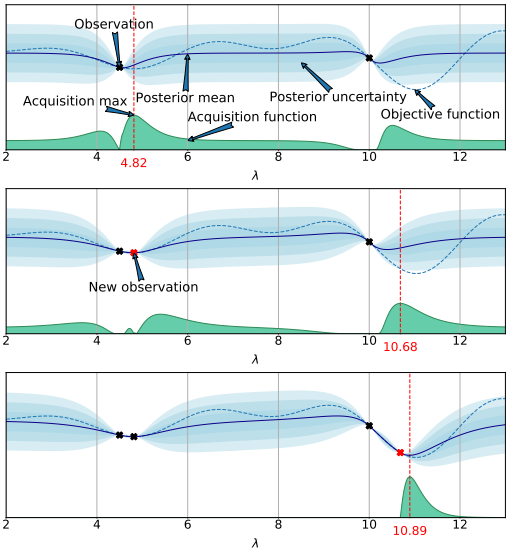
Popular approach in the statistics literature since Mockus et al. [1978]

- Efficient in #function evaluations
- Works when objective is nonconvex, noisy, has unknown derivatives, etc.
- Recent convergence results
  [Srinivas et al. 2009; Bull et al. 2011; de Freitas et al. 2012; Kawaguchi et al. 2015]



Bayesian Optimization: Pseudocode

BO loop

Require: Search space $\mathbf{\Lambda}$, cost function c, acquisition function u, predictive model $\hat{c}$, maximal number of function evaluations T

Result : Best configuration $\hat{\boldsymbol{\lambda}}$ (according to $\mathcal{D}$ or $\hat{c}$)

1 Initialize data $\mathcal{D}^{(0)}$ with initial observations

2 **for** $t = 1$ **to** T **do**

3 Fit predictive model $\hat{c}^{(t)}$ on $\mathcal{D}^{(t-1)}$

4 Select next query point: $\boldsymbol{\lambda}^{(t)} \in \arg\max_{\boldsymbol{\lambda} \in \mathbf{\Lambda}} u(\boldsymbol{\lambda}; \mathcal{D}^{(t-1)}, \hat{c}^{(t)})$

5 Query $c(\boldsymbol{\lambda}^{(t)})$

6 Update data: $\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{\lambda}^{(t)}, c(\boldsymbol{\lambda}^{(t)}) \rangle\}$

Bayesian Optimization: Origin of the Name

- Bayesian optimization uses Bayes' theorem:

$$P(A|B) = \frac{P(B|A) \times P(A)}{P(B)} \propto P(B|A) \times P(A)$$

- Bayesian optimization uses this to compute a posterior over functions:

$$P(f|\mathcal{D}_{1:t}) \propto P(\mathcal{D}_{1:t}|f) \times P(f), \qquad \text{where } \mathcal{D}_{1:t} = \{\boldsymbol{\lambda}_{1:t}, c(\boldsymbol{\lambda}_{1:t})\}$$

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- Meaning of the individual terms:
  - $P(f)$ is the prior over functions, which represents our belief about the space of possible objective functions before we see any data
  - $\mathcal{D}_{1:t}$ is the data (or observations, evidence)
  - $P(\mathcal{D}_{1:t}|f)$ is the likelihood of the data given a function
  - $P(f|\mathcal{D}_{1:t})$ is the posterior probability over functions given the data

Bayesian Optimization: Advantages and Disadvantages

Advantages

- Sample efficient
- Can handle noise
- Native incorporation of priors
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Disadvantages

- Overhead because of model training in each iteration
- Crucially relies on robust surrogate model

Questions to Answer for Yourself / Discuss with Friends

- Repetition. What is Bayesian about Bayesian optimization?
- Repetition. Write down the steps of the BO loop.
- Discussion. Can you think of an expensive blackbox optimization problem other than hyperparameter optimization?

Learning Goals of this Lecture

After this lecture, students can ...

- Explain the basics of Bayesian optimization
- Derive simple acquisition functions
- Describe complex lookahead acquisition functions
- Describe possible surrogate models and their pros and cons
- Discuss the limits of Bayesian optimization and extensions to tackle these
- Discuss success stories of Bayesian optimization