Efficient algorithm design via automated algorithm selection and configuration

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Euro PhD School Data Science Meets Combinatorial Optimisation

Story Line This Session

- What do we optimize?
  - Parameters vs. Hyperparameters
  - Challenges for AutoML
- How do we optimize it?
  - Grid Search
  - Random Search
- How do we optimize it efficiently?
  - Bayesian Optimization
- How do we optimize across many problem instances?
  - Algorithm Configuration
  - Aggressive Racing
  - Other Racing Strategies
- Outlook and Software Packages

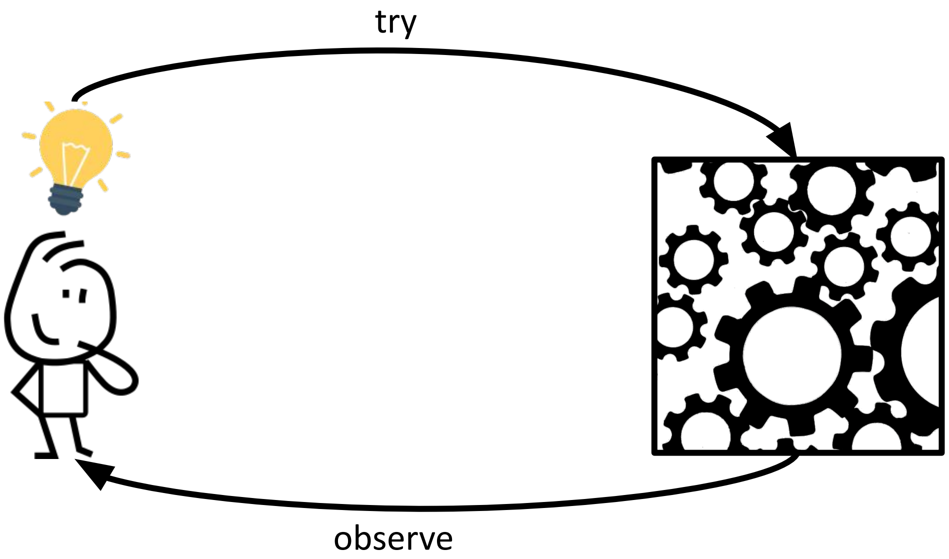
Note: This lecture is partially based on the free online lecture "Automated Machine Learning" at https://learn.ki-campus.org/courses/automl-luh2021

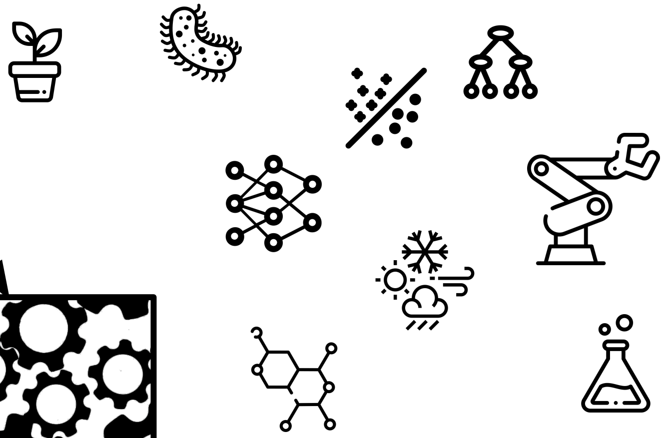
- Basics of HPO
- Bayesian Optimization for HPO

What do we optimize?

>> Here's my algorithm and data, what should I do?

Sequential Experimentation

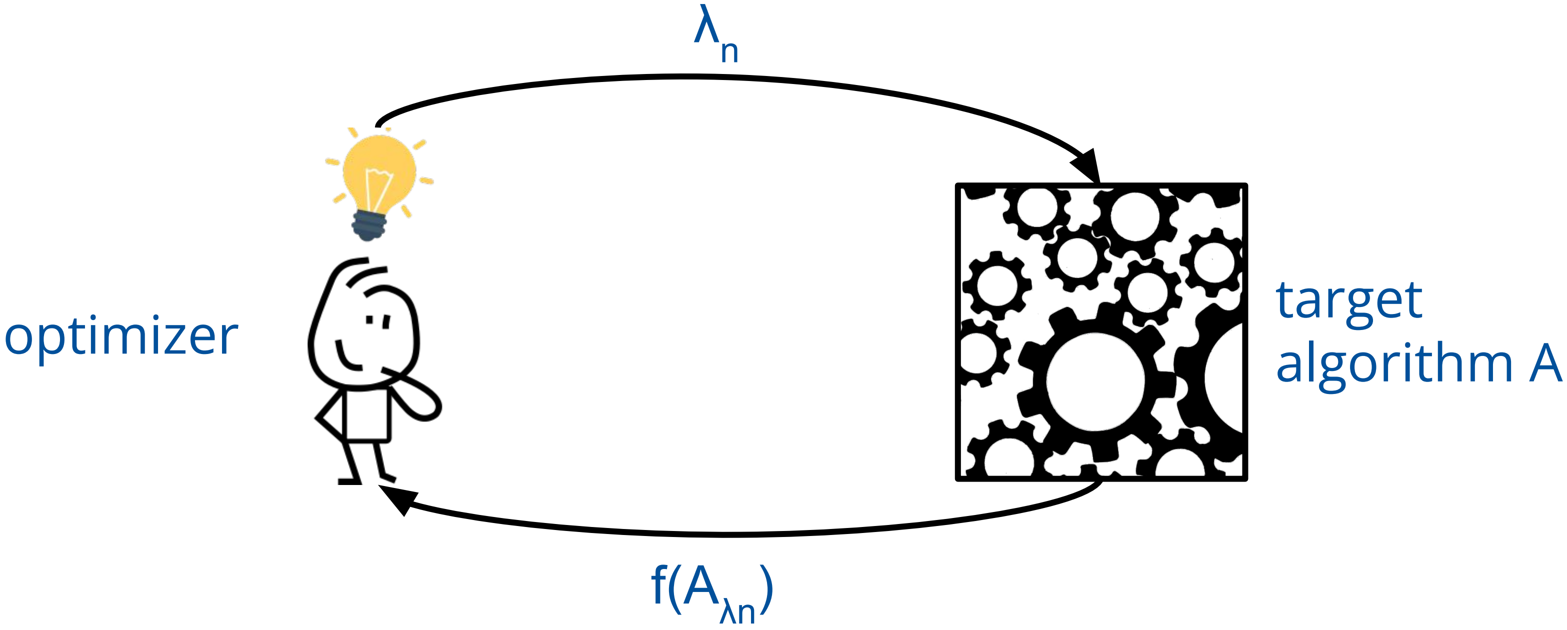




- Algorithm
- Neural Architecture
- Network Training
- Data Science Pipeline
- Simulator
- Robot

Hyperparameter Optimization

Goal: Find the best performing configuration: $\boxed{\lambda^* \in \arg\min_{\lambda \in \Lambda} f(\mathcal{A}_\lambda)}$



Example: Machine Learning

- **Given a dataset**, we want to train a neural network
- We need to choose a **learning rate and architecture**
- The “learner” takes the input data, and returns a fitted network

→ We are interested in **generalization error**!

→ We need to look at how our trained model **performs on “unseen” data**

→ We evaluate different settings and select the one that **performs best w.r.t generalization error**.

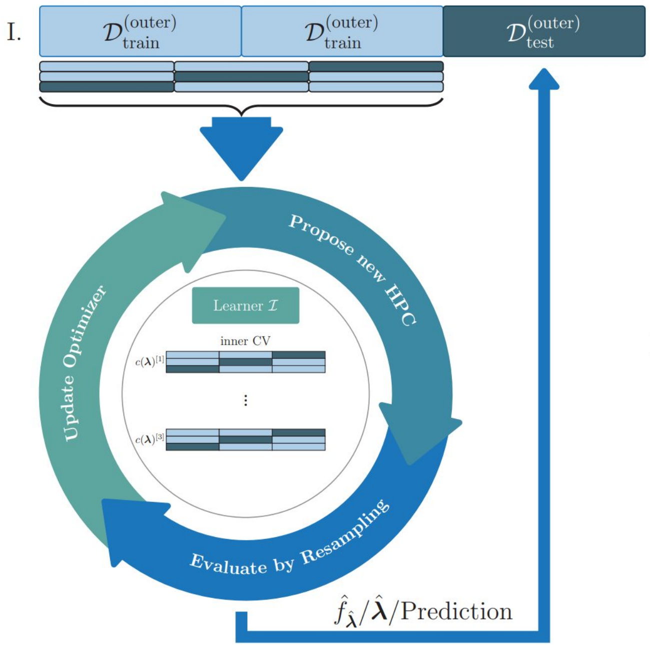


Image: Bischl et al. 2023

Hyperparameters and Parameters

Model parameters can be optimized during training and are the output of the training. Examples:

- Splits of a Decision Tree
- Weights of a Neural Network
- Coefficients of a linear model

Hyperparameters need to be set manually before training. They control the flexibility, structure and complexity of the model and training procedure. Examples:

- Max. depth of a Decision Tree
- Number of layers of a Neural Network
- K for K-Nearest Neighbours

Types of Algorithm Parameters (Hyperparameters)

Real-valued

- Learning rate for SGD to train NNs
- Bandwidth of kernel density estimates in Naive Bayes

Integer

- #Neurons in a layer of a NN
- maximum depth of a Decision Tree

Categorical

- Training Algorithm for NNs
- Split criterion for Decision Trees

Can also be on a log-scale

+ Hyperparameters can be **hierarchically dependent** on each other

Why is Hyperparameter Optimization Challenging?

Goal: Find the best performing configuration:

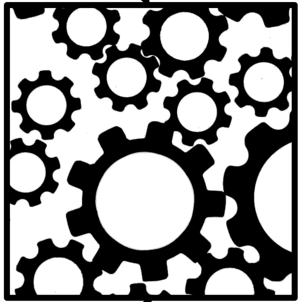
$$\boxed{\lambda^* \in \arg\min_{\lambda \in \Lambda} f(\mathcal{A}_\lambda)}$$

complex search space

No gradients
No prior knowledge

λ_n

optimizer



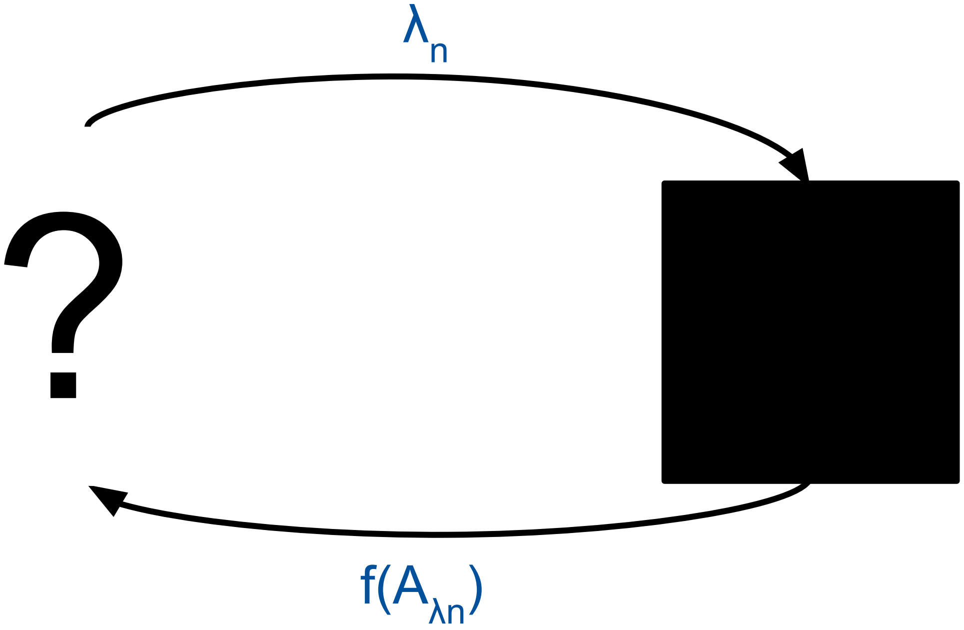
target algorithm A

$f(A_{\lambda n})$

noisy
expensive-to-evaluate

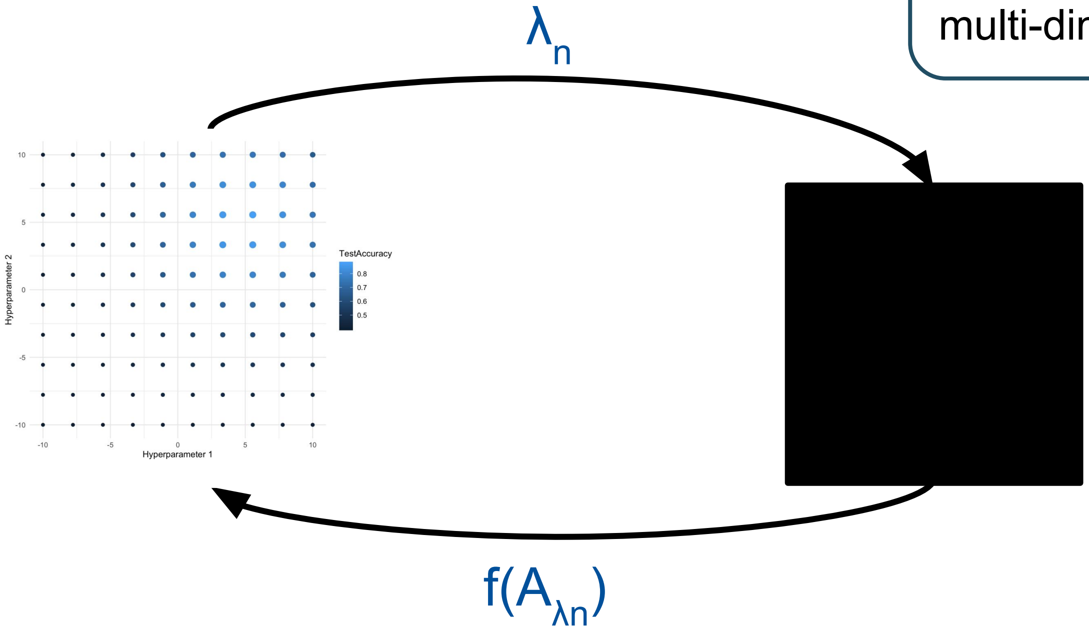
How do we optimize it?

