Bayesian Optimization

fundamentals, implementations, and practice

Quan Nguyen

Who am I?

- **Quan Nguyen**
- Ph.D. student – Bayesian machine learning, decision-making under uncertainty

krisnguyen135.github.io

github.com/KrisNguyen135/Talks

@the_subtrahend

What you will learn today

Bayesian optimization (BayesOpt) essentials

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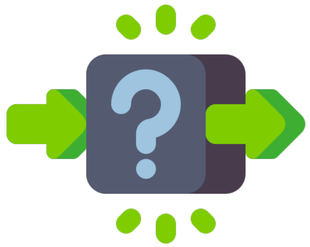
expensive black-box optimization



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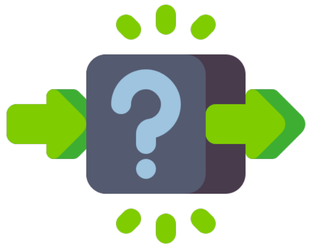

high-level overview of BayesOpt

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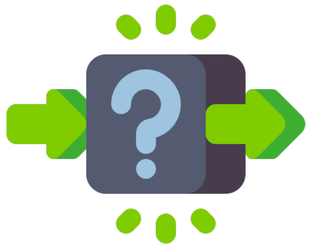

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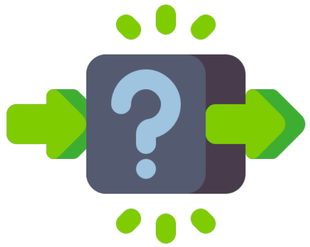

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BayesOpt in practice

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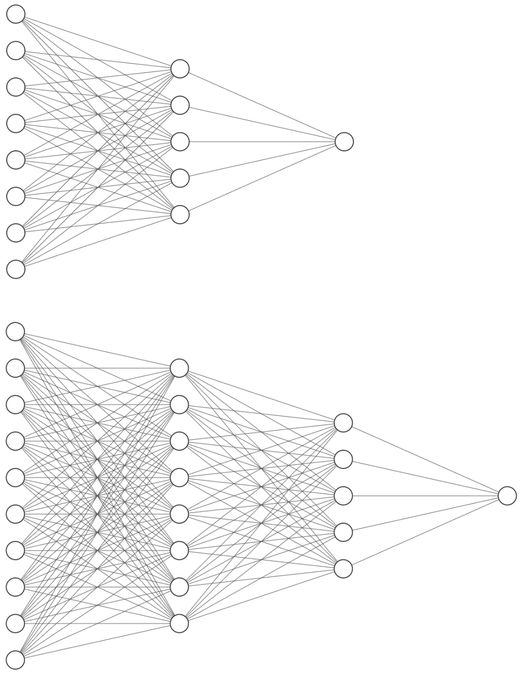
Examples

- *Hyperparameter tuning*: choose parameters for ML models

which model gives higher accuracy?



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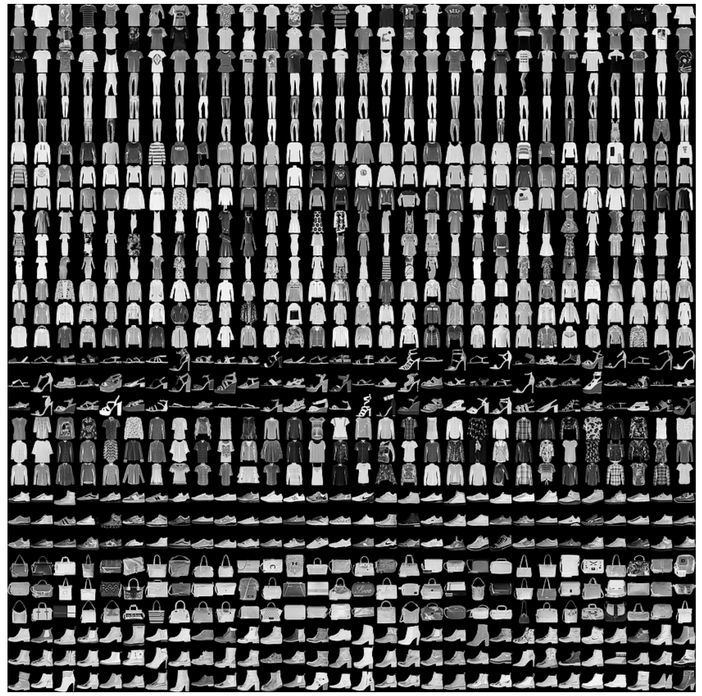

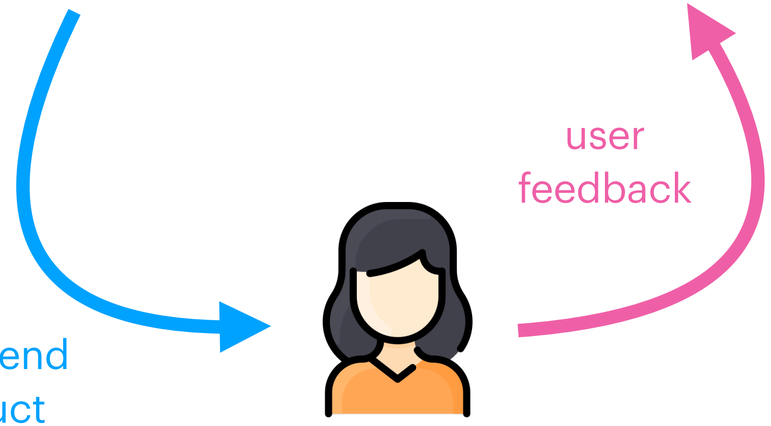

FashionMNIST https://github.com/zalandoresearch/fashion-mnist

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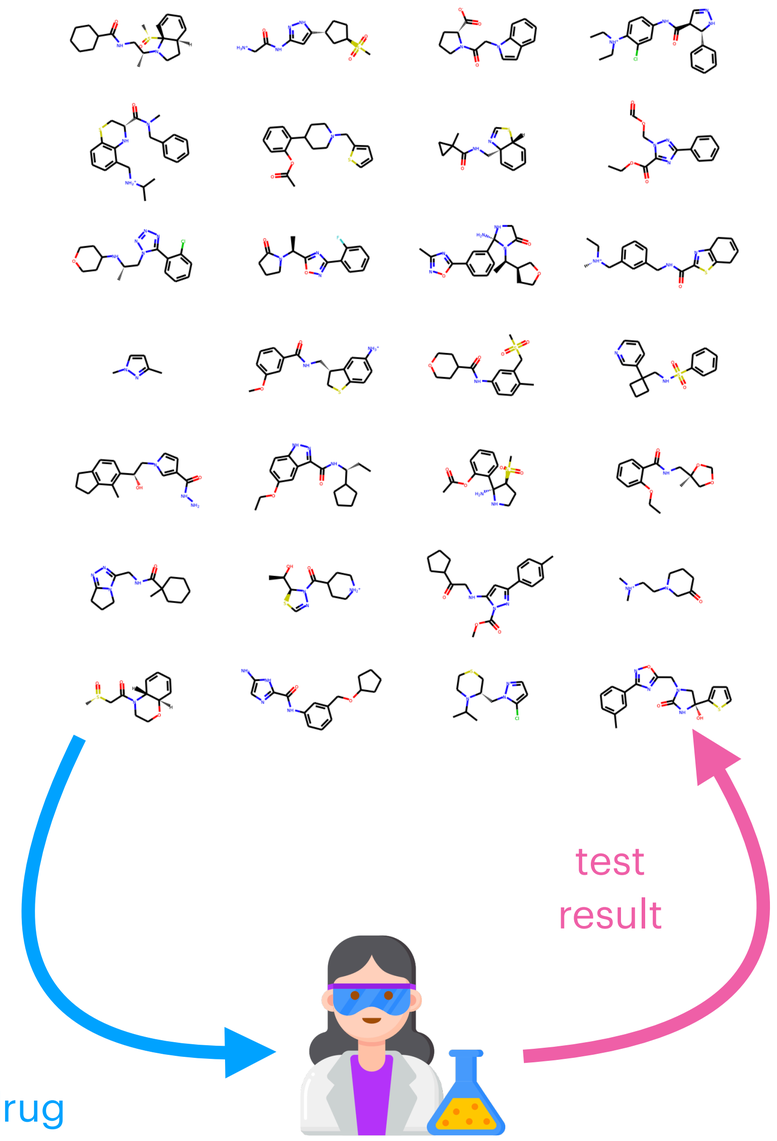
- *Product recommendation*: find products customers want
- *Drug discovery*: discover effective drugs against diseases



Naïve strategies might waste resources

example: finding the best neural network architecture

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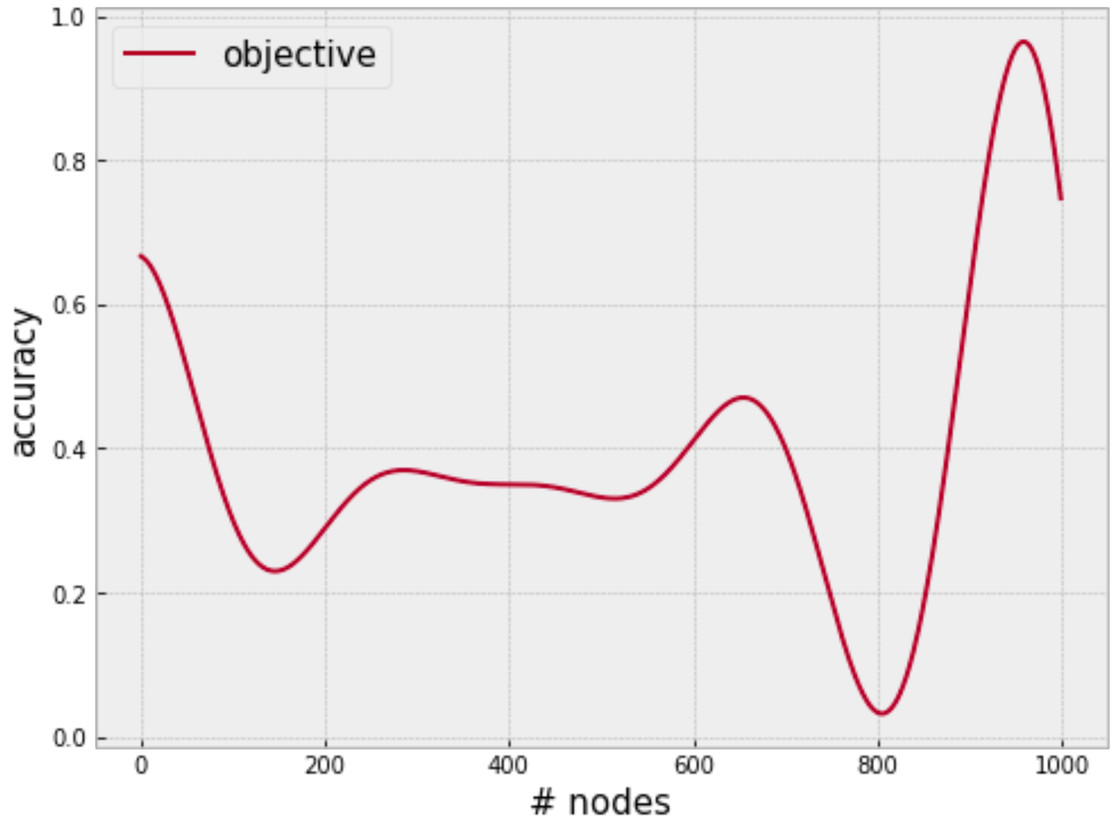

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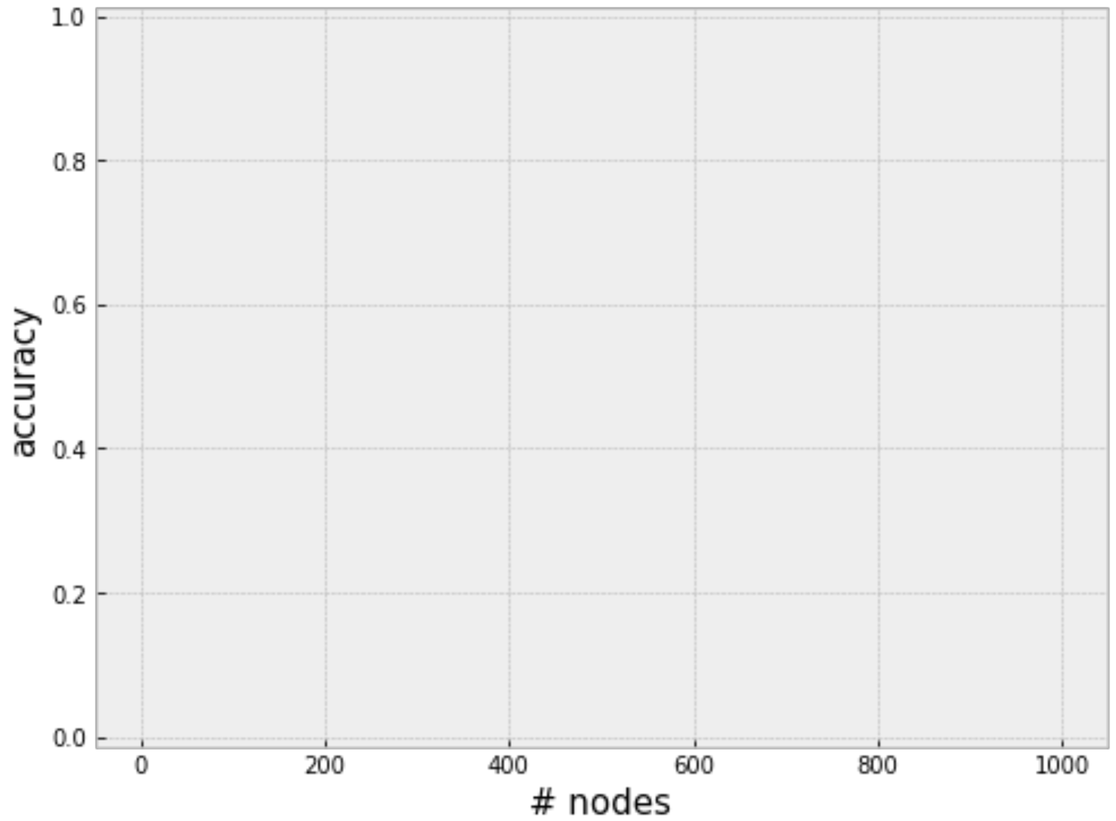

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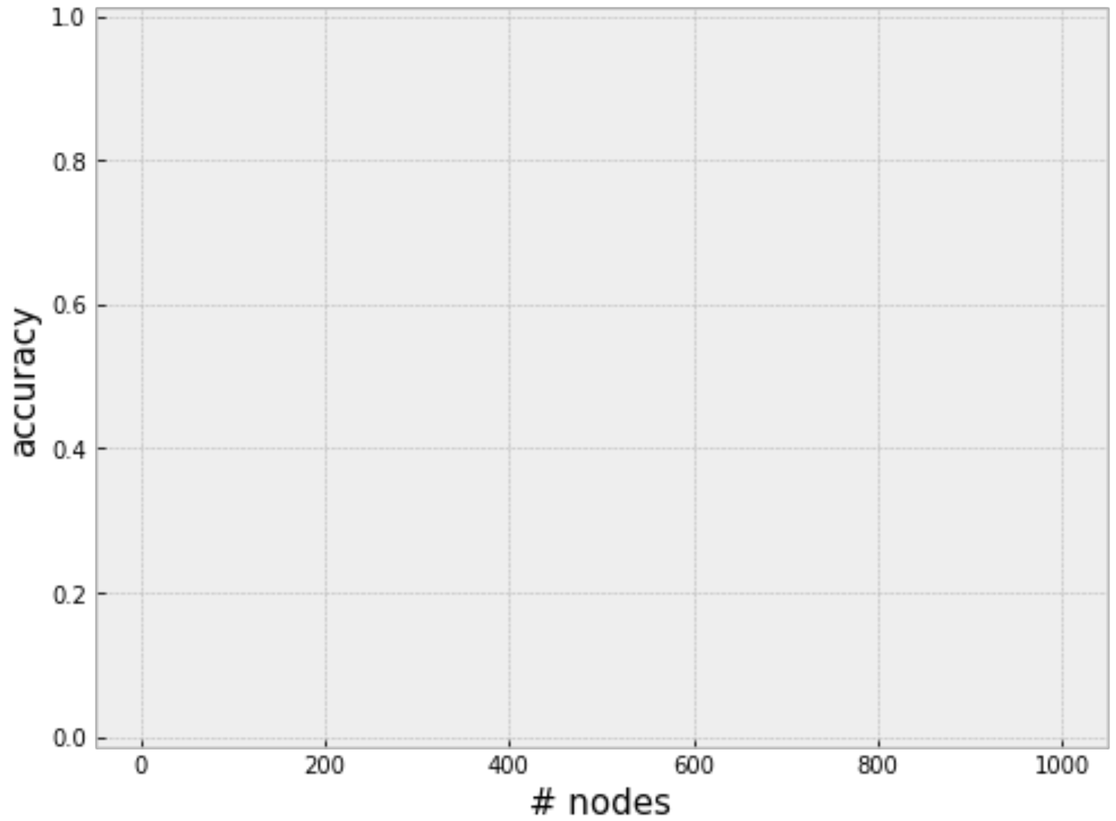

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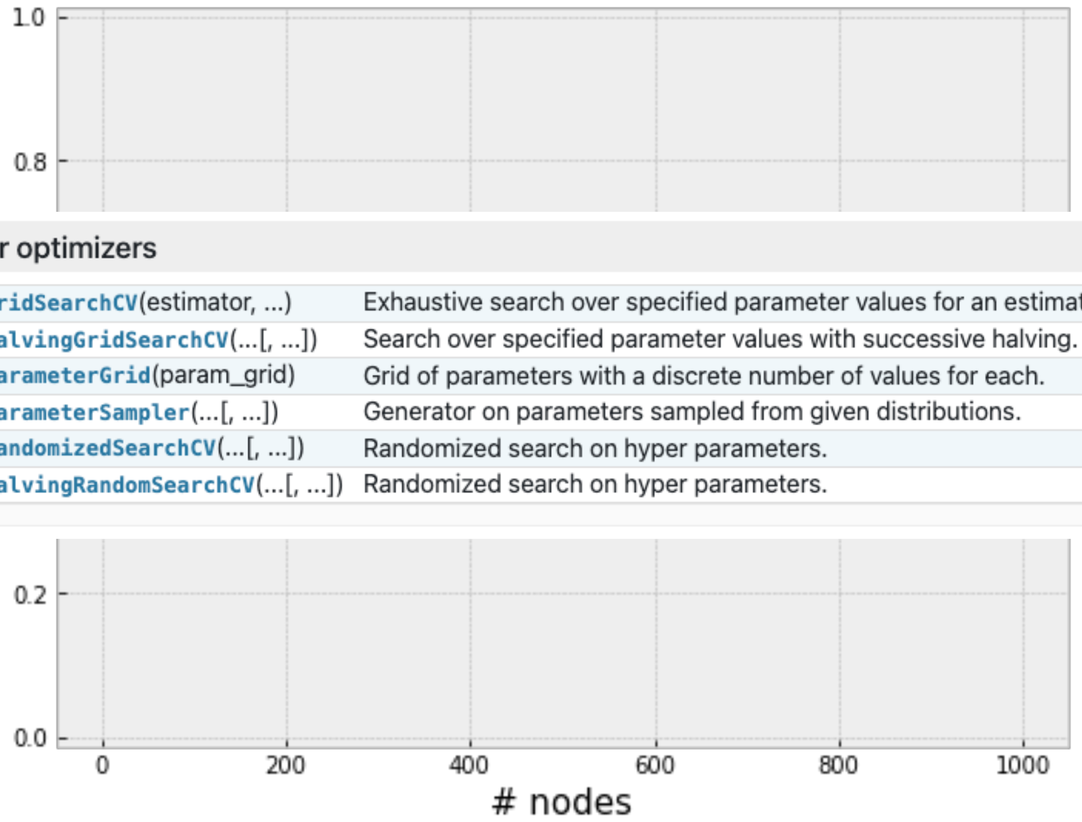

Hyper-parameter optimizers

`model_selection.GridSearchCV`(estimator, ...)	Exhaustive search over specified parameter values for an estimator.
`model_selection.HalvingGridSearchCV`(...[, ...])	Search over specified parameter values with successive halving.
`model_selection.ParameterGrid`(param_grid)	Grid of parameters with a discrete number of values for each.
`model_selection.ParameterSampler`(...[, ...])	Generator on parameters sampled from given distributions.
`model_selection.RandomizedSearchCV`(...[, ...])	Randomized search on hyper parameters.
`model_selection.HalvingRandomSearchCV`(...[, ...])	Randomized search on hyper parameters.

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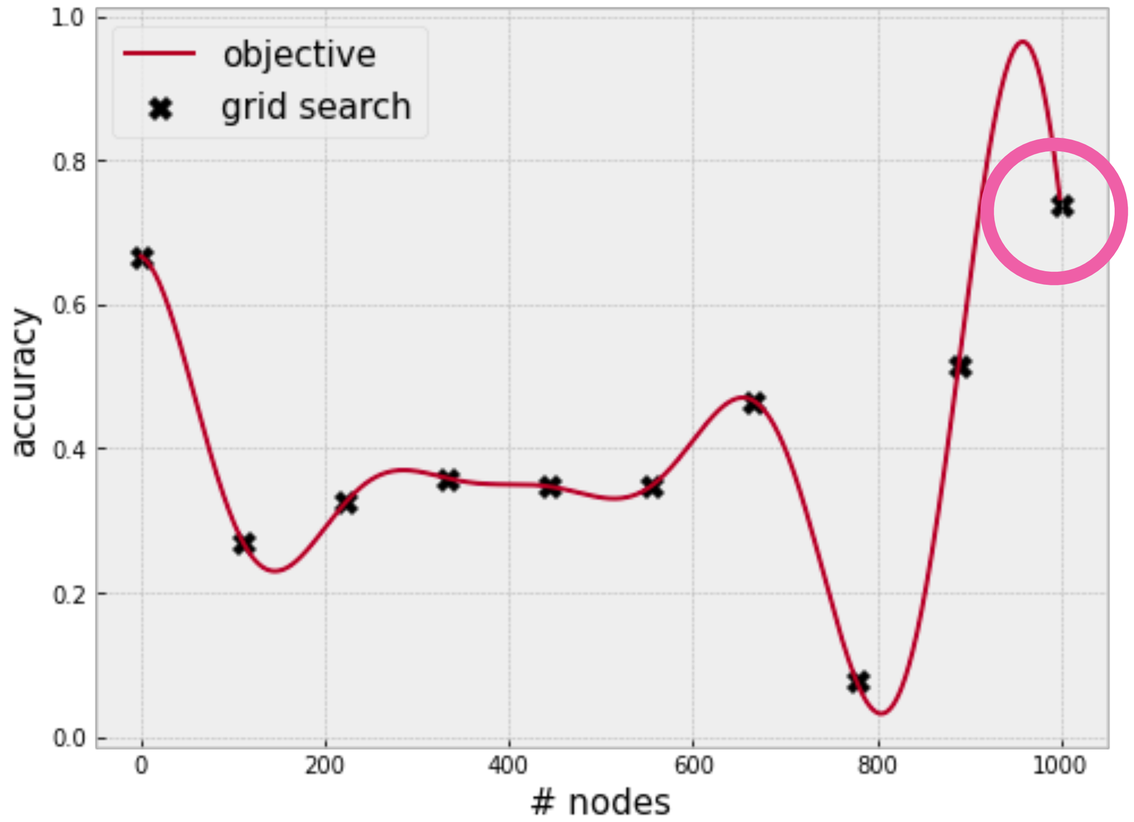

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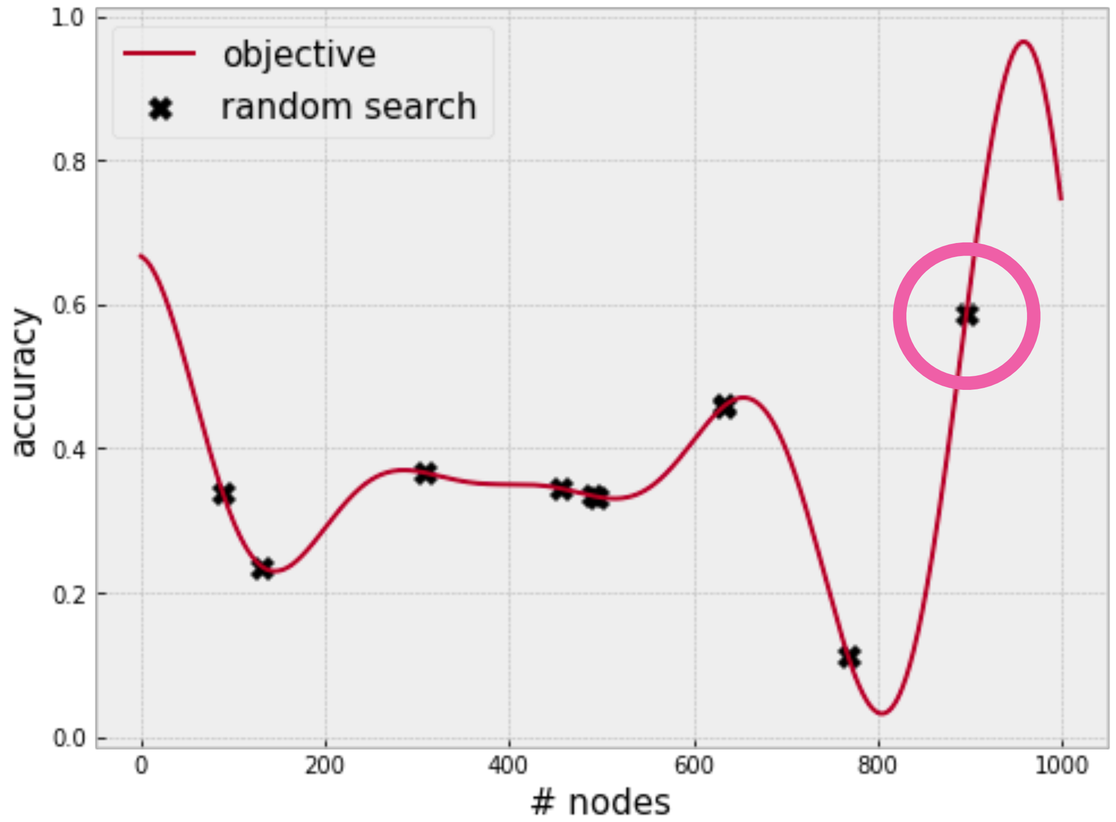

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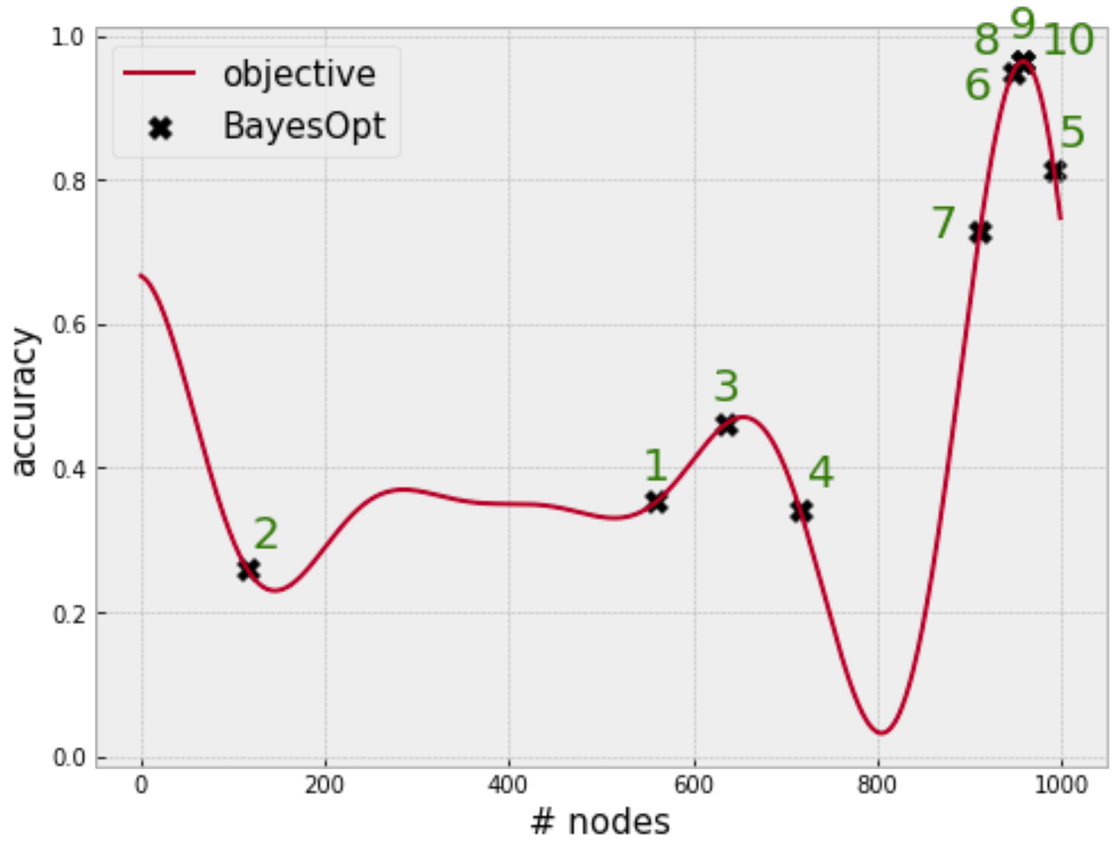


Introducing Bayesian optimization

the main components

and how they work

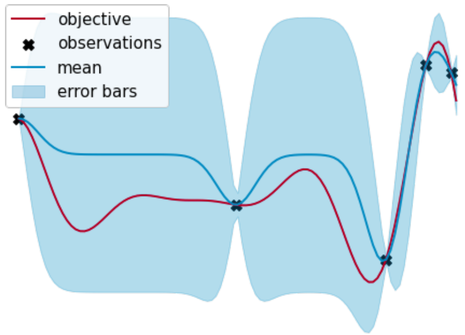
The Bayesian optimization loop

a virtuous cycle of optimization

The Bayesian optimization loop

a virtuous cycle of optimization

ML model (Gaussian process)
with uncertainty quantification



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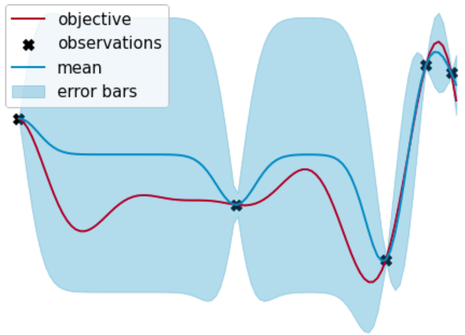
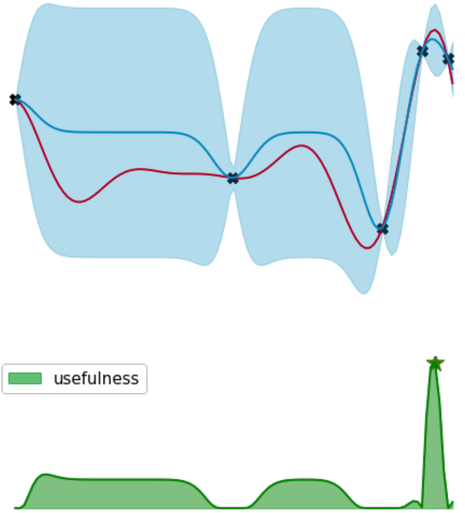


inform decisions

decision-making policy
finds the next point to label



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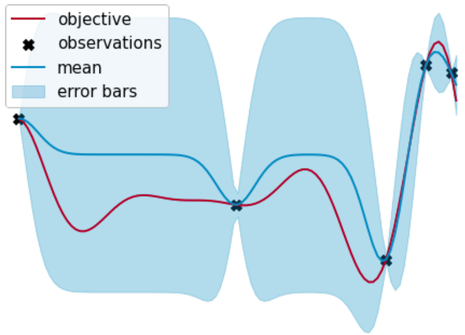

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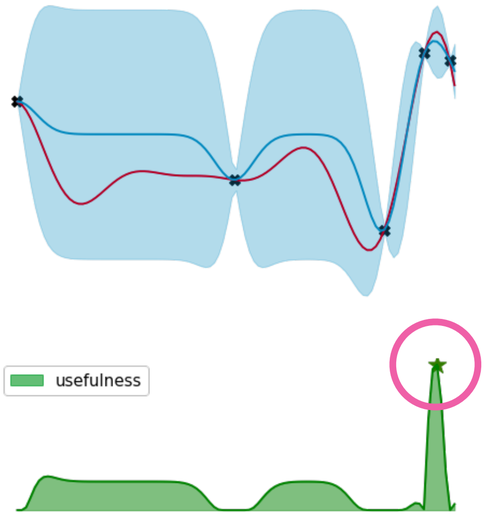

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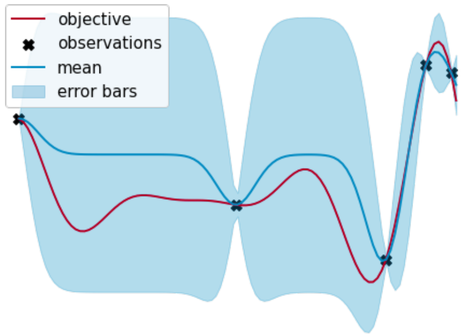

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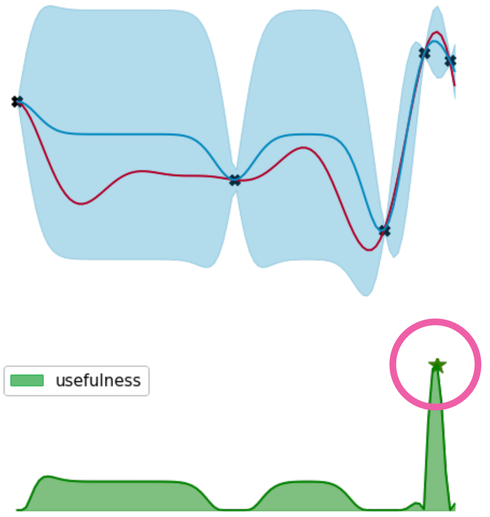

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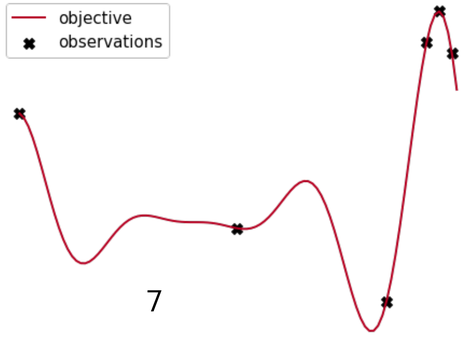
training data is updated



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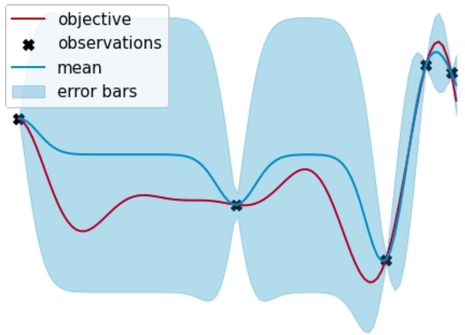

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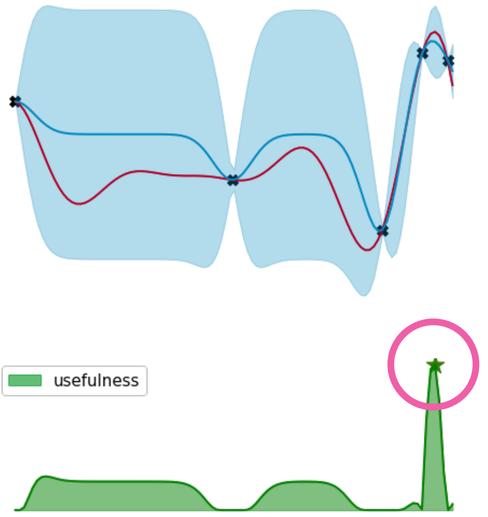

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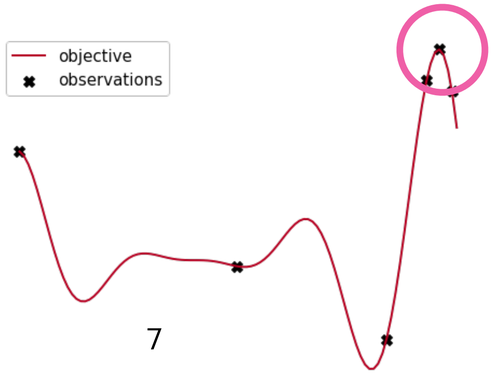

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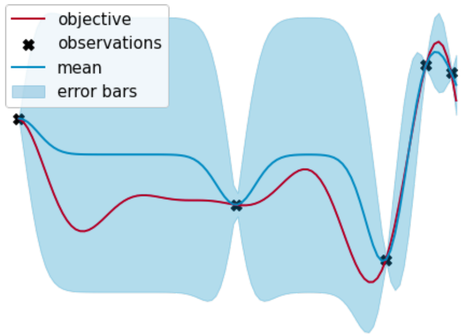

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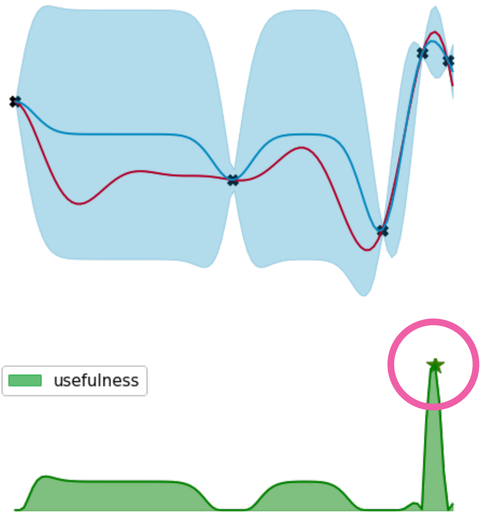

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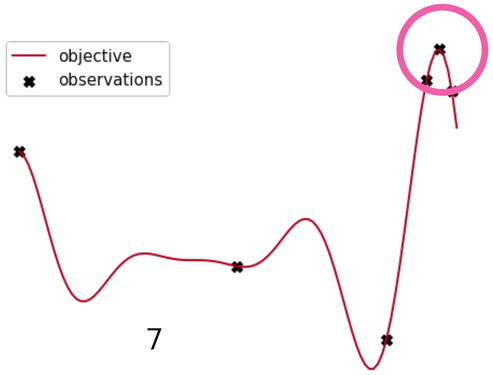
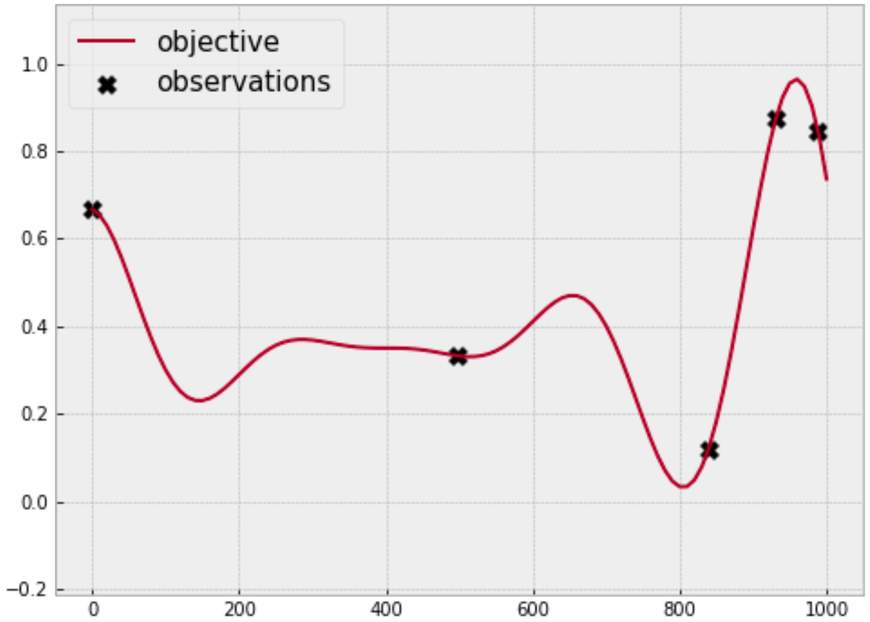


retrain the
ML model

Gaussian process as the predictive model

predictions with confidence levels



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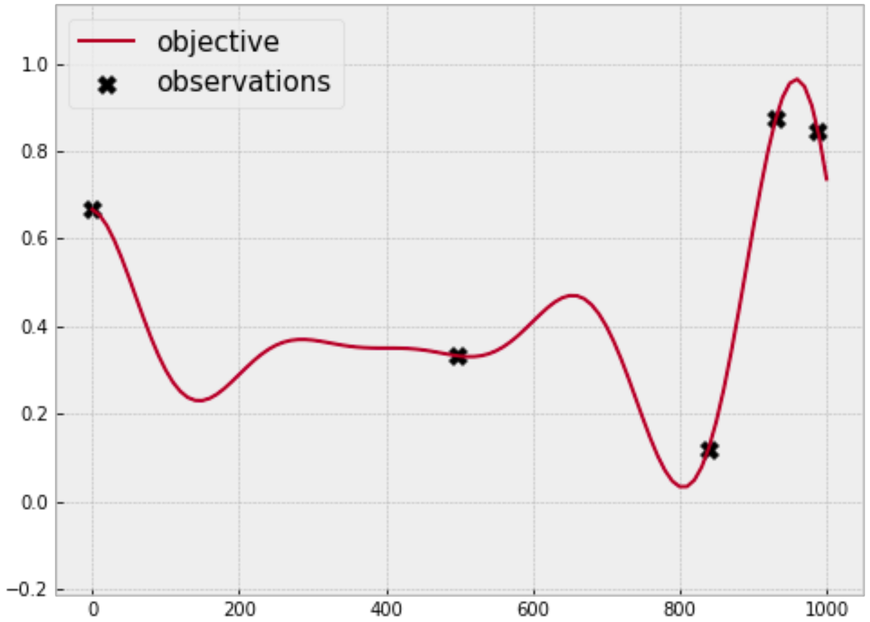