Black-Box Optimization Problem

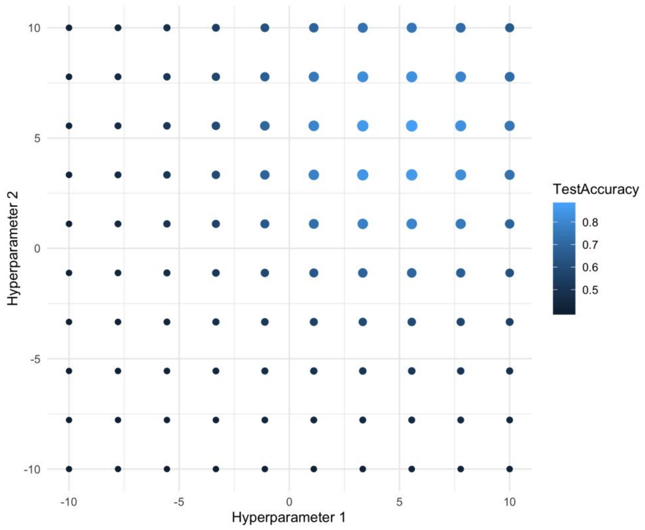


Option 1: Grid Search

Popular technique: Evaluates all combinations on a pre-defined multi-dimensional grid



Option 1: Grid Search II



Advantages

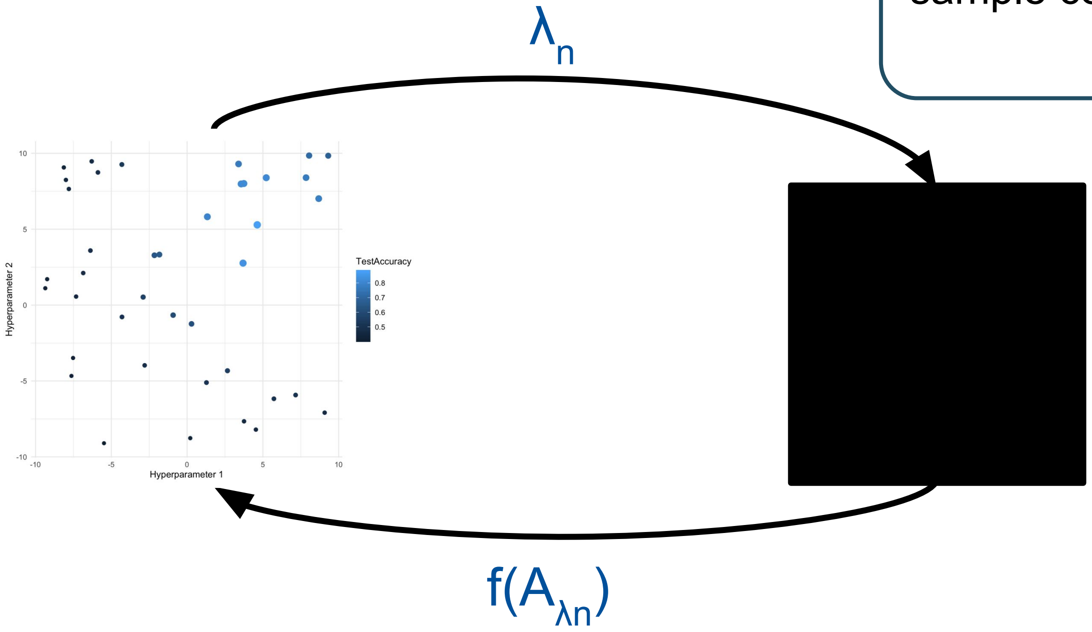
- Very easy to implement
- Very easy to parallelize
- Can handle all types of hyperparameters

Disadvantages

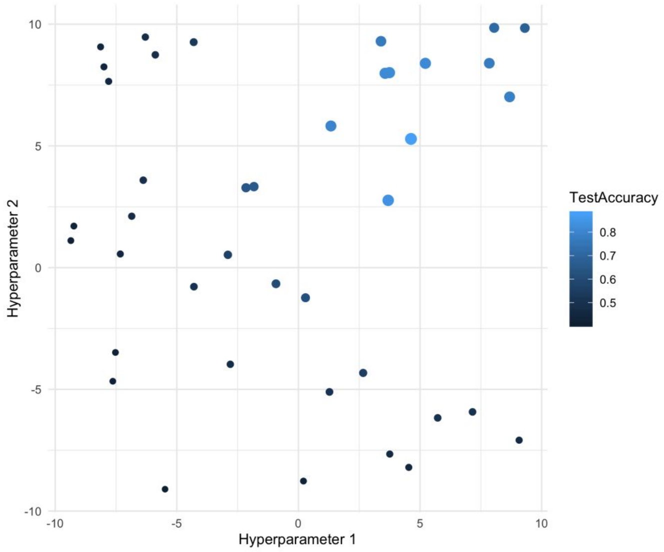
- Scales badly with #dimensions
- Inefficient: Searches irrelevant areas
- Requires to manual define discretization
- All grid points need to be evaluated

Option 2: Random Search

Variation of Grid Search: Uniformly sample configurations at random



Option 2: Random Search II



Advantages

- Very easy to implement
- Very easy to parallelize
- Can handle all types of hyperparameters
- No discretization required
- Anytime algorithm: Can be stopped and continued based on the available budget and performance goal.

Disadvantages

- Scales badly with #dimensions
- Inefficient: Searches irrelevant areas

Grid Search vs. Random Search

With a **budget** of T iterations:

Grid Search evaluates only $T^{\frac{1}{d}}$ unique values per dimension

Random Search evaluates (most likely) T different values per dimension

→ Grid search can be disadvantageous if some hyperparameters have little of no impact on the performance [Bergstra et al. 2012]

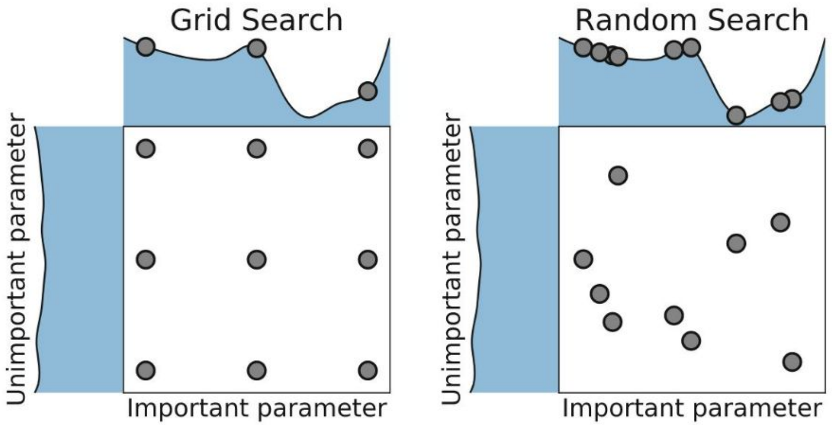


Image source: [Hutter et al. 2019]

Questions?

Kahoot Quiz I

How do we optimize it efficiently?

Model-based Optimization

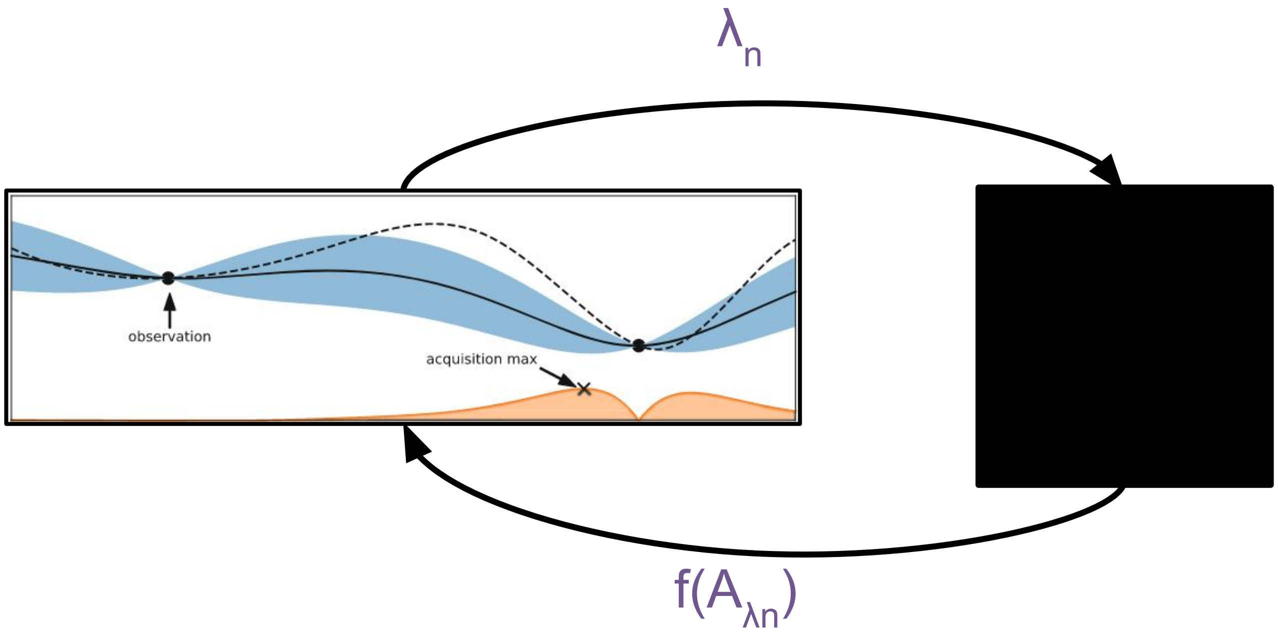
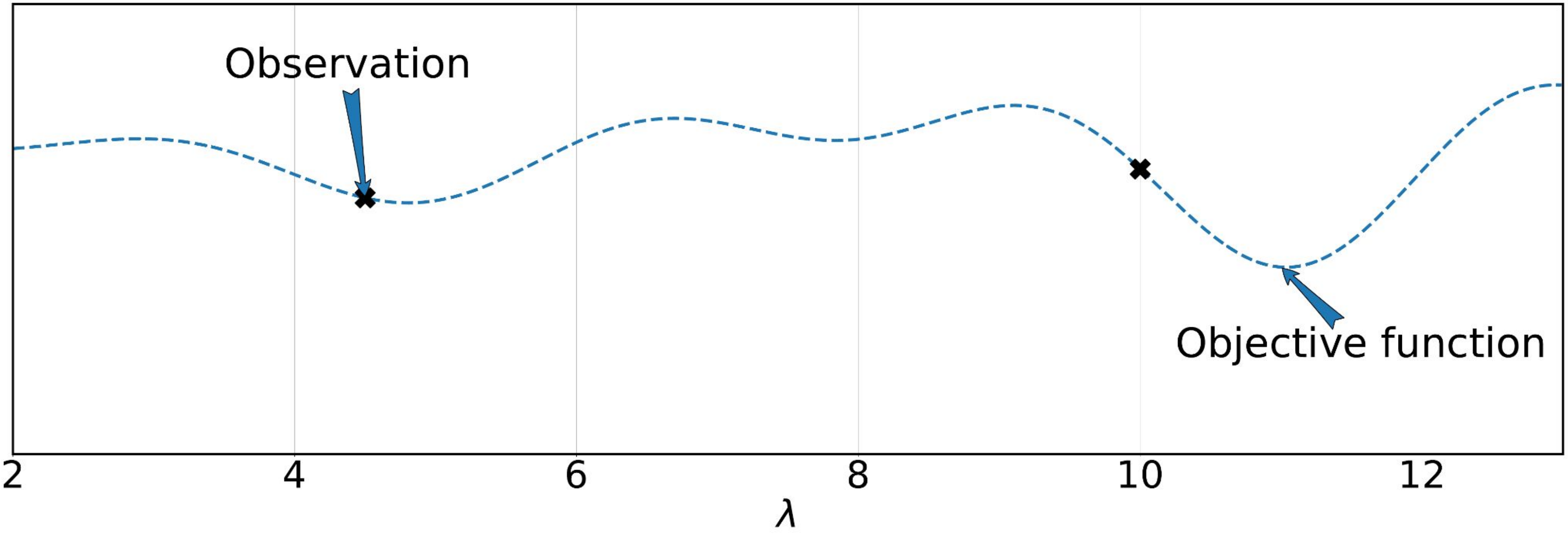


Photo by Wilhelm Gunkel on Unsplash
Image by Feurer, Hutter: Hyperparameter Optimization.
In: Automated Machine Learning