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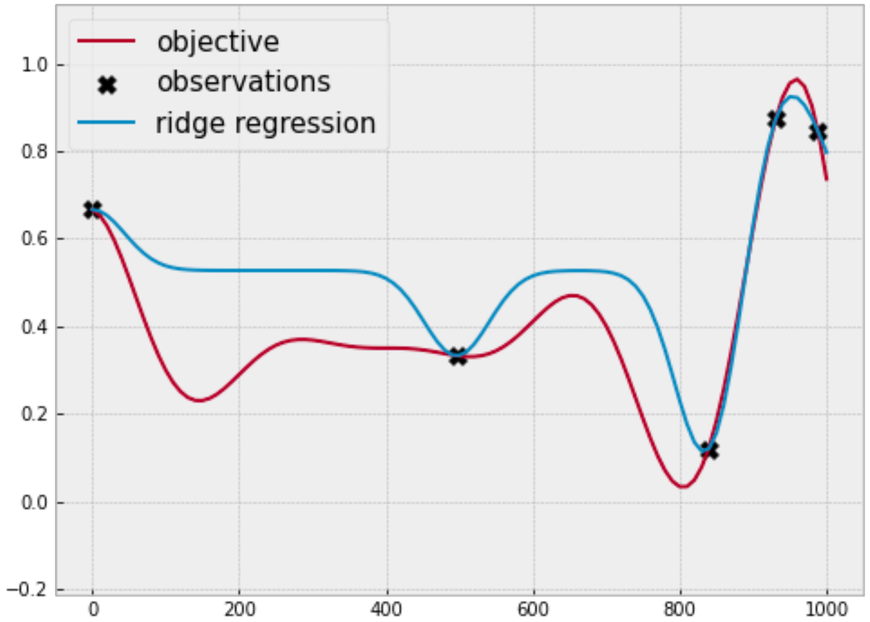

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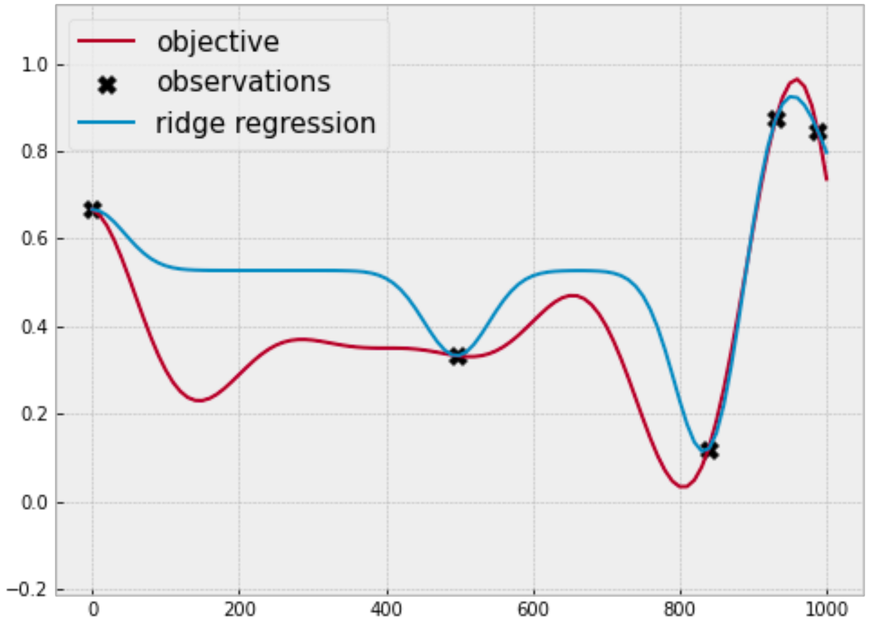

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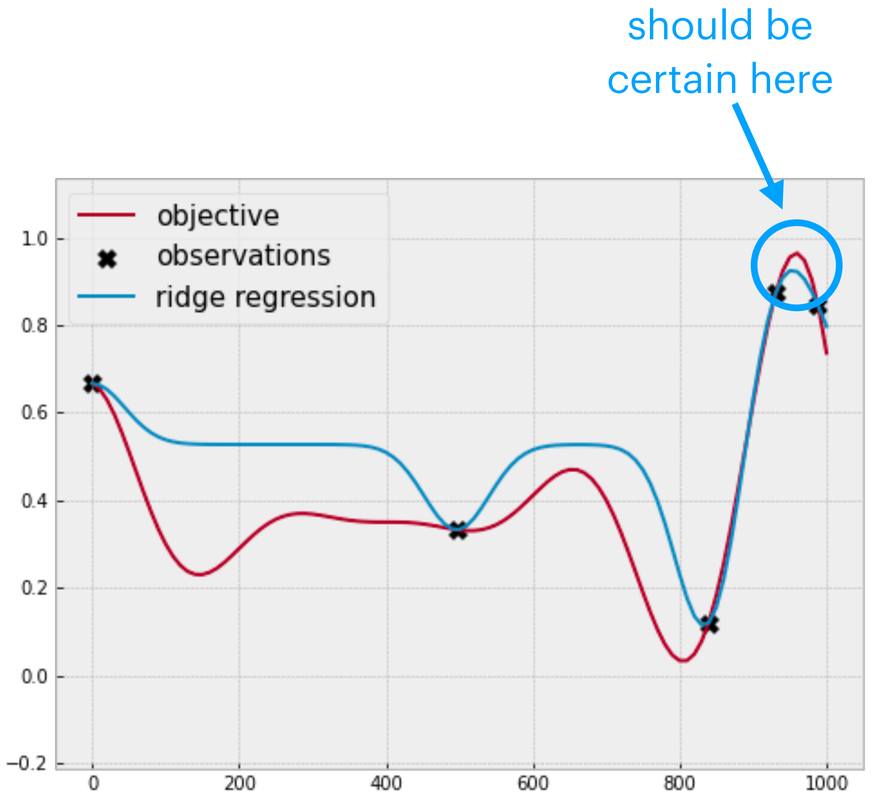

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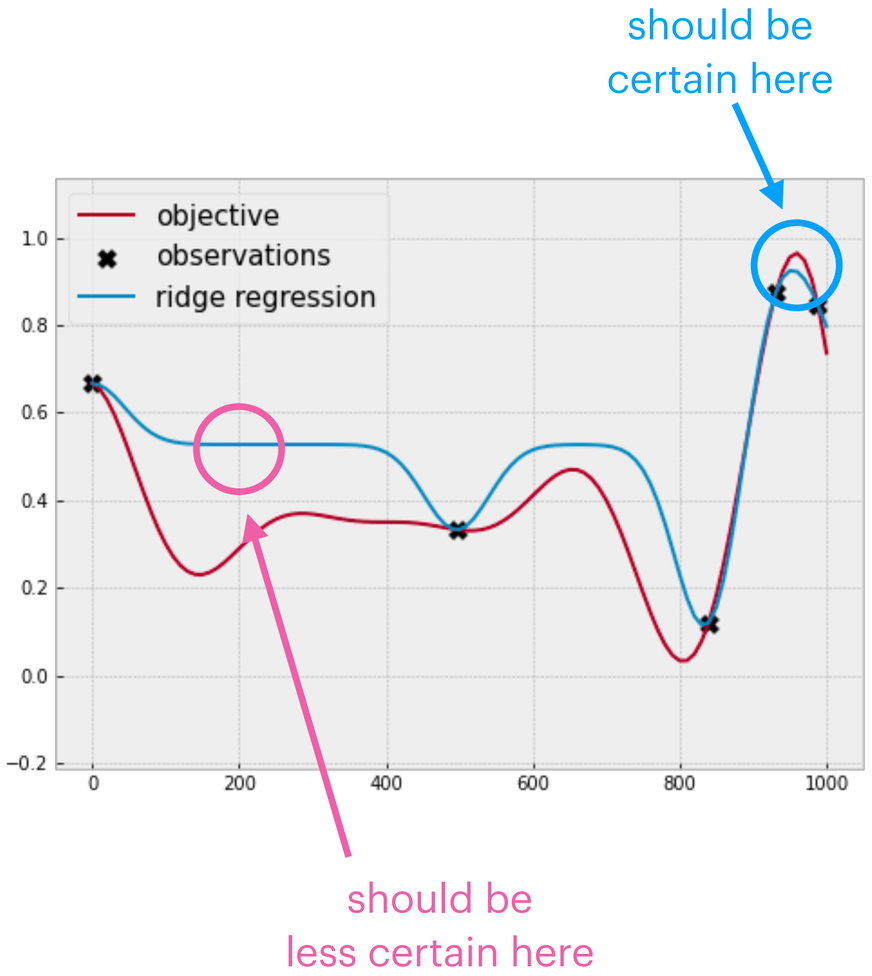

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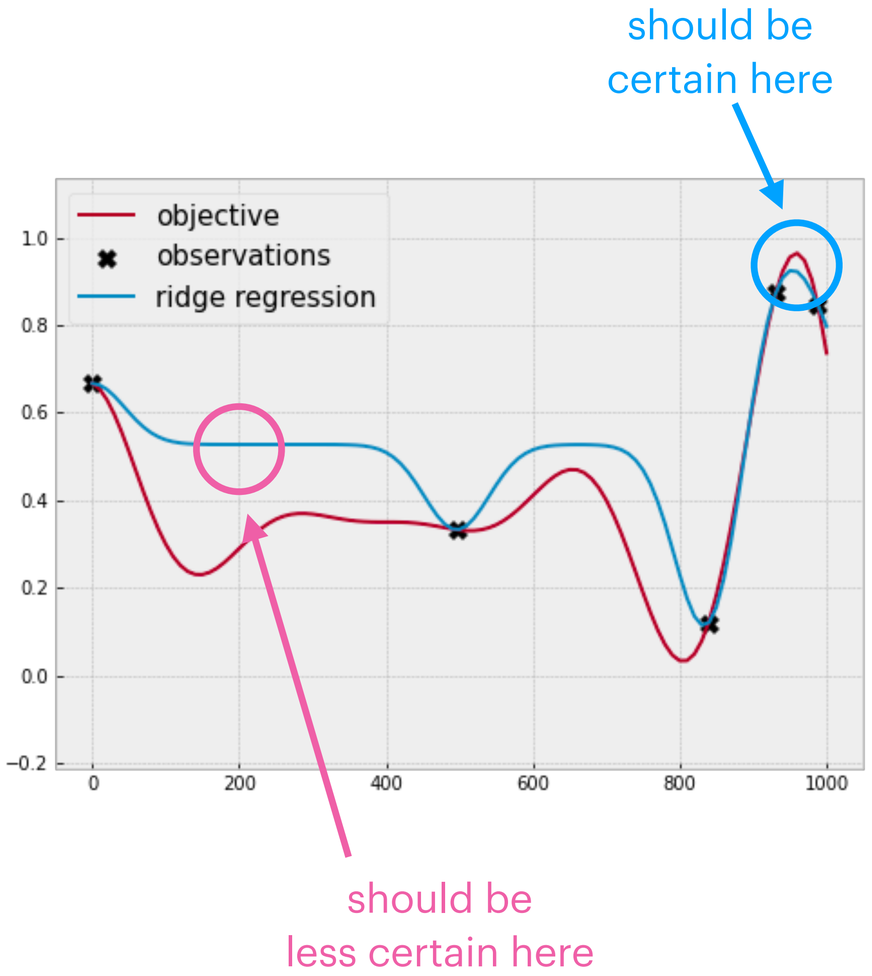

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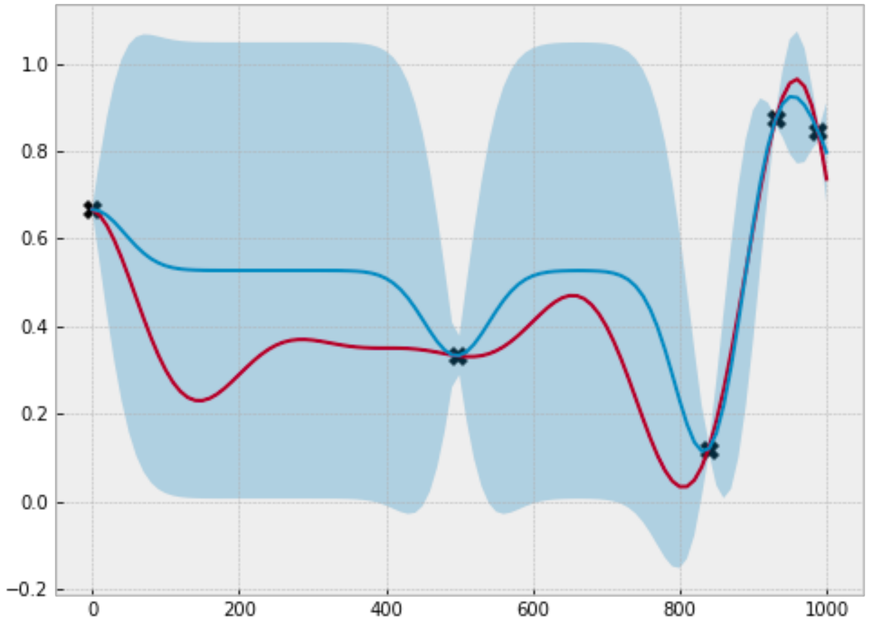

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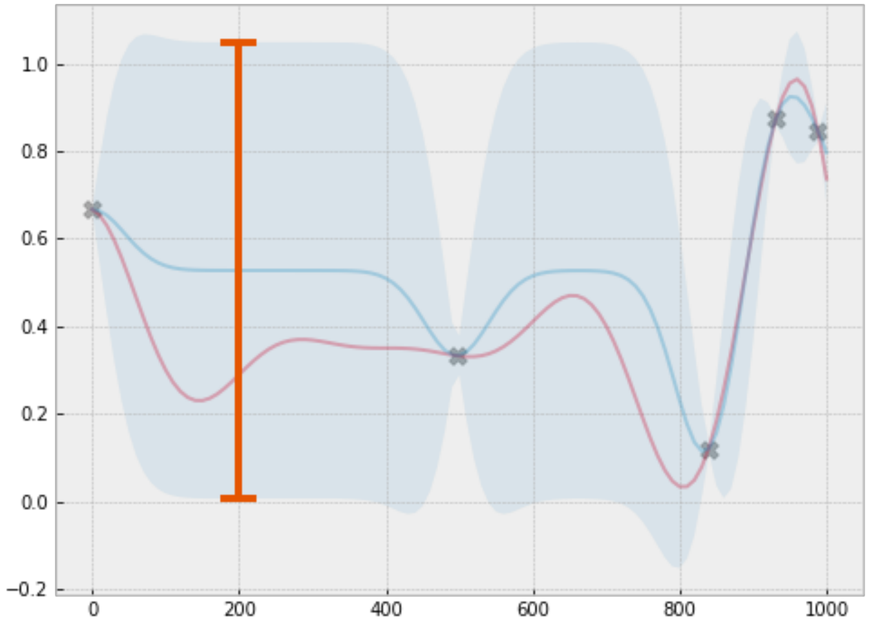

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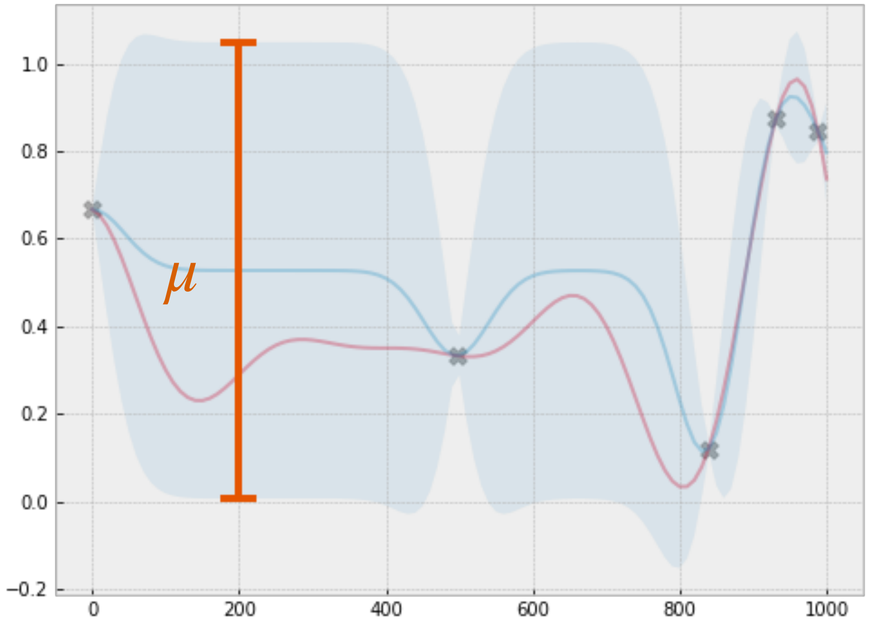

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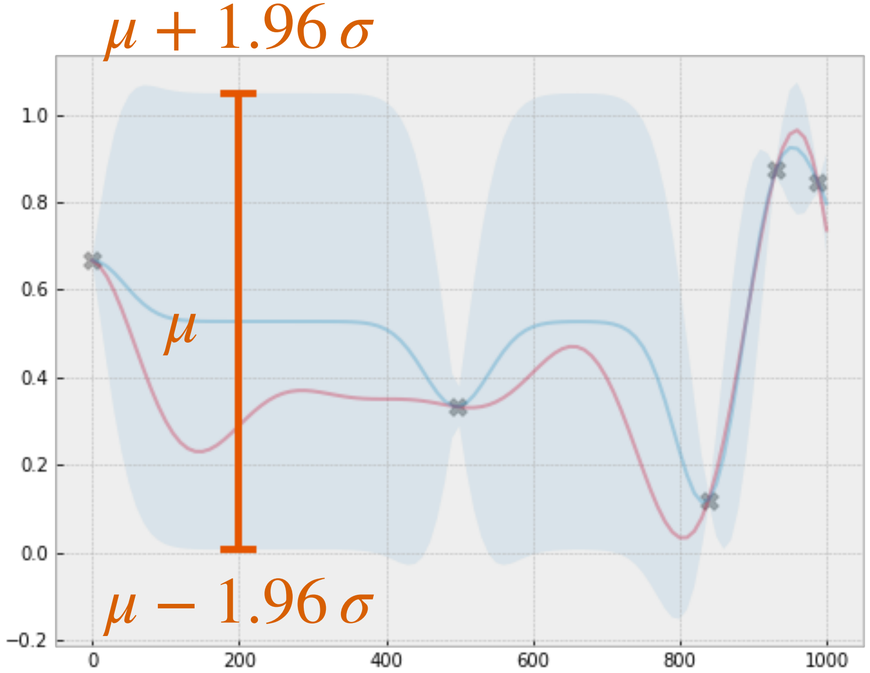

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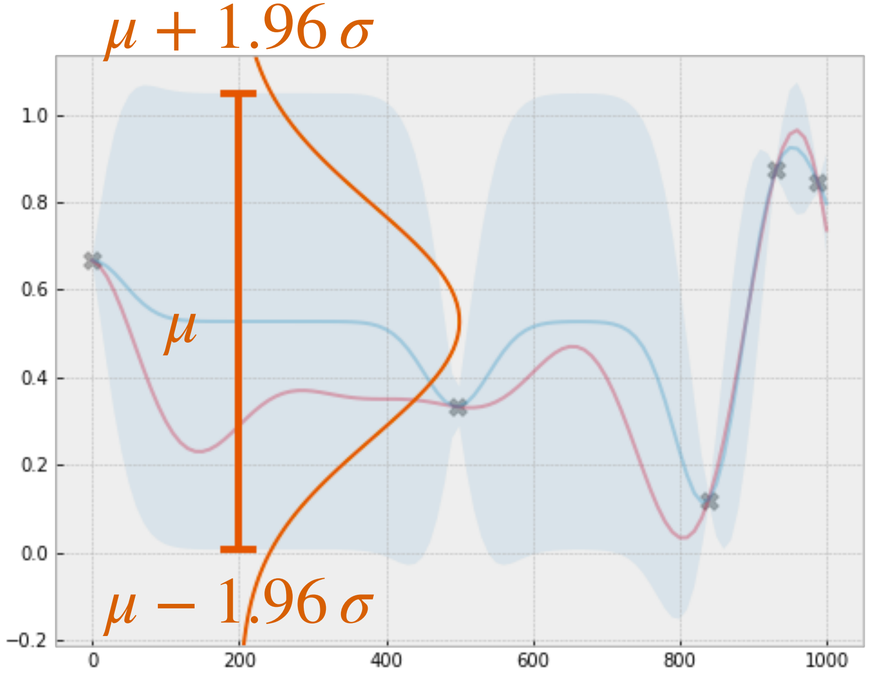

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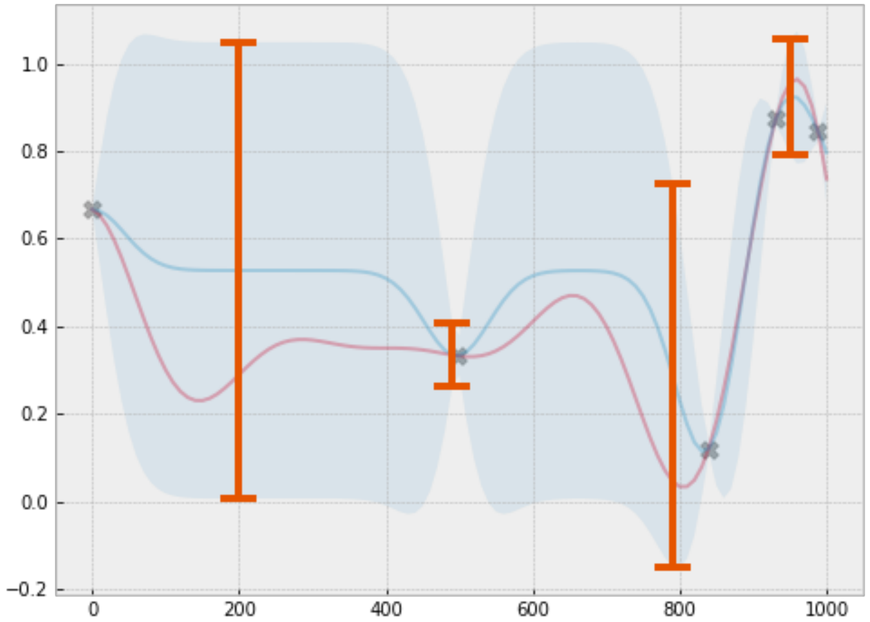

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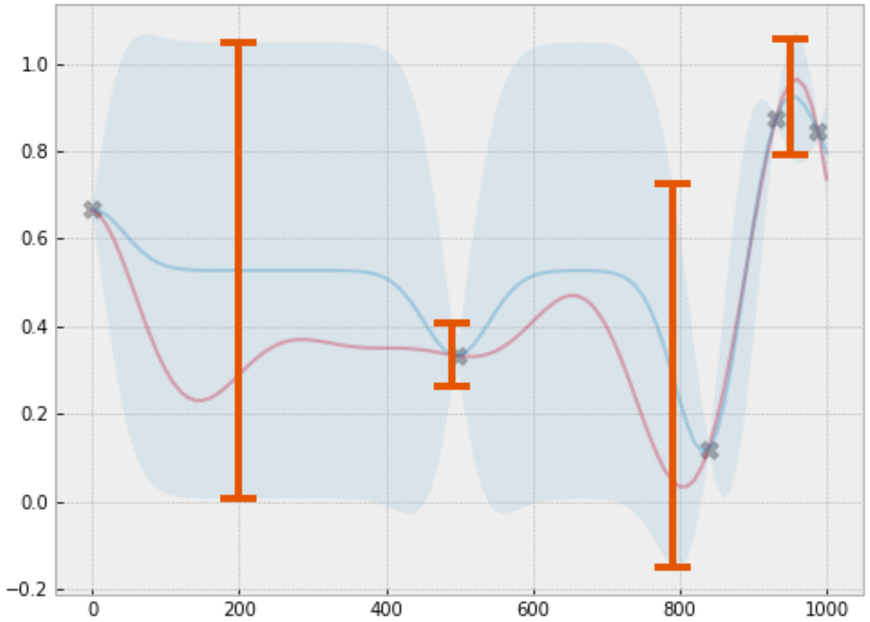

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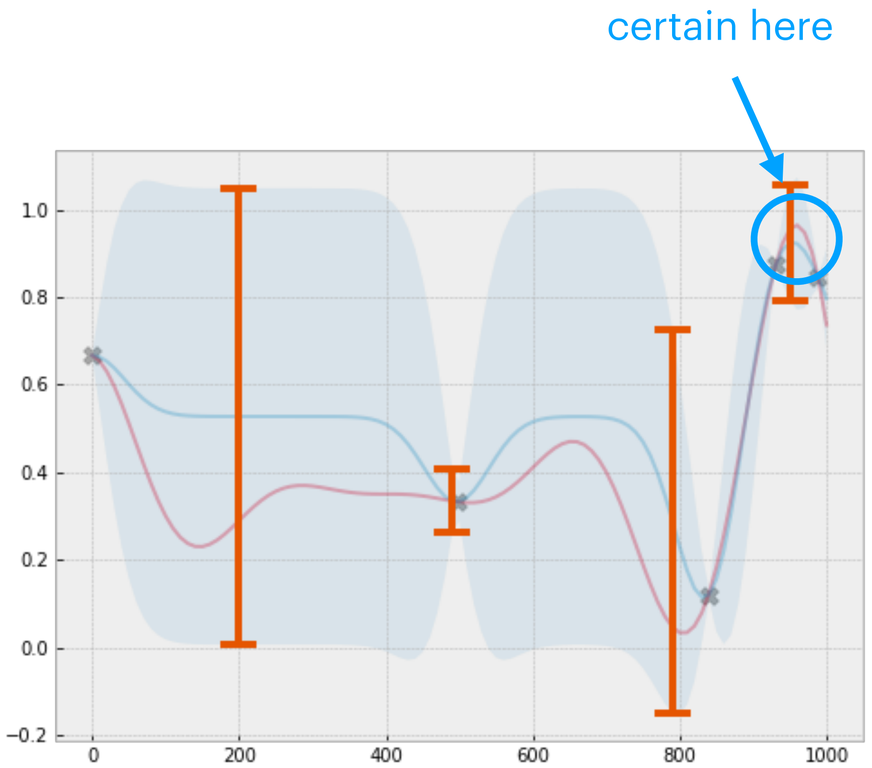

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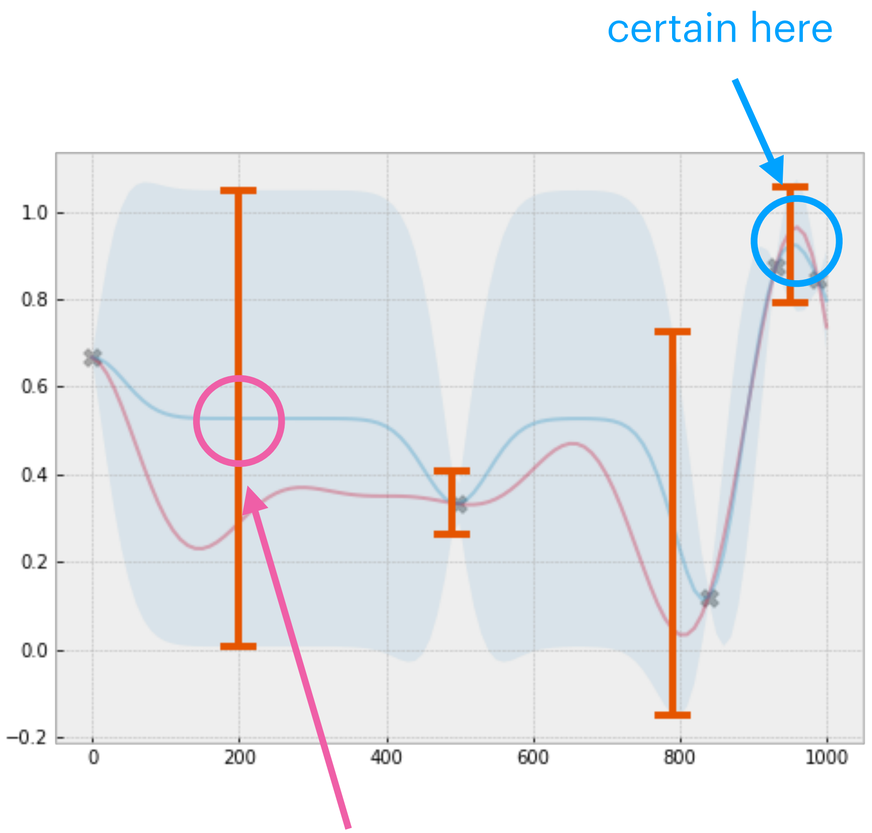

The exploitation–exploration trade-off

sticking to what we know vs. taking a risk

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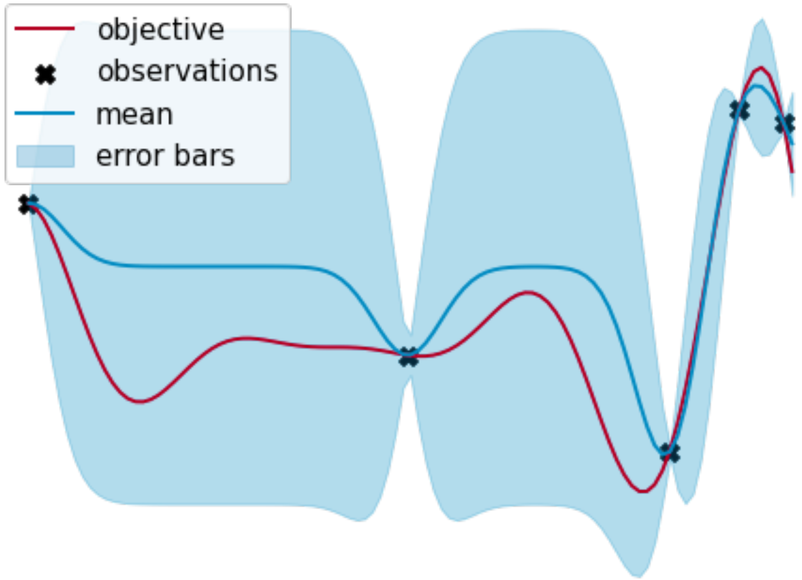

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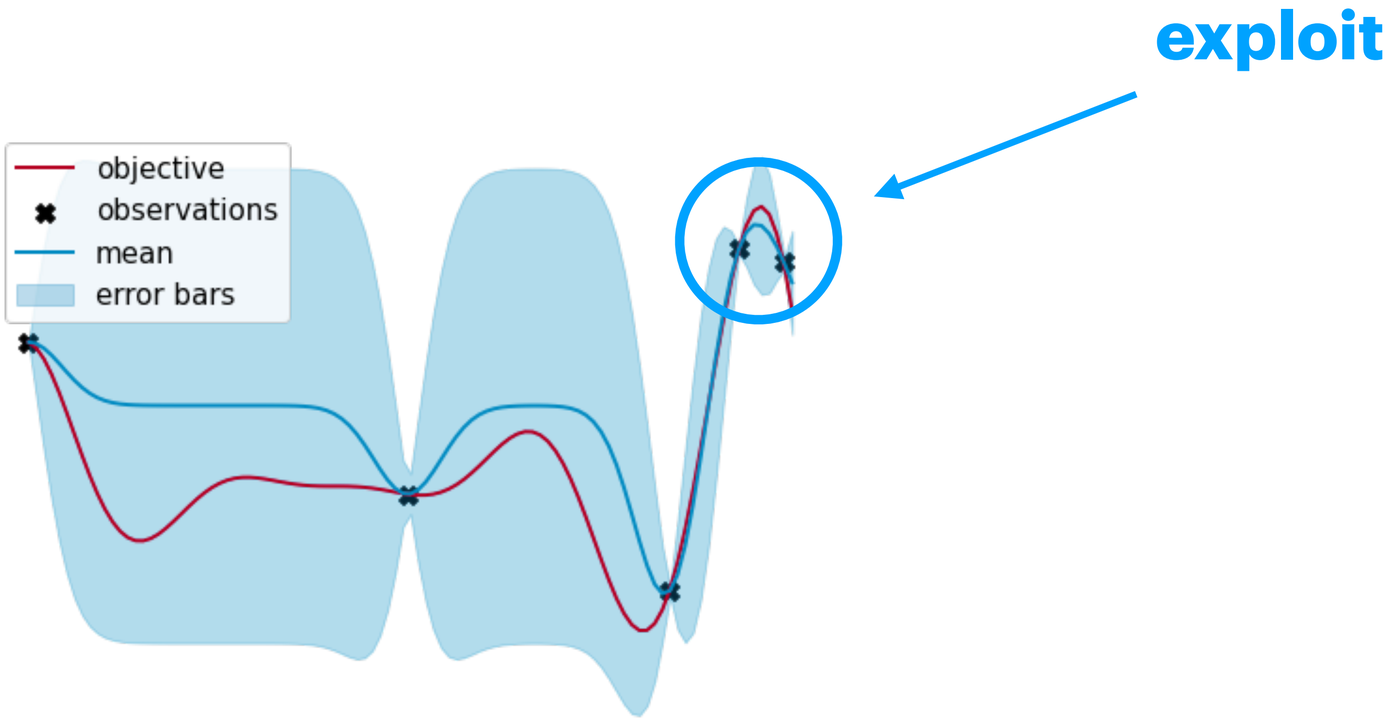

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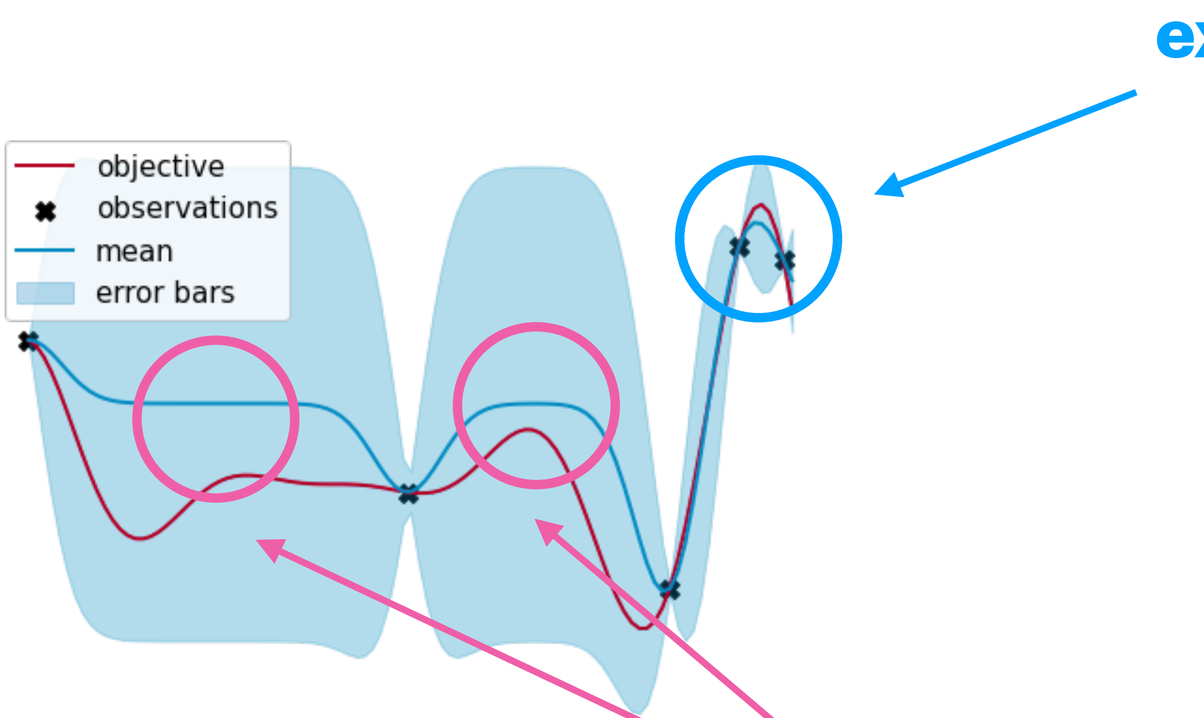

exploit

explore

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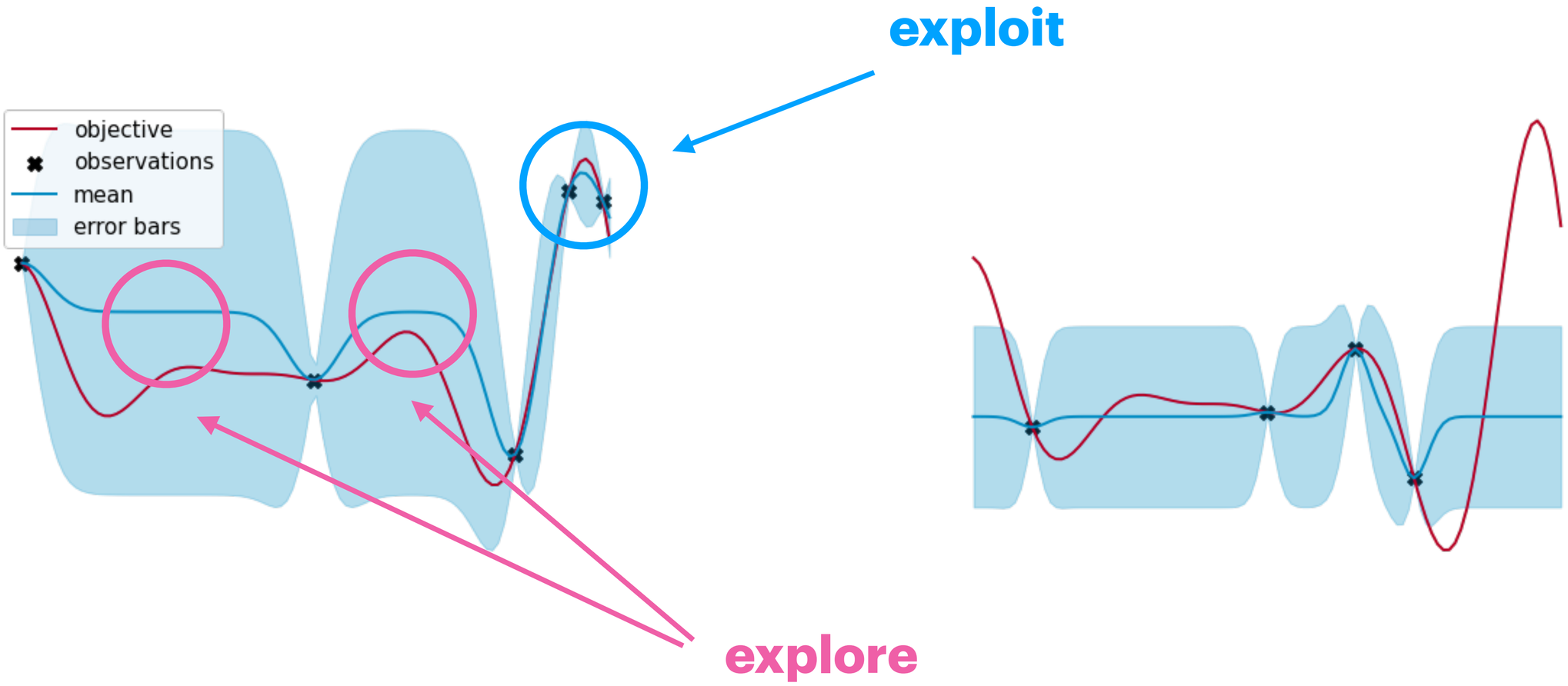