Bayesian Optimization in a Nutshell



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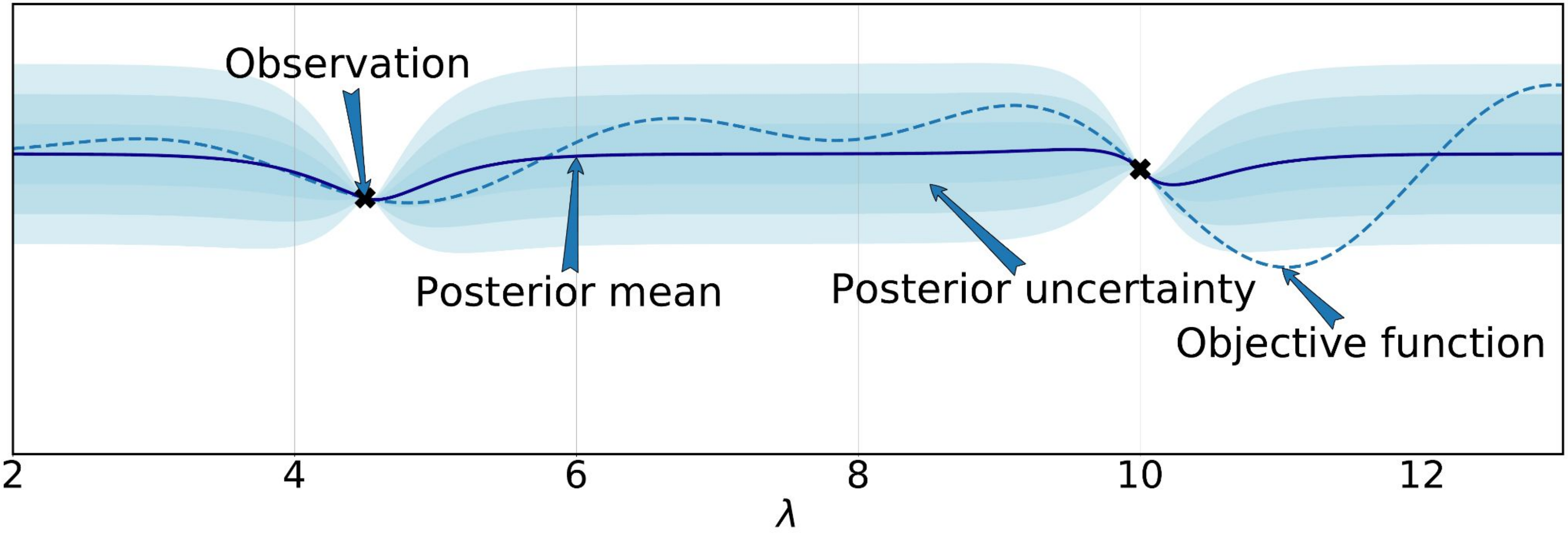

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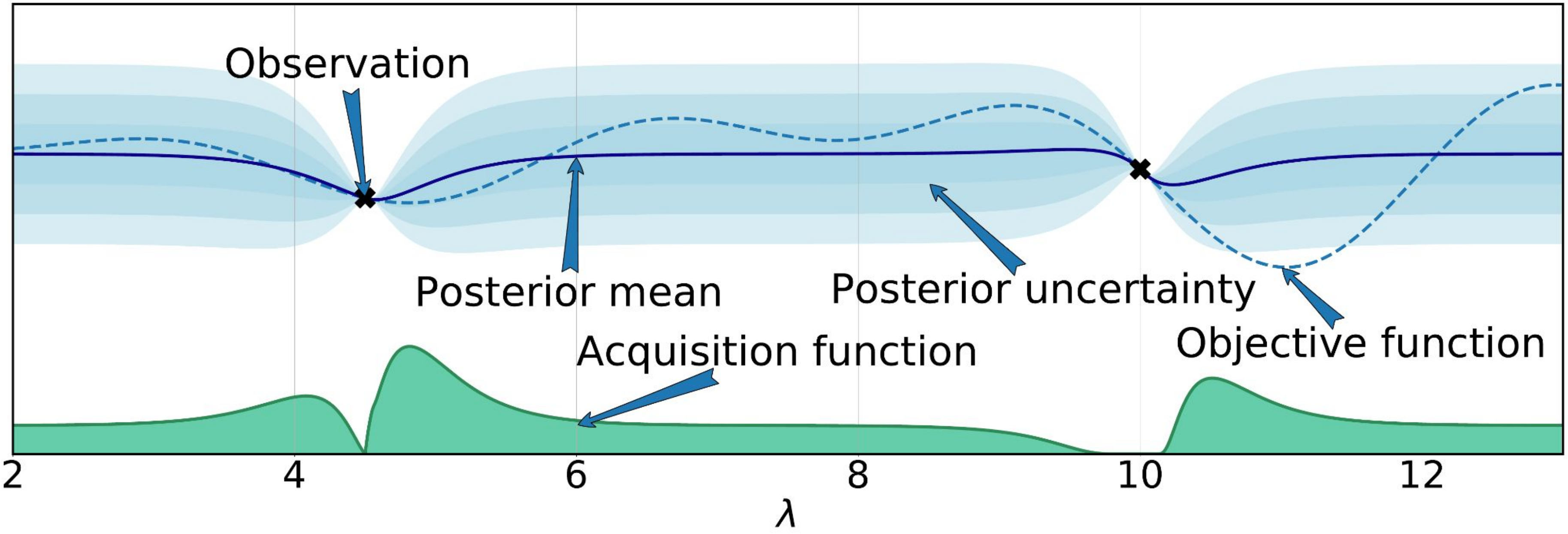

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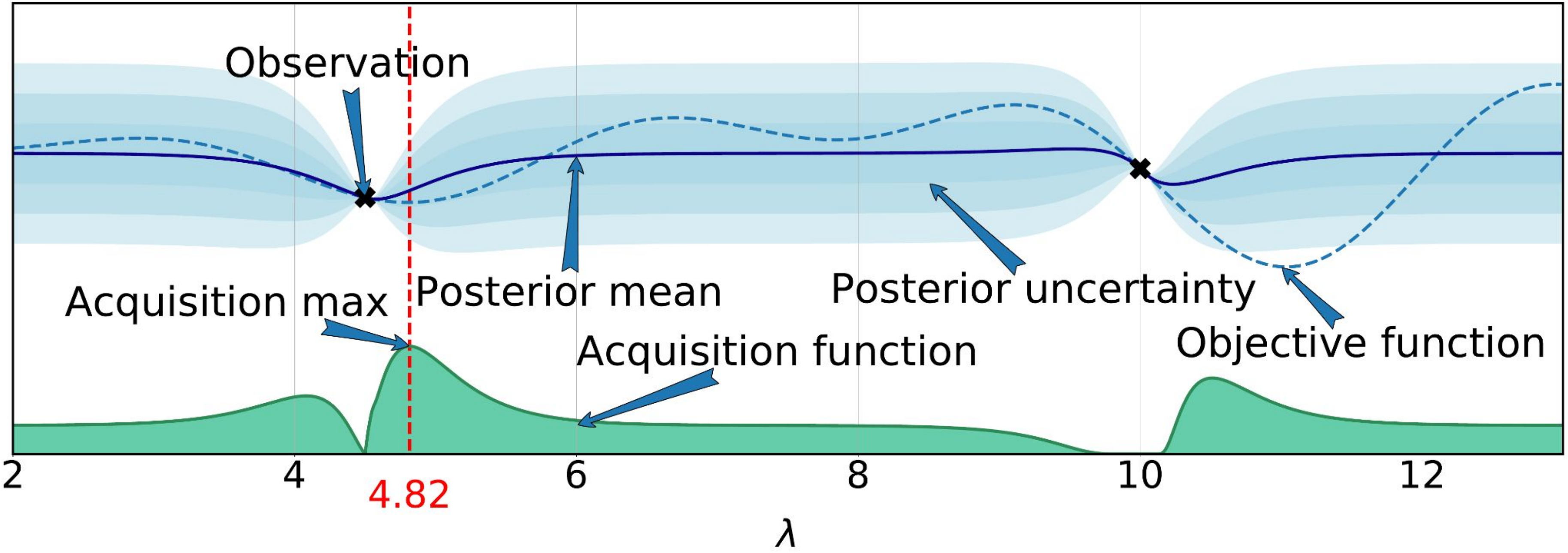