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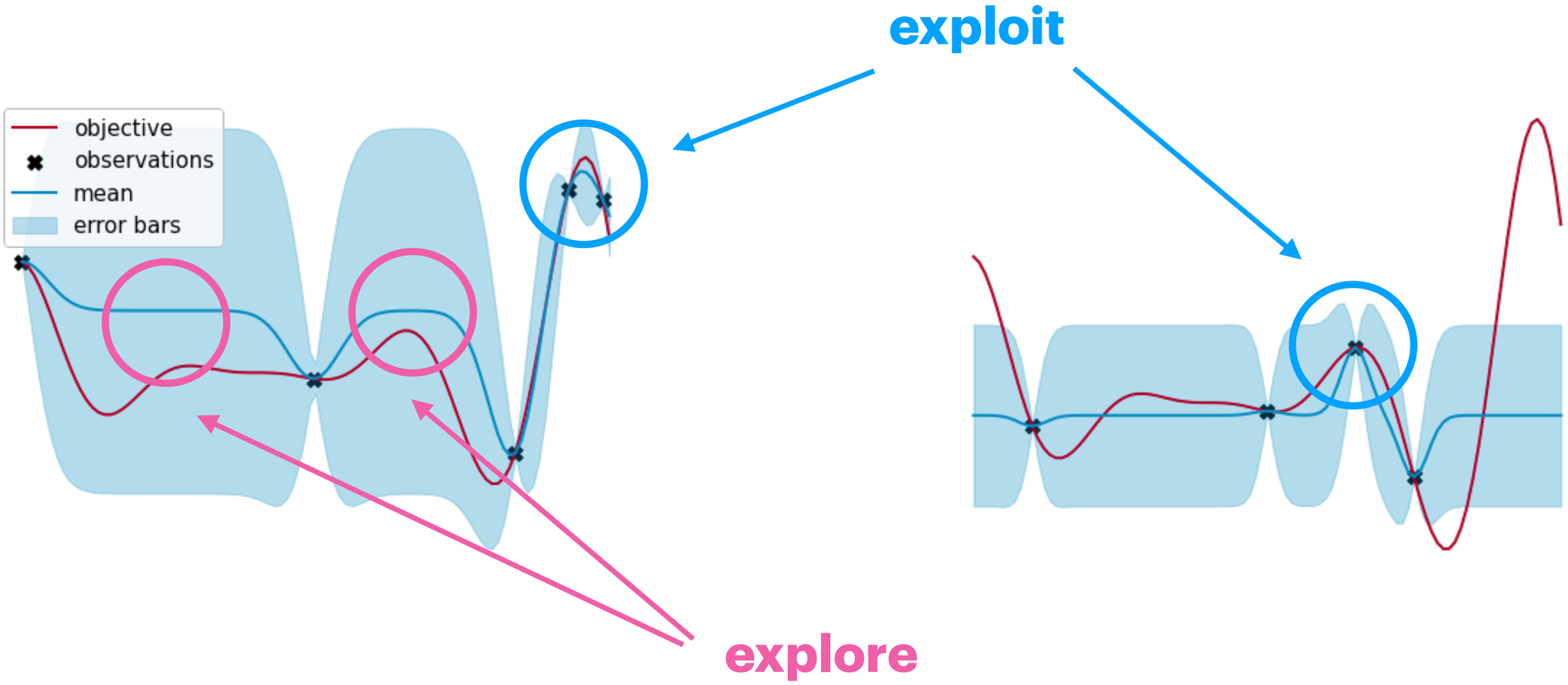

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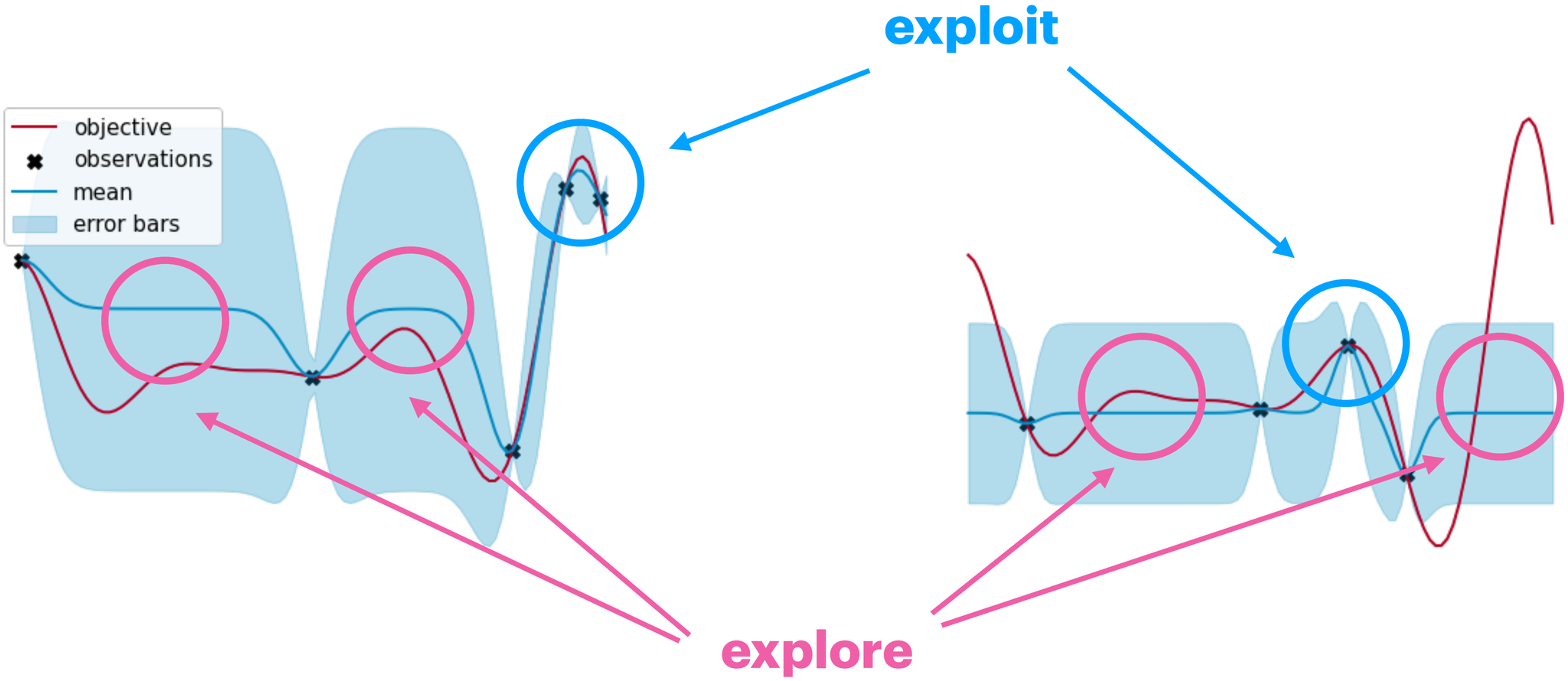

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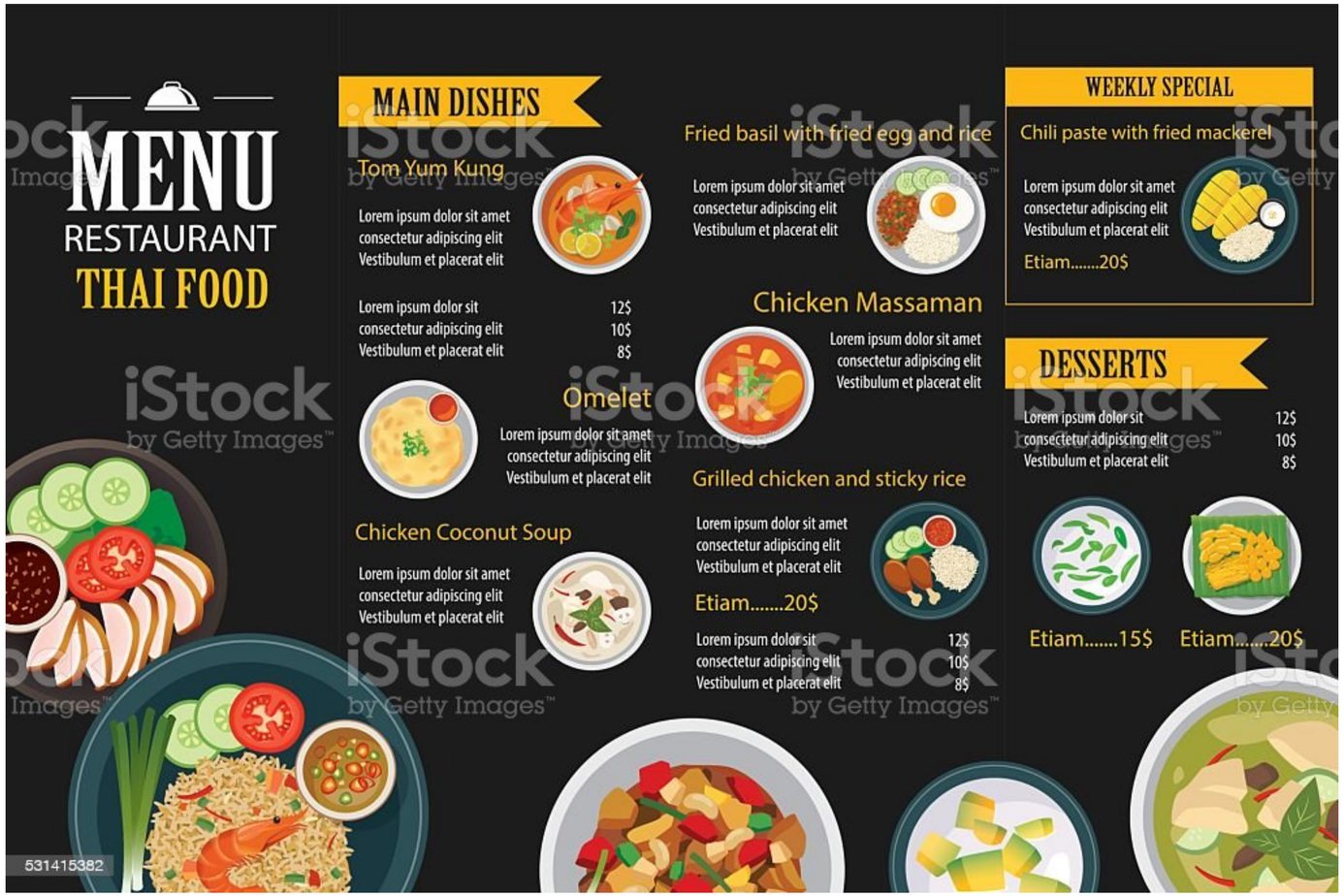

Optimization policy for decision making

choosing the best course of action, the Bayesian way

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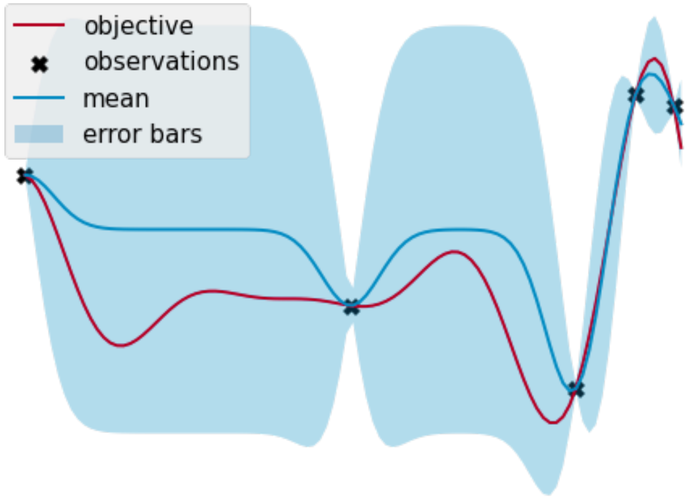

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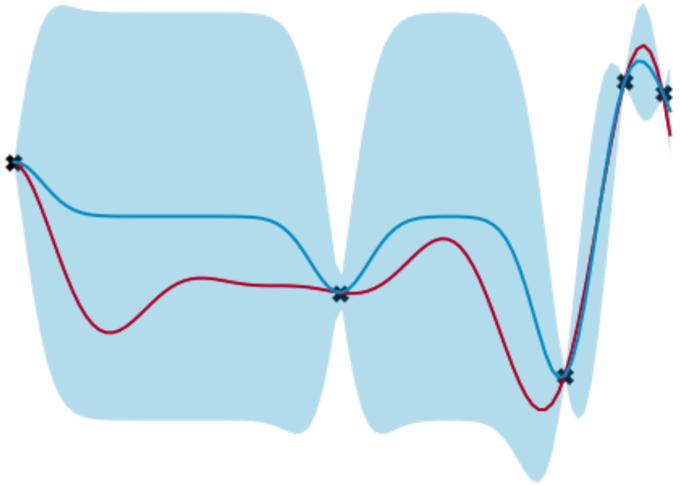

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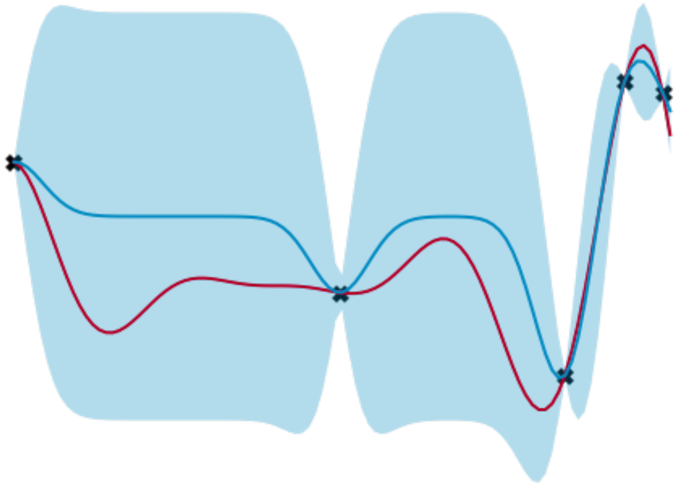

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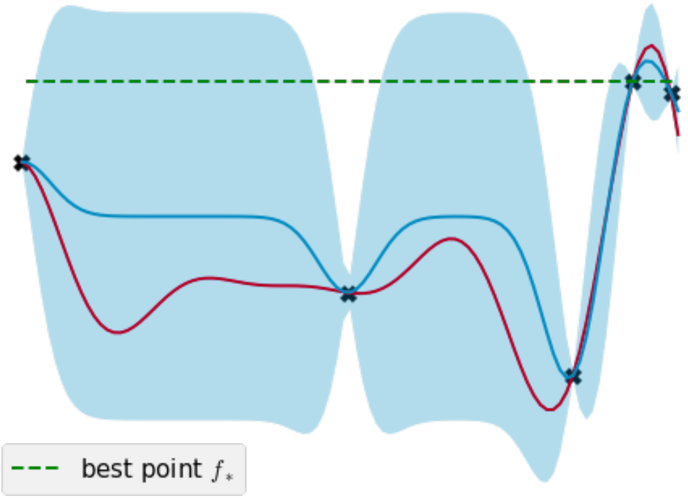

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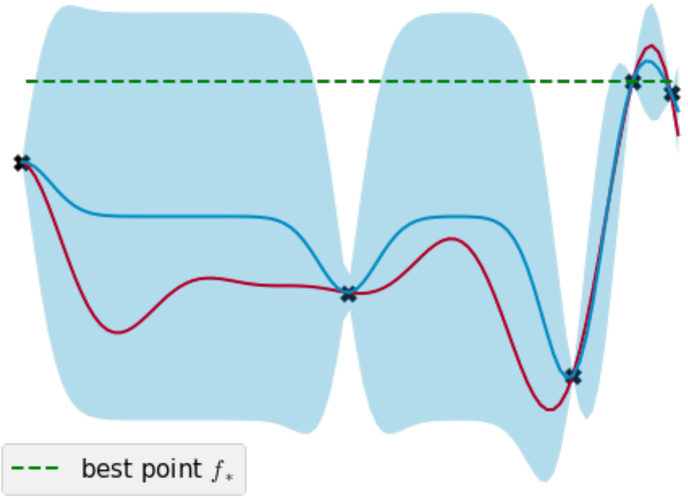

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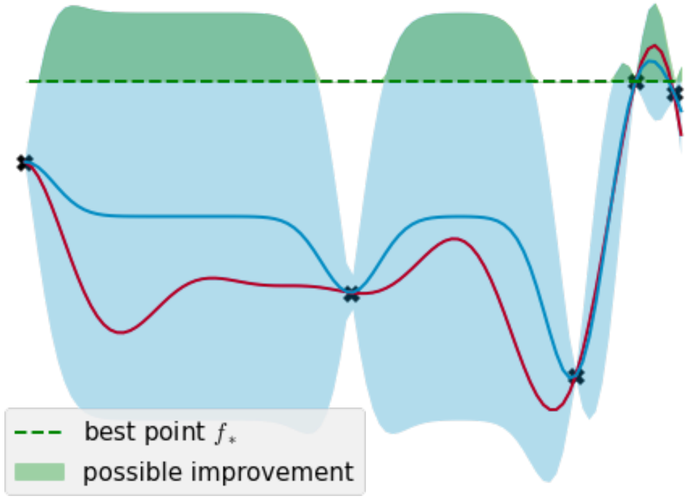

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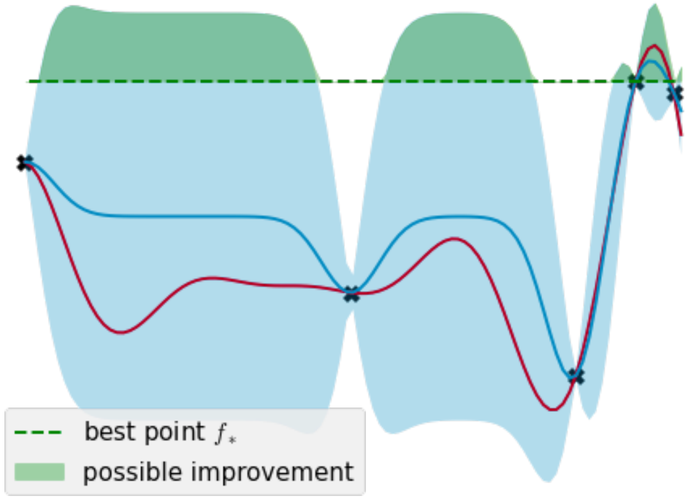

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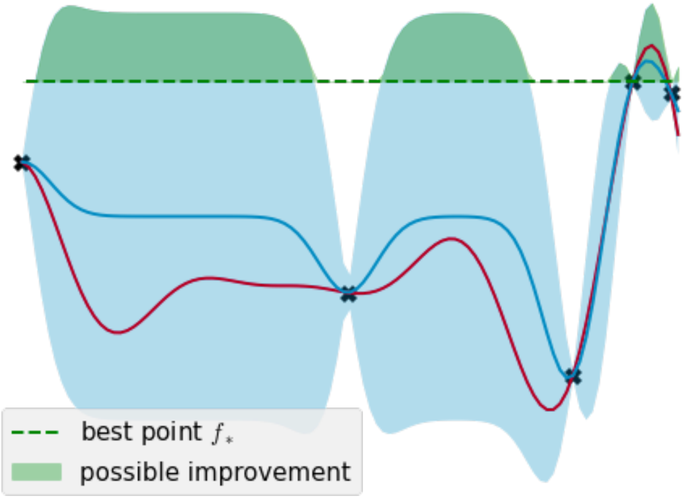

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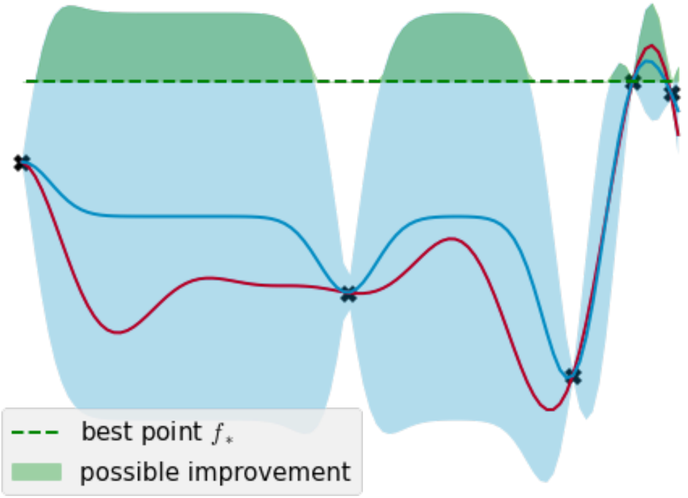

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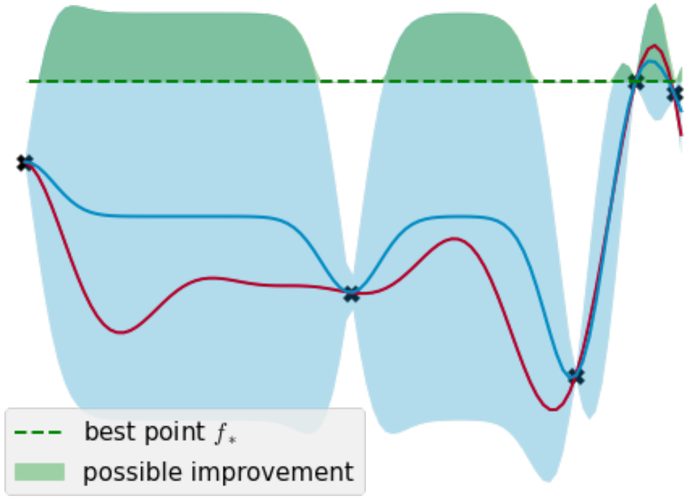

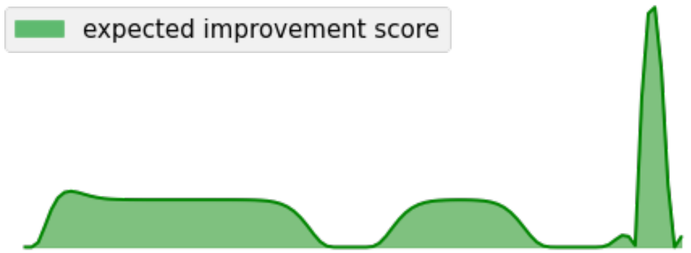

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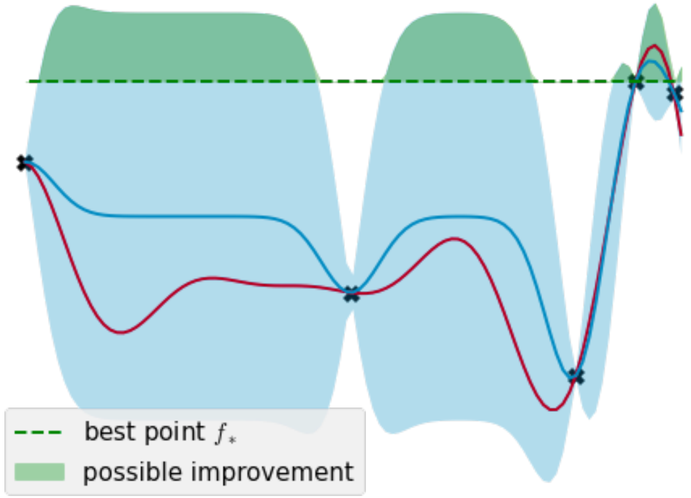

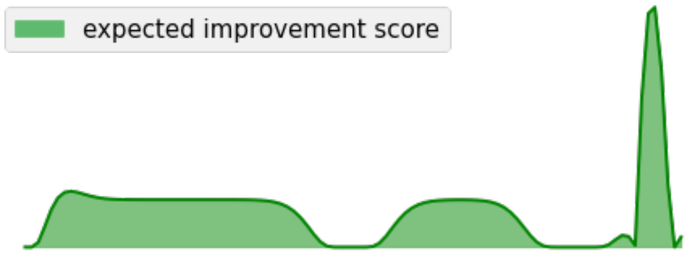

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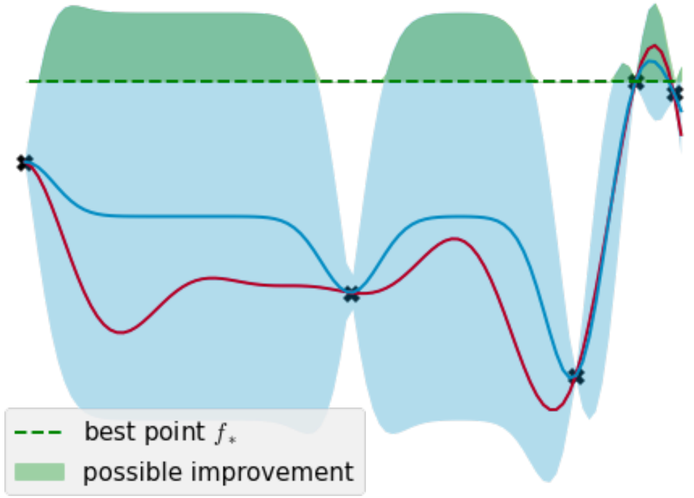

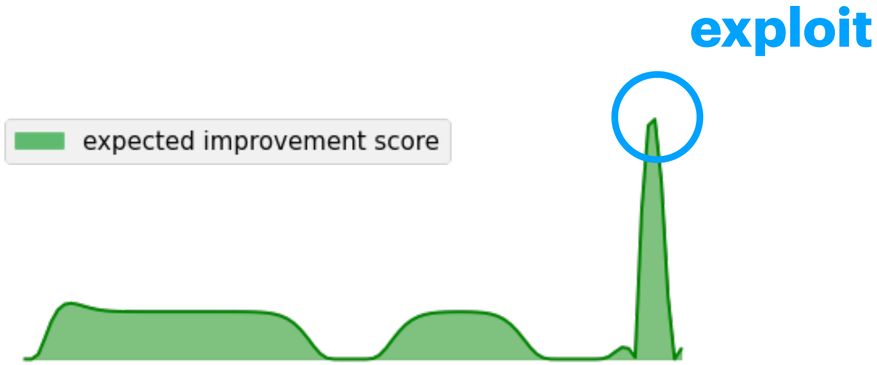

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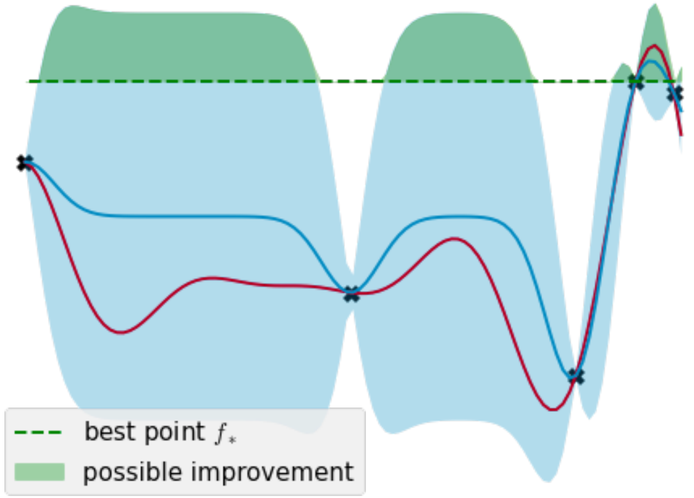

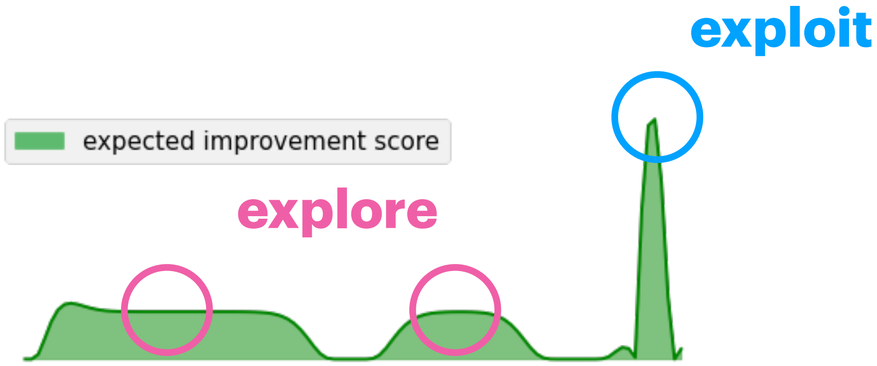

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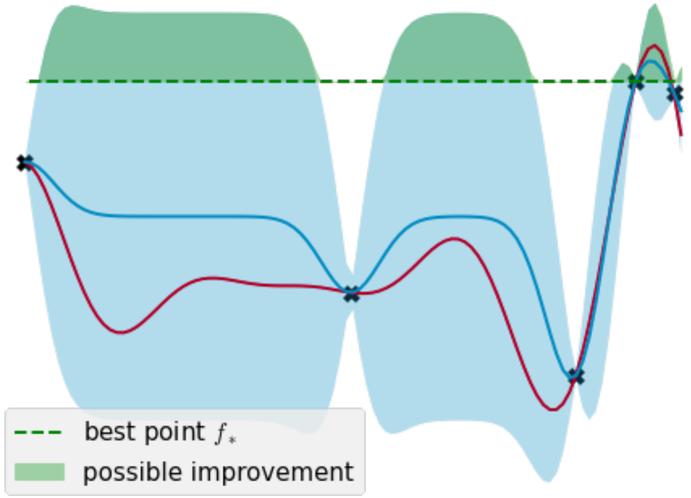
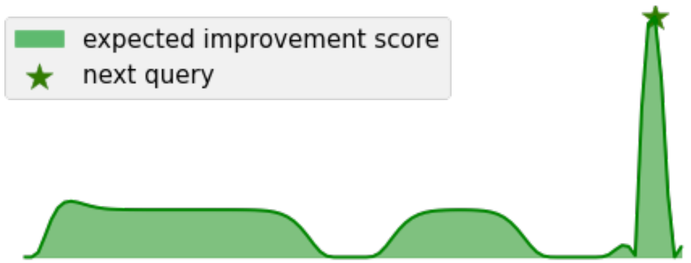
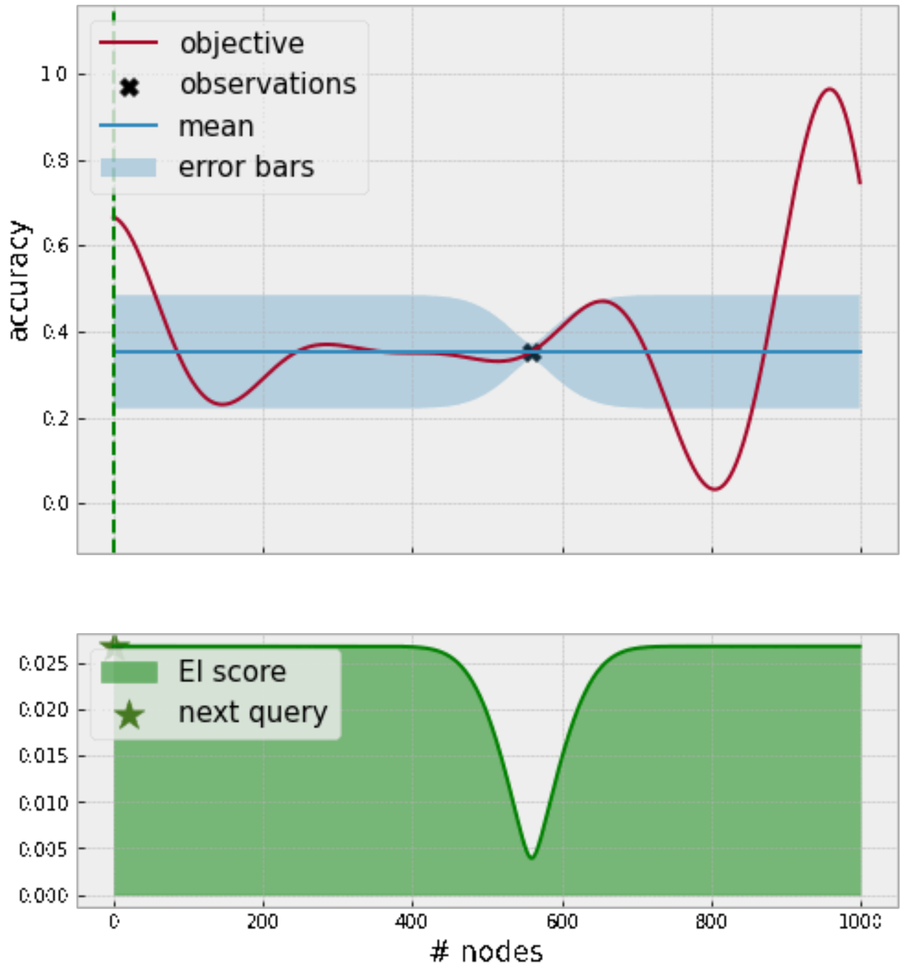




Bayesian optimization in action

benefits from adaptive decision-making



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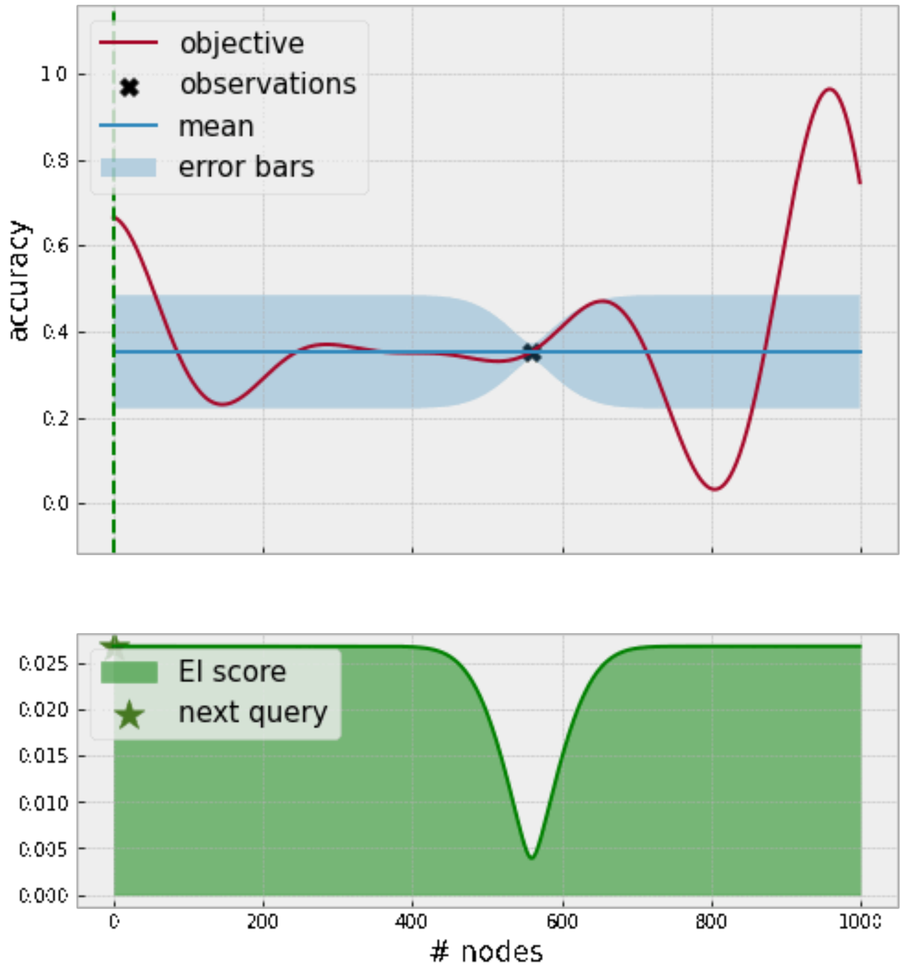

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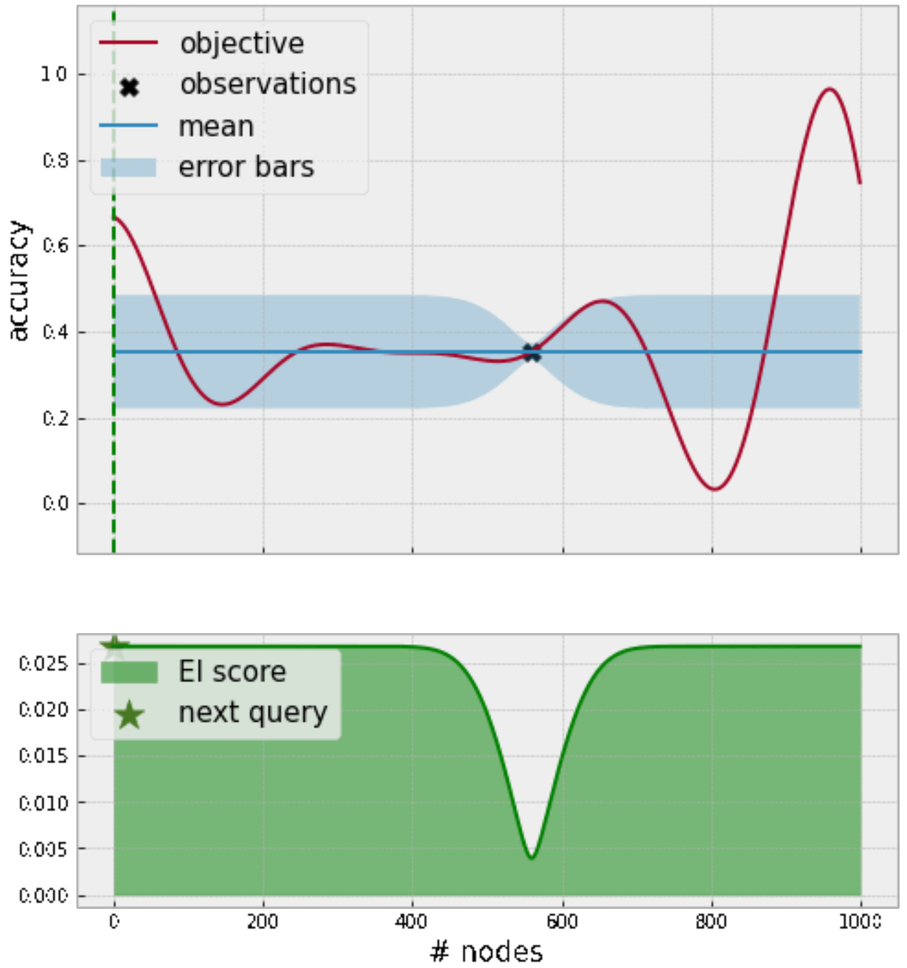

Bayesian optimization in action

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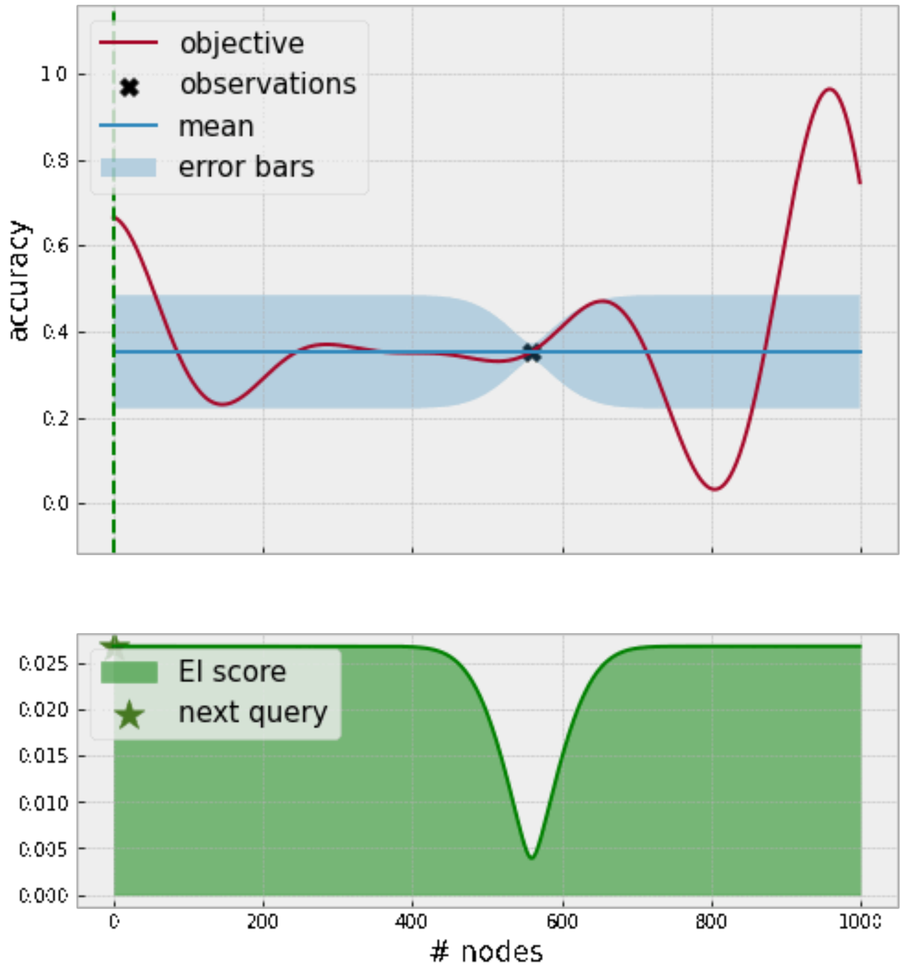
- Leverages *past observations to inform future decisions*
- Doesn't get *stuck in local optima*