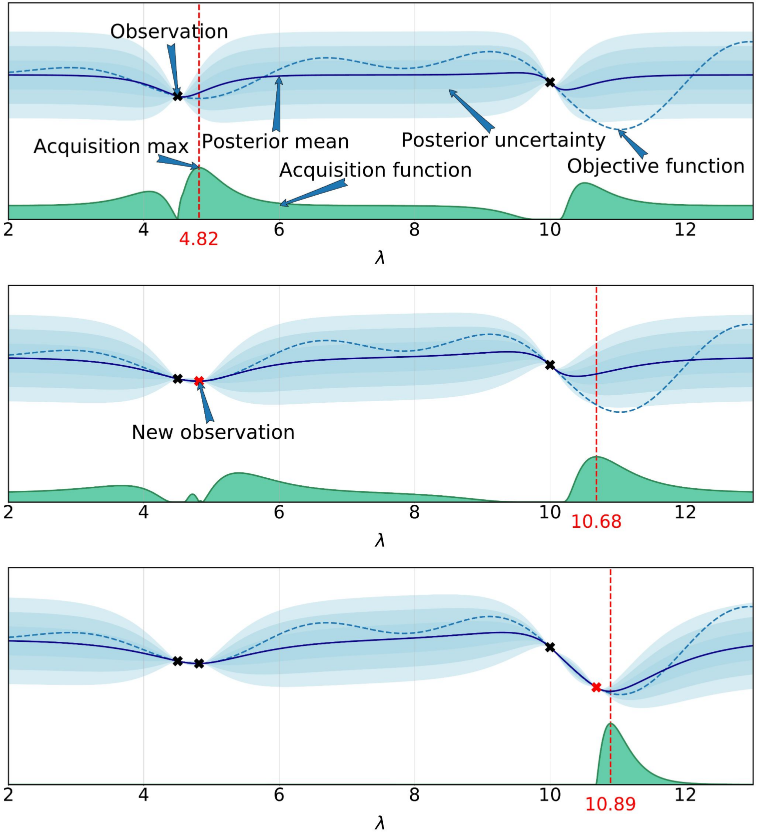
Bayesian Optimization in a Nutshell

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

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 Λ, cost function c, acquisition function u, predictive model ĉ, maximal number of function evaluations T
Result  : Best configuration λ̂ (according to D or ĉ)
Initialize data D^(0) with initial observations
for t = 1 to T do
    Fit predictive model ĉ^(t) on D^(t−1)
    Select next query point: λ^(t) ∈ arg max_{λ∈Λ} u(λ; D^(t−1), ĉ^(t))
    Query c(λ^(t))
    Update data: D^(t) ← D^(t−1) ∪ {⟨λ^(t), c(λ^(t))⟩}
```

BO loop

Require: Search space $\boldsymbol{\Lambda}$, 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 $\hat{c}$)

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

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

- Fit predictive model $\hat{c}^{(t)}$ on $\mathcal{D}^{(t-1)}$
- Select next query point: $\boldsymbol{\lambda}^{(t)} \in \arg\max_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} u(\boldsymbol{\lambda}; \mathcal{D}^{(t-1)}, \hat{c}^{(t)})$
- Query $c(\boldsymbol{\lambda}^{(t)})$
- Update data: $\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{\lambda}^{(t)}, c(\boldsymbol{\lambda}^{(t)})\rangle\}$

Why is it called Bayesian Optimization?

- 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:

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

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: Pros and Cons

Advantages

- Sample efficient
- Can handle noise
- Priors can be incorporated
- Does not require gradients
- Theoretical guarantees

Many extensions available:
Multi-Objective | Multi-Fidelity |
Parallelization | Warmstarting | etc.

Disadvantages

- Overhead because of model training
- Crucially relies on robust surrogate model
- Has quite a few design decisions

Main Ingredient I: The Acquisition Function

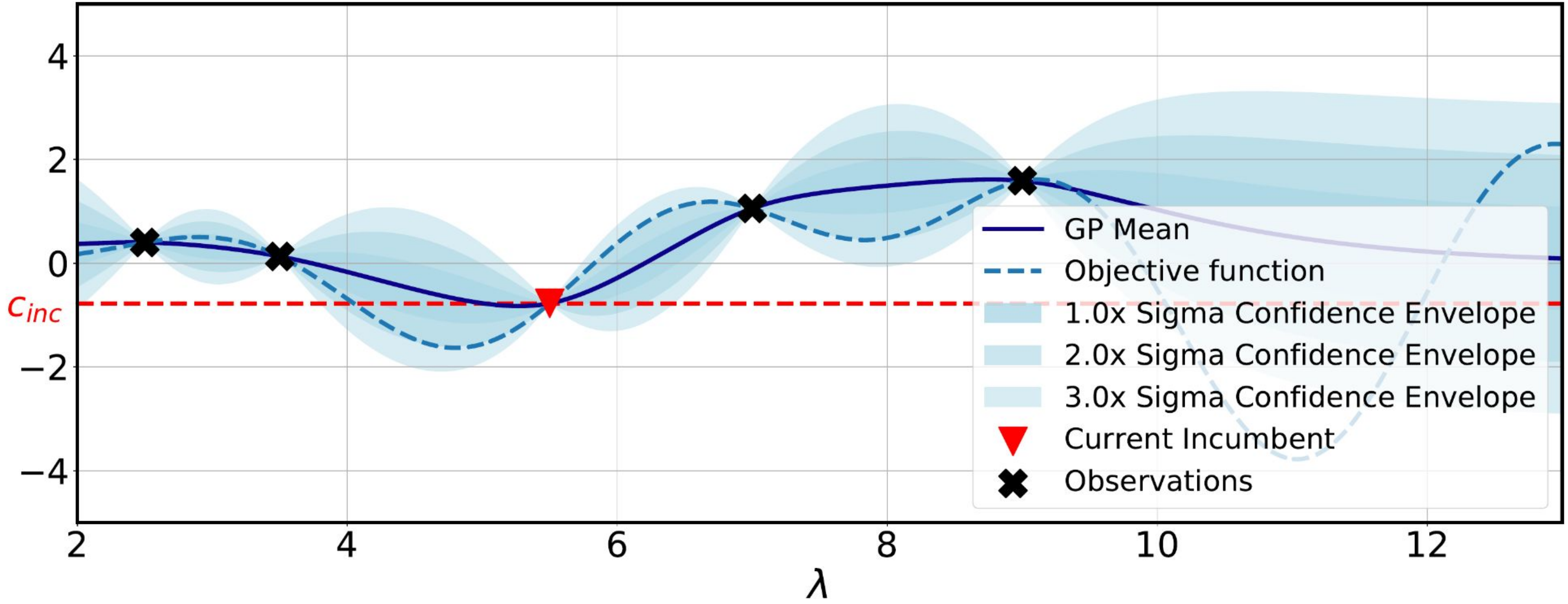
The acquisition function

- decides which configuration to evaluate next
- judges the **utility** (or **usefulness**) of evaluating a configuration (based on the surrogate model)

→ It needs to trade-off **exploration and exploitation**

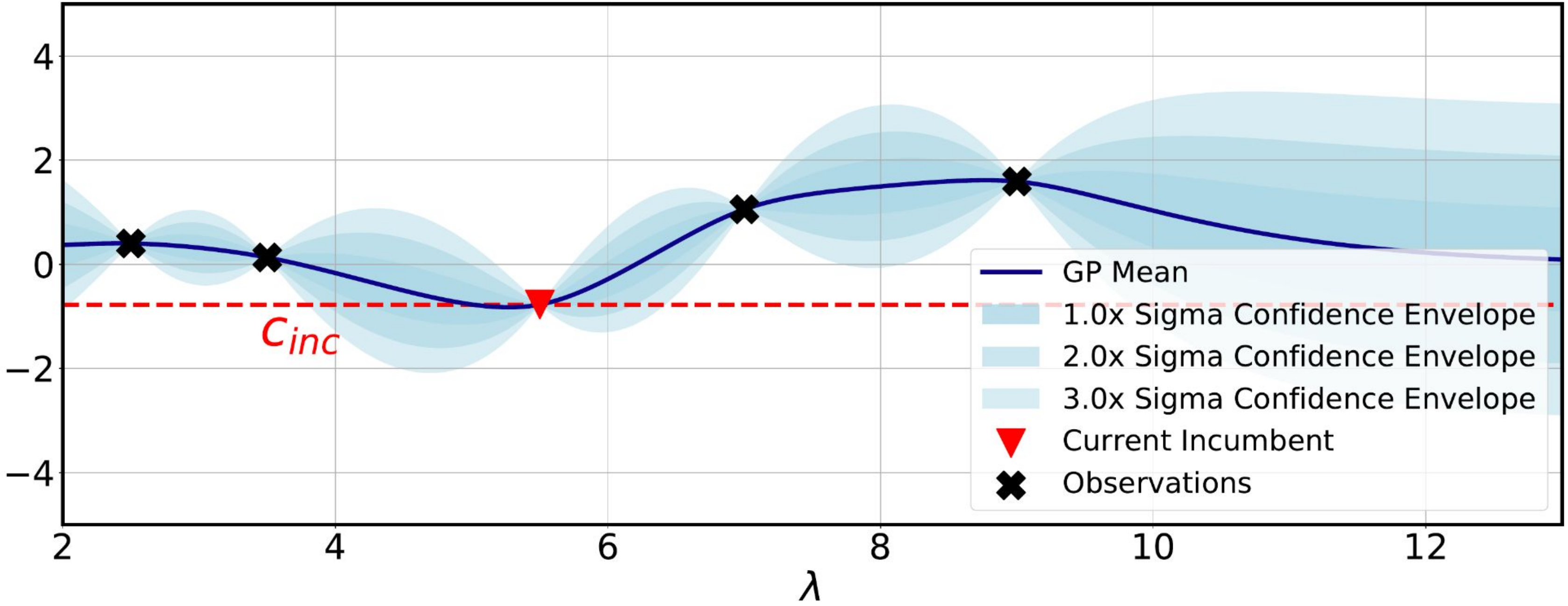
- Just picking the configuration with the lowest prediction would be too greedy
- It needs to consider the uncertainty of the surrogate model

Expected Improvement (EI)



Given some observations and a fitted surrogate,

Expected Improvement (EI)



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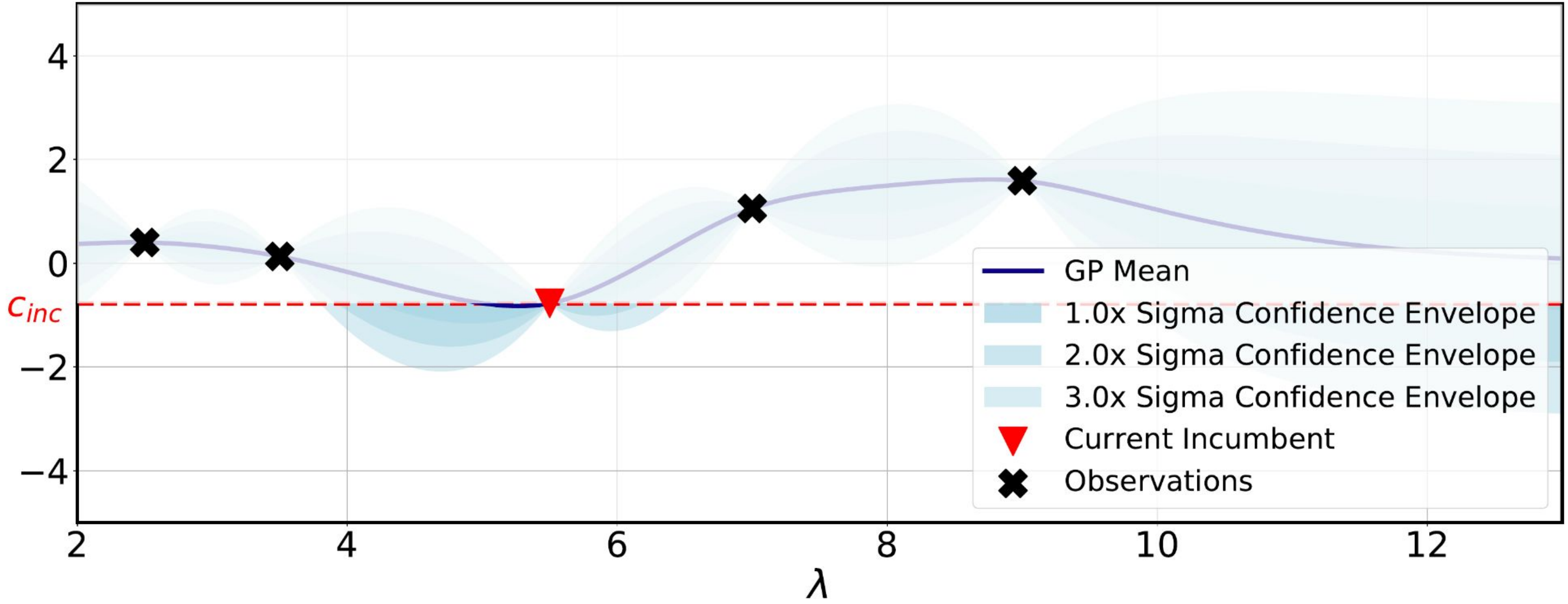
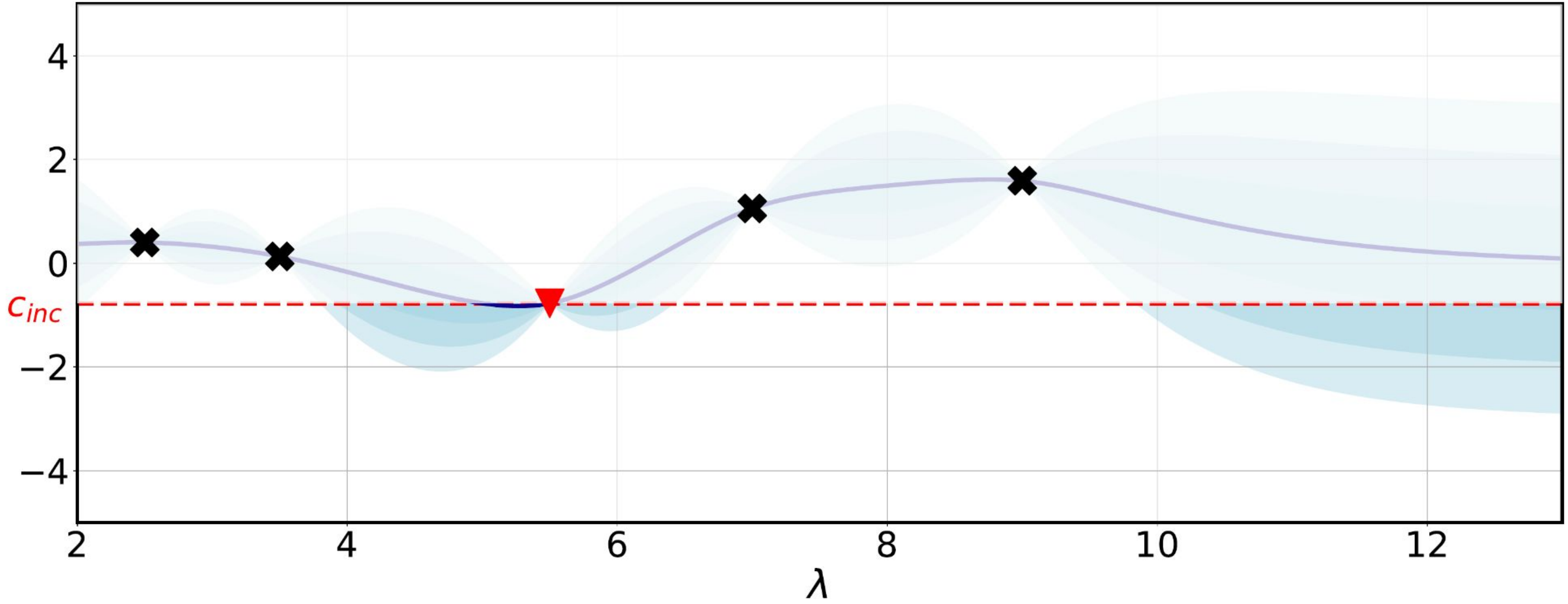


We care about *improving* over the c_{inc}.

Expected Improvement (EI)



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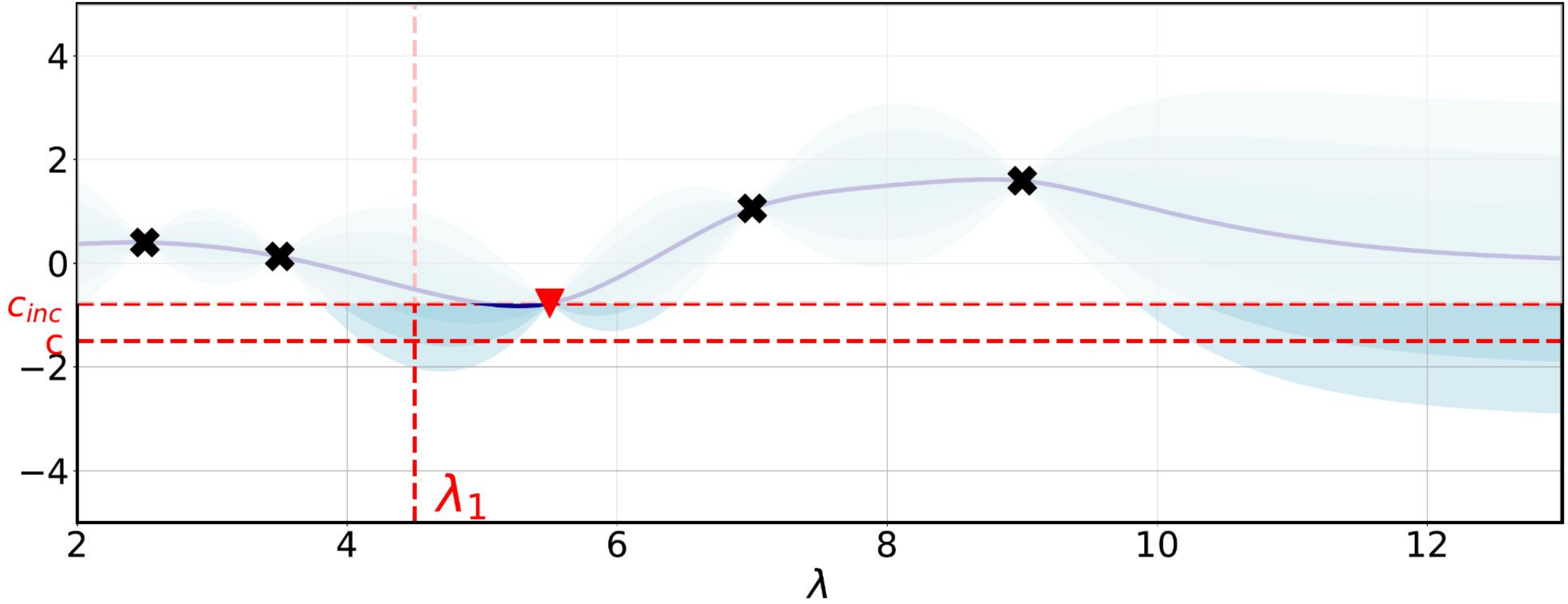
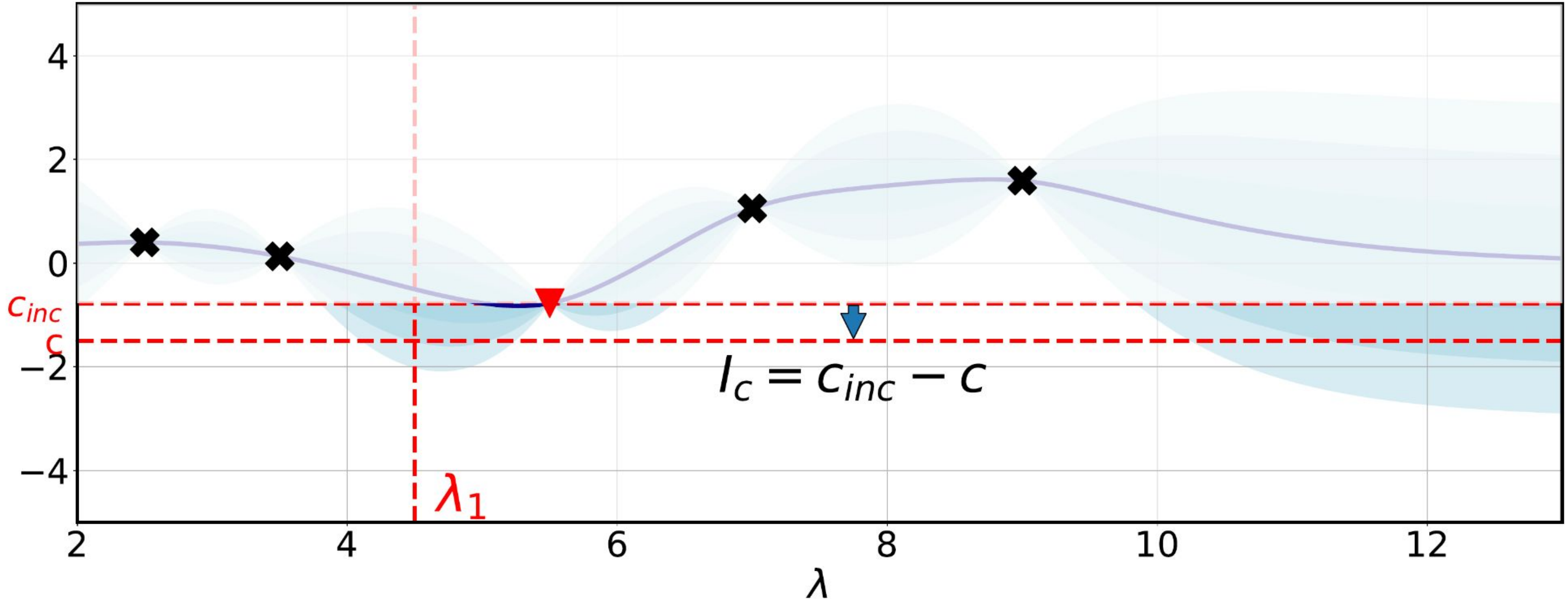


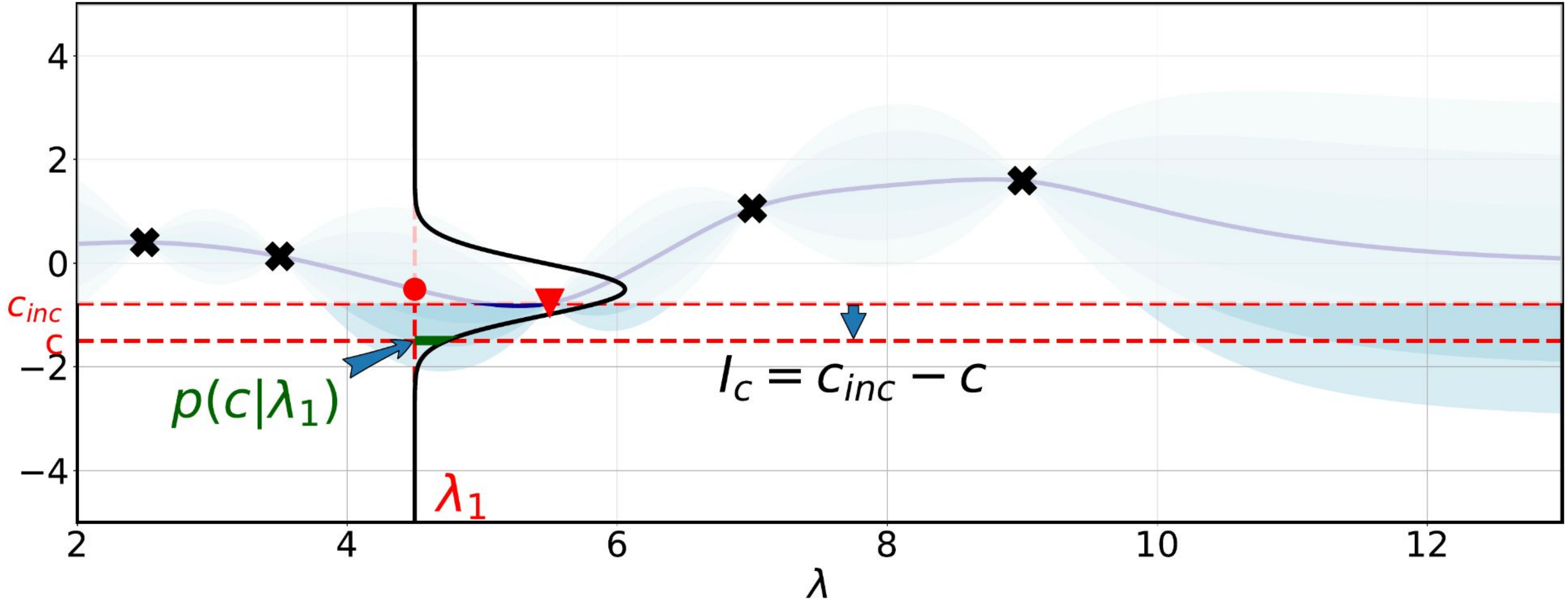
Let's look at a candidate configuration λ_1 and its hypothetical cost c.

Expected Improvement (EI)



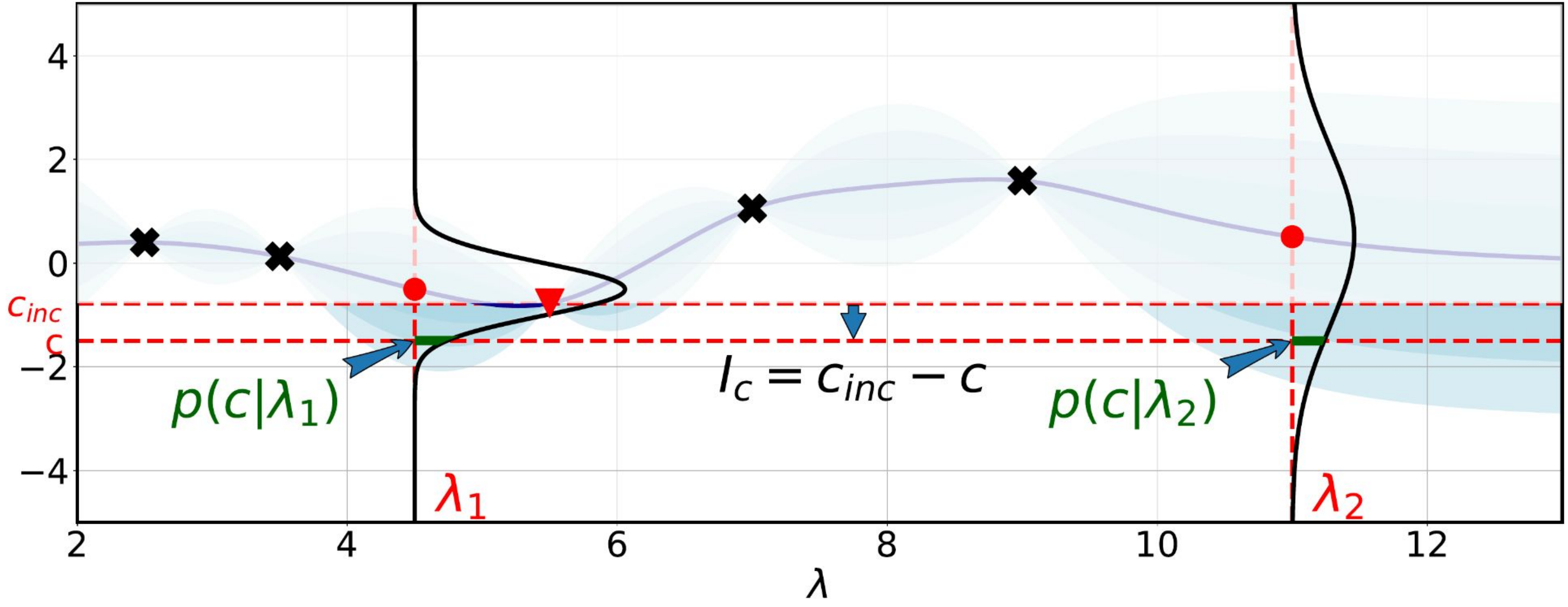
We can compute the improvement $I_c(\lambda_1)$. But how likely is it?

Expected Improvement (EI)



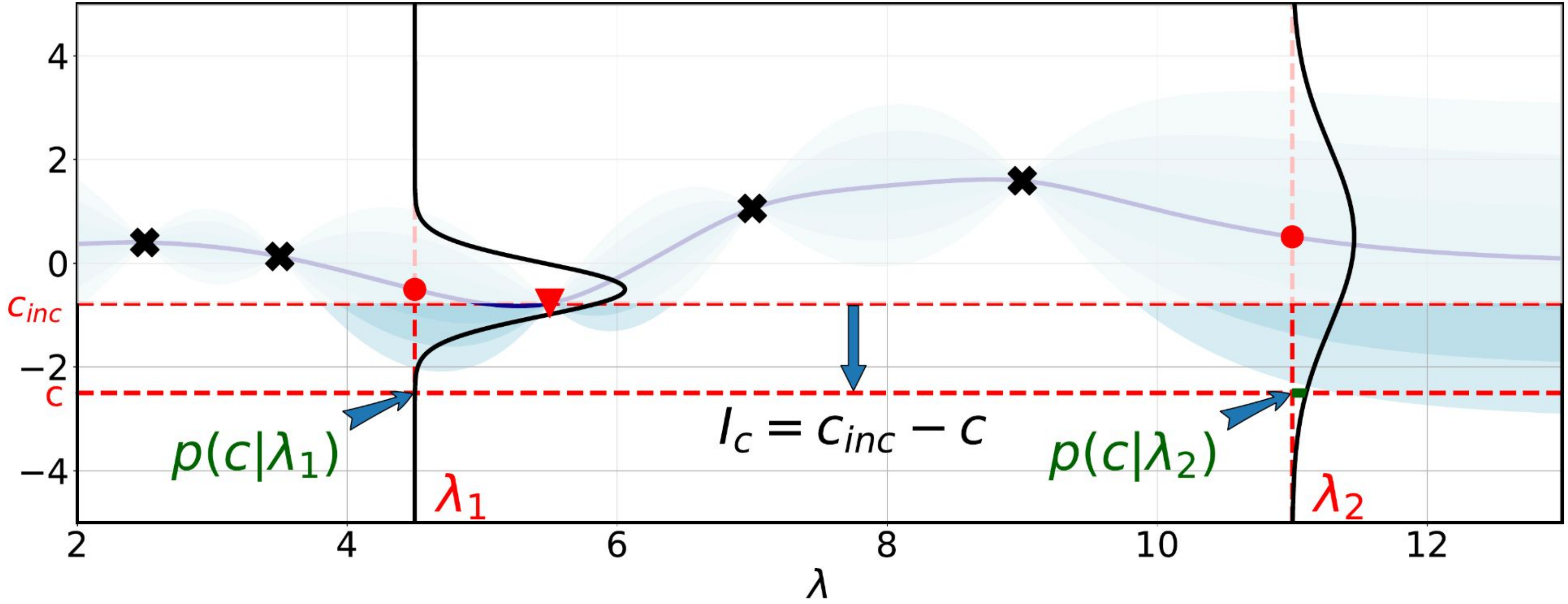
Knowing that $\hat{c}(\boldsymbol{\lambda}) = \mathcal{N}(\mu(\boldsymbol{\lambda}), \sigma^2(\boldsymbol{\lambda}))$, we can compute $p(c|\boldsymbol{\lambda})$

Expected Improvement (EI)



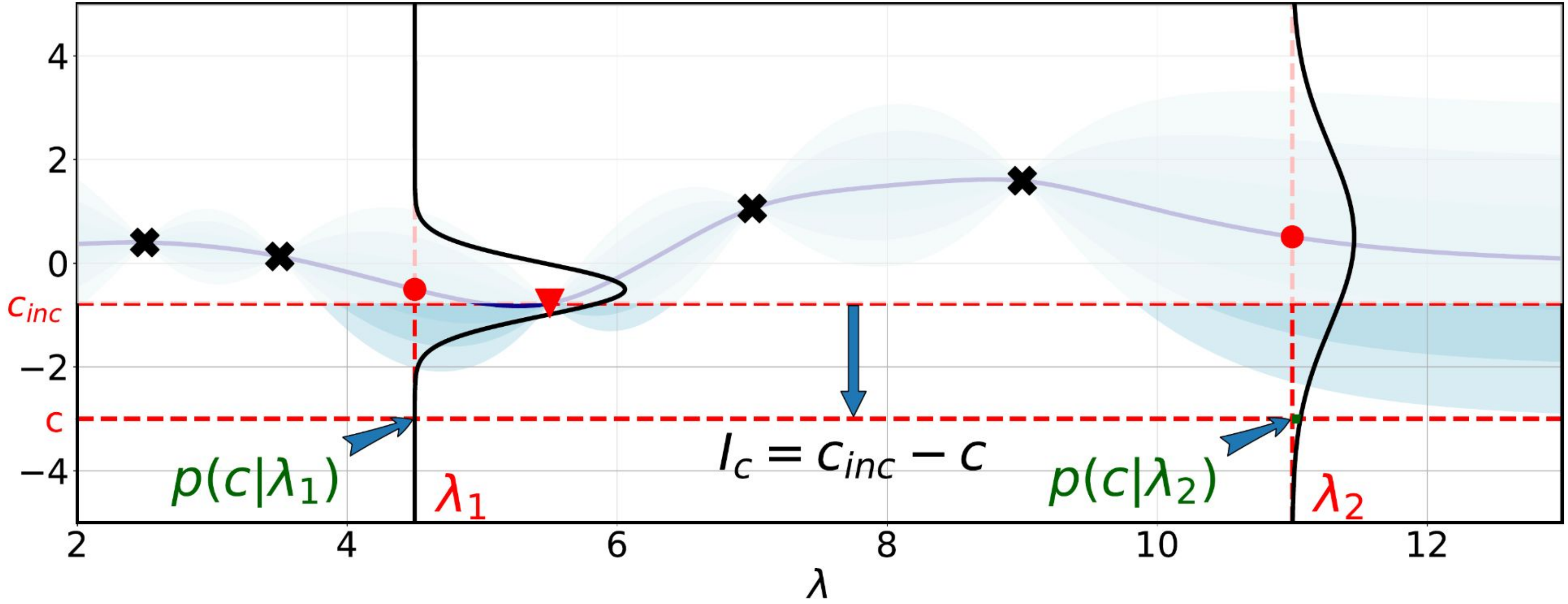
Comparing this for different configurations

Expected Improvement (EI)



and costs.

Expected Improvement (EI)



To compute EI, we sum all $p(c \mid \boldsymbol{\lambda}) \times I_c$ over all possible cost values.

Expected Improvement (EI)-Formal Definition

We define the one-step positive improvement over the current incumbent as

$$I^{(t)}(\boldsymbol{\lambda}) = \max(0, c_{inc} - c(\boldsymbol{\lambda}))$$

Expected Improvement is then defined as

$$u_{EI}^{(t)}(\boldsymbol{\lambda}) = \mathbb{E}[I^{(t)}(\boldsymbol{\lambda})] = \int_{-\infty}^{\infty} p^{(t)}(c \mid \boldsymbol{\lambda}) \times I^{(t)}(\boldsymbol{\lambda}) \; dc.$$

Since posterior is Gaussian, EI can be computed in closed form.

$$\boxed{\text{Choose } \boldsymbol{\lambda}^{(t)} \in \arg\max_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}}(u_{EI}^{(t)}(\boldsymbol{\lambda}))}$$

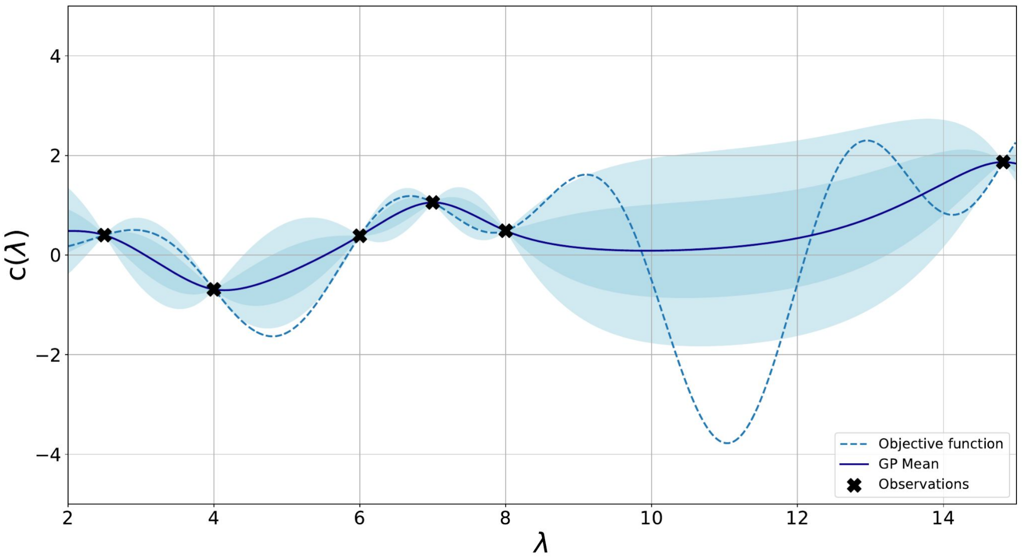
Main Ingredient II: The Surrogate Model

Required in all cases

- Regression model with uncertainty estimates
- Accurate predictions

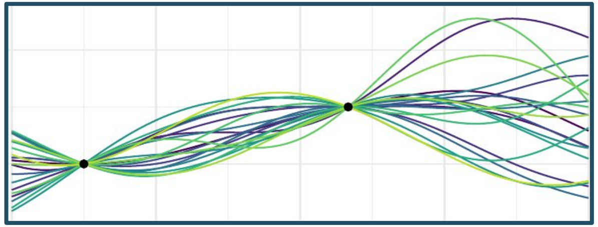
Depending on the application

- Cheap to train
- Scales well with #observations and #dimensions
- Can handle different types of hyperparameters



Types of Surrogates Models

- Gaussian Processes



- Random Forests

- Bayesian Neural Networks

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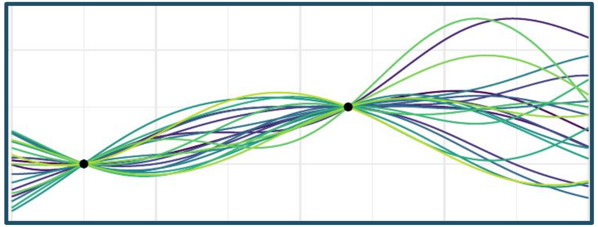
Gaussian Processes

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})]$$
$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}\left[(f(\mathbf{x}) - \mathbb{E}[f(\mathbf{x})])\,(f(\mathbf{x}') - \mathbb{E}[f(\mathbf{x}')])\right]$$
$$f(\mathbf{x}) \sim \mathcal{G}\left(m(\mathbf{x}), k\left(\mathbf{x}, \mathbf{x}'\right)\right)$$



Advantages

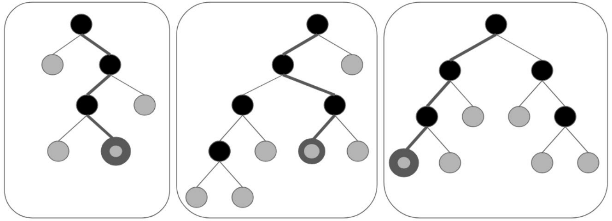
- Smooth uncertainty estimates
- Strong sample efficiency
- Expert knowledge can be encoded in the kernel
- Accurate predictions

Disadvantages

- Cost scales cubically with #observations
- Weak performance for high dimensionality
- Not easily applicable in discrete, categorical or conditional spaces
- Sensitive wrt its own hyperparameters

→ These make GPs the most commonly used model for Bayesian optimization

Tree-Based Methods



Advantages

- Scales well with #dimensions and #observations
- Training can be parallelized and is fast
- Can easily handle discrete, categorical and conditional spaces
- Robust wrt. its own hyperparameters

Disadvantages

- Poor uncertainty estimates
- Poor extrapolation (constant)
- Expert knowledge can not be easily incorporated

→ These make RFs a robust option in high dimensions, a high number of evaluations and for mixed spaces

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Bayesian Neural Networks

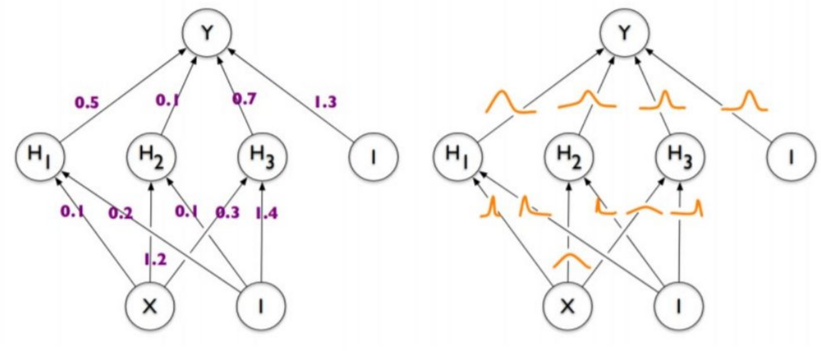

Image source: [Blundell et al. 2015]

Advantages

- Scales linear #observations
- (Can yield) smooth uncertainty estimates
- Flexibility wrt. discrete and categorical spaces

Disadvantages