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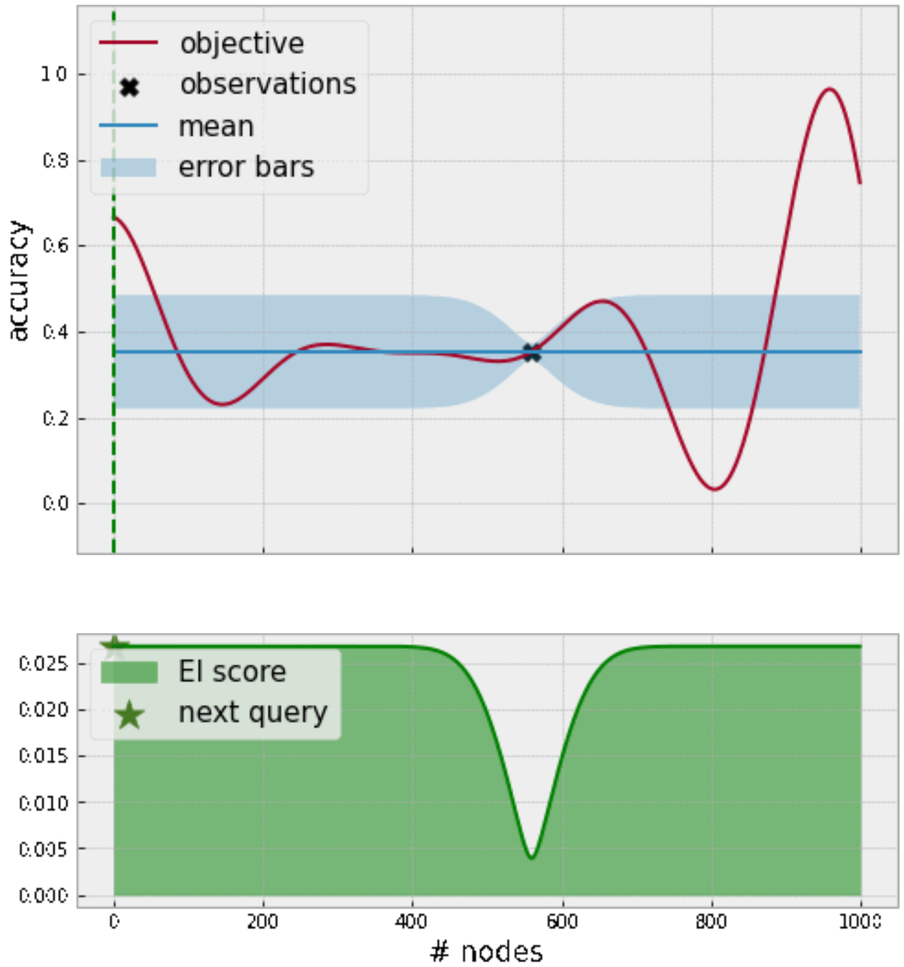

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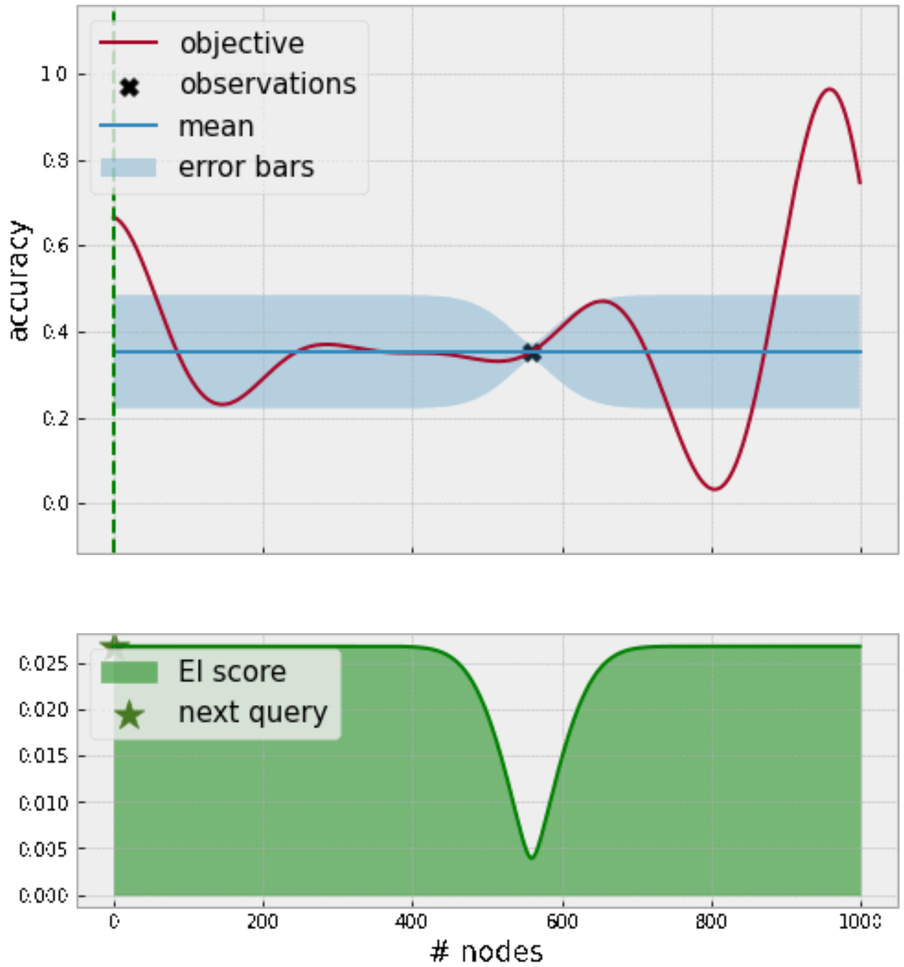

Other Bayesian optimization policies

different heuristics to decision-making

Other Bayesian optimization policies

different heuristics to decision-making

- From reinforcement learning's multi-armed bandit:

Other Bayesian optimization policies

different heuristics to decision-making

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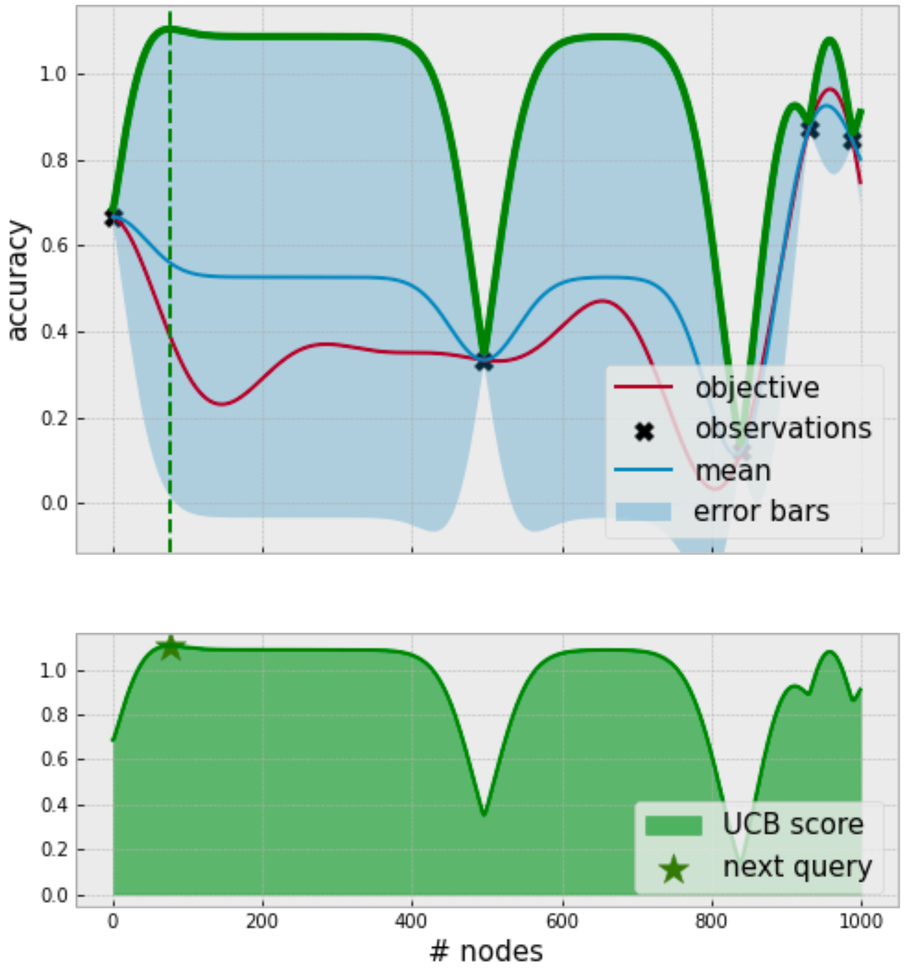

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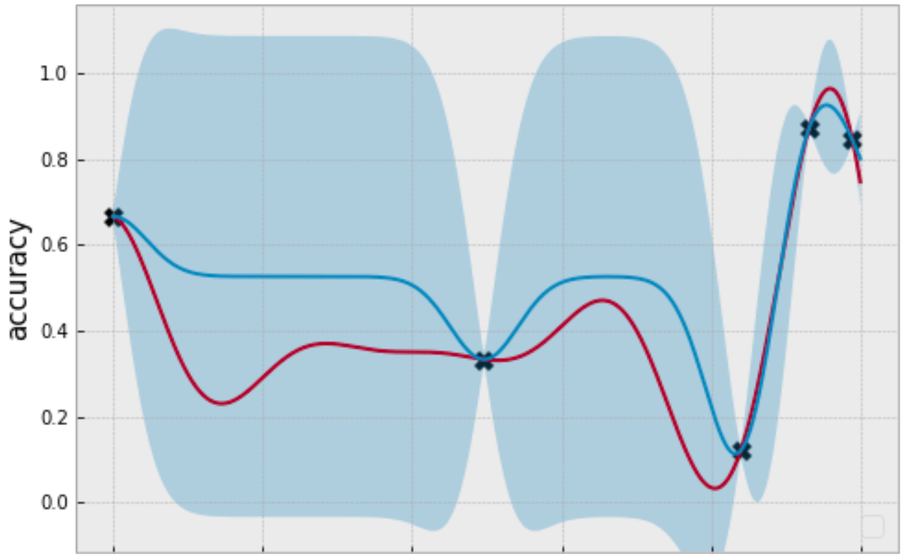

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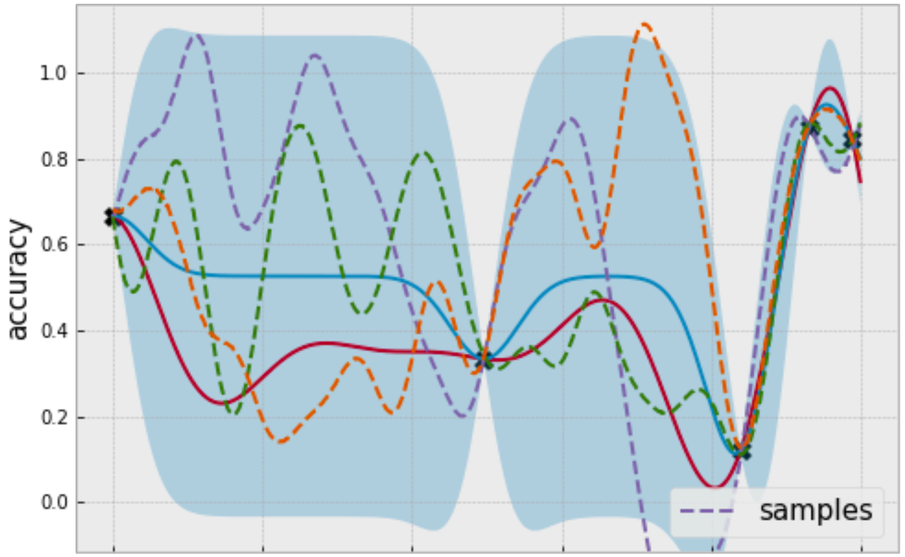

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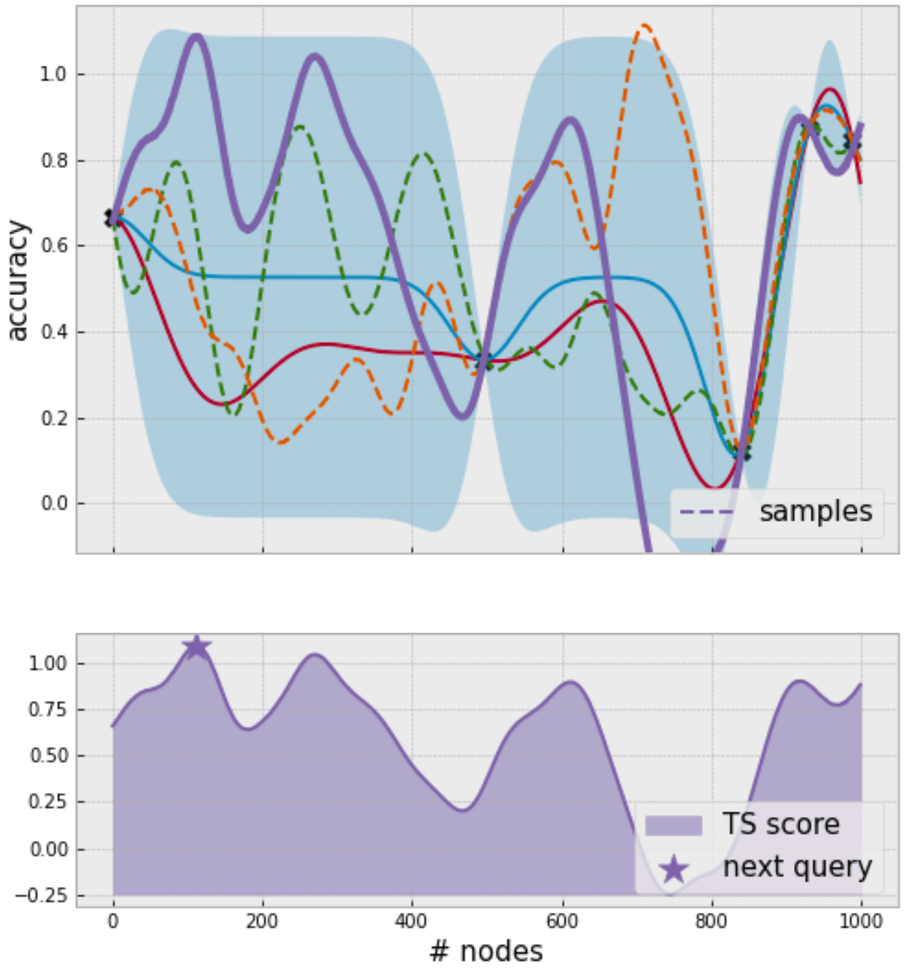

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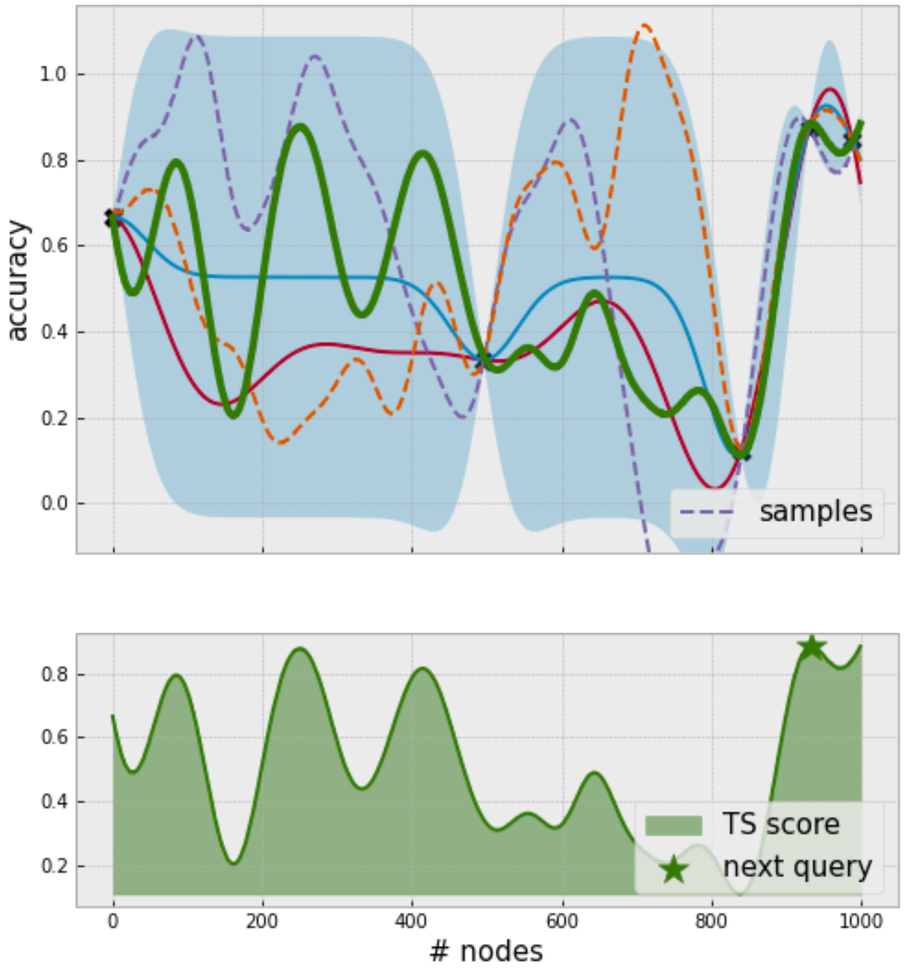

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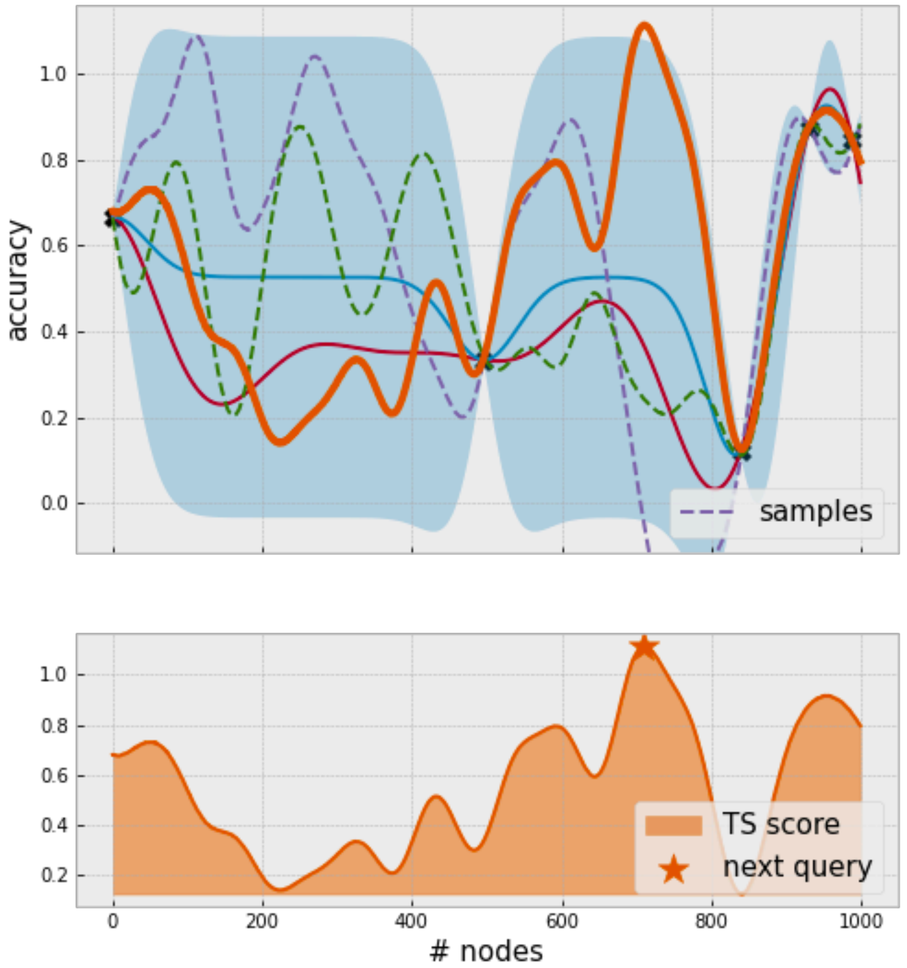

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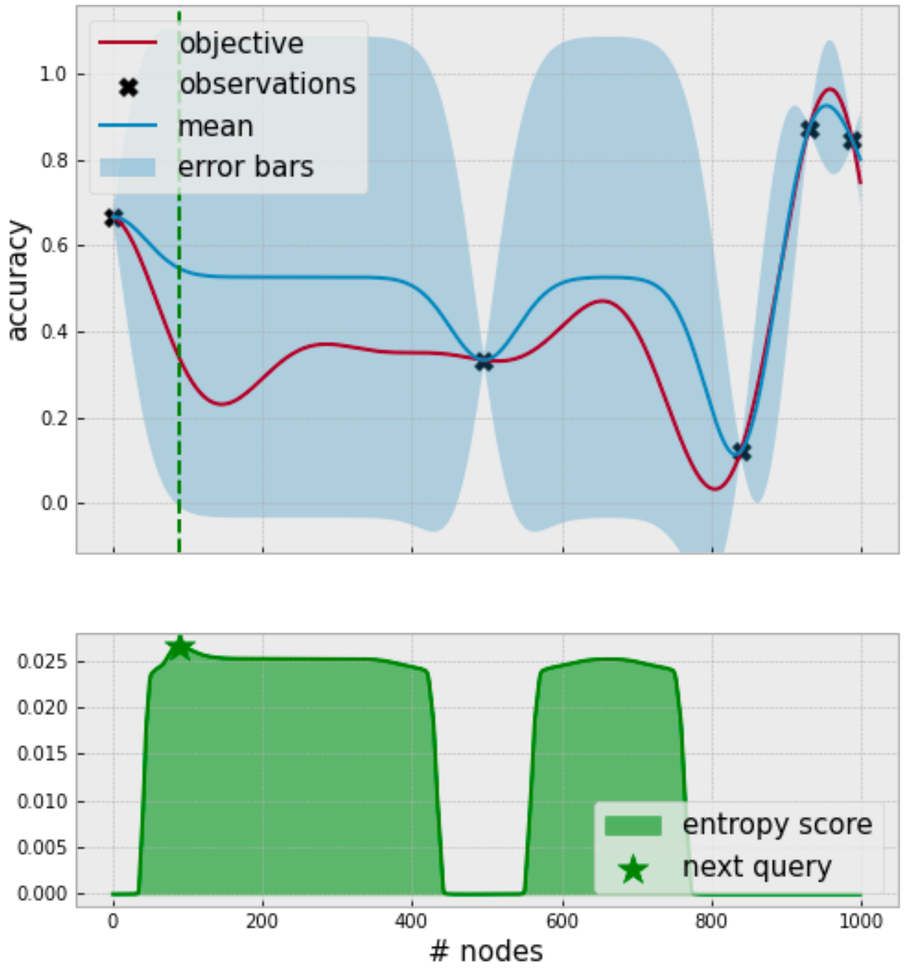

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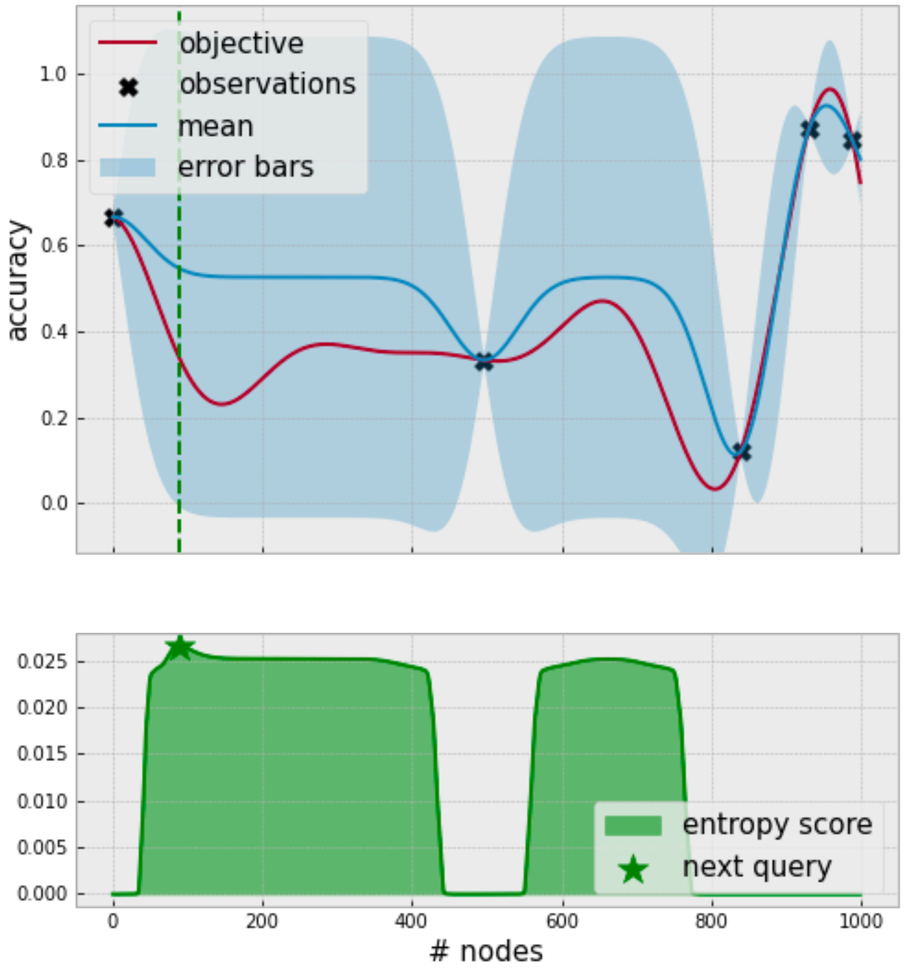
- Each policy balances between exploitation and exploration

no one-size-fits-all policy



Success stories

how others have used Bayesian optimization

Success stories

how others have used Bayesian optimization

- *Conclusive success* at

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Bayesian Optimization is Superior to Random Search for Machine Learning Hyperparameter Tuning: Analysis of the Black-Box Optimization Challenge 2020

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4Paradigm

Isabelle Guyon
guyon@chalearn.org
ChaLearn

Turner et al. https://arxiv.org/pdf/2104.10201.pdf

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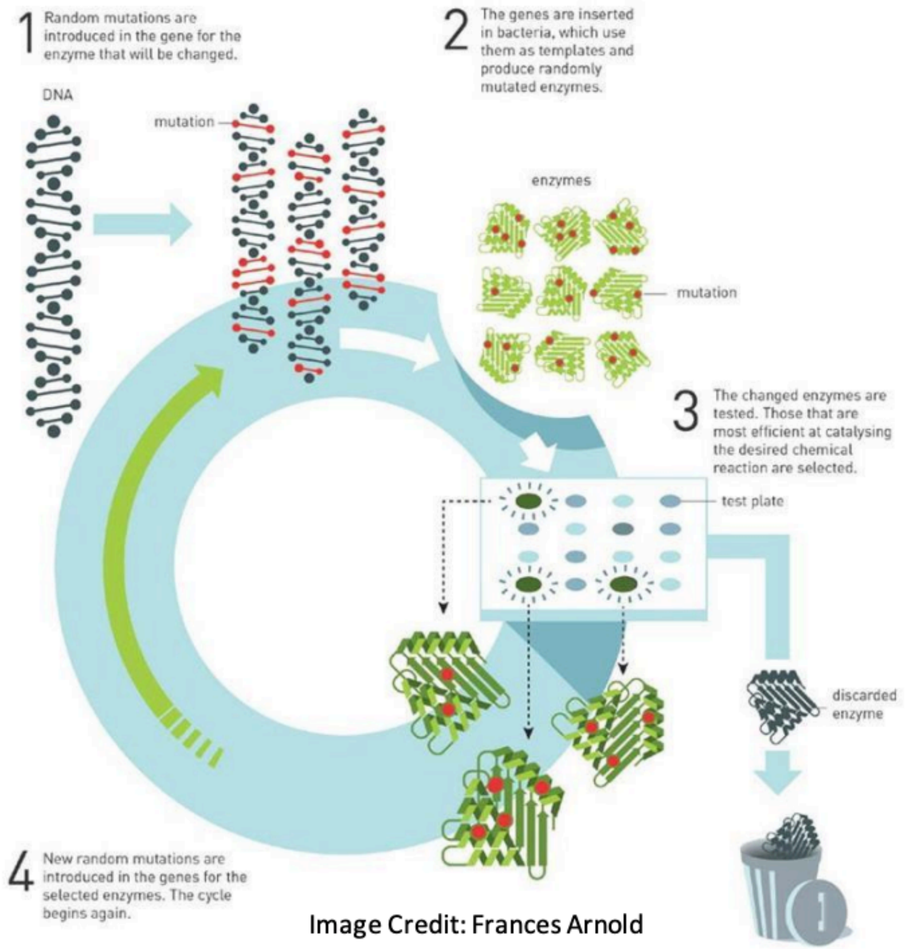

Image Credit: Frances Arnold

http://www.yisongyue.com/talks/real_world_bo.pdf

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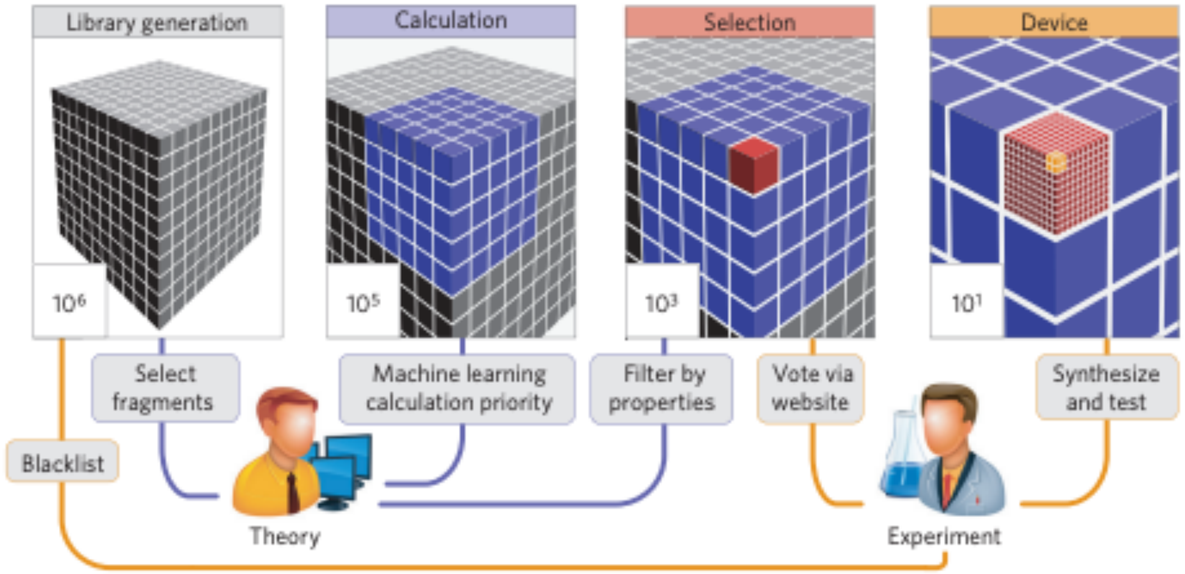


Gómez-Bombarelli et al. https://www.nature.com/articles/nmat4717

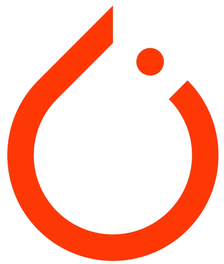
Implementing Bayesian optimization in Python

using a cohesive software ecosystem

The Torch ecosystem of Bayesian optimization

The Torch ecosystem of Bayesian optimization

PyTorch for
tensor manipulation



The Torch ecosystem of Bayesian optimization

PyTorch for
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GPyTorch for
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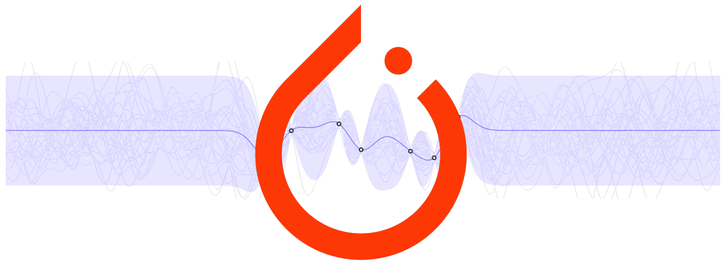

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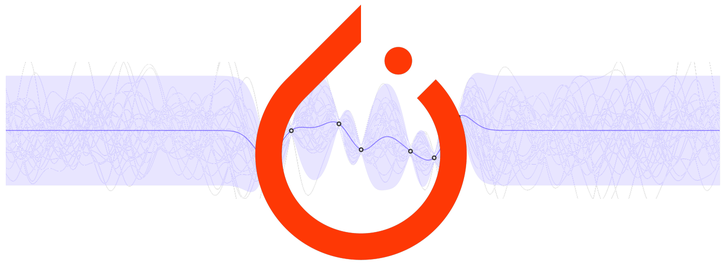

BoTorch for
BayesOpt policies

GPyTorch for Gaussian process modeling

modular implementation of Gaussian processes

Need to declare two components:

- **Mean function** models the *expected trend*
- **Kernel** models *smoothness*

GPyTorch for Gaussian process modeling

modular implementation of Gaussian processes

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```
class GPModel(ExactGP):
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = ConstantMean()
        self.covar_module = RBFKernel()

    def forward(self, x):
        mean_x = self.mean_module(x)
        covar_x = self.covar_module(x)
        return MultivariateNormal(mean_x, covar_x)
```

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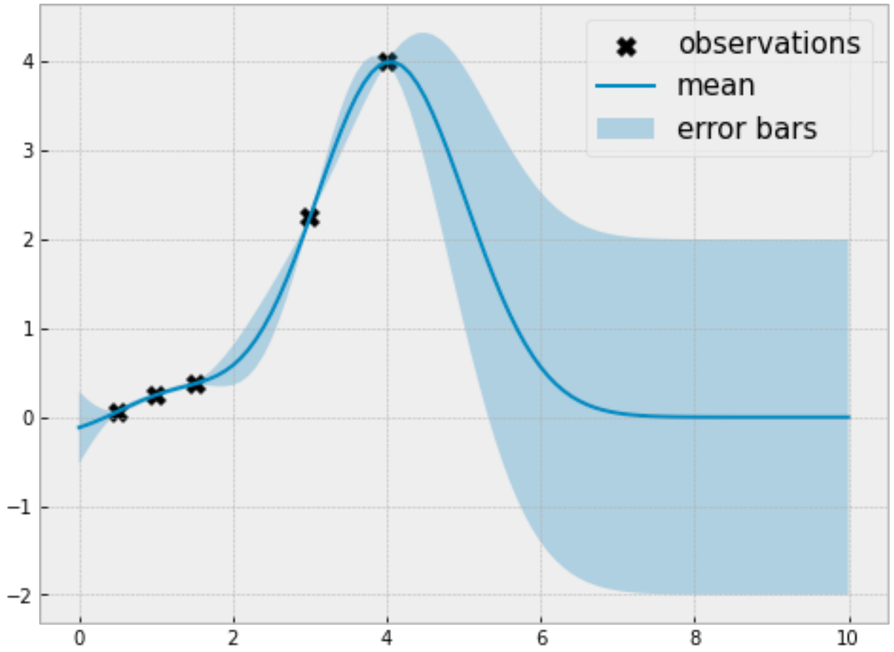

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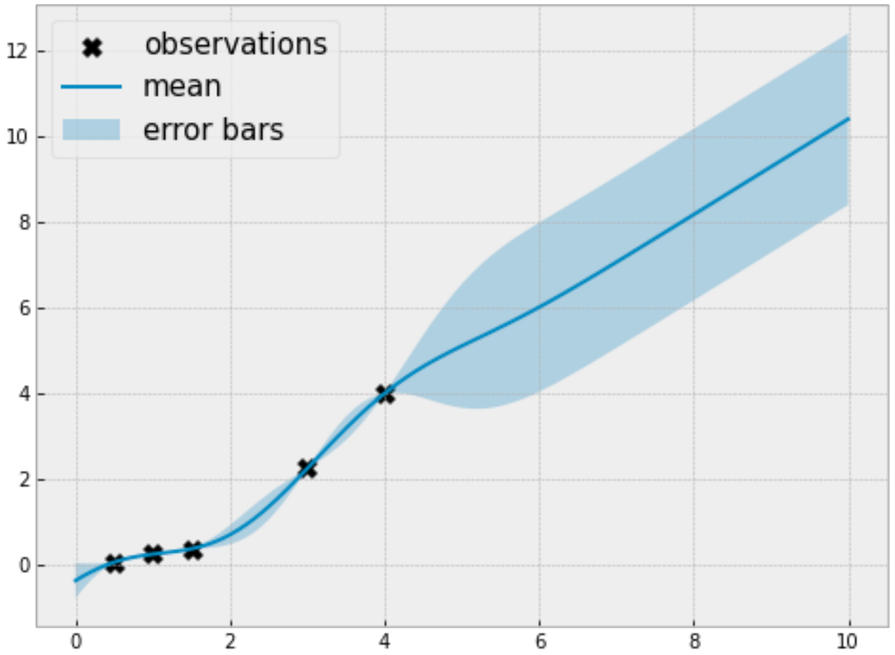
```
class GPModel(ExactGP):
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = LinearMean(1)
        self.covar_module = RBFKernel()
```



GPyTorch for Gaussian process modeling

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Need to declare two components:

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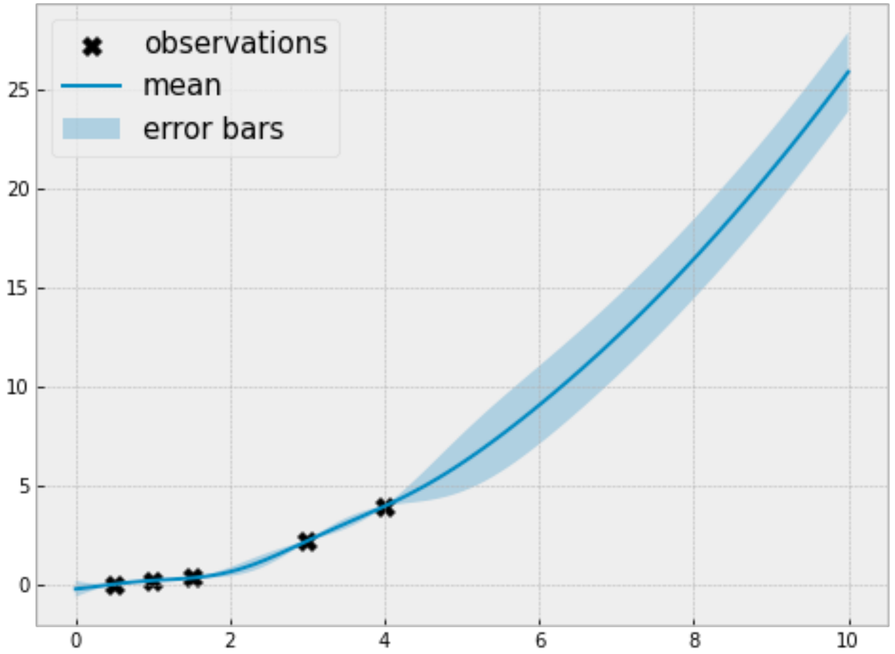
```
class QuadraticMean(Mean):
    def forward(self, x):
        res = (
            x.pow(2).matmul(self.second)
            + x.matmul(self.first)
            + self.bias
        )
        return res
```



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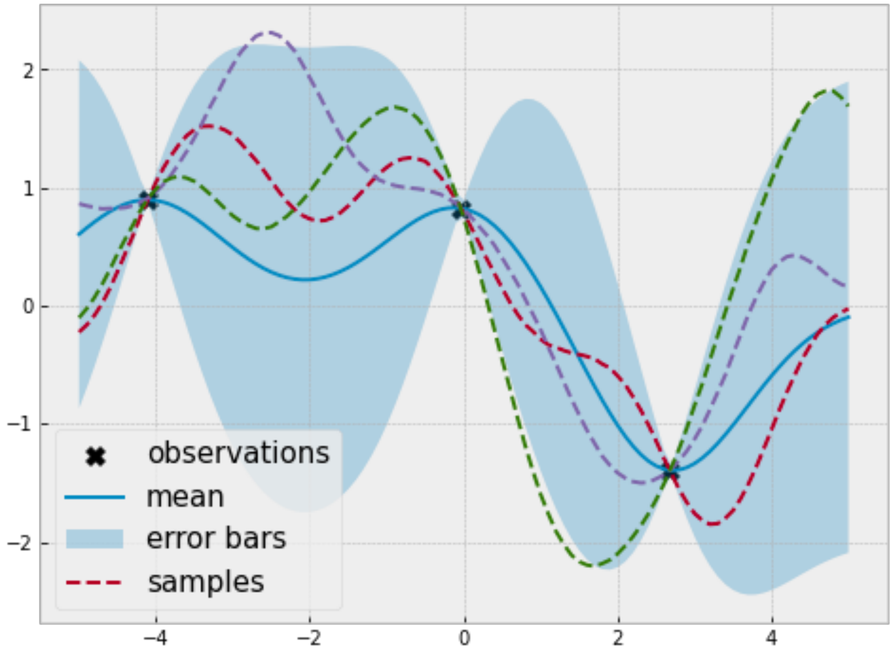

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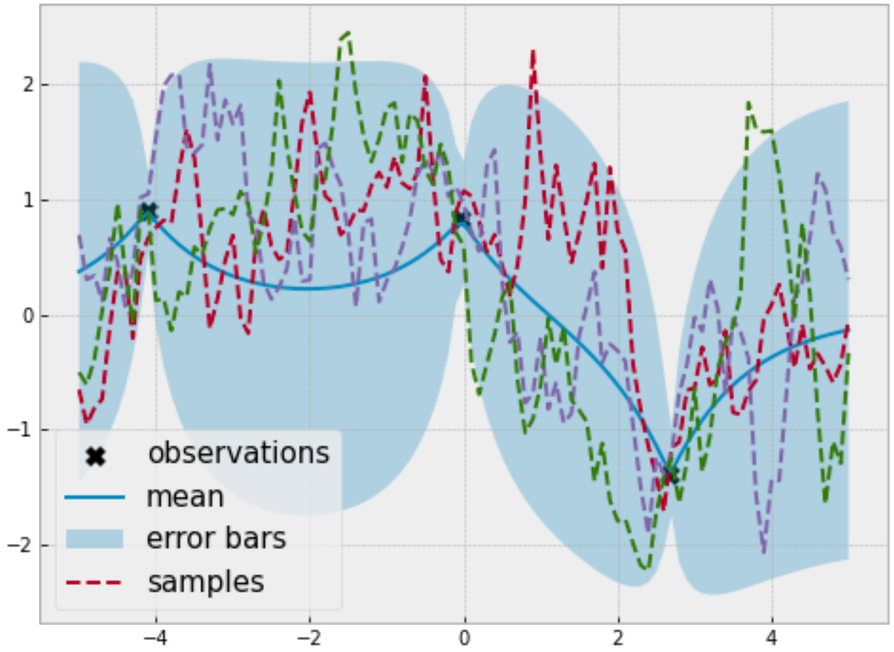
    def __init__(self, train_x, train_y, likelihood):
        super().__init__(train_x, train_y, likelihood)
        self.mean_module = ConstantMean()
        self.covar_module = MaternKernel(nu=0.5)
```