- Needs many #observations
- Uncertainty estimates often worse than for GPs
- Many hyperparameters
- No robust off-the-shelf model

→ These make BNNs a promising alternative. [Li et al. 2023]

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Alternatives to Bayesian Optimization

- Genetic Algorithms / Evolutionary Algorithms
  - E.g., GGA [Ansótegui et al. 2009, Ansótegui et al. 2015, Ansótegui et al. 2021]
- Estimation of Distributions
  - E.g., irace [López-Ibáñez et al. 2016]
- Reinforcement Learning
  - E.g., Neural architecture search with RL [Zoph and Le. 2017]
- Golden Parameter Search [Pushak and Hoos. 2020]
  - Assumes a benign landscape [Pushak and Hoos. 2018]

Are AC Landscapes Benign? [Pushak and Hoos, 2018]

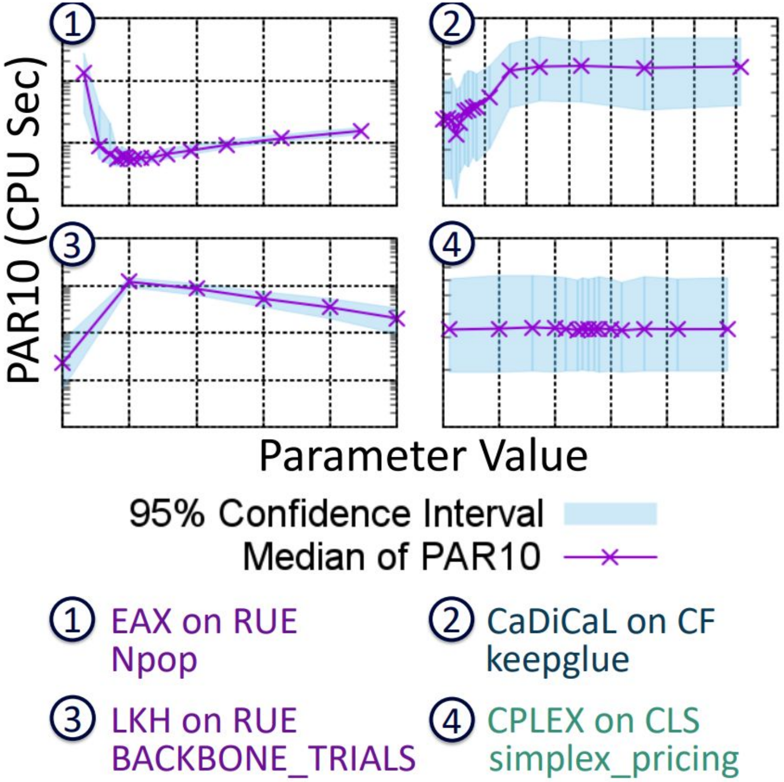
Instance set responses:

- Nearly all unimodal
- Nearly all convex
- Relatively “smooth”

Individual instance responses:

- Mostly uni-modal
- Mostly convex
- More “noisy

⇒ What kind of optimizers do we really need?



Questions?

Kahoot Quiz II

How to optimize across instances?

The Problem of Generalization & Instances

- **So far**: Obtaining a single configuration performing well on a single task (e.g., dataset, SAT instances, MIP instance, …)
  - **Problem**: Why should we search for a well-performing configuration if we have solved the task already?
    - This makes sense for optimization tasks (e.g., machine learning) where we might find better solutions.
    - Makes little to no sense for decision problems (e.g., SAT, ASP, Planning, …)
- **New Objective**:

  <u>Find a configuration that performs well on a distribution of instances</u>

  - The obtained configuration should also perform well on new instances
    → Generalization of the configuration's performance

The Algorithm Configuration Problem

Given:

- A configuration space
- A set of instances (drawn from some instance distribution)
- A cost metric (wlog. to be minimized)

The configuration problem is:

$$\operatorname{argmin}_{\lambda \in \Lambda} \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} c(\lambda, i)$$

⇒ Assumes that there is a single good configuration for all (homogeneous) instances!

How to find good configuration we know already.

But how do we compare n configurations across instances?

Naive Algorithm Configuration

- Comparing two configurations against each other on set of instances (being sampled from the underlying instance distribution)

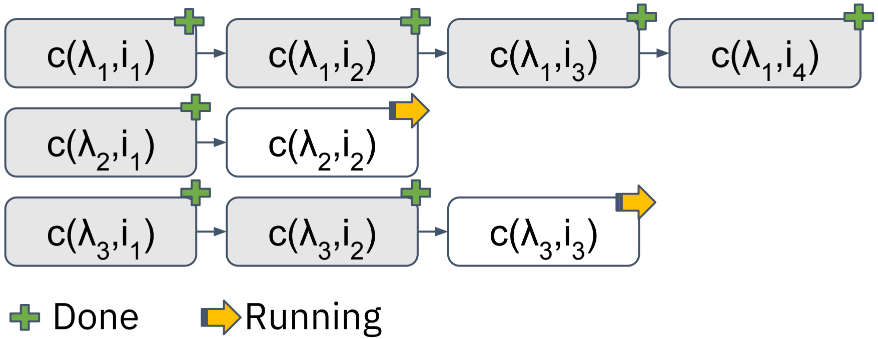
$c(\lambda_1, i_1)$	$c(\lambda_1, i_2)$	$c(\lambda_1, i_3)$	$c(\lambda_1, i_4)$	$c(\lambda_1, i_5)$	$c(\lambda_1, i_6)$	$c(\lambda_1, i_7)$	…
$c(\lambda_2, i_1)$	$c(\lambda_2, i_2)$	$c(\lambda_2, i_3)$	$c(\lambda_2, i_4)$	$c(\lambda_2, i_5)$	$c(\lambda_2, i_6)$	$c(\lambda_2, i_7)$	…

- If we consider runtime as our cost c, then we pay for evaluation two configurations:

$$\sum_{i \in \mathcal{I}} c(\lambda_1, i) + \sum_{i \in \mathcal{I}} c(\lambda_2, i)$$

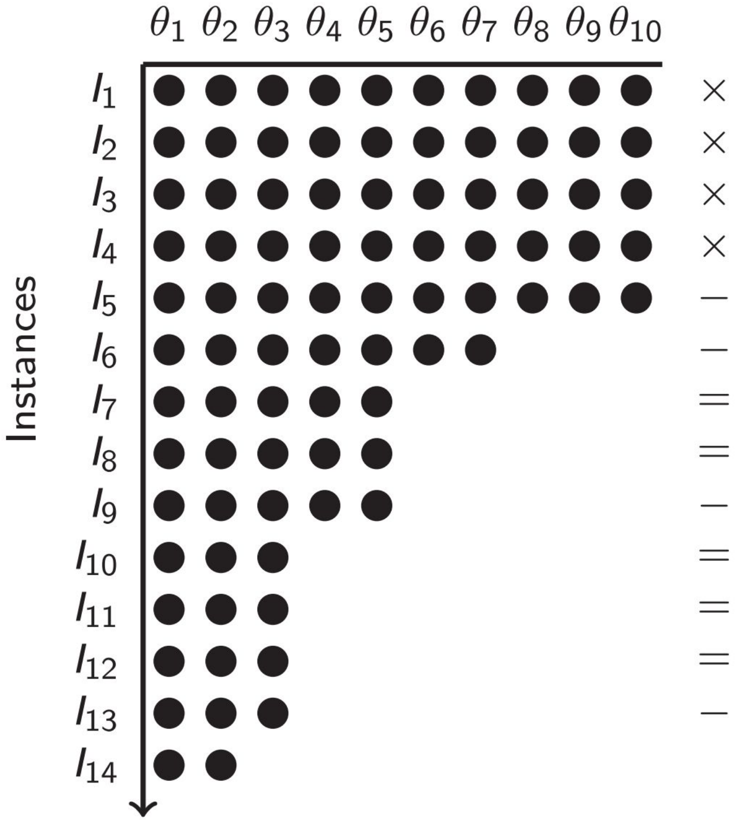
- If we have a few thousand instances and each of them takes minutes, it is crazy expensive to only compare two configurations

Simple Parallel Racing [Ansotegui et al. 2009]



- Run *n* configurations in parallel on *k* instances
- Whoever is done first, won the race
  - primarily, designed for runtime as cost metric
- Increase the number of instances for next race (e.g., geometric schedule)

Racing with Statistical Tests [López-Ibáñez et al. 2016]



- “X” no statistical test to collect sufficient evidence first
- “–” at least one underperforming configuration was discarded
- “=” no configuration was discarded

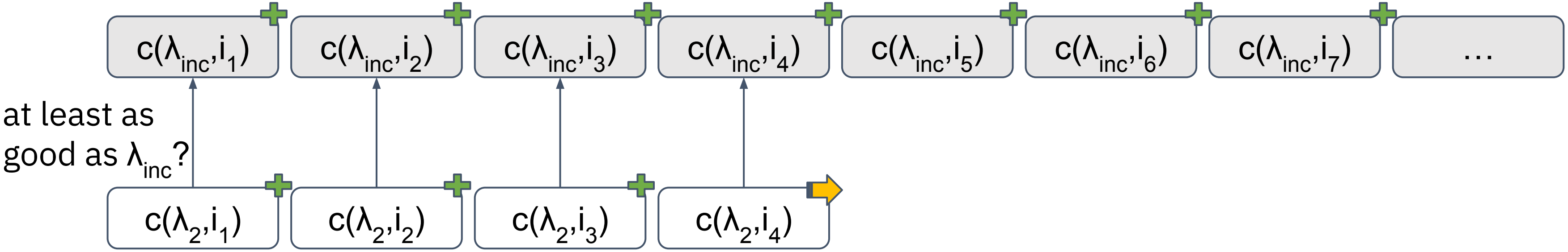
⇒ irace

— — —

- Refresh the slots of discarded configurations to have efficient parallelization [Xiao et al. 2023]

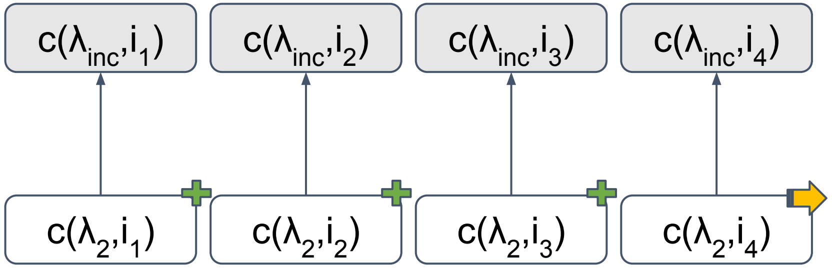
Aggressive Racing [Hutter et al. 2009]

- Idea: If a configuration underperforms compared to the current incumbent configuration, directly reject it.



- For n instances being evaluated on λ_2 (and λ_{inc})
  - **if** $\frac{1}{|\mathcal{I}_n|}\sum_{i\in\mathcal{I}_n} c(\lambda_{\text{inc}}, i) \geq \frac{1}{|\mathcal{I}_n|}\sum_{i\in\mathcal{I}_n} c(\lambda_2, i)$
    - Evaluate λ_2 on more instances (doubling the amount each time)
  - **otherwise**
    - Reject λ_2 and sample a new configuration to challenge λ_{inc}

Adaptive Capping for Aggressive Racing



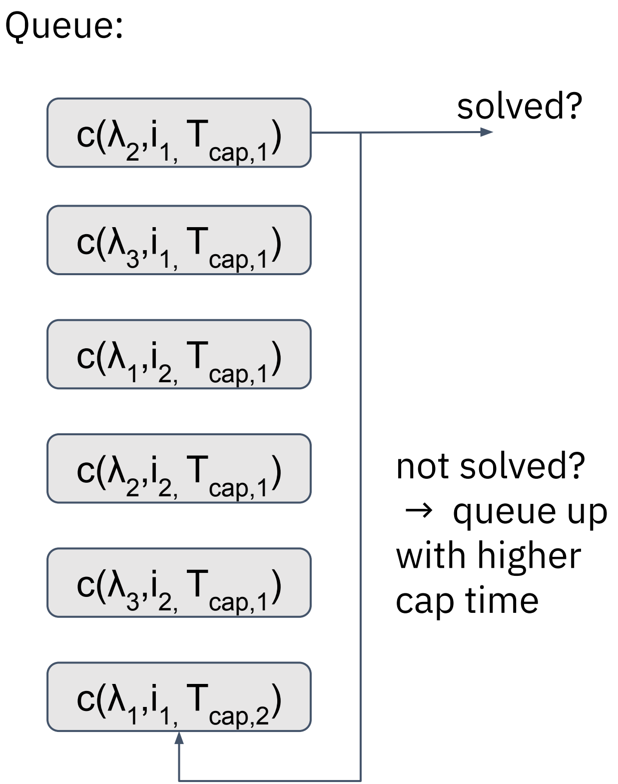
- Assuming, runtime optimization
- If we know the runtime of λ_{inc} on all *k* instances, and the runtime for λ_2 on some instances, how much time (captime) do we need at most to invest to check whether λ_2 can outperform λ_{inc}?

$$\sum_{i \in \mathcal{I}_1} c(\lambda_{\text{inc}}, i) - \sum_{i \in \mathcal{I}_2} c(\lambda_2, i) \text{ where } \mathcal{I}_1 \supseteq \mathcal{I}_2$$

Structured Procrastination

[Klein et al. 2017, 2019, Weisz et al. 2021]

- **Assumptions**:
  - Runtime optimization
  - Identify the best configurations on arbitrarily many instances
- **Problem** with previous approaches:
  - If assume a maximal captime for each configuration run, the algorithm configurator can waste arbitrarily much time on bad configurations
  - No theoretical guarantees on efficiency
- **Idea**: Instead of top-down capping runs, start with very small captimes and increase them iteratively
  - → unsuccessful runs will be procrastinated in favor of short runs of other configurations
- **⇒ Theoretical guarantees!**



AC-Band [Brandt et al. 2023]

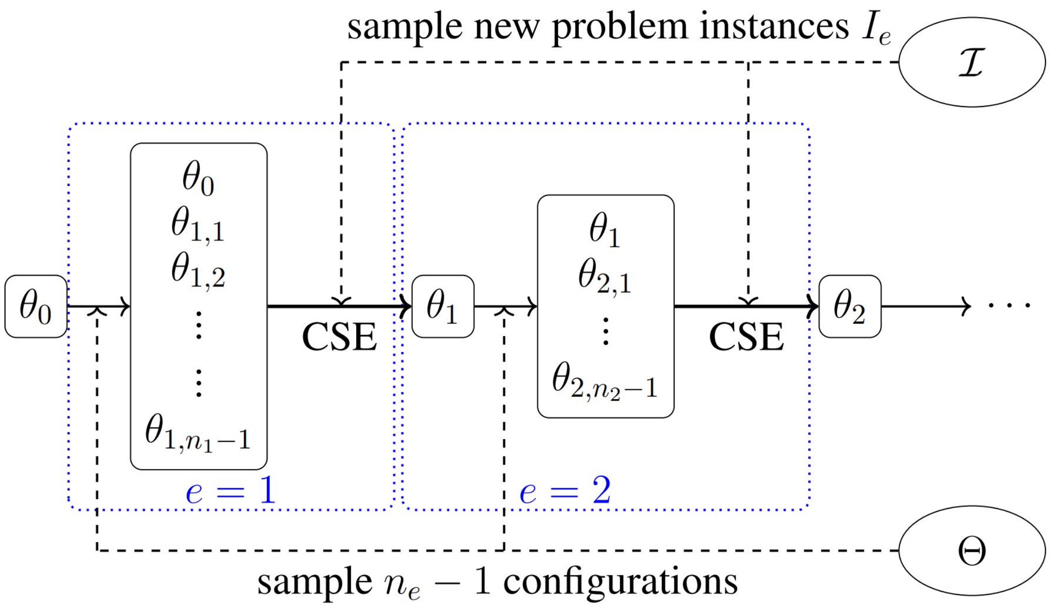
Tradeoff:

- too aggressive: rejecting good configurations
- too gracious: wasting compute time

Idea:

- motivated by Hyperband, start with many configurations on few instances → decrease number of configurations and increase number of instances

⇒ theoretical guarantees



Recommended Software

- SMAC [Hutter et al. 2011, Lindauer et al. 2021]
  - SMAC2 in Java [not maintained anymore]
  - SMAC3 in Python [active development]
- GGA [Ansótegui et al. 2009, Ansótegui et al. 2015, Ansótegui et al. 2021]
  - GGA in Python → PyDGGA
- irace [López-Ibáñez et al. 2016]
  - irace in R [active development]
  - irace in Python WIP
- AClib [Hutter et al. 2014]
  - Benchmark library for AC problems

Beyond traditional AC

Further Variations

- Real-time AC [Fitzgerald et al. 2014, Weiss & Tierney. 2022]
  - stream of instances
- Multi-objective algorithm configuration [Blot et al. 2016]