BoTorch for Bayesian optimization policies

modular decision making

changing the policy == replacing one line of code (most of the time)

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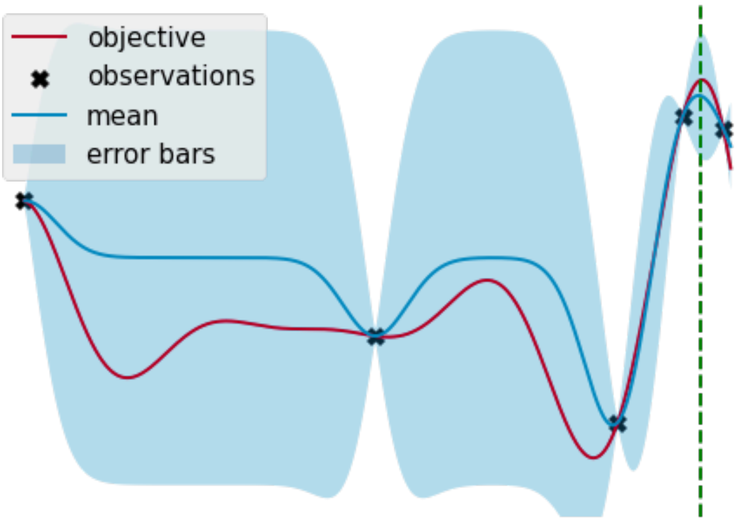
```
policy = ExpectedImprovement(
    model, best_f=train_y.max()
)
```



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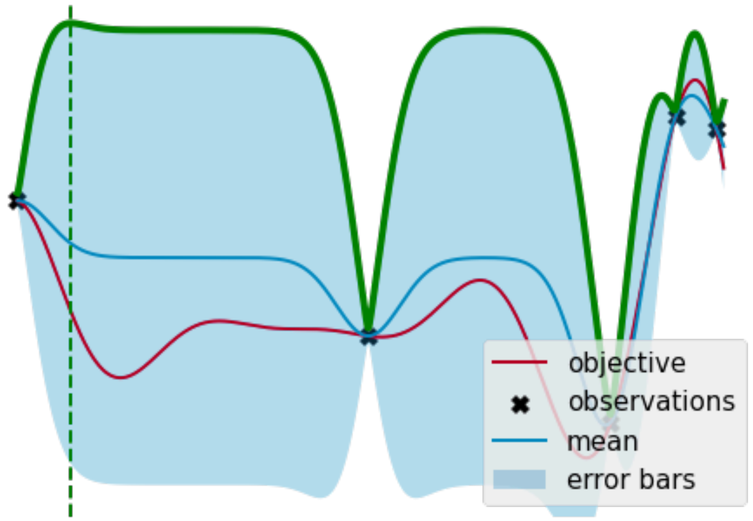
```
policy = UpperConfidenceBound(
    model, beta=2
)
```



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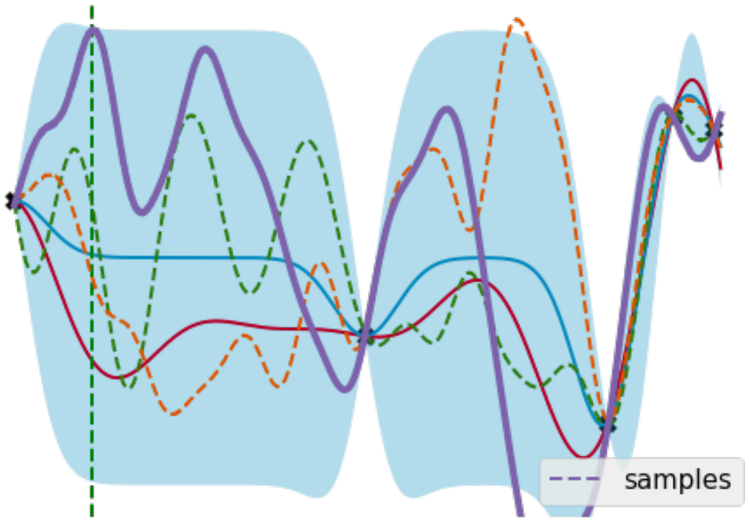
```
sobol = SobolEngine(1, scramble=True)
candidate_x = sobol.draw(1000)
ts = MaxPosteriorSampling(
    model, replacement=False
)
```



Bayesian optimization in practice

using Bayesian optimization in the real world

Bayesian optimization in practice

using Bayesian optimization in the real world

- **Batch optimization** to maximize throughput

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  - Making multiple evaluations *at the same time*

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All handled by **BayesOpt**!

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a hands-on guide to Python implementation

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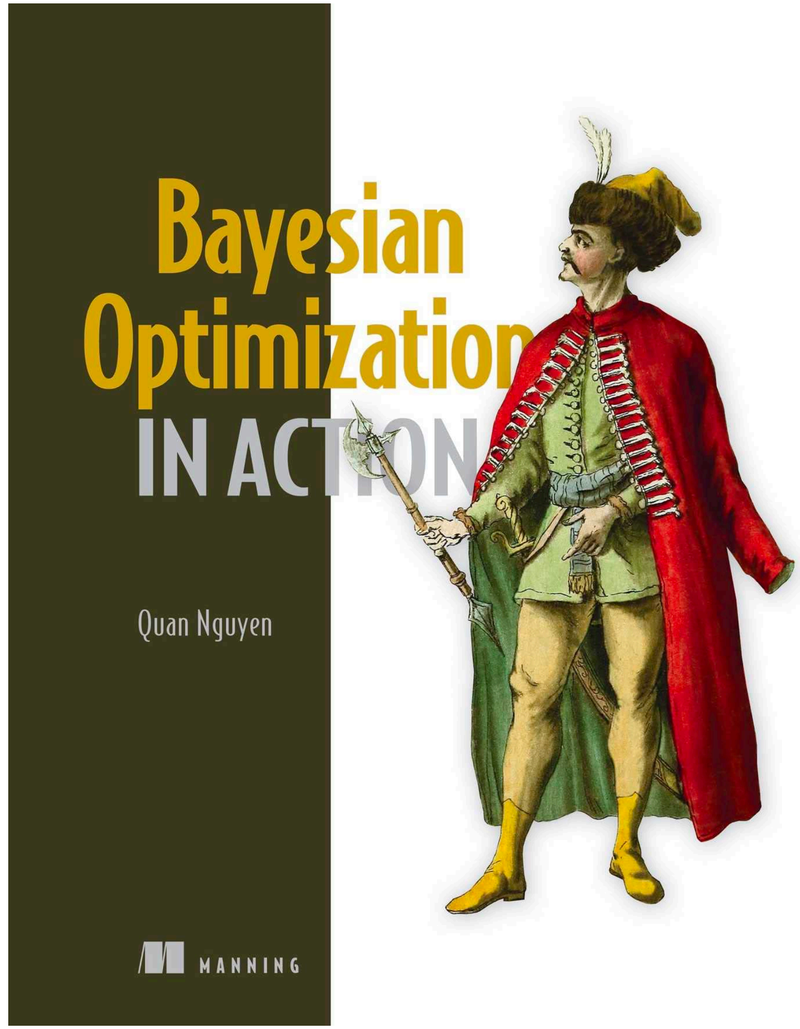

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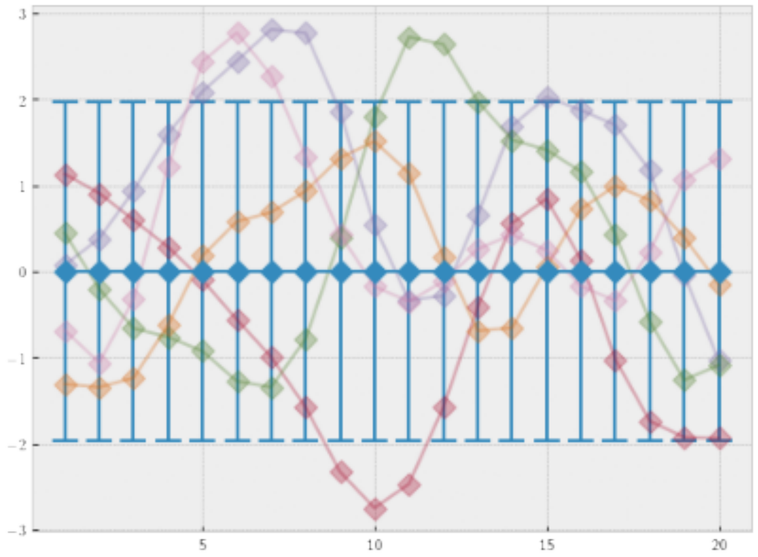

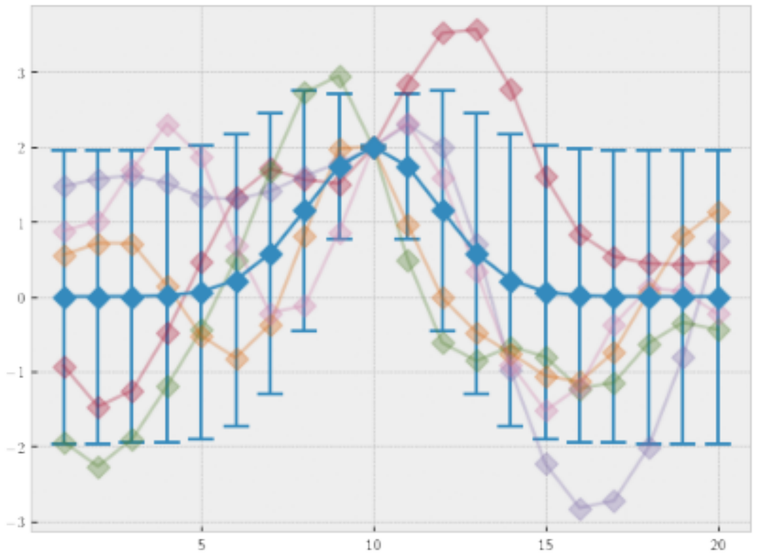

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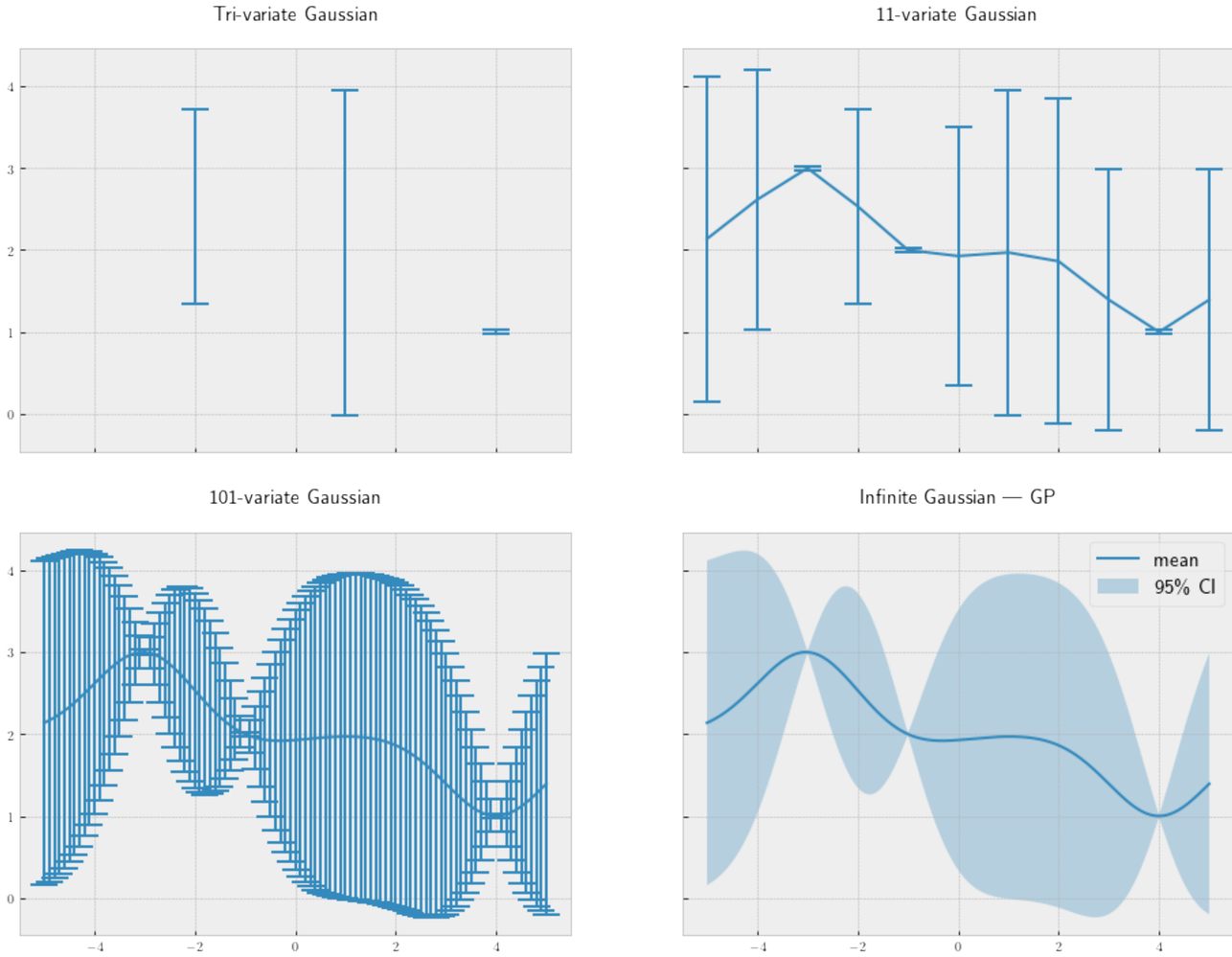

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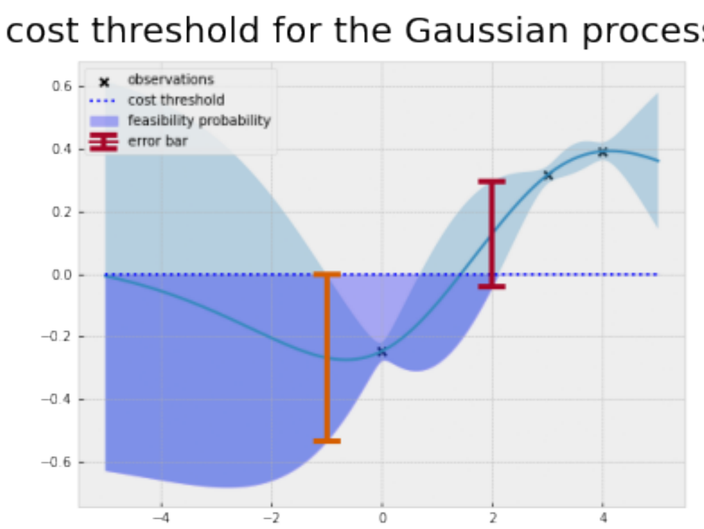

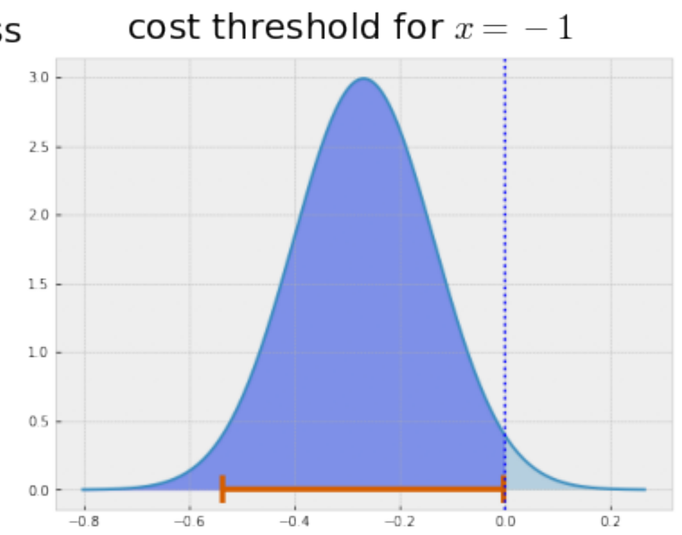

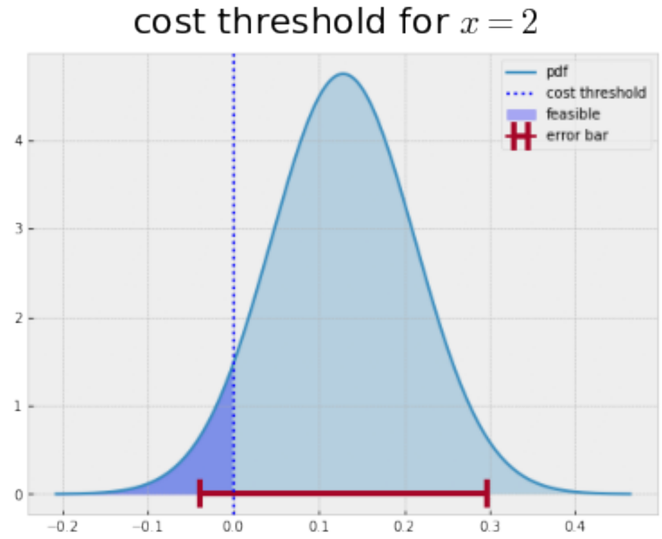

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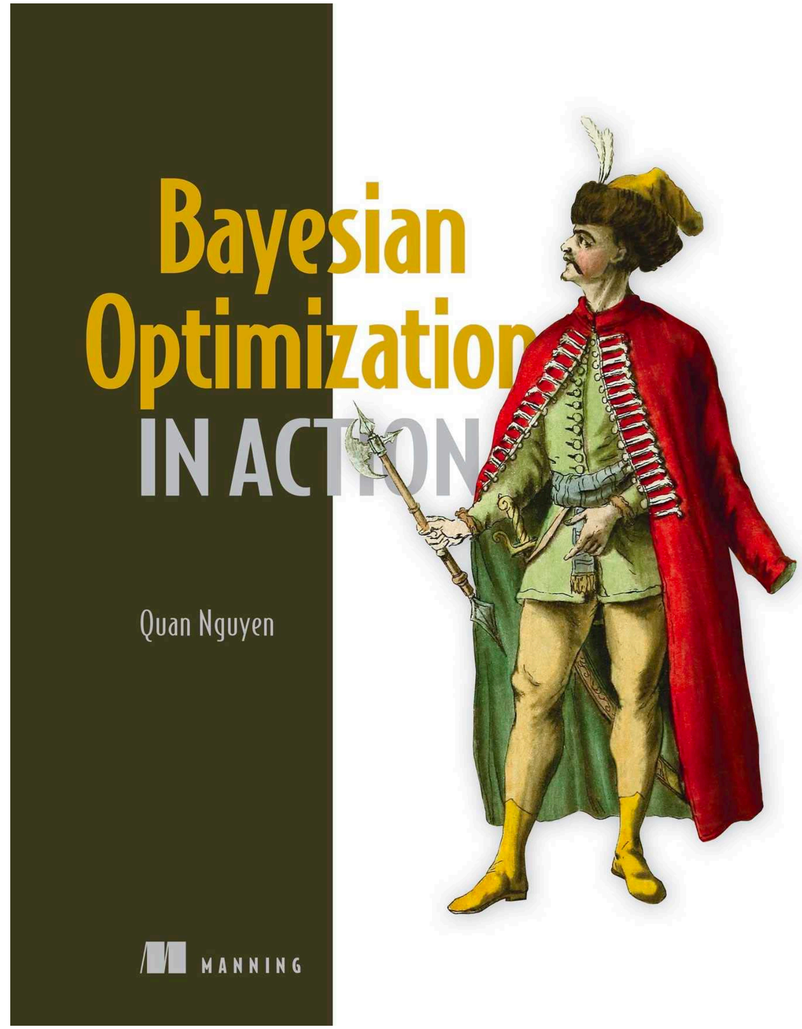

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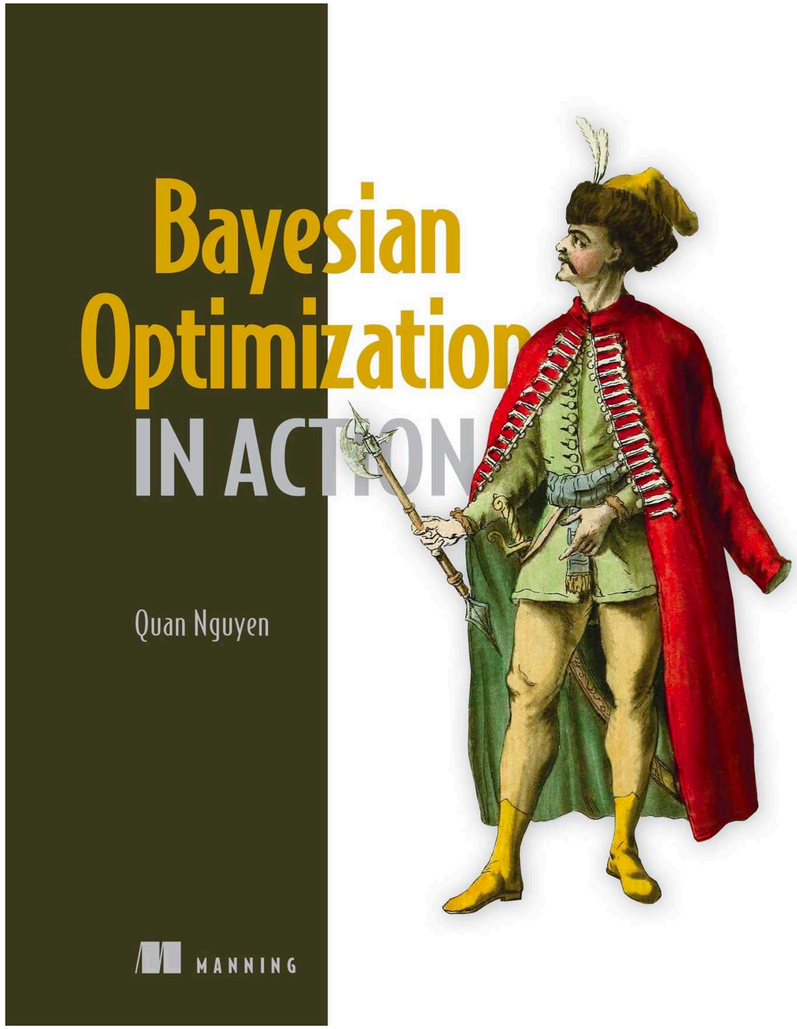

Bayesian optimization in practice

using Bayesian optimization in the real world

Optimization policy for decision making

choosing the best course of action, the Bayesian way

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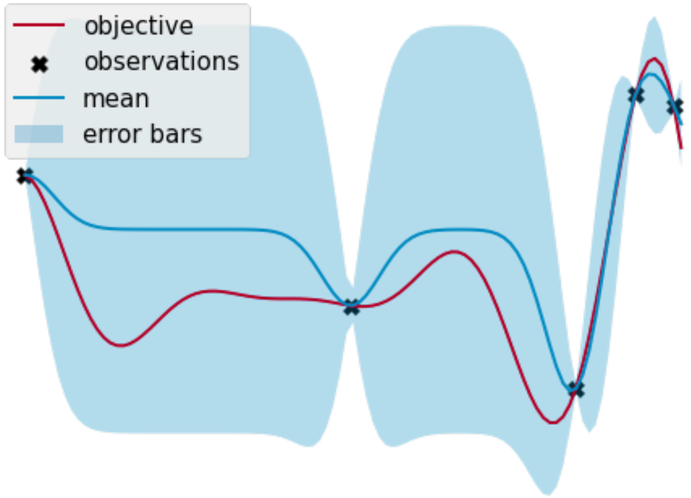
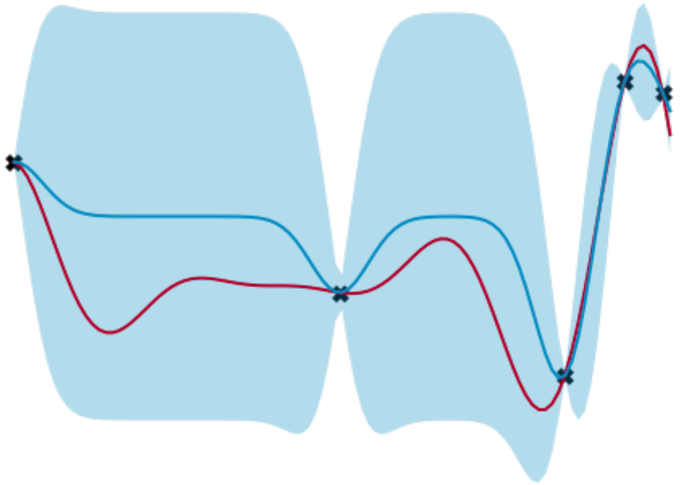


Optimization policy for decision making

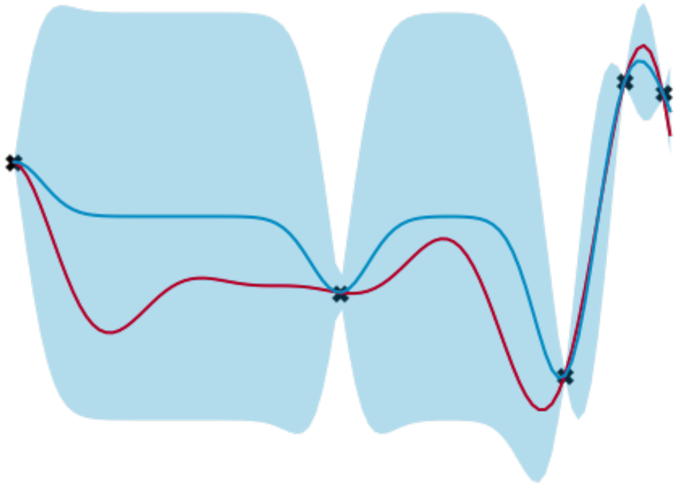
choosing the best course of action, the Bayesian way



Optimization policy for decision making

choosing the best course of action, the Bayesian way

- **Goal**: pick x to improve from the best point f_*



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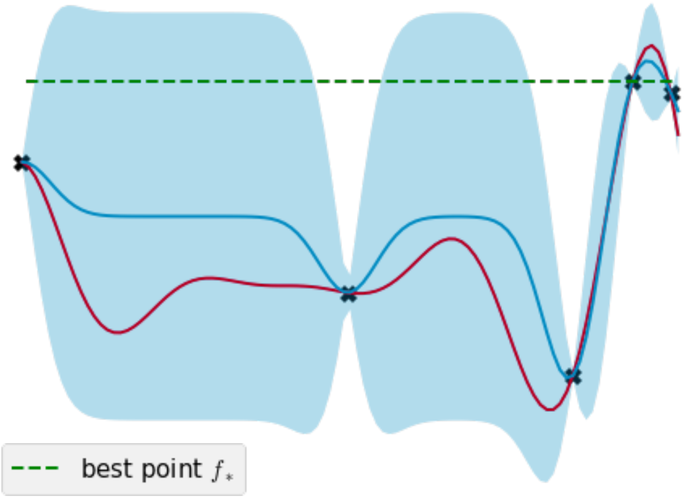

Optimization policy for decision making

choosing the best course of action, the Bayesian way

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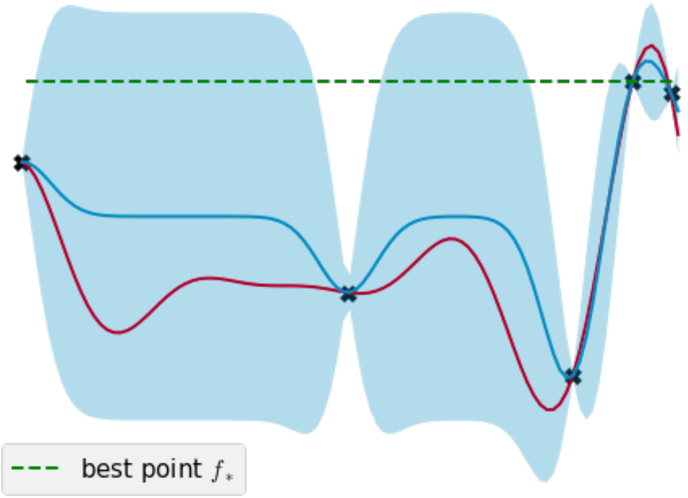

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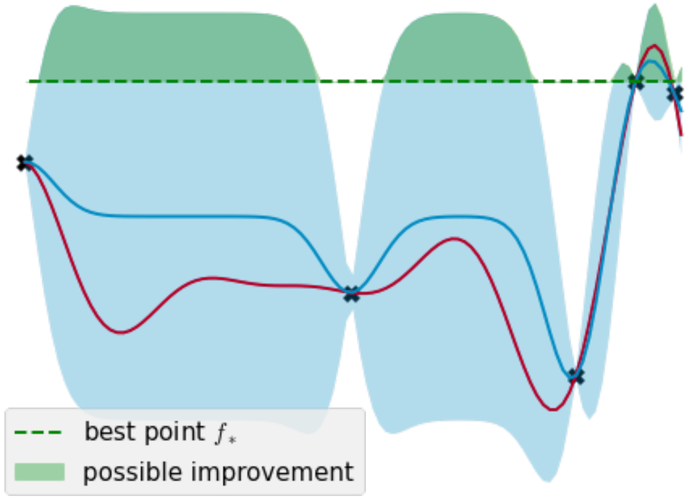

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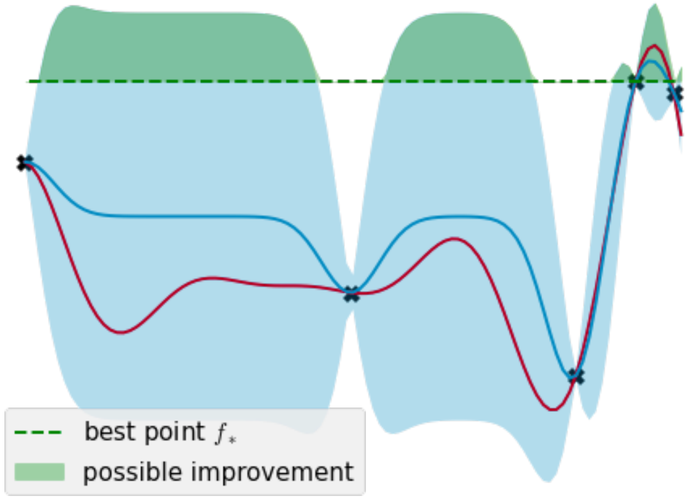

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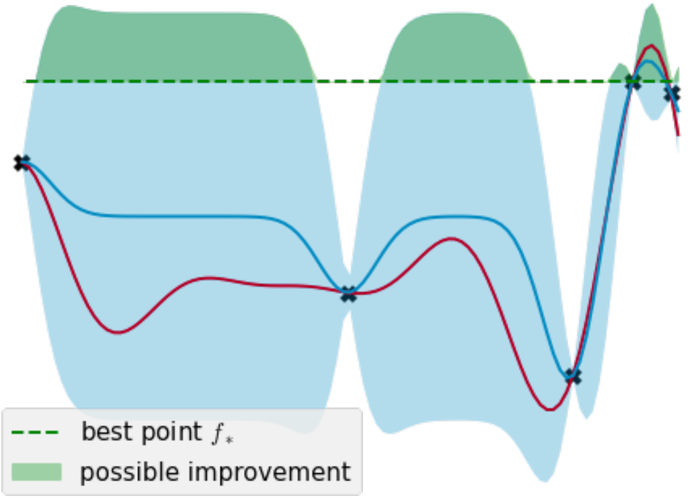

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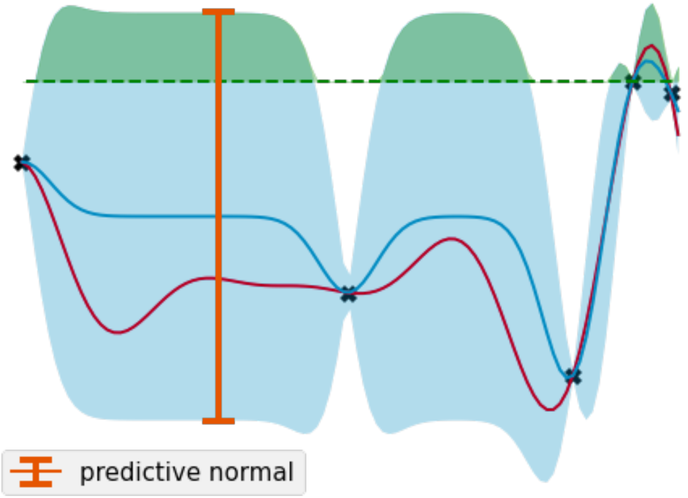

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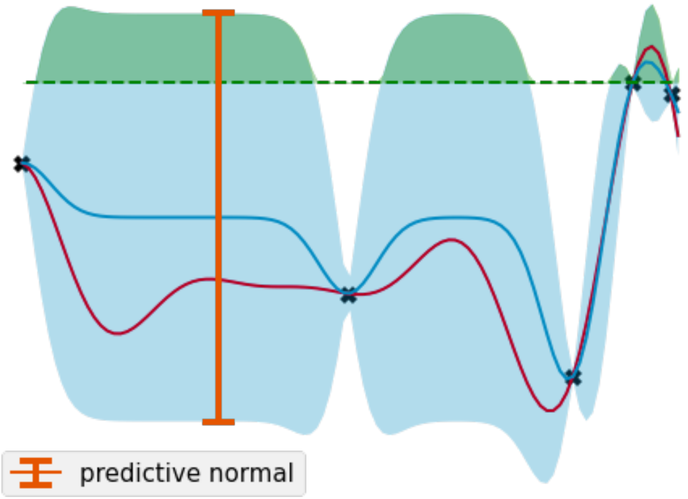

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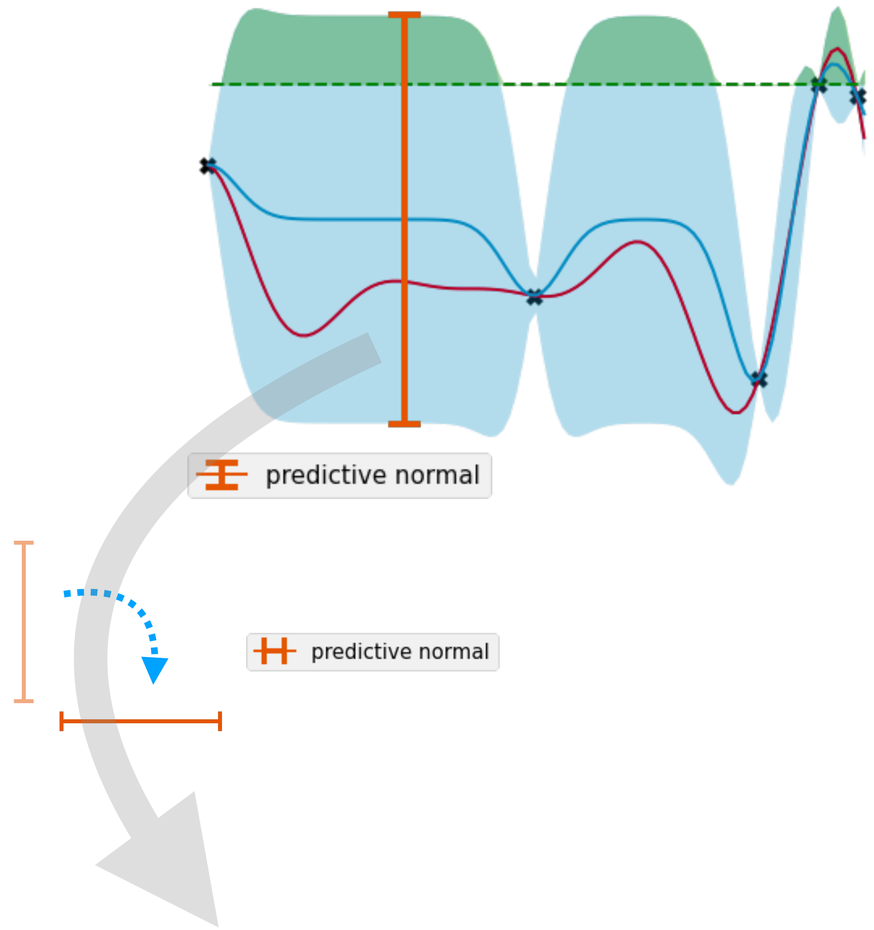