  - several objectives, such as runtime, memory, CO2-footprint, ...
  - Soon, there will be a multi-objective configurator based on Bayesian Optimization
- Dynamic algorithm configuration [Adriansen et al. 2022]
  - dynamically adapt configuration while the algorithm is running
- Per-Instance Algorithm Configuration e.g. [Xu et al. 2011]
  - Learn to map instance features to configurations
- Neural Architecture Search [Elsken et al. 2019]
  - Finding a well-performing architecture of a deep neural network
- CASH [Thornton et al. 2013]
  - Structured search spaces for AutoML (pipelines)

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A Survey of Methods for Automated Algorithm Configuration

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Join our COSEAL network on algorithm selection, configuration and related topics, if you are interested to work more on these topics:

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Niedersachsen

Backup Slides

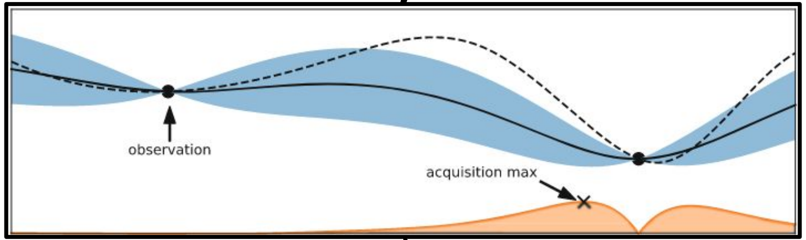
Bayesian Optimization: Extensions

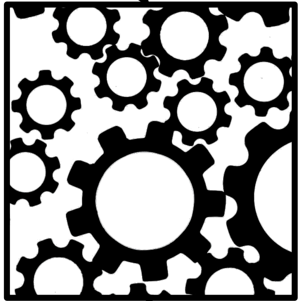
Different models to handle new design spaces

λ_n

Increase efficiency by using lower fidelities

Multi-objective





Consider constraints

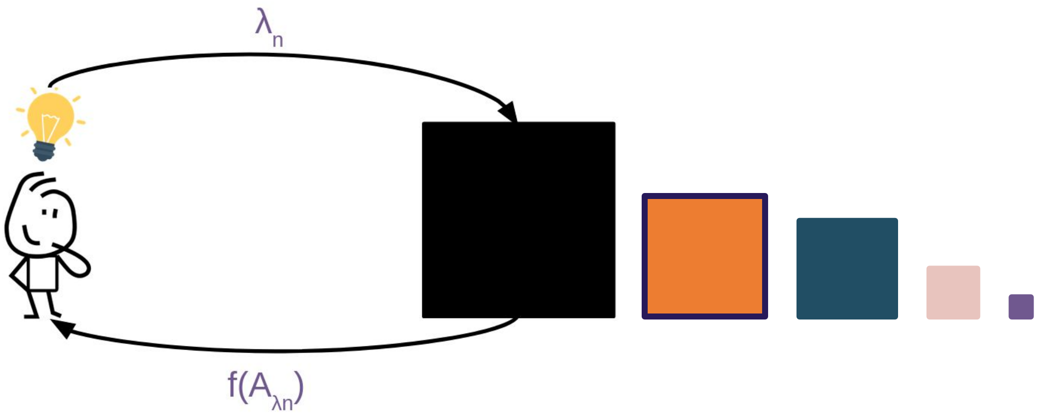
Leverage observations across experiments

$f(A_{\lambda n})$

Take user priors into account

Photo by Wilhelm Gunkel on Unsplash
Image by Feurer, Hutter: Hyperparameter Optimization
In: Automated Machine Learning

Multi-Fidelity Bayesian Optimization



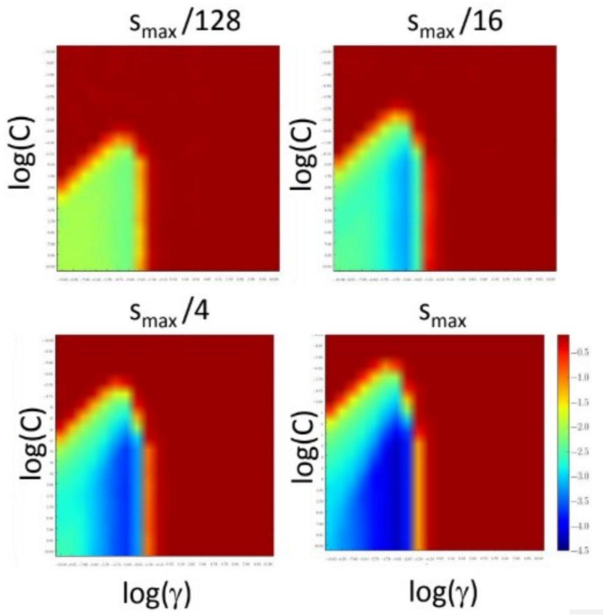
Often, the black-box

- is an **iterative** process,
- has **cheaper approximations** available,
- or can be evaluated **partially**

→ We can collect information about the actual objective value with less costly evaluations

Two Motivating Examples

Performance of a SVM on different subsets of MNIST



Learning curves of fully connected NNs on CIFAR-10

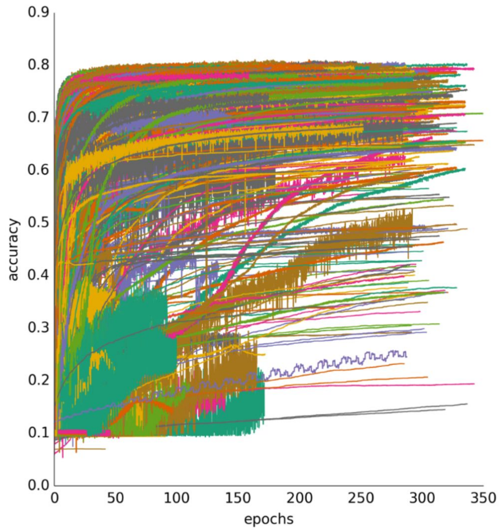
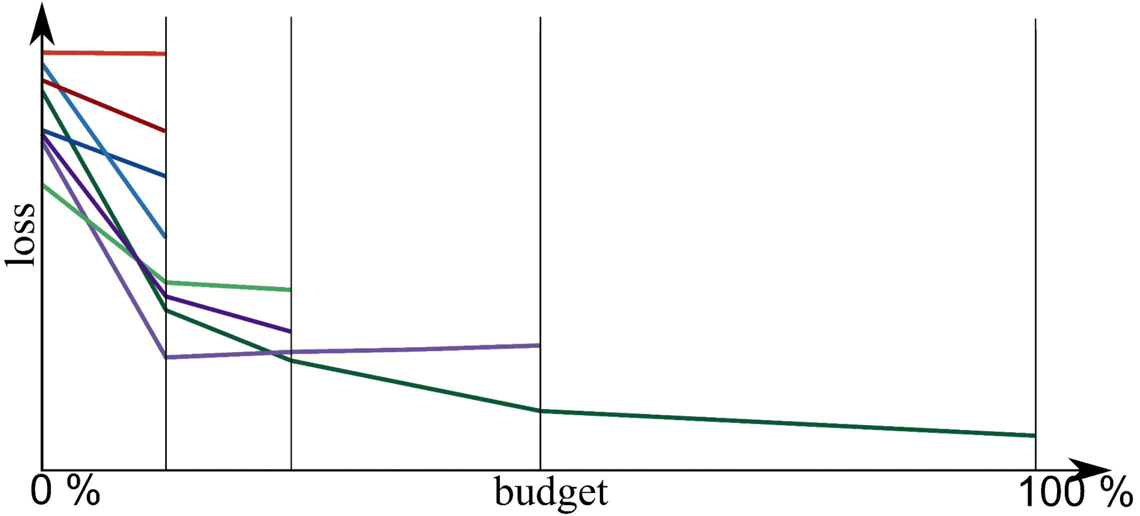


Image Source: [Domhan et al., 2015]

Successive Halving



[Jamieson and Talwalkar. 2016]

- A very simple algorithm:
  - Sample N configurations uniformly at random & evaluate them on the cheapest fidelity
  - Keep the best half (or third), move them to the next fidelity
  - Iterate until the most expensive fidelity (= original expensive black box)

Hyperband

What if the information on the lowest fidelity is not informative?

→ Run multiple iterations of SH, starting at different “lowest” fidelities.

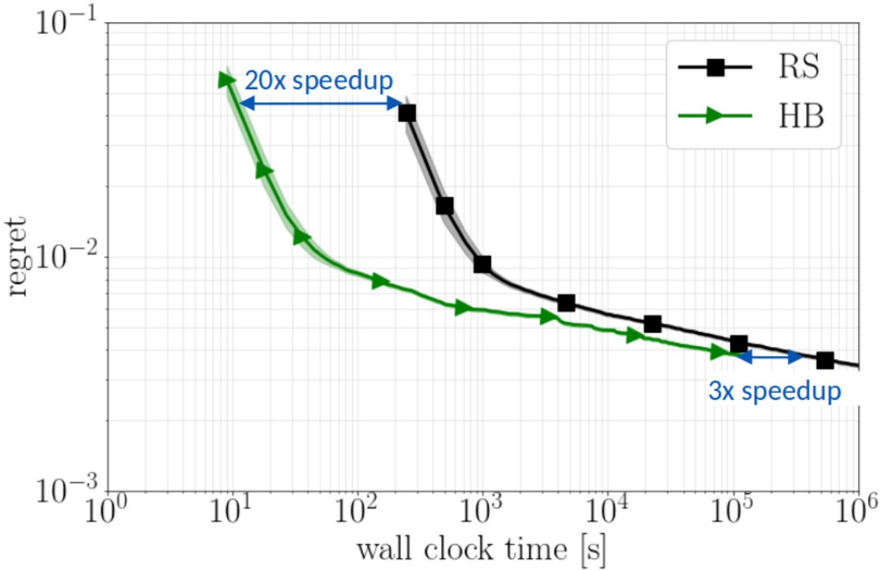


image credit: [Falkner et al. 2018]

BOHB: Hyperband X Bayesian Optimization

Idea: Use Bayesian Optimization to choose configurations [Falkner et al. 2018]

- BO to achieve strong performance
- HB to achieve good anytime performance

→ easy parallelization

→ with interleaved random sampling it keeps theoretical guarantees of HB

→ with RFs as surrogate model, it performs better than with TPE [Lindauer et al. 2022]

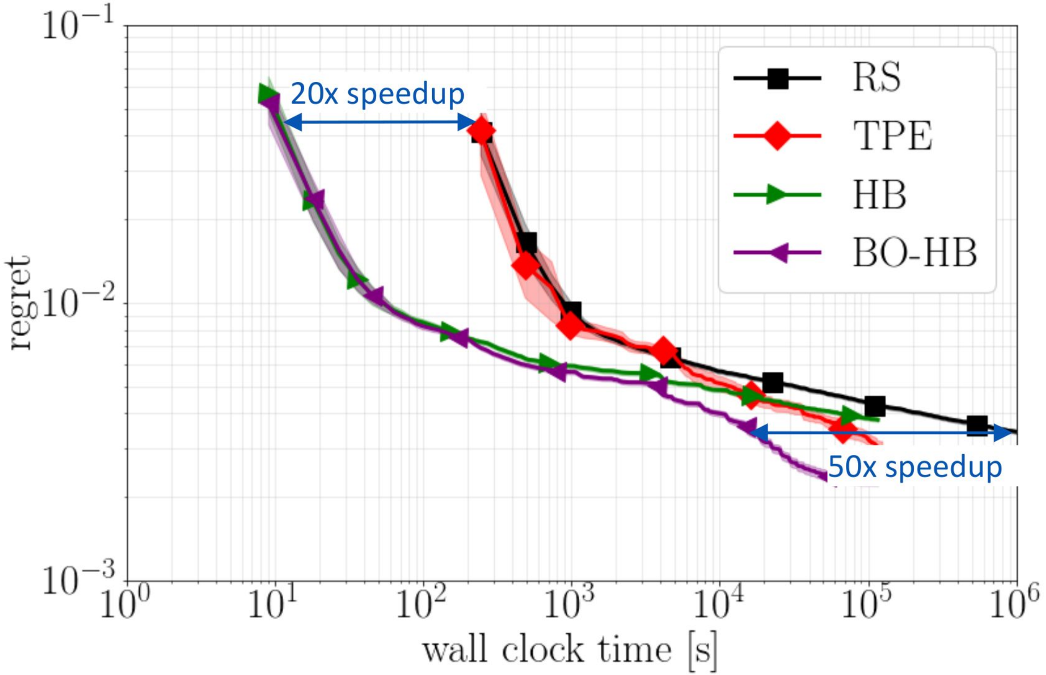


image credit: [Falkner et al. 2018]

Landscape of Multi-Fidelity HPO Methods

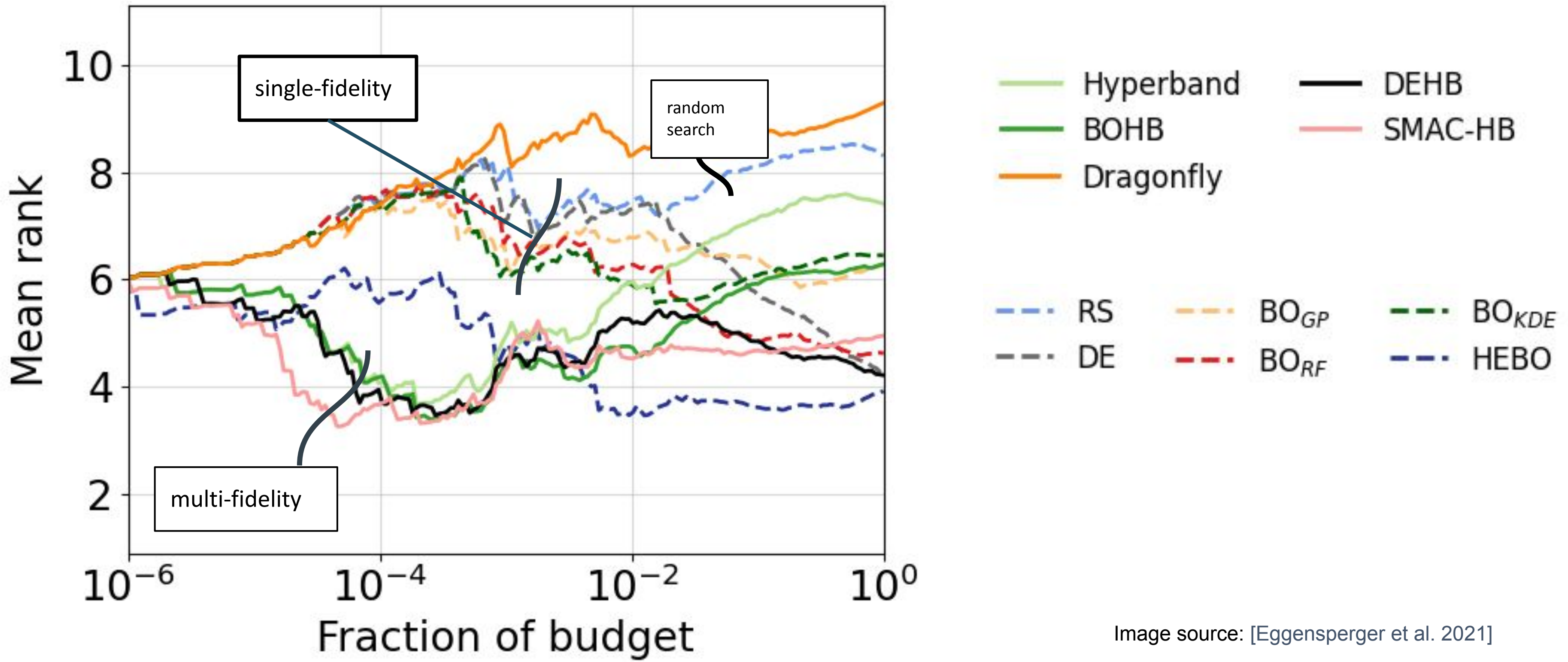


Image source: [Eggensperger et al. 2021]