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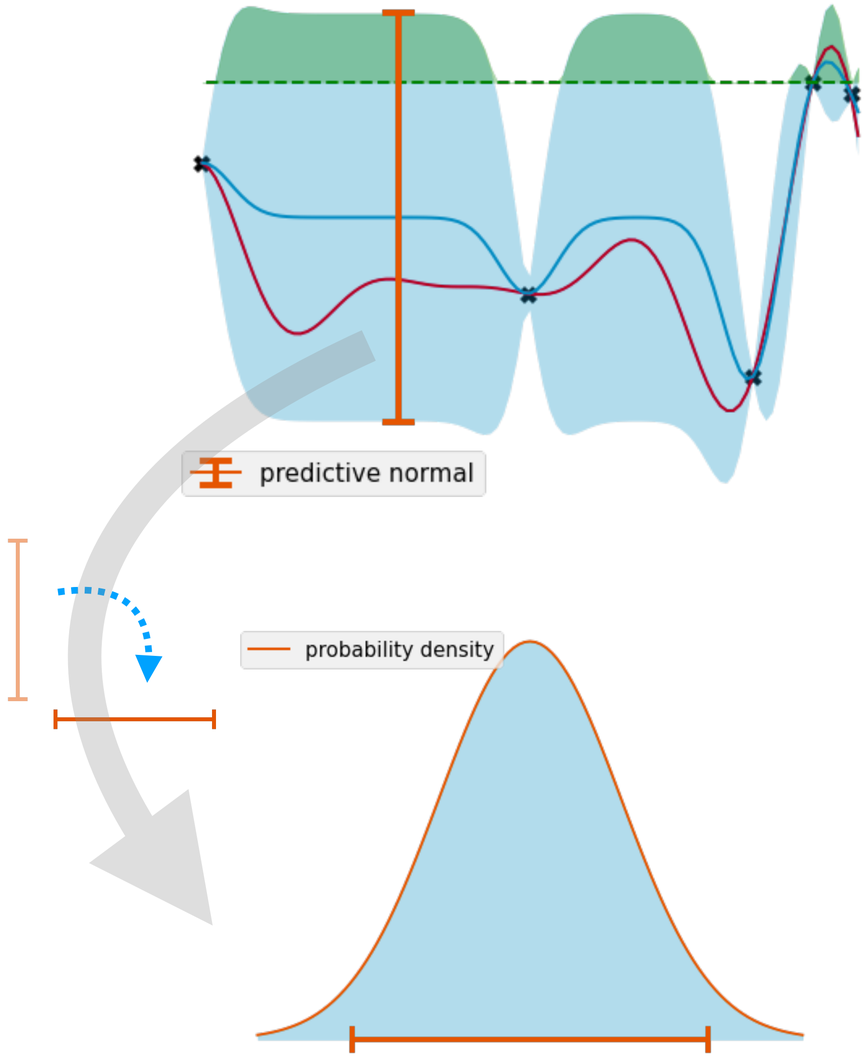

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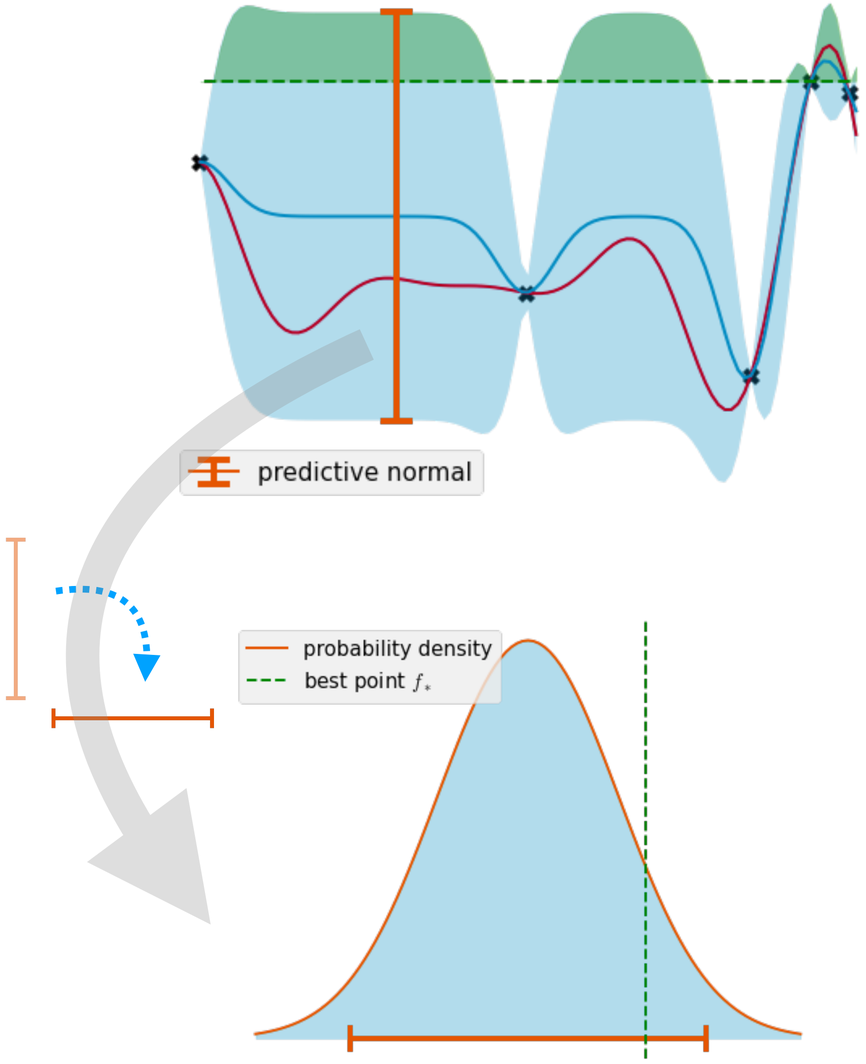

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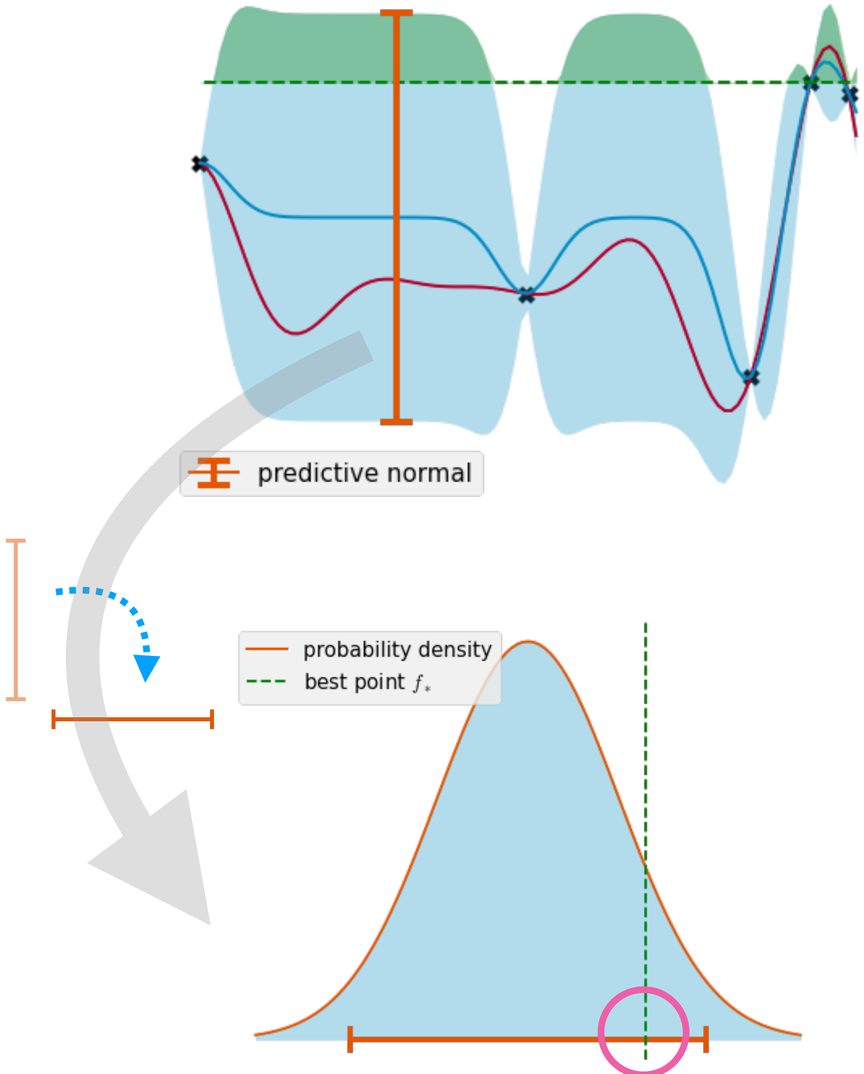

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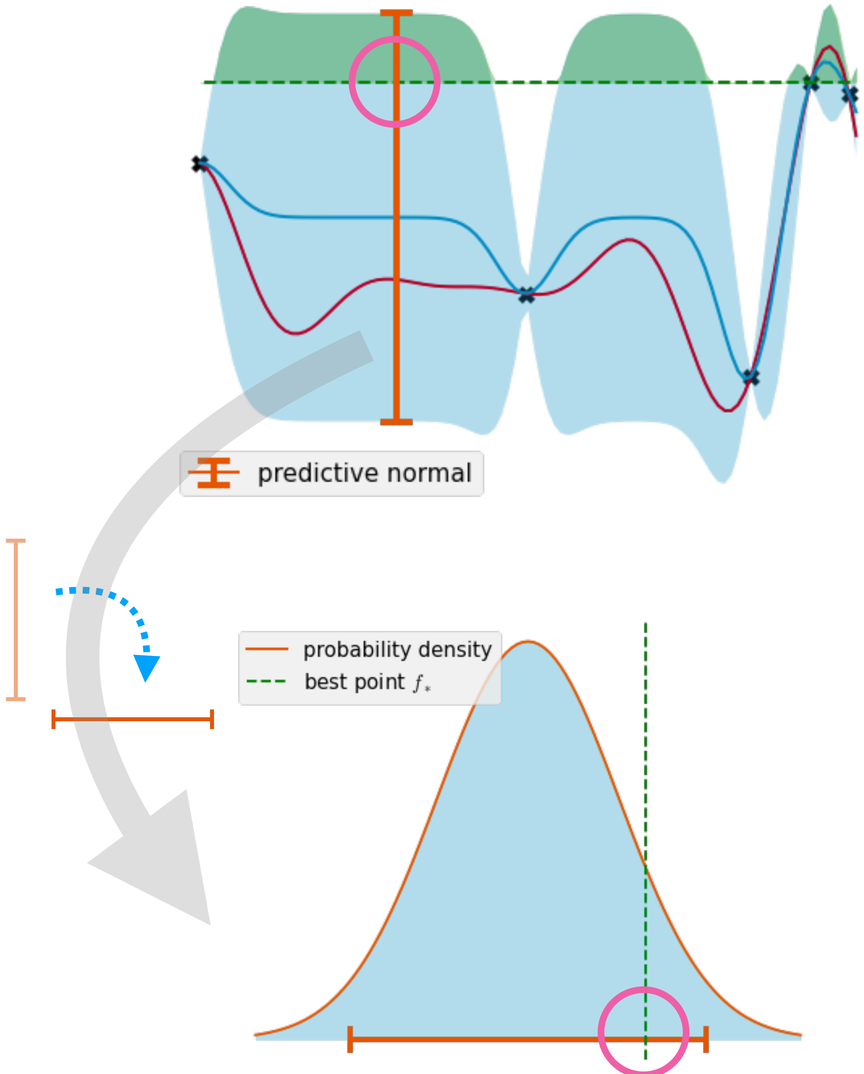

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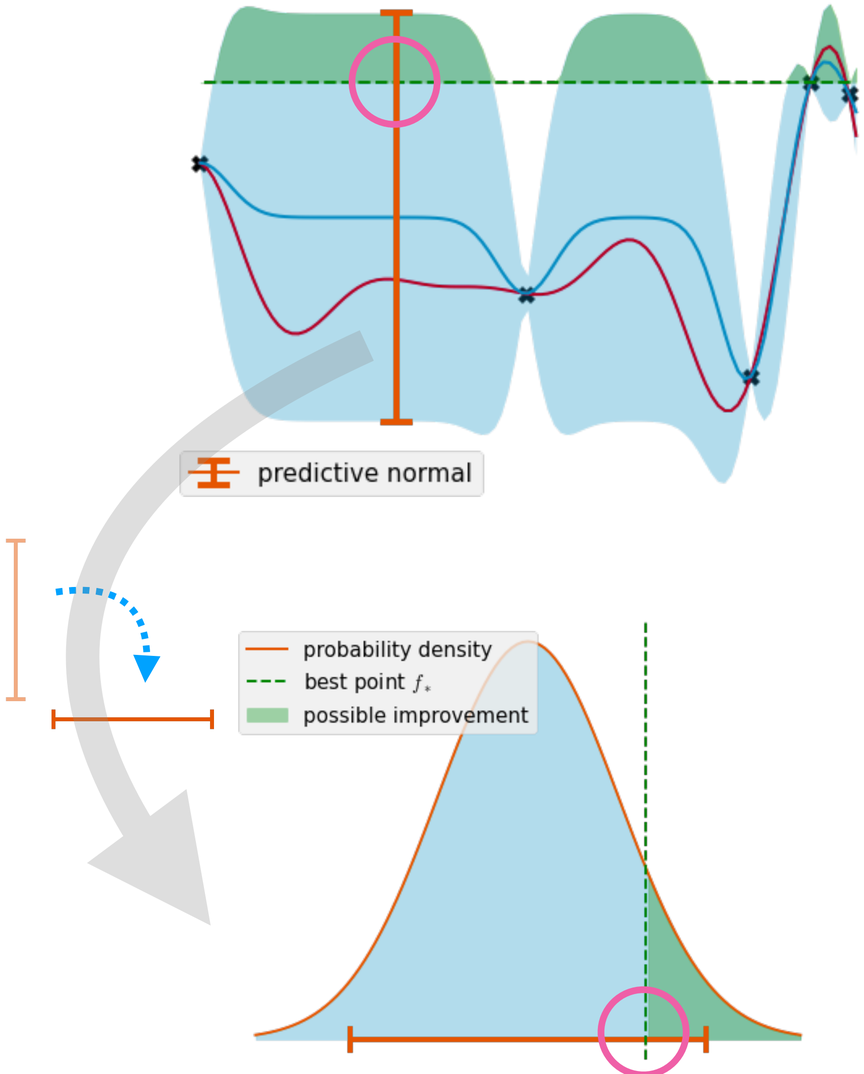

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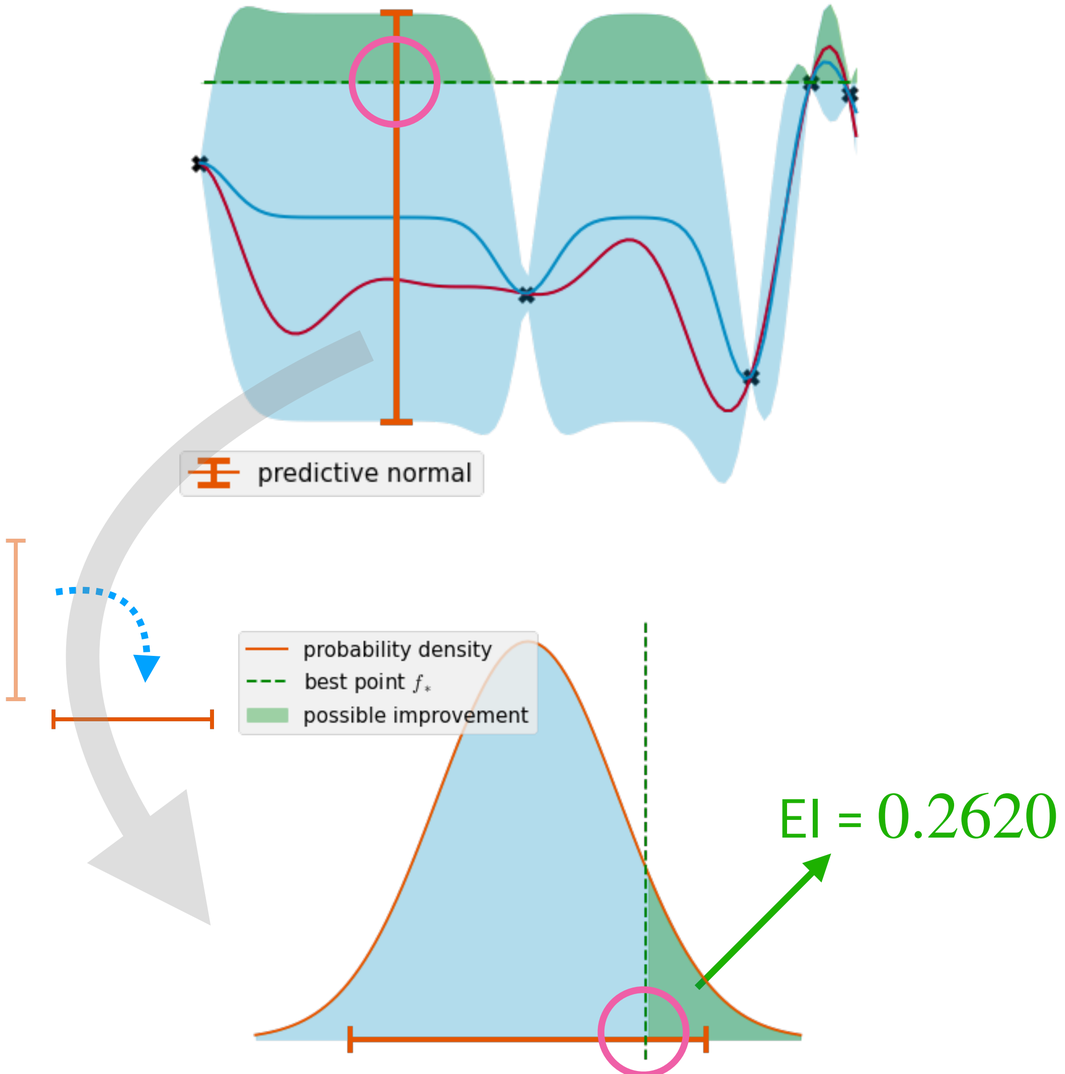

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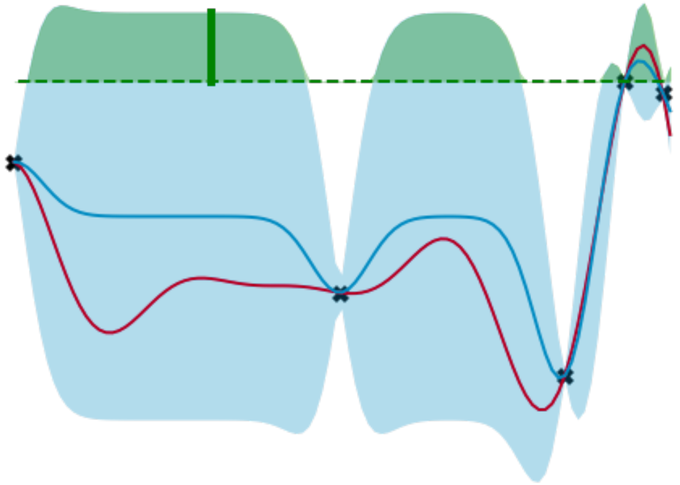

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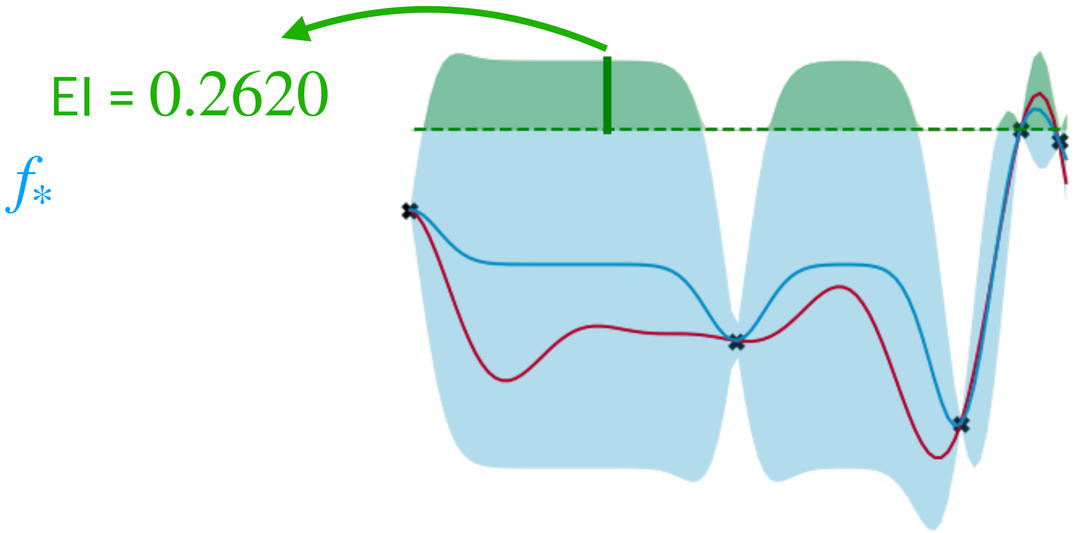

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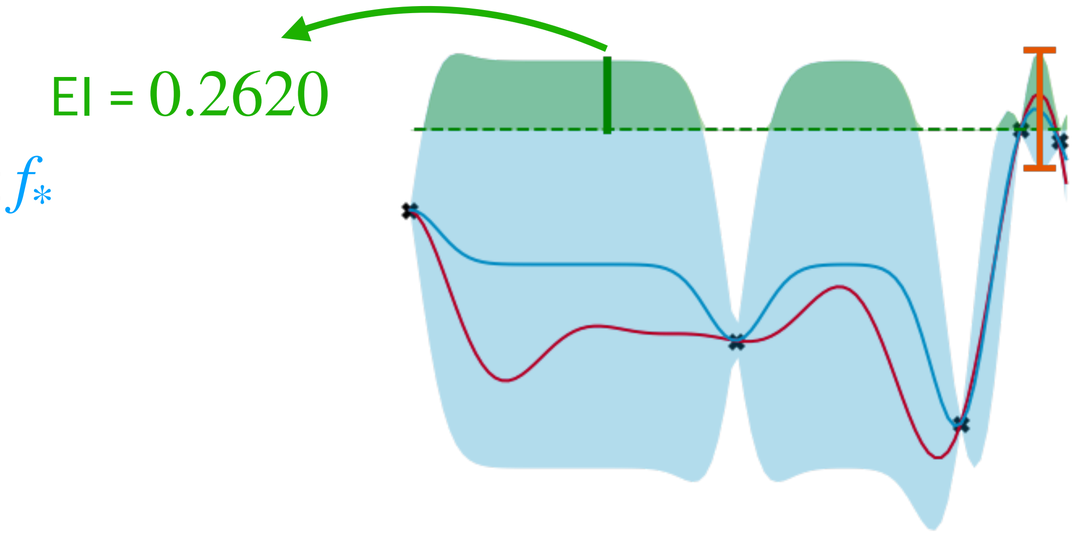

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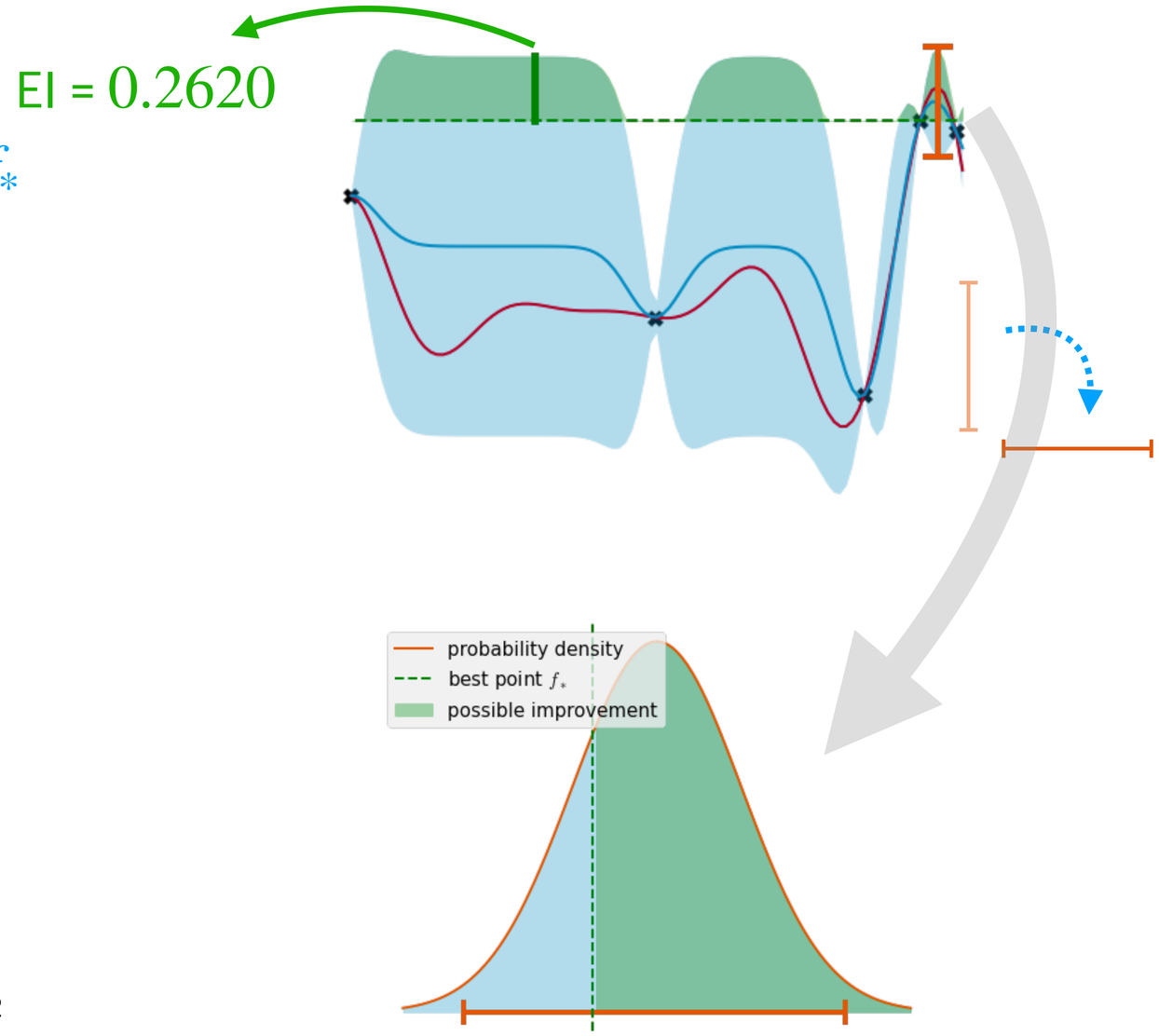

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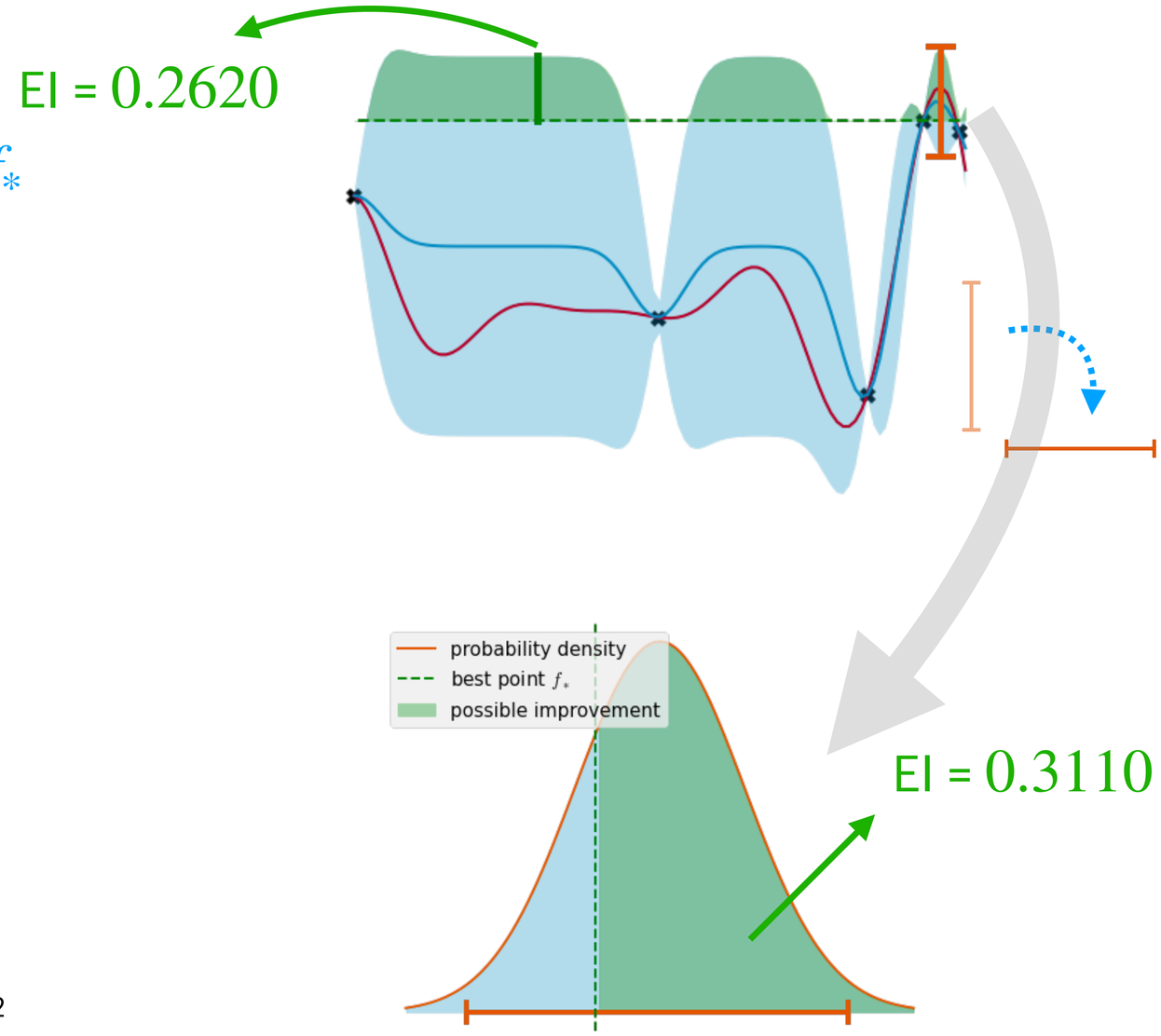

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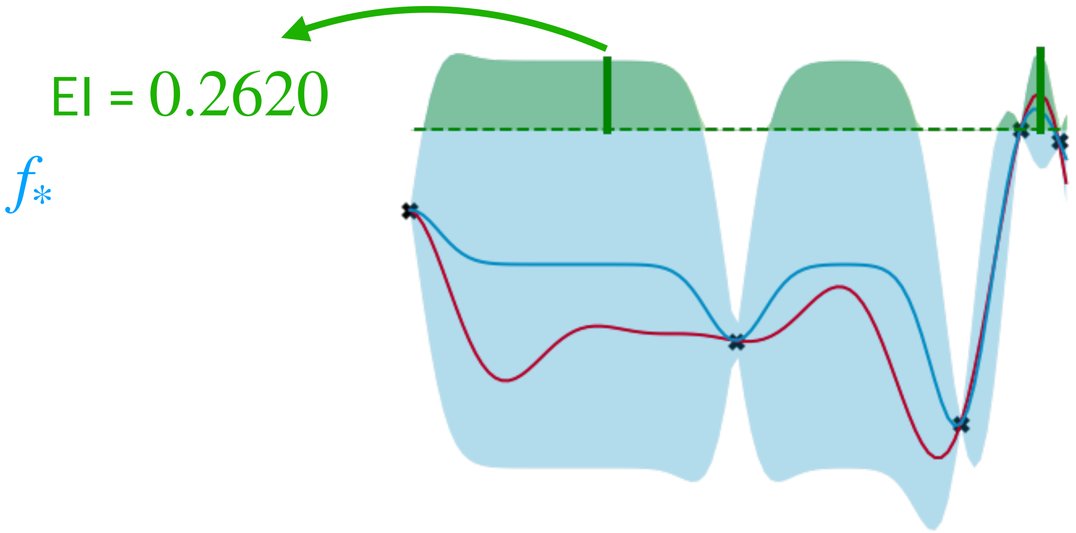

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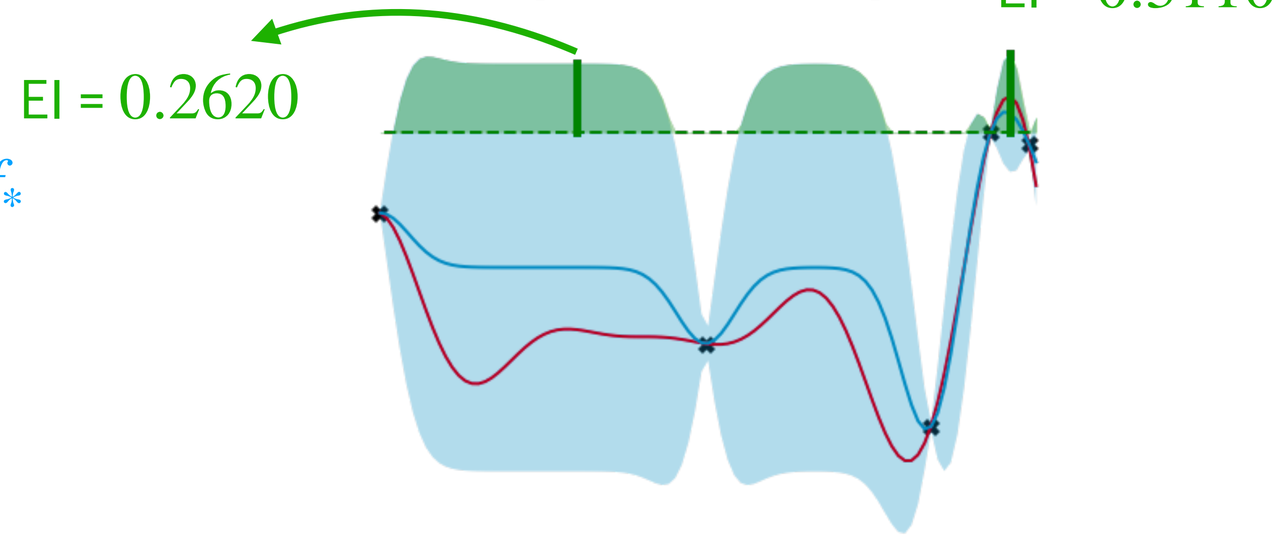

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Optimization policy for decision making

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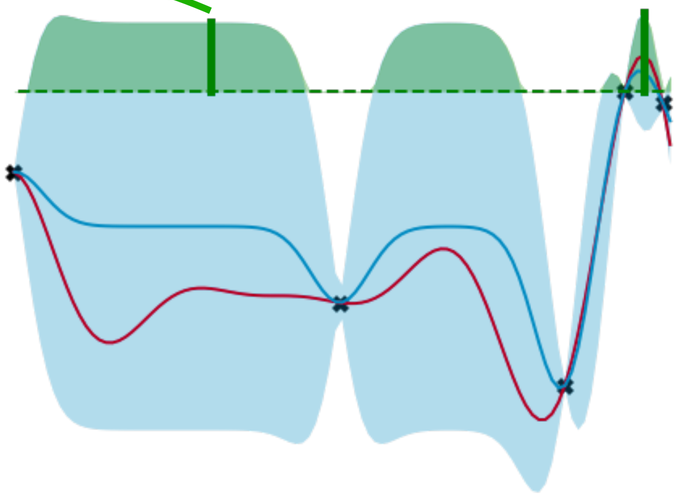
EI = 0.3110

EI = 0.2620



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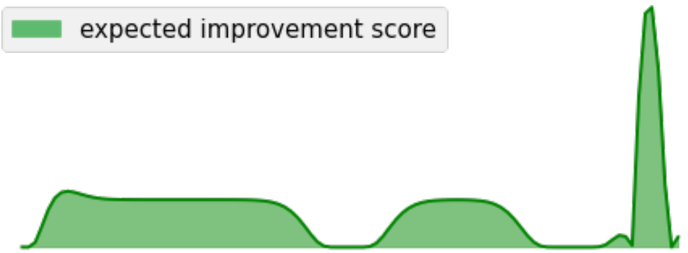

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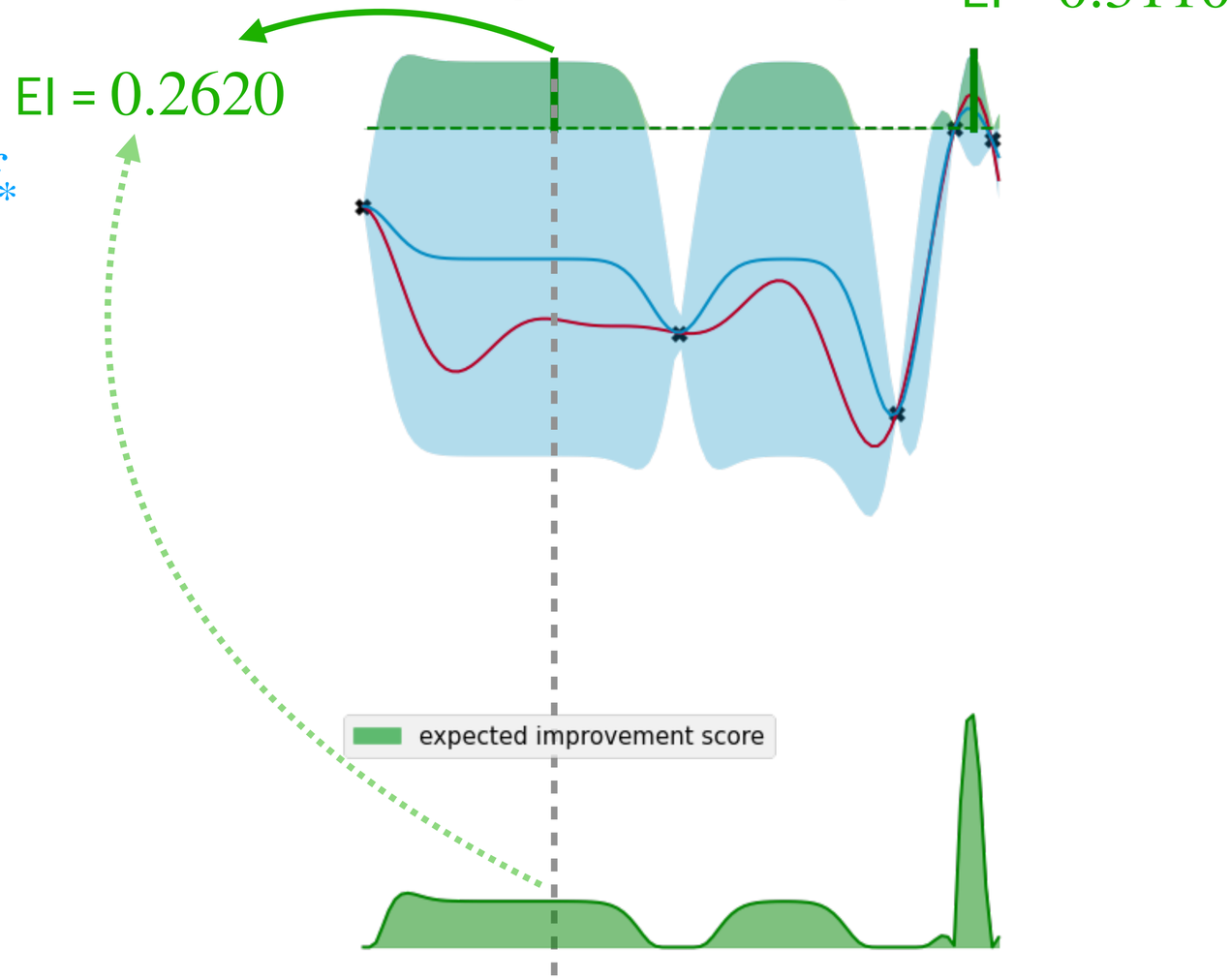

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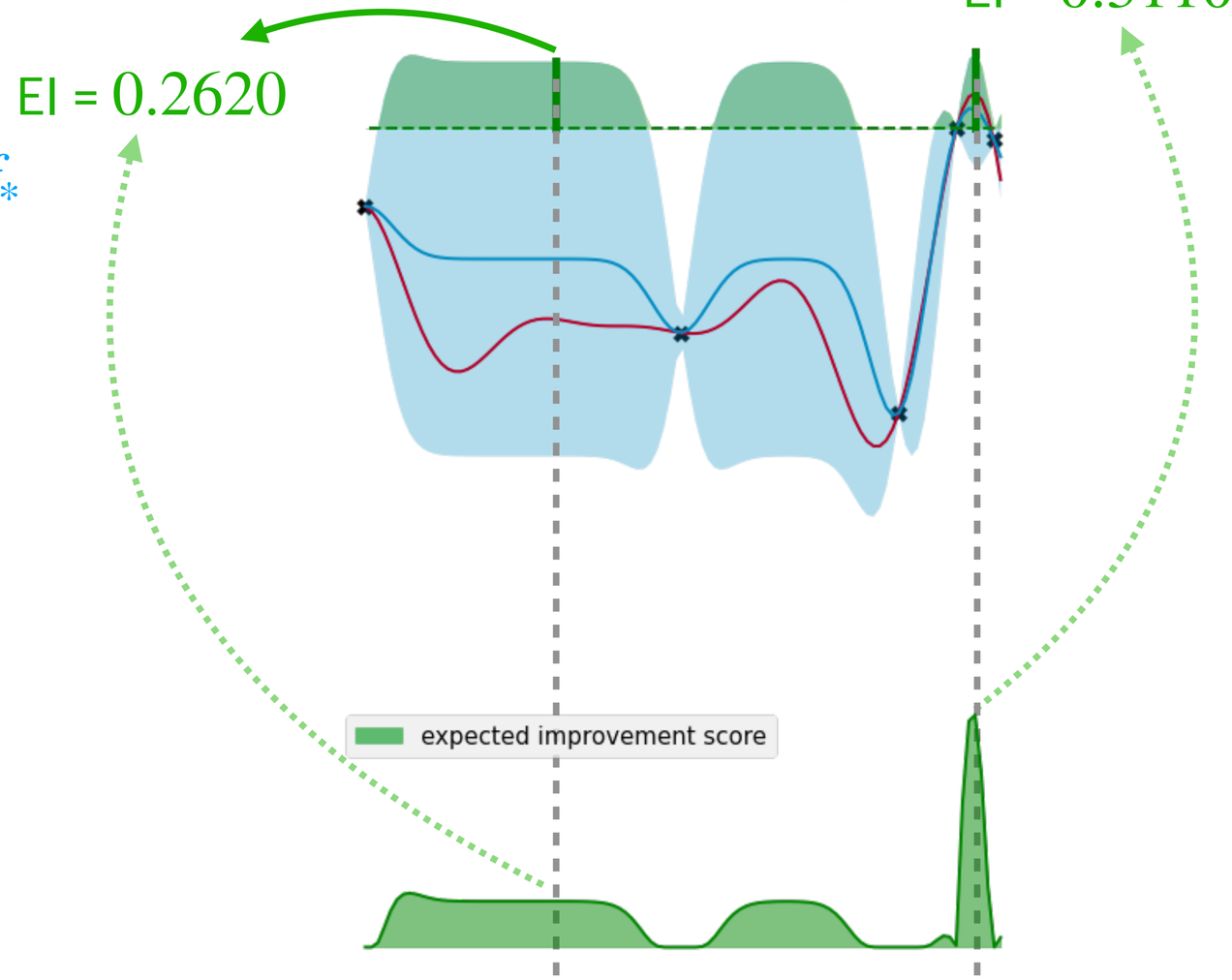

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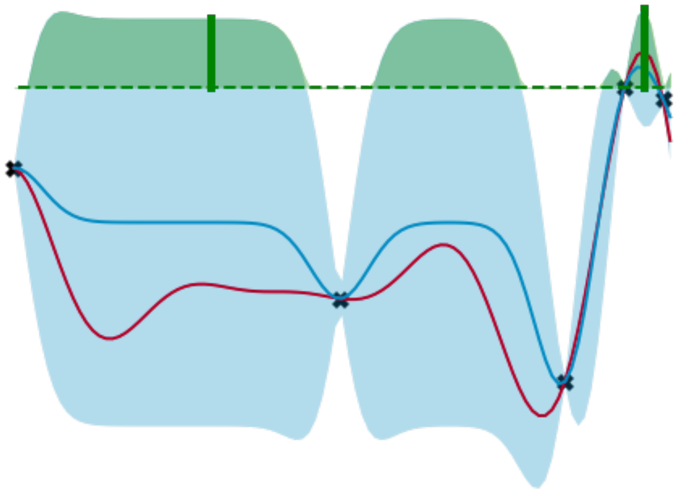

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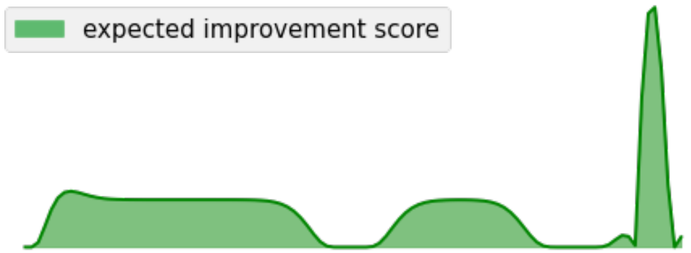

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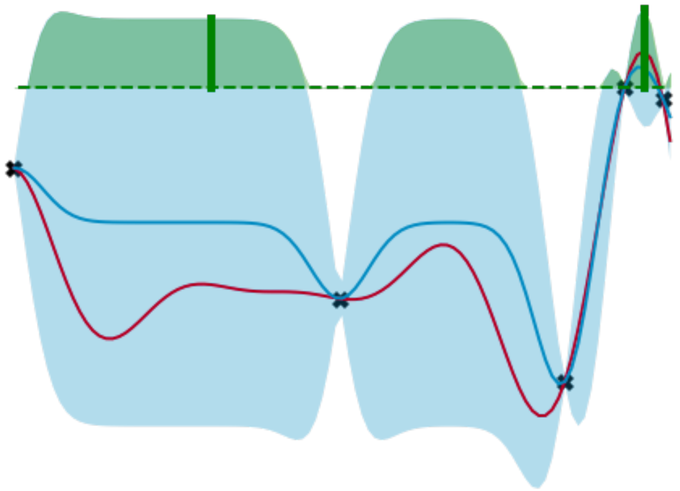

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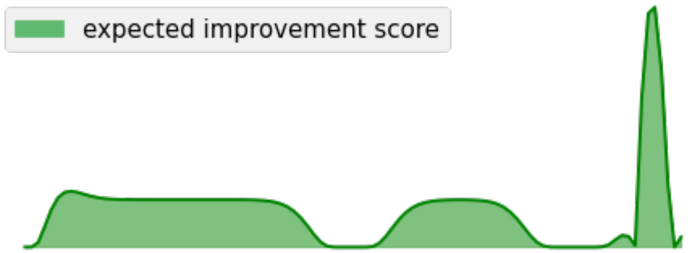

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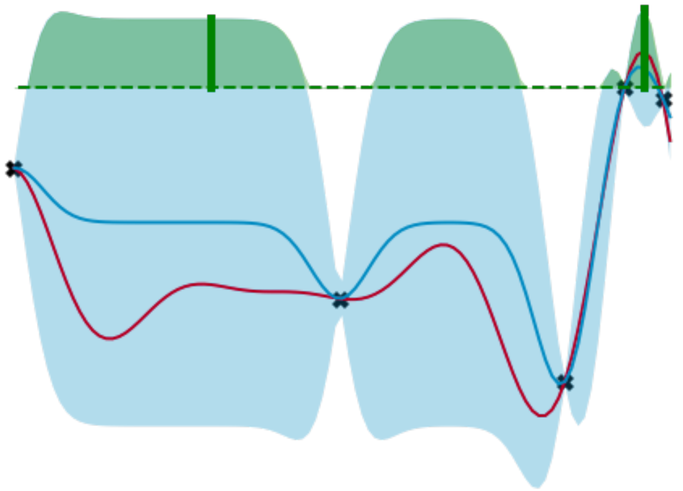

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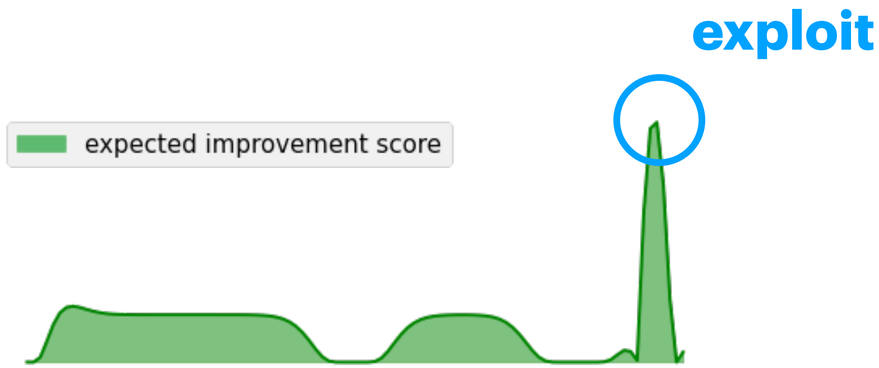

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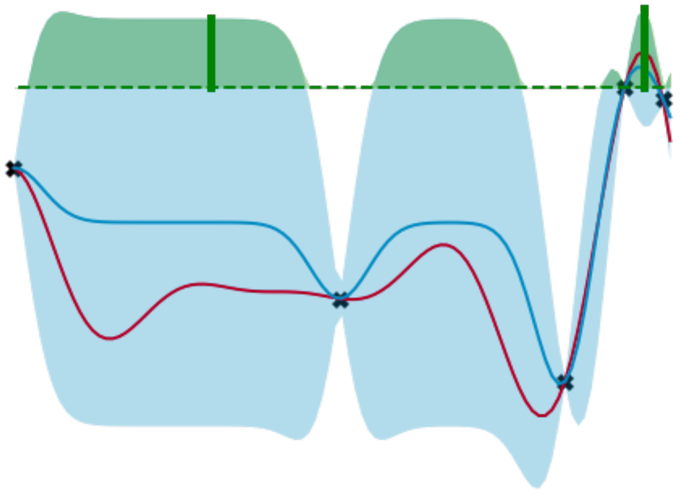

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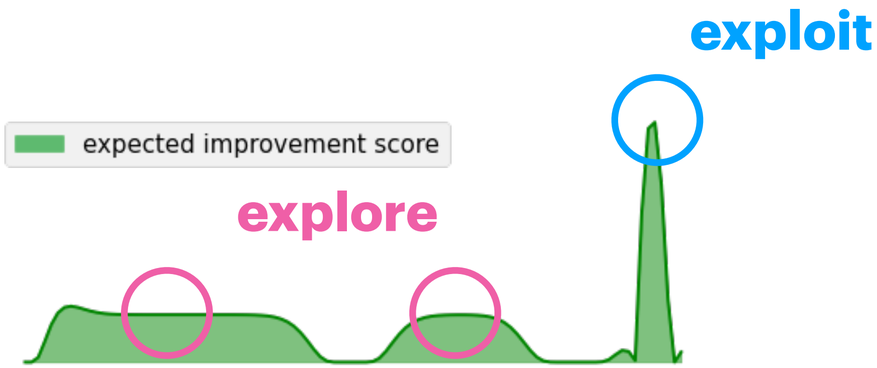
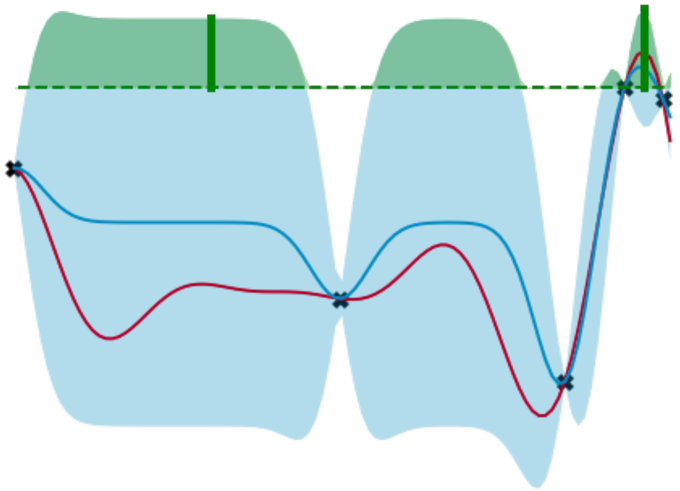
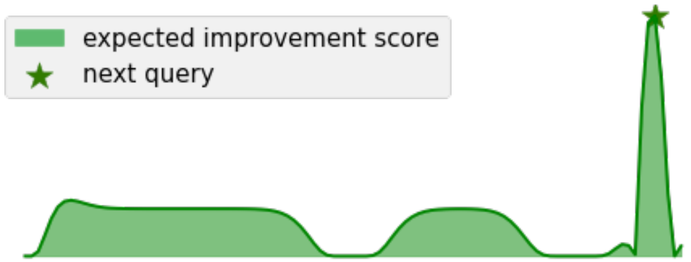


Optimization policy for decision making

choosing the best course of action, the Bayesian way



- **Goal**: pick x to improve from the best point f_*
  - Want to maximize $\max\{0, f(x) - f_*\}$
- **Problem**: $f(x)$ is unknown
- **Solution**: $f(x)$ follows a normal distribution
  - Can compute the expected improvement (**EI**) value $\mathbb{E}\left[\max\{0, f(x) - f_*\}\right]$
    - Balances large *means (exploit)* and *standard deviations (explore)*



Batch optimization to maximize throughput

making multiple queries at the same time

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Bayesian Optimization for a Better Dessert

Greg Kochanski, Daniel Golovin, John Karro, Benjamin Solnik, Subhodeep Moitra, and D. Sculley
{gpk, dgg, karro, bsolnik, smoitra, dsculley}@google.com; Google Brain Team

Abstract

We present a case study on applying Bayesian Optimization to a complex real-world system; our challenge was to optimize chocolate chip cookies. The process was a mixed-initiative system where both human chefs, human raters, and a machine optimizer participated in 144 experiments. This process resulted in highly rated cookies that deviated from expectations in some surprising ways – much less sugar in California, and cayenne in Pittsburgh. Our experience highlights the importance of incorporating domain expertise and the value of transfer learning approaches.

Kochanski et al. (2017) https://static.googleusercontent.com/media/research.google.com/en//pubs/archive/46507.pdf

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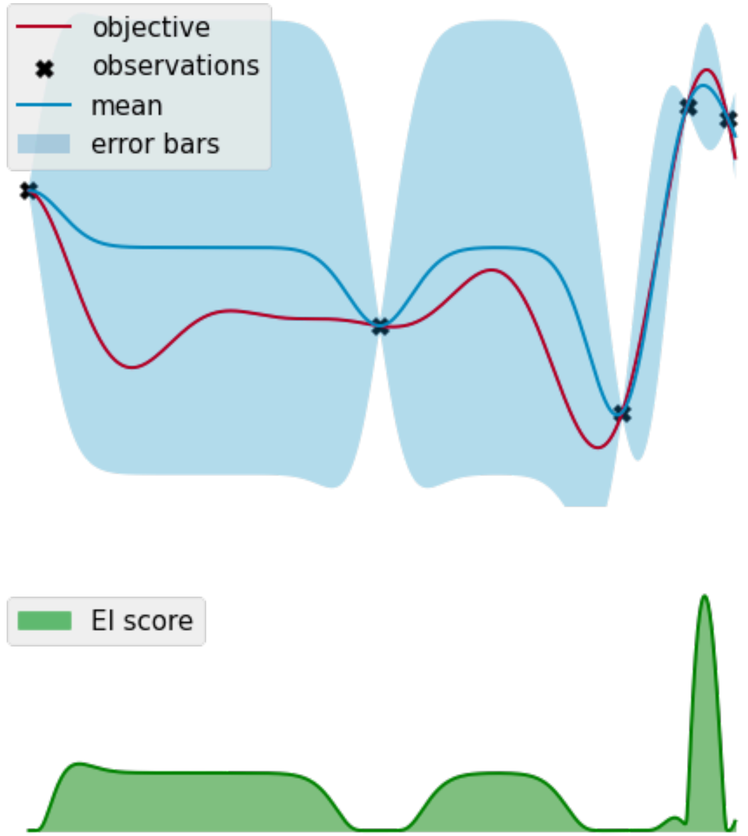

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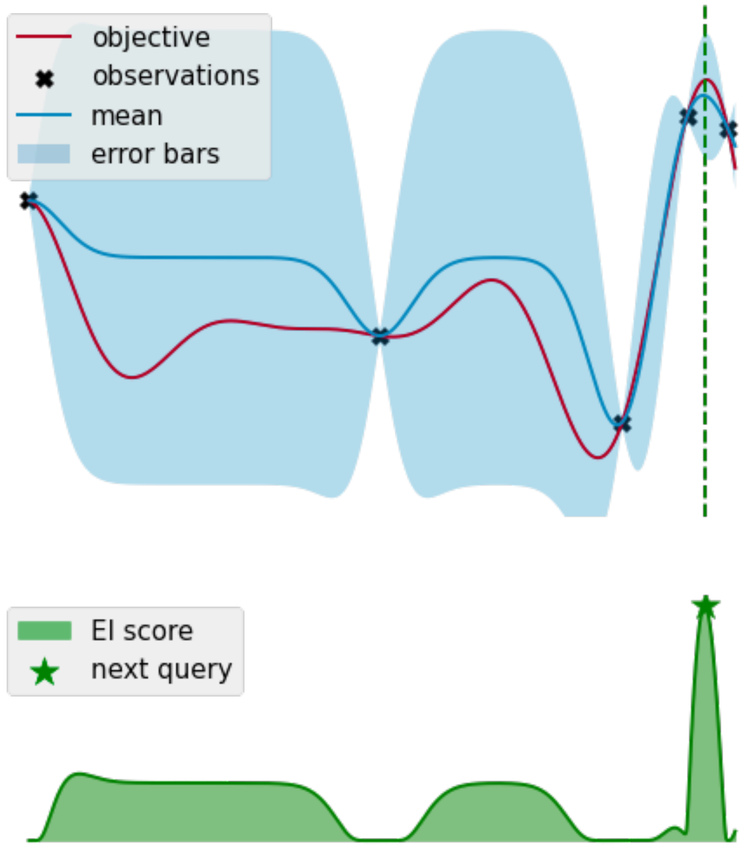

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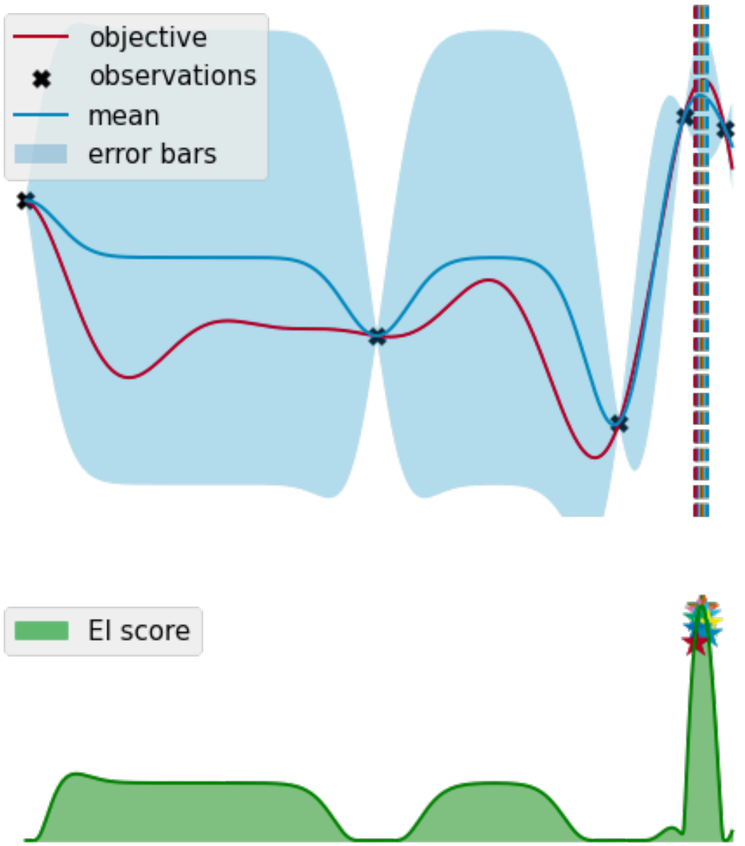

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policy = qExpectedImprovement(
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Constrained optimization for safe solutions

satisfying outcome constraints during exploration

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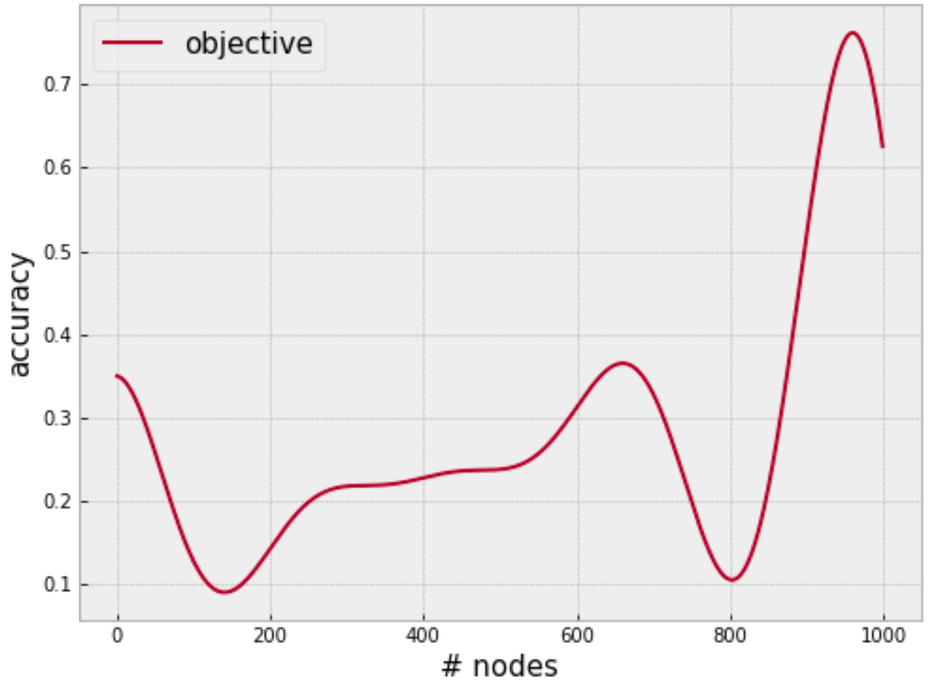

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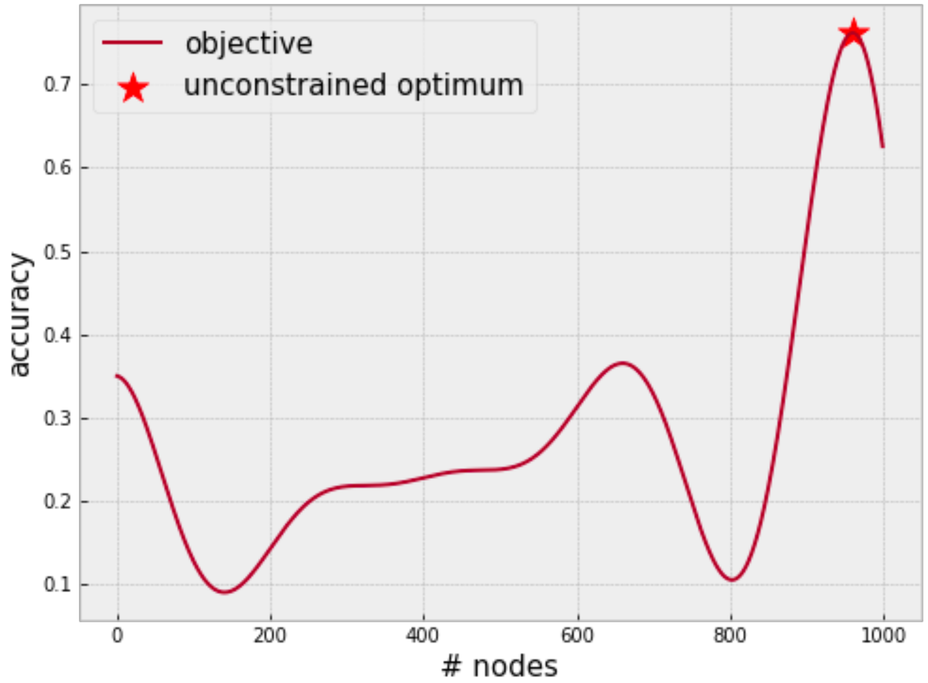

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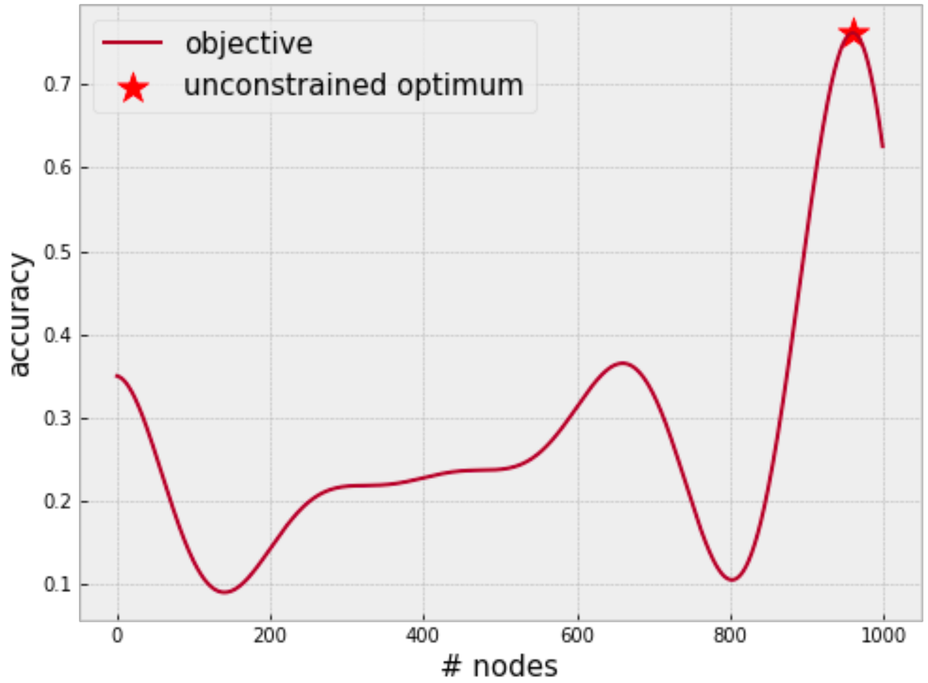

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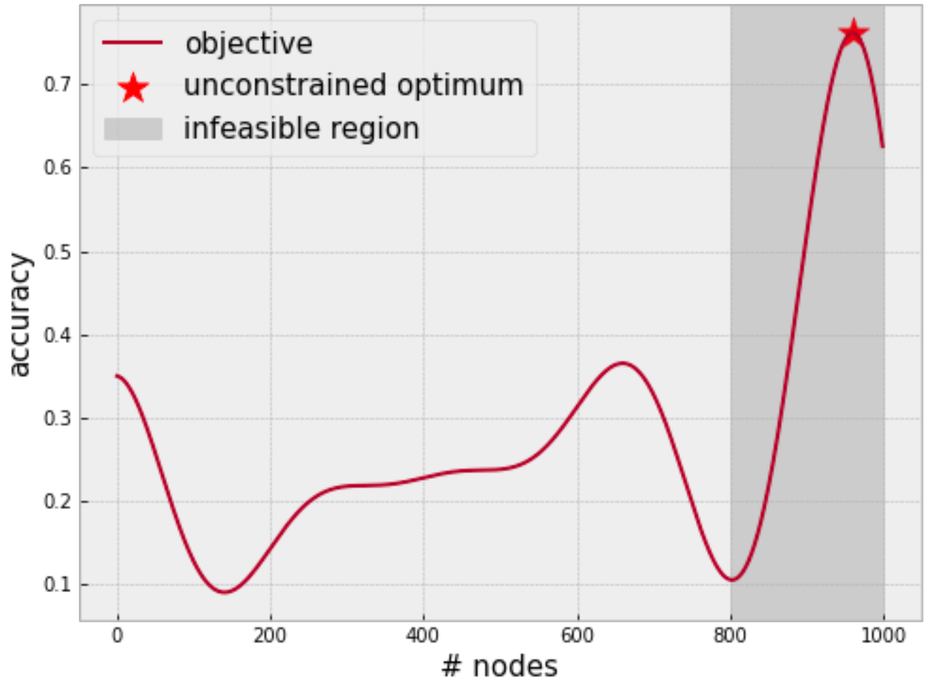

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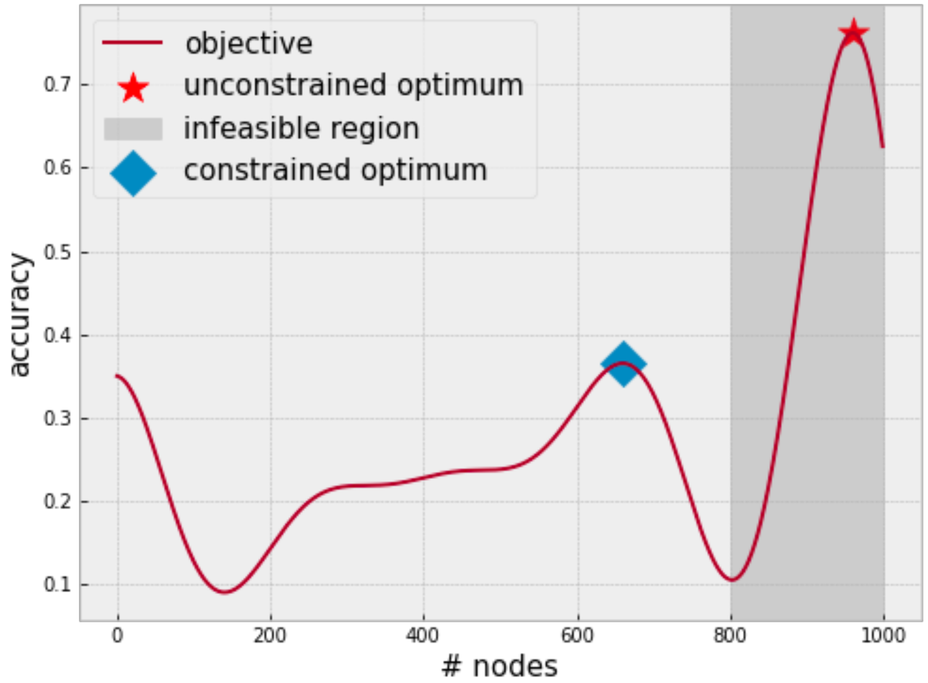

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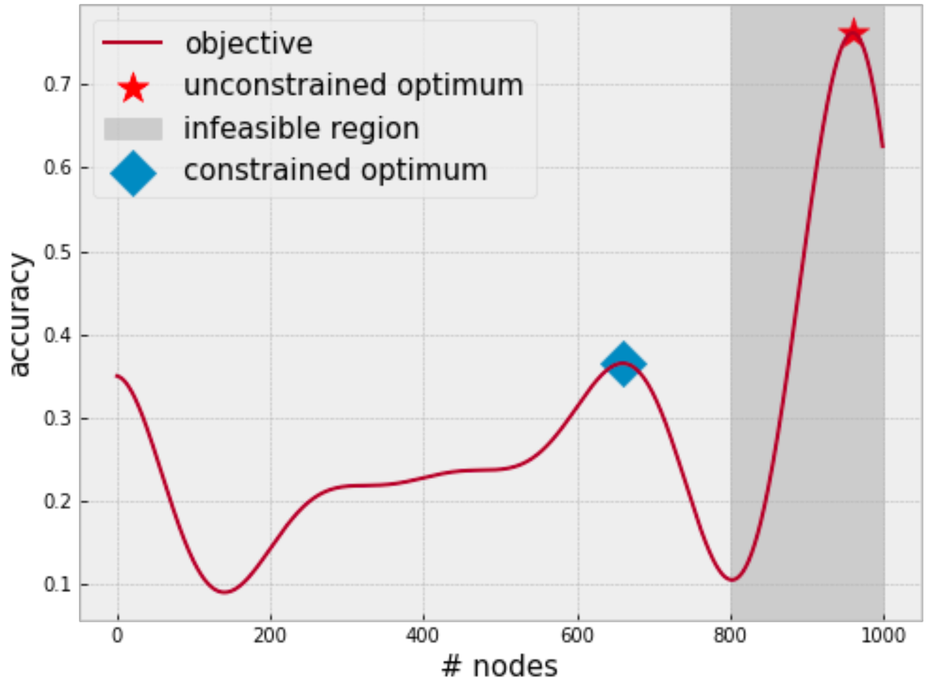

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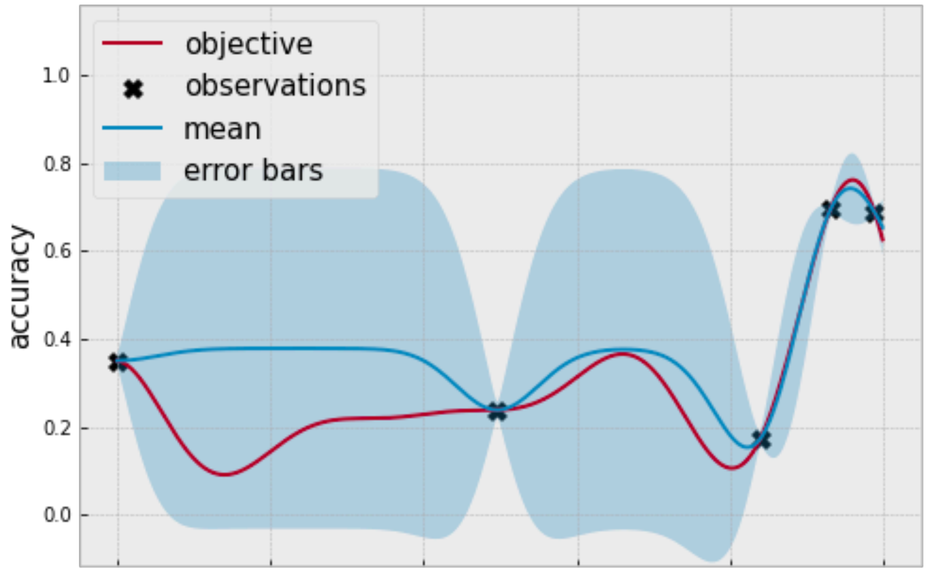

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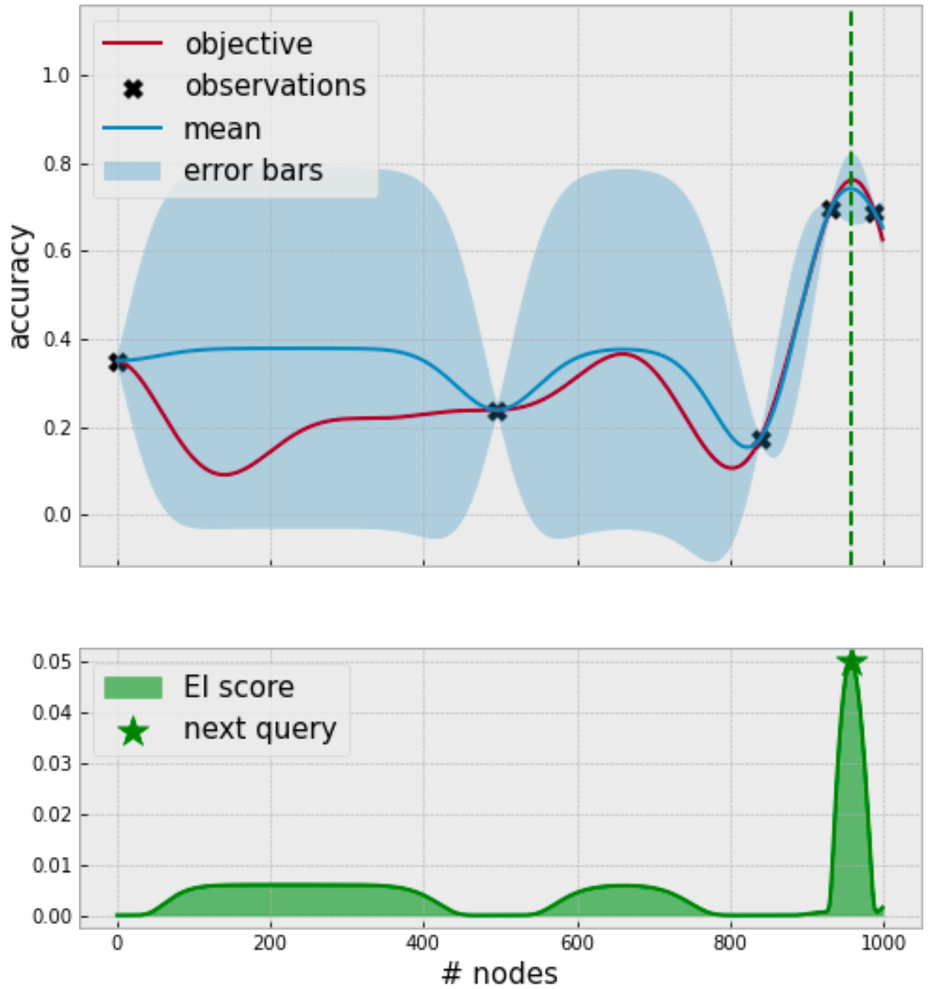

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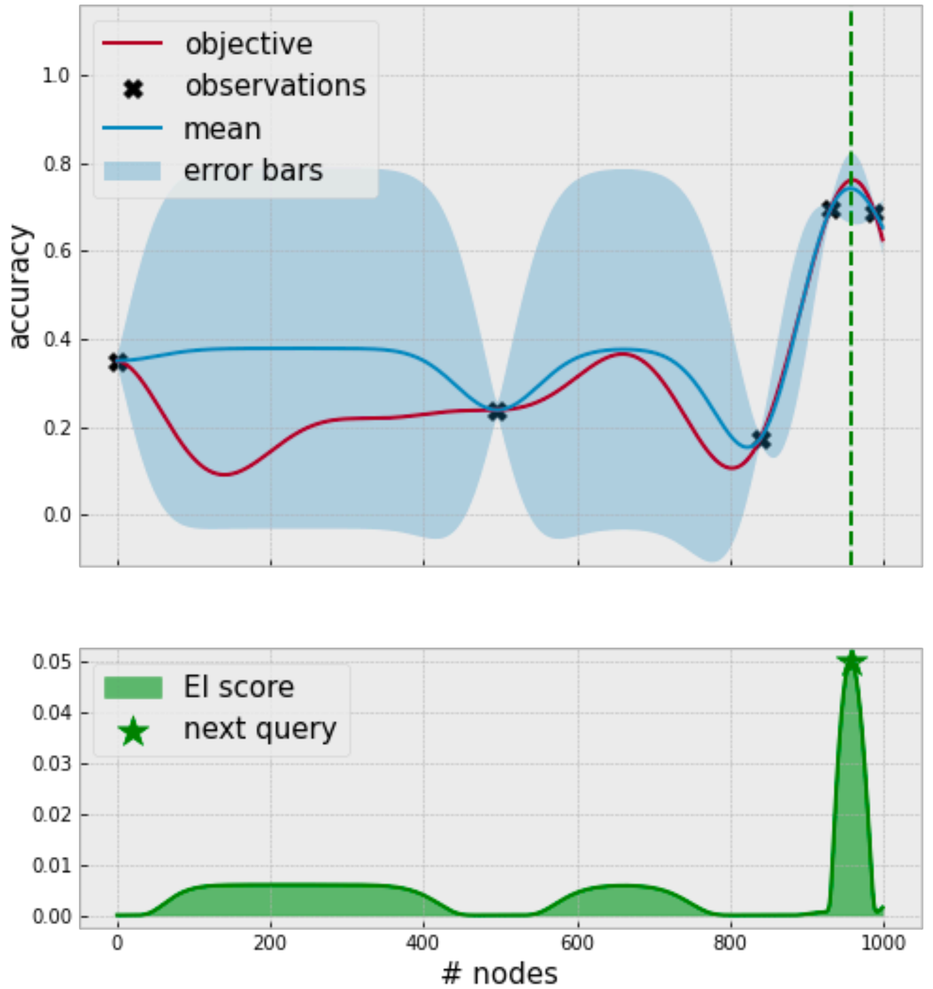

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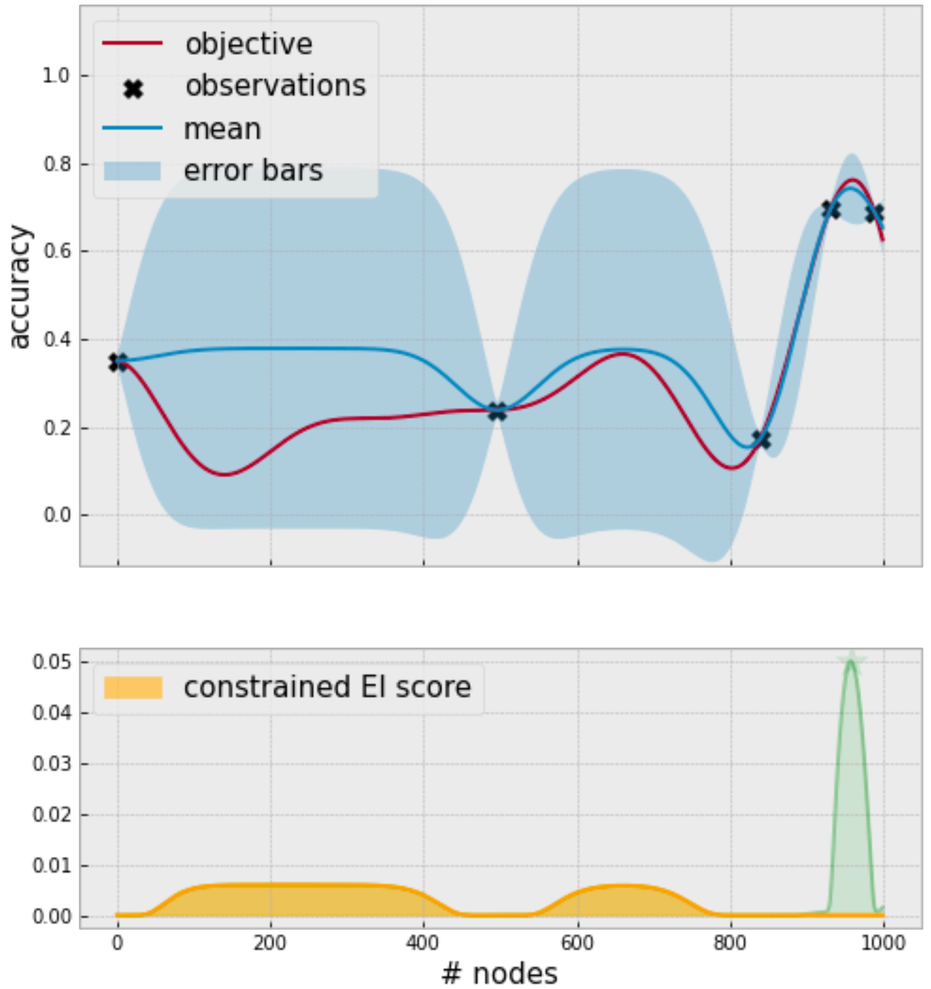

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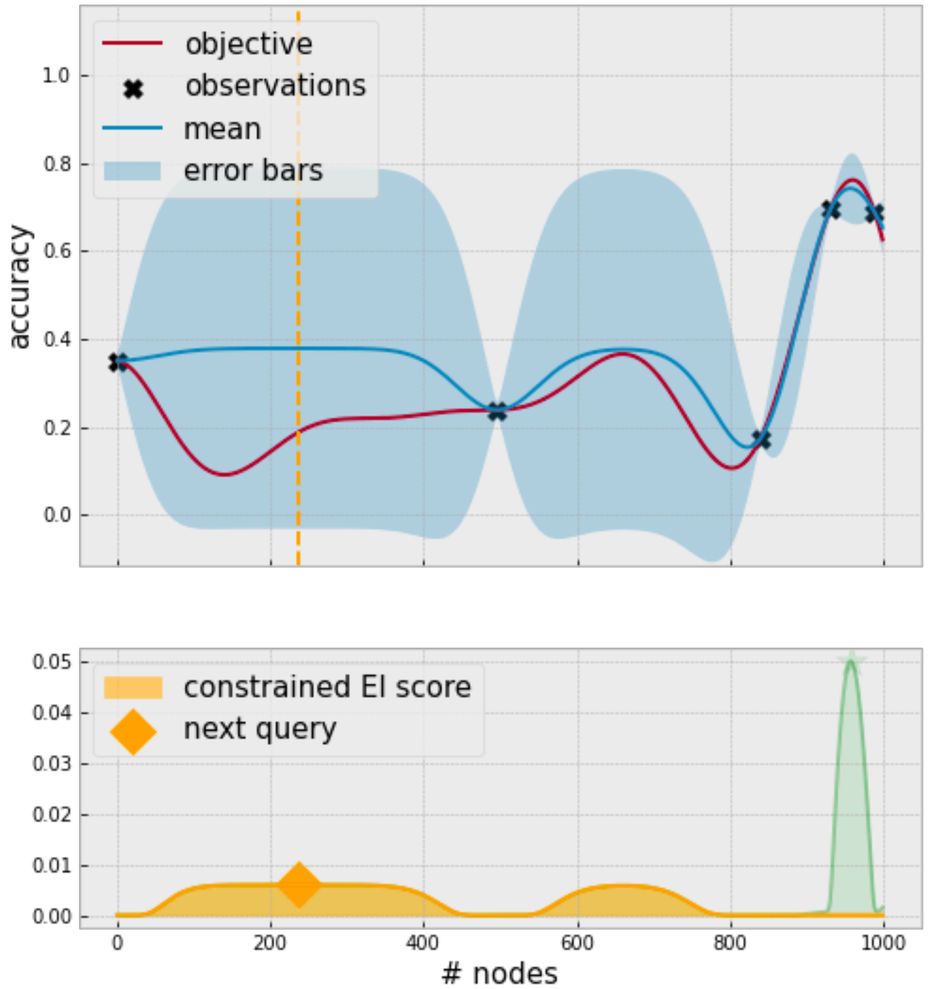

Gardner et al. (2014) http://proceedings.mlr.press/v32/gardner14.pdf

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```
policy = ConstrainedExpectedImprovement(
    model=ModelListGP(utility_model, cost_model),
    best_f=best_f,
    objective_index=0,
    constraints={1: [None, 800]}  # upper-bounded at 800
)
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Multi-objective optimization for balanced solutions

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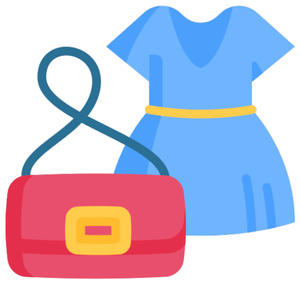

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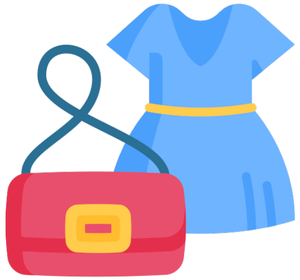

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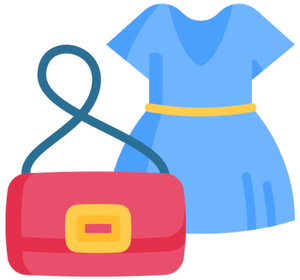

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collected data	objective value 1	objective value 2
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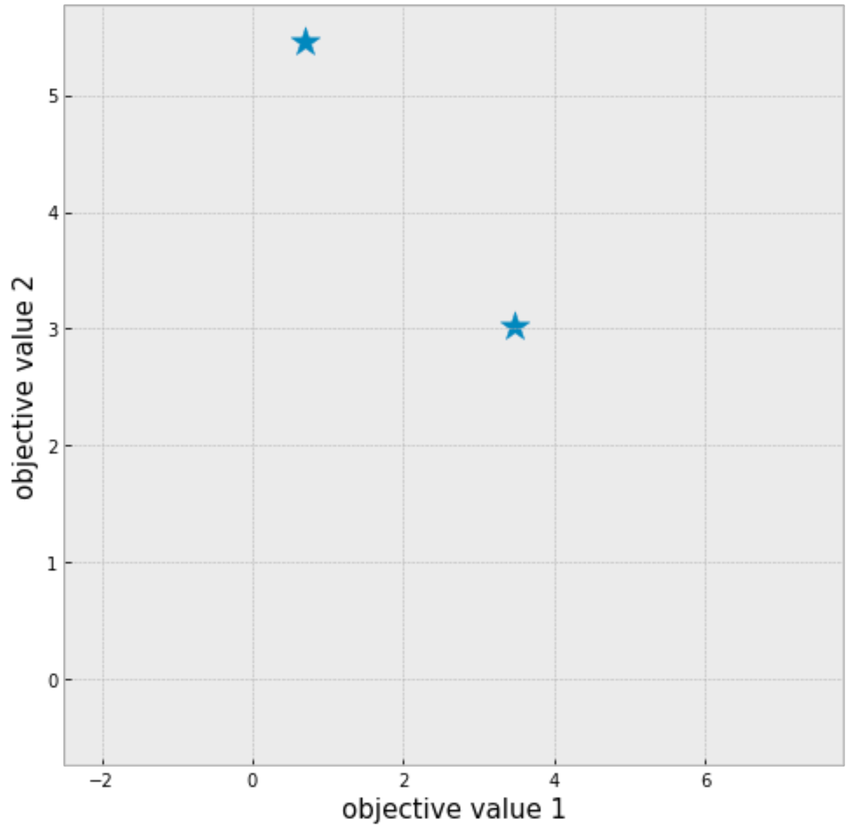

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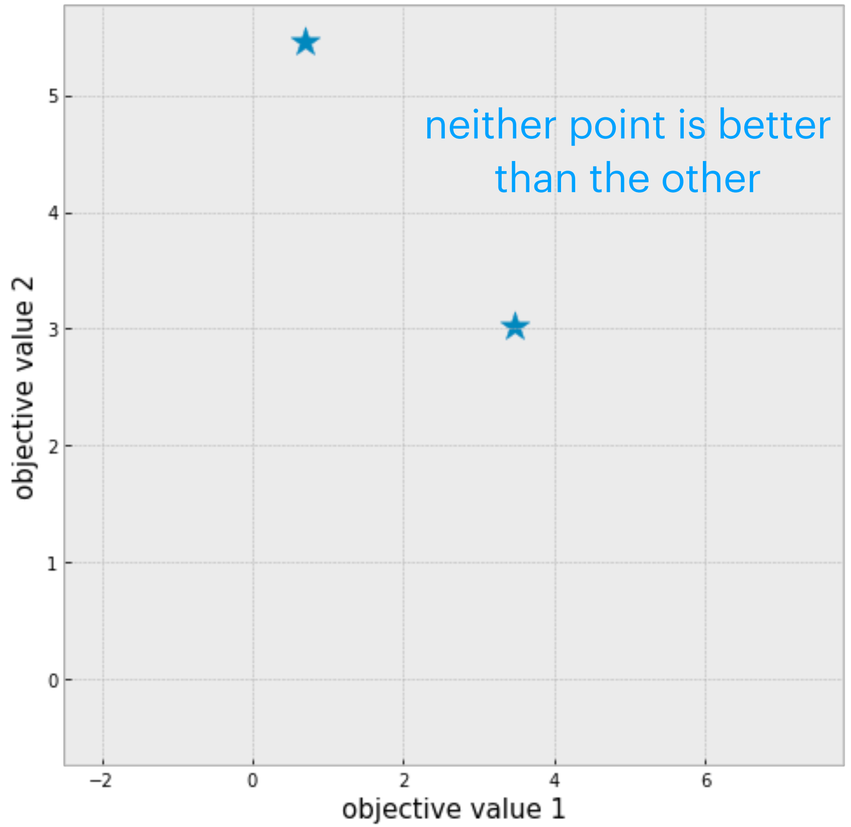

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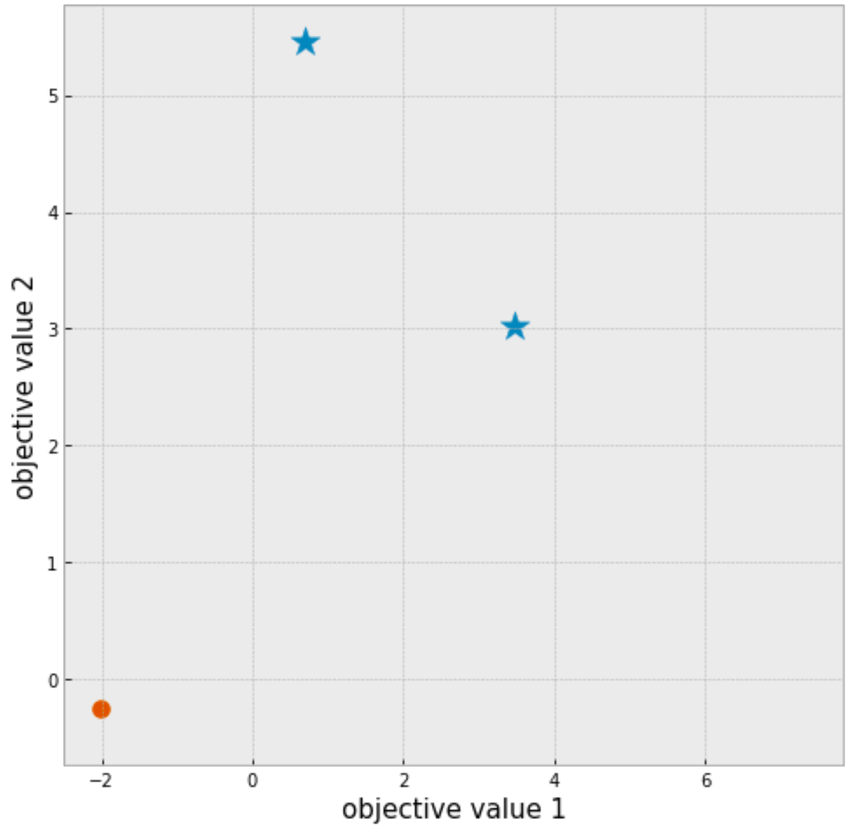

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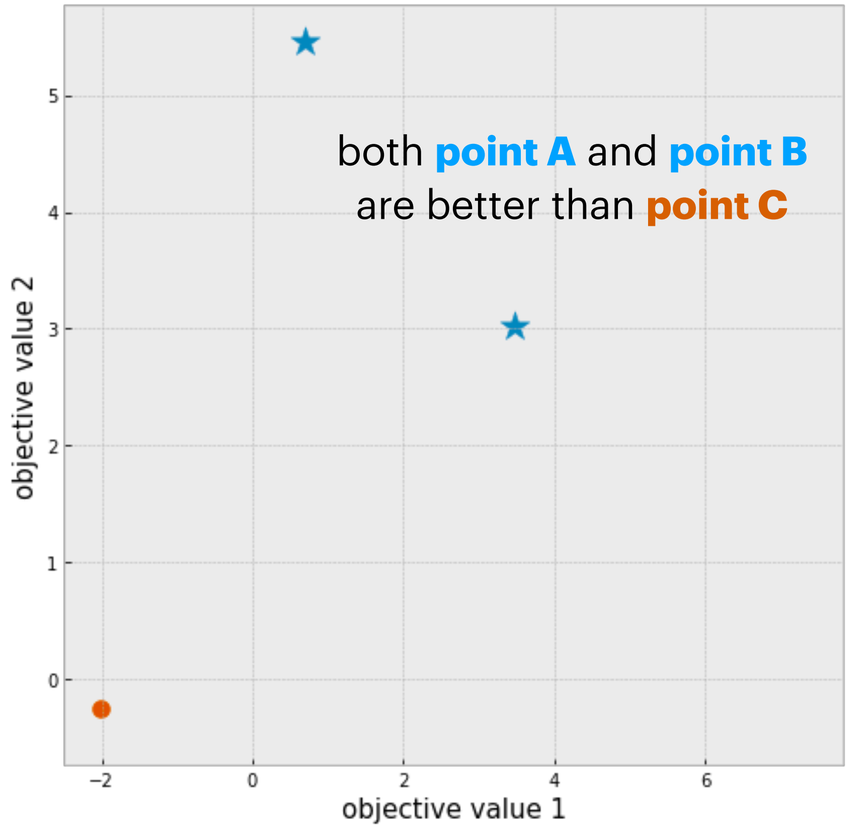

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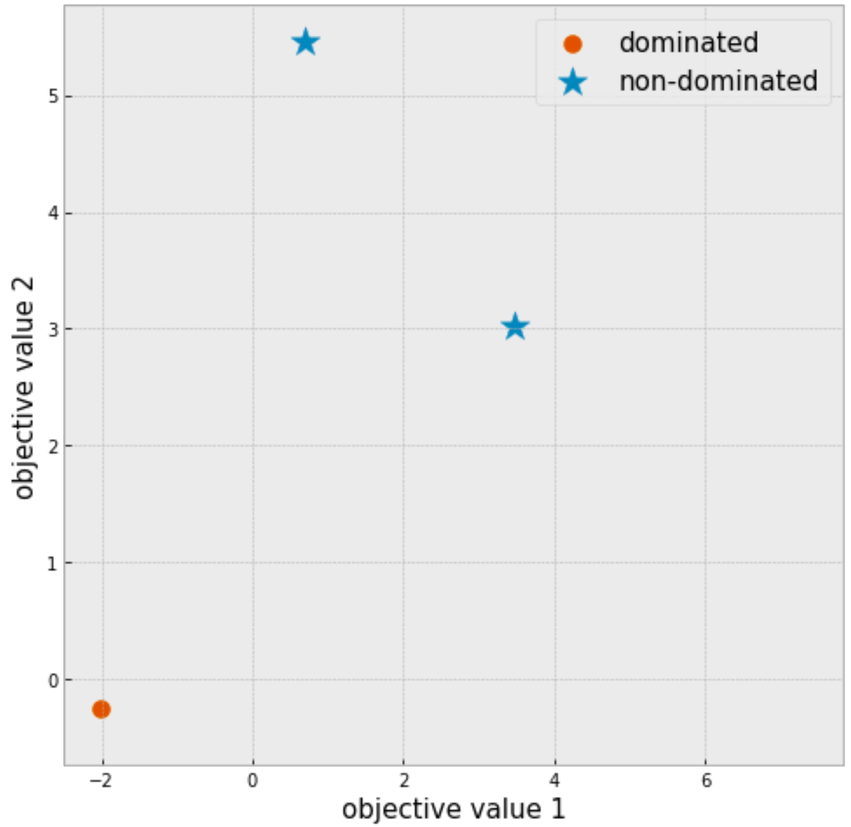

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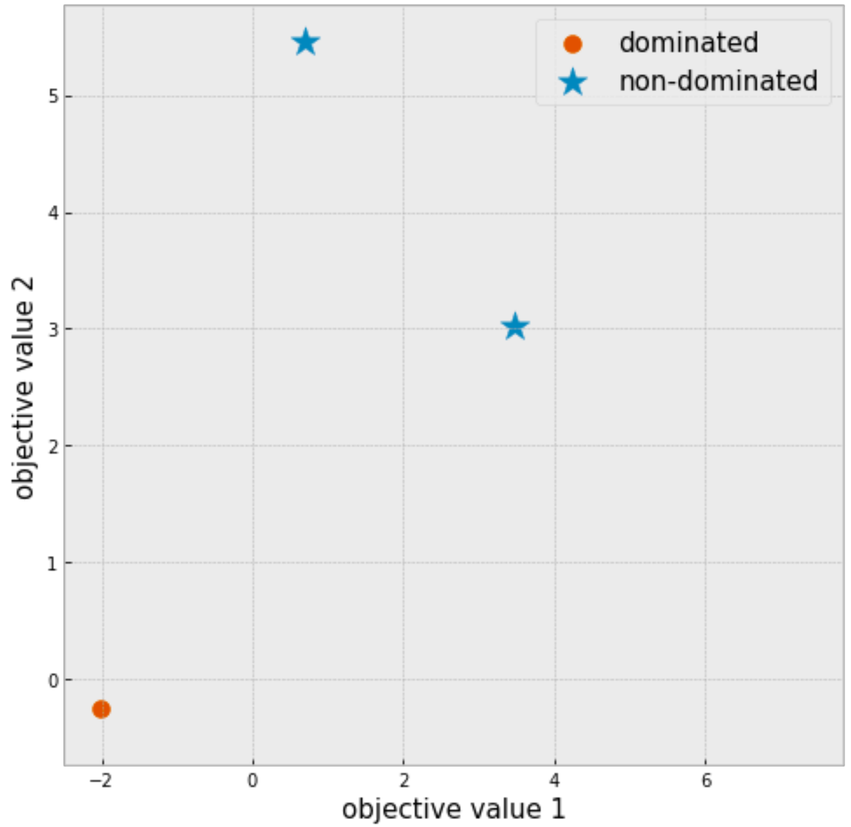

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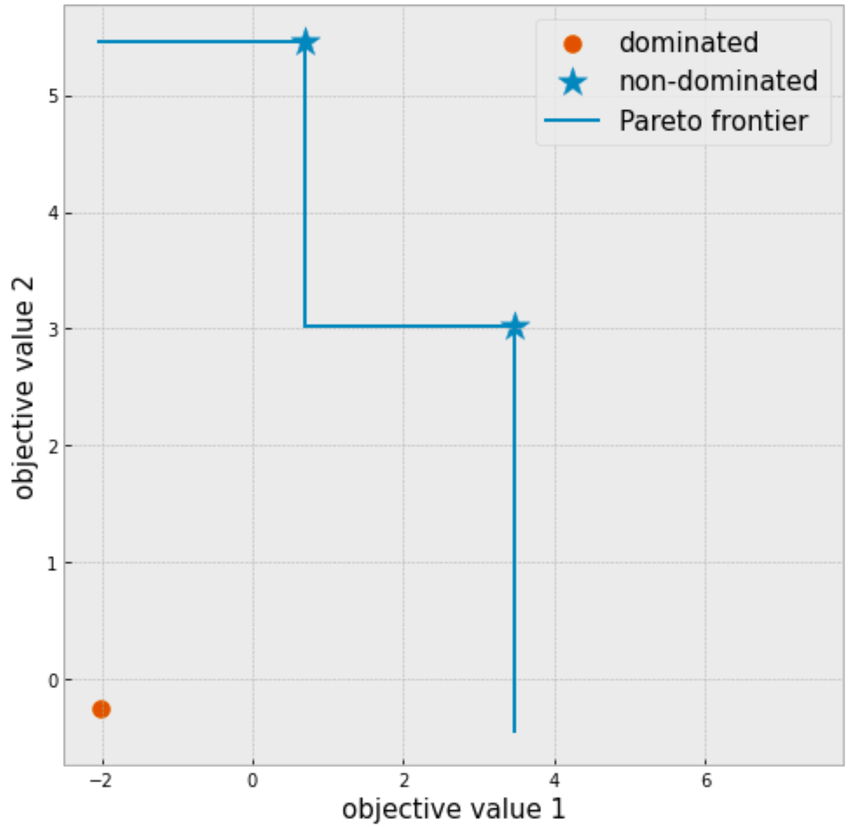

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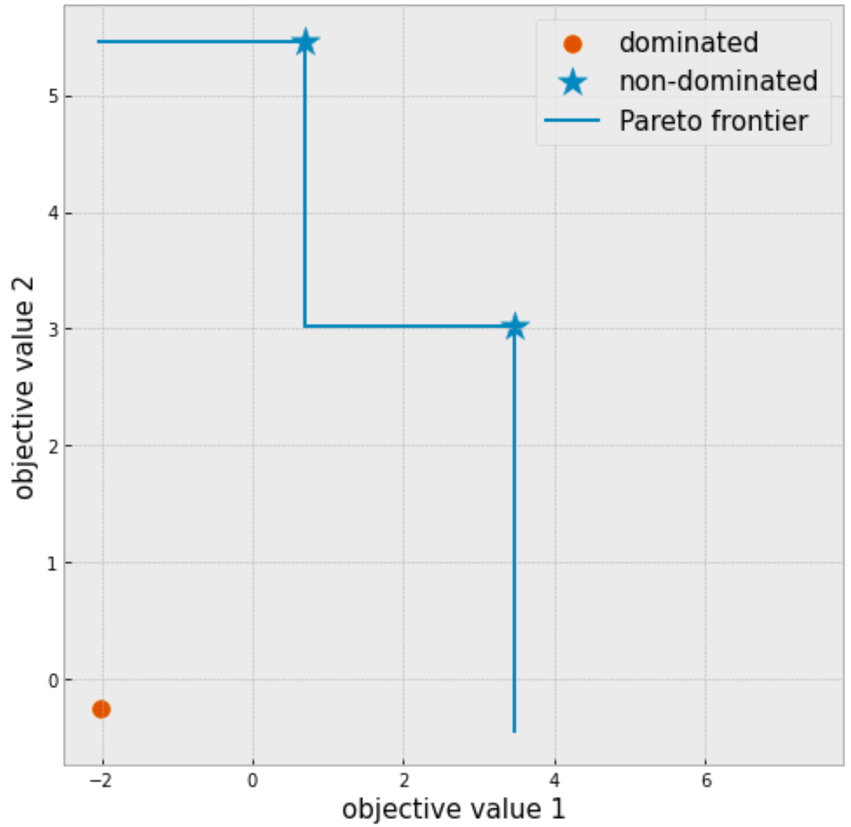

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policy = ExpectedHypervolumeImprovement(
    model=ModelListGP(model1, model2),
    ref_point=ref_point,
    partitioning=FastNondominatedPartitioning(
        ref_point, train_y
    )  # computes the Pareto frontier
)
```

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balancing between learning and cost

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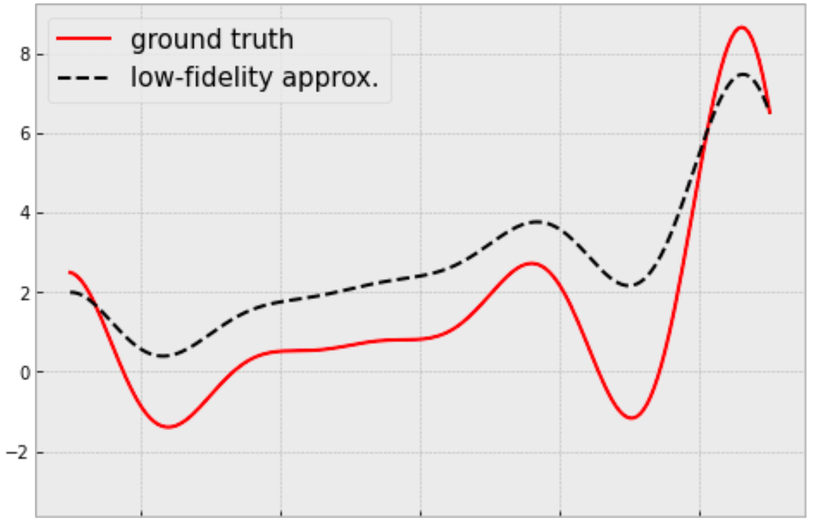

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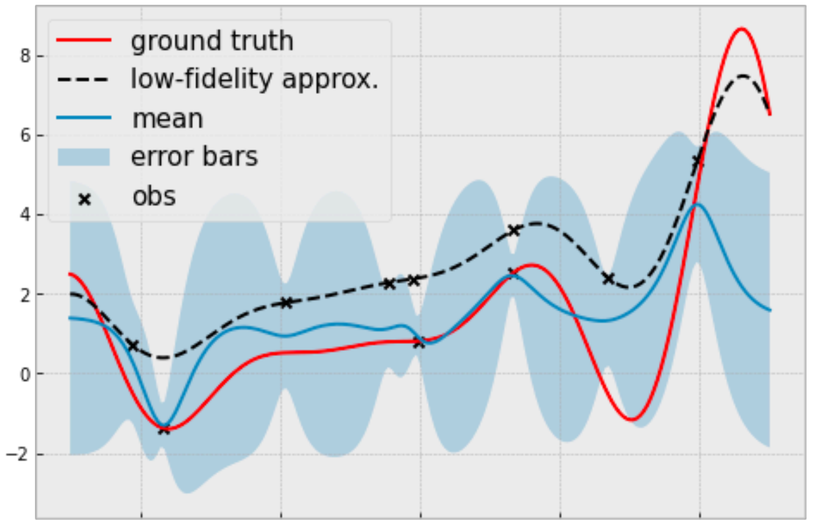

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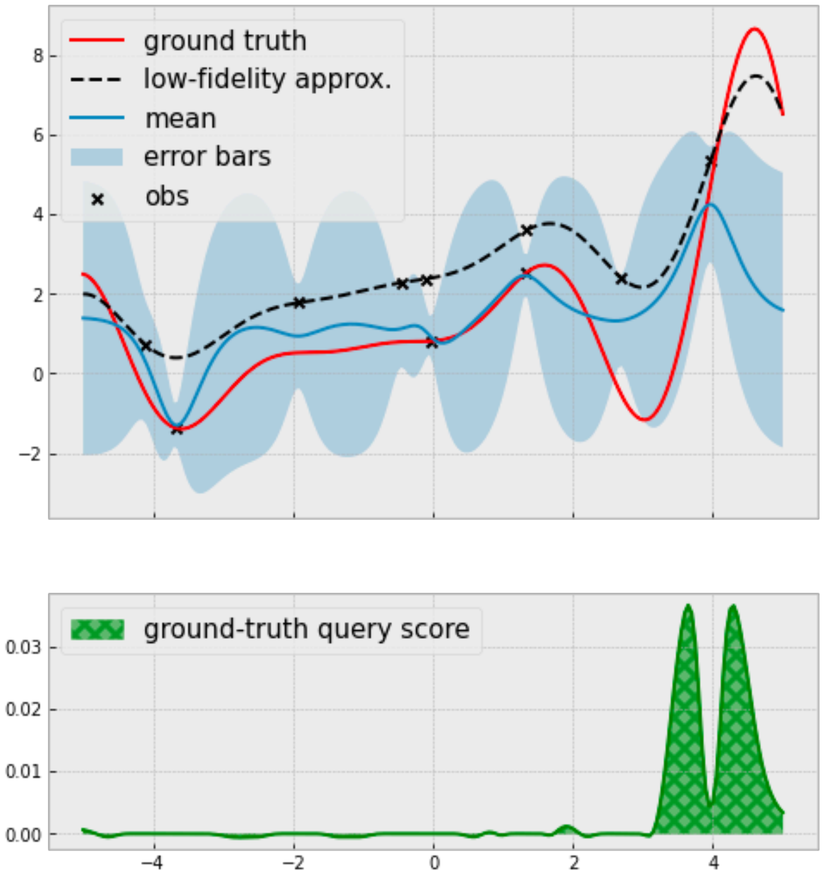

Multi-fidelity optimization to minimize cost

balancing between learning and cost

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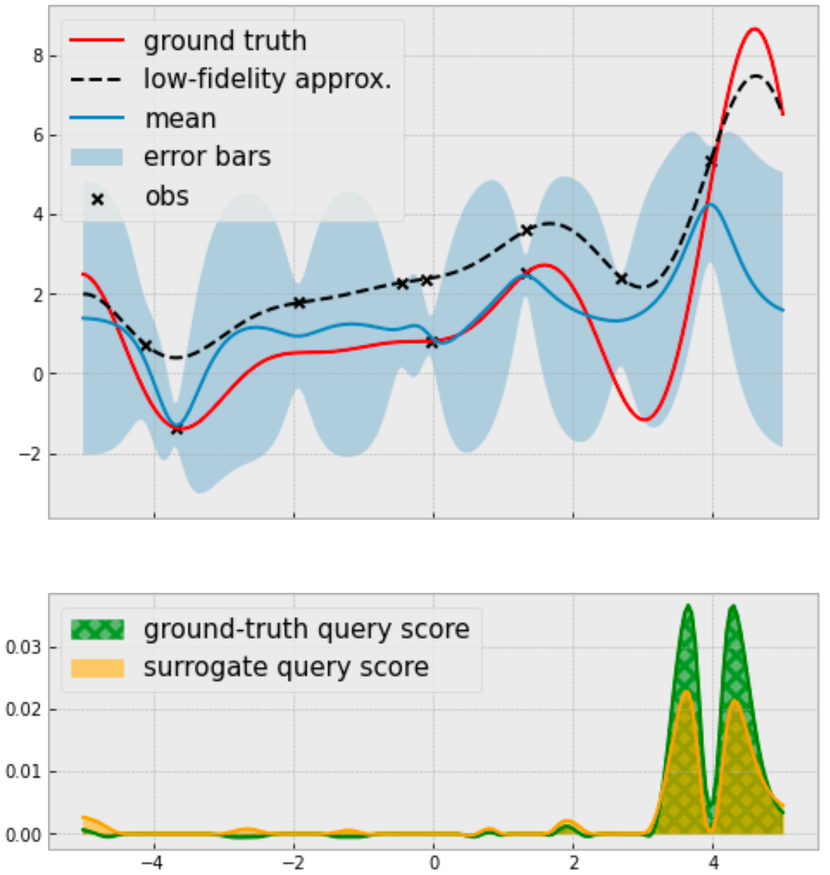

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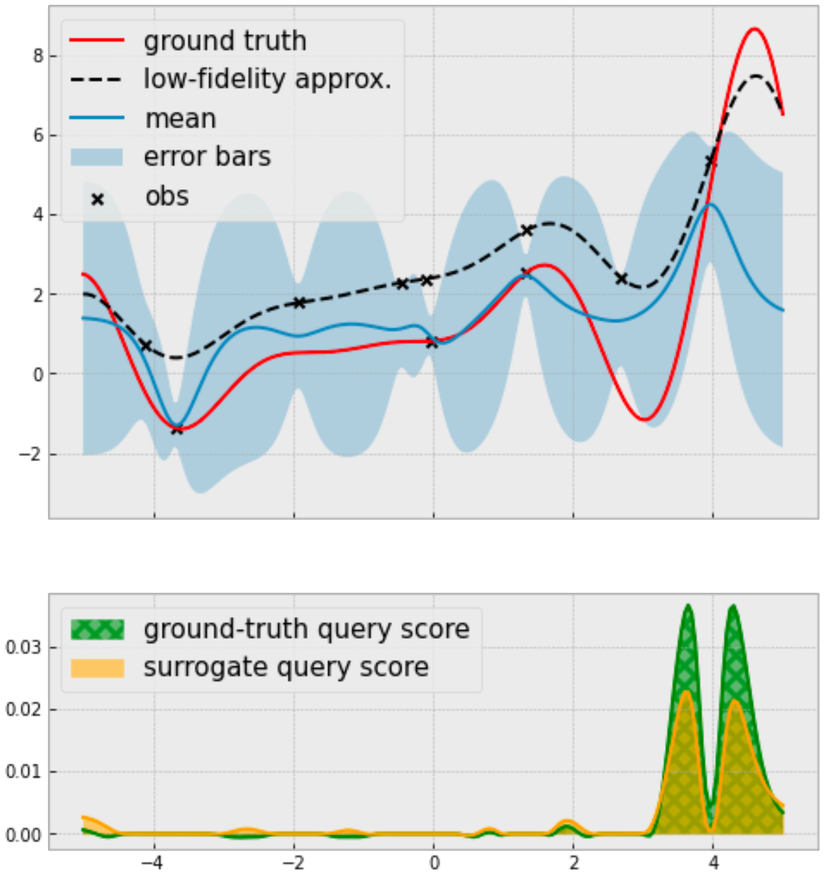

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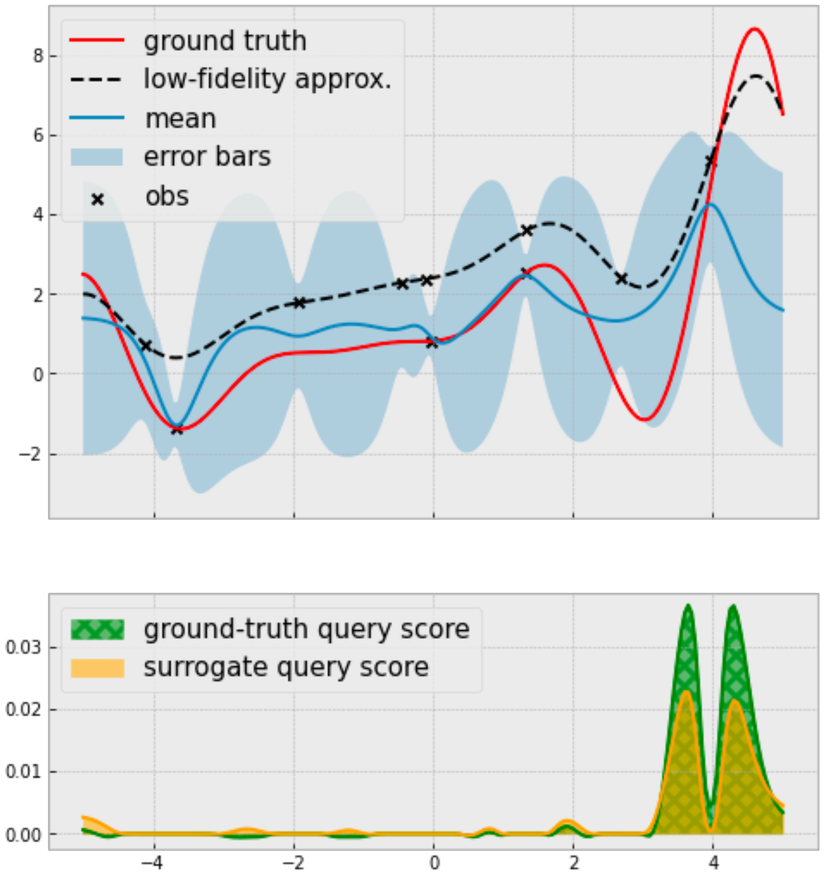

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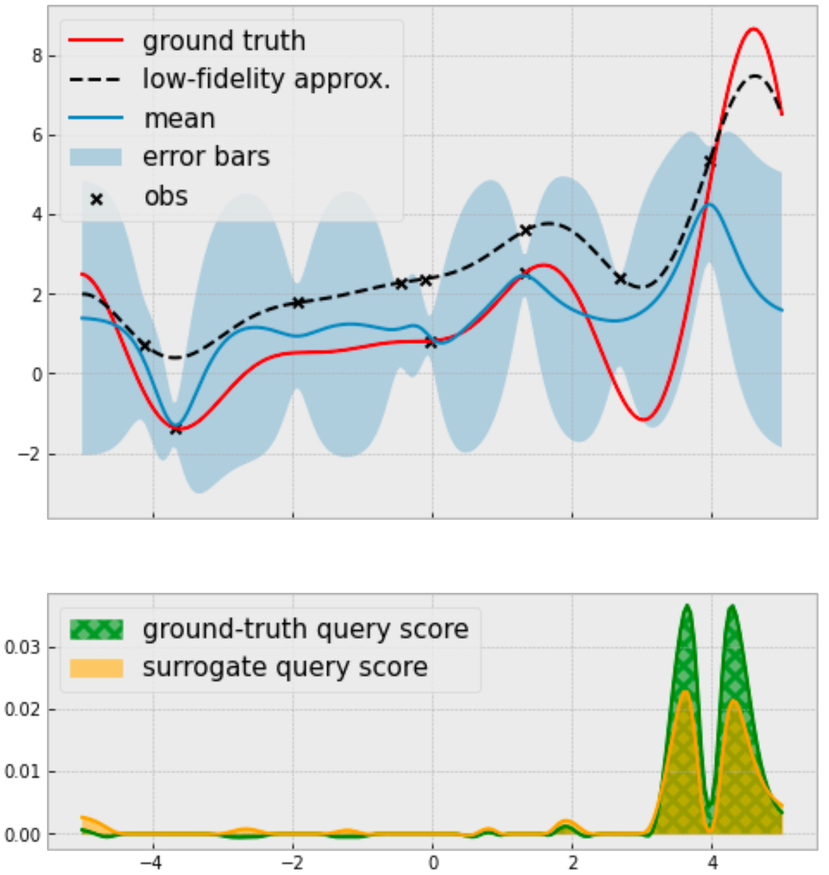

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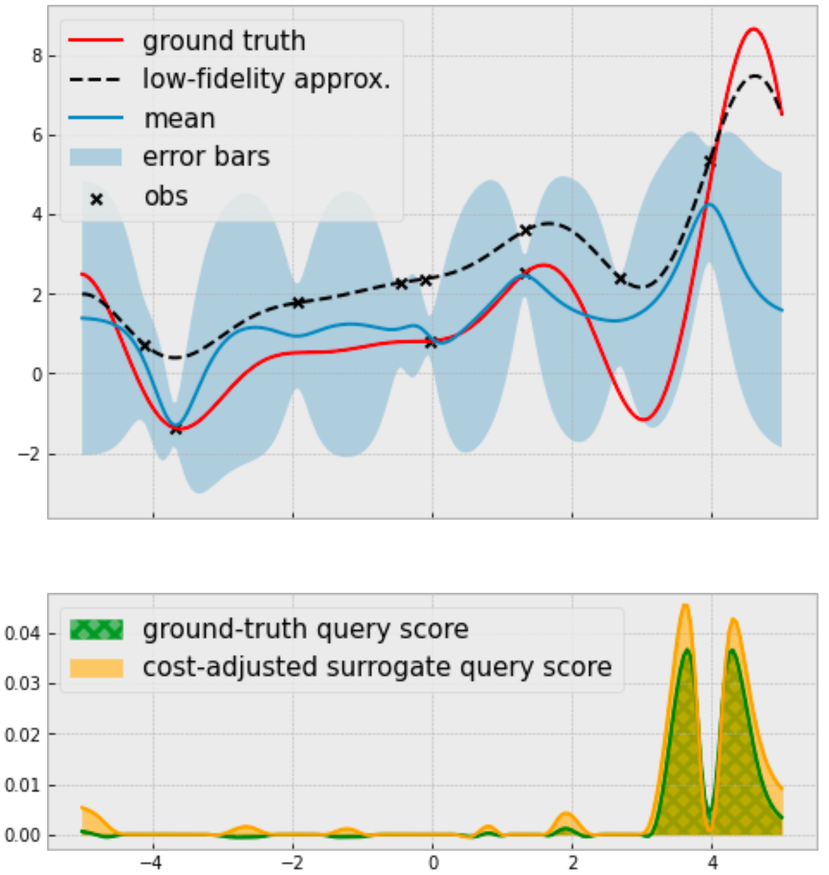

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```
policy = qMultiFidelityMaxValueEntropy(
    model,
    candidate_x,
    cost_aware_utility=cost_aware_utility,  # ROI
    project=project_to_target_fidelity,
)
```