Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index

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Joint work with Raul Astudillo, Peter Frazier, Ziv Scully, and Alexander Terenin

INFORMS'24 Data Mining Best General Paper Competition

Coauthors
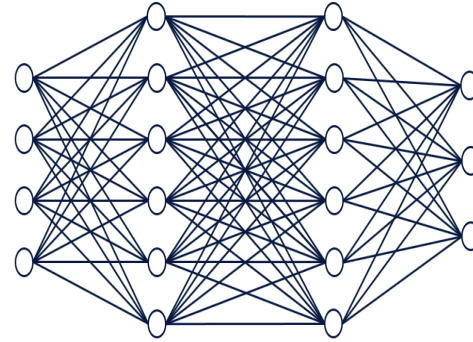

Raul Astudillo

Peter Frazier

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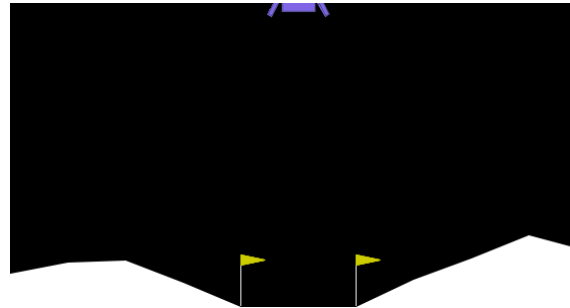
World of Parameter Optimization

Hyperparameter tuning:

Training parameters → Accuracy
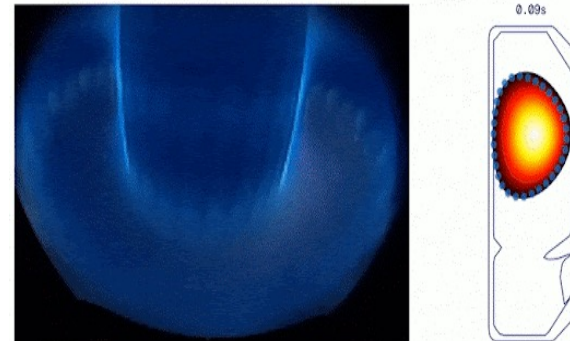
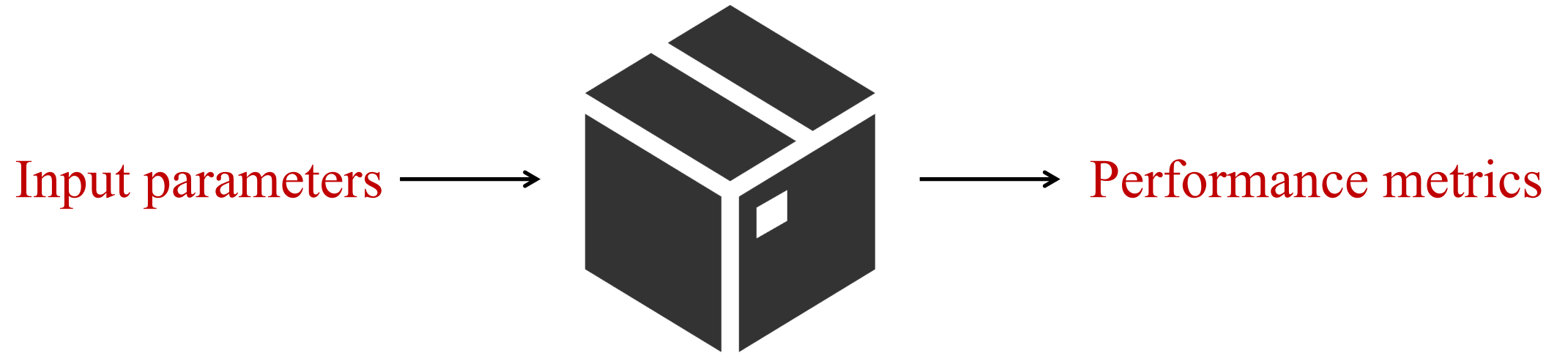Control optimization:

Control parameters → Reward

Plasma physics:

Reactor parameters → Stability

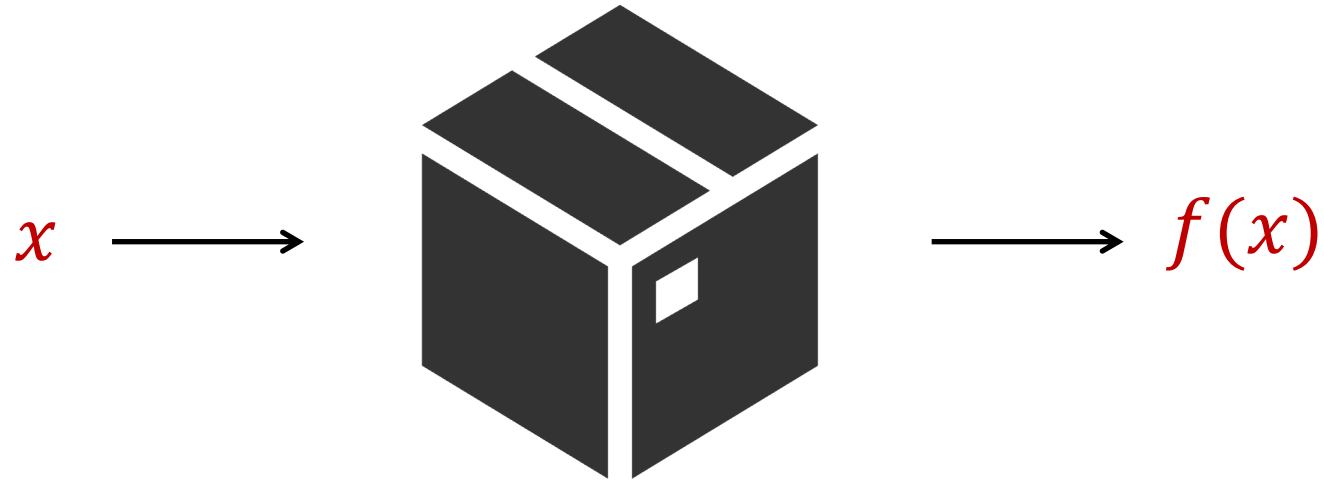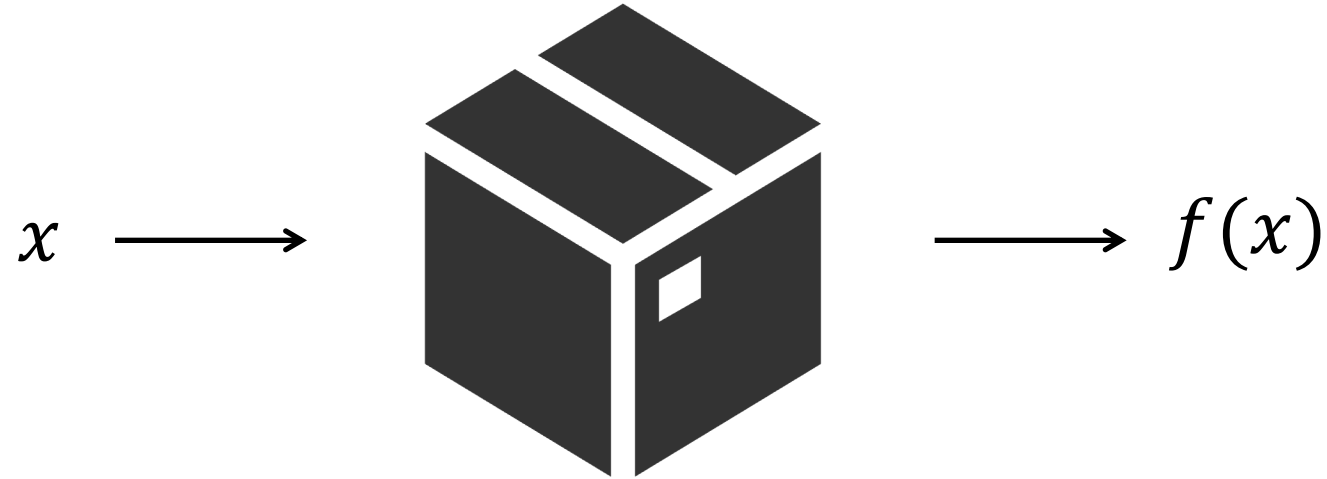# World of Parameter Optimization

Black-box optimization:

Input parameters $\longrightarrow$ $\longrightarrow$ Performance metrics

World of Parameter Optimization

Black-box optimization:

x ⟶ ⟶ $f(x)$

Optimizing Black-box Functions

$x \longrightarrow$ ☐ $\longrightarrow f(x)$

Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

Optimizing Black-box Functions
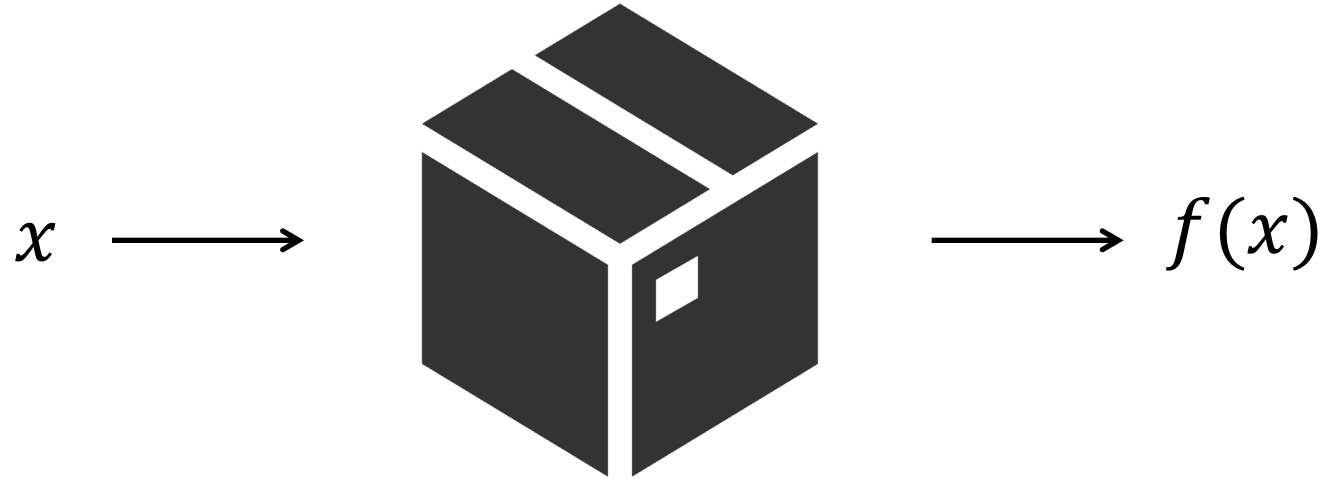
$x \longrightarrow$ [black box] $\longrightarrow f(x)$

Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

$f \sim$ Stochastic Process

Optimizing Black-box Functions

$x \longrightarrow$ [black box] $\longrightarrow f(x)$

expensive-to-evaluate

Goal: $\mathbf{max}_{x \in \mathcal{X}} \, f(x)$

Optimizing Black-box Functions

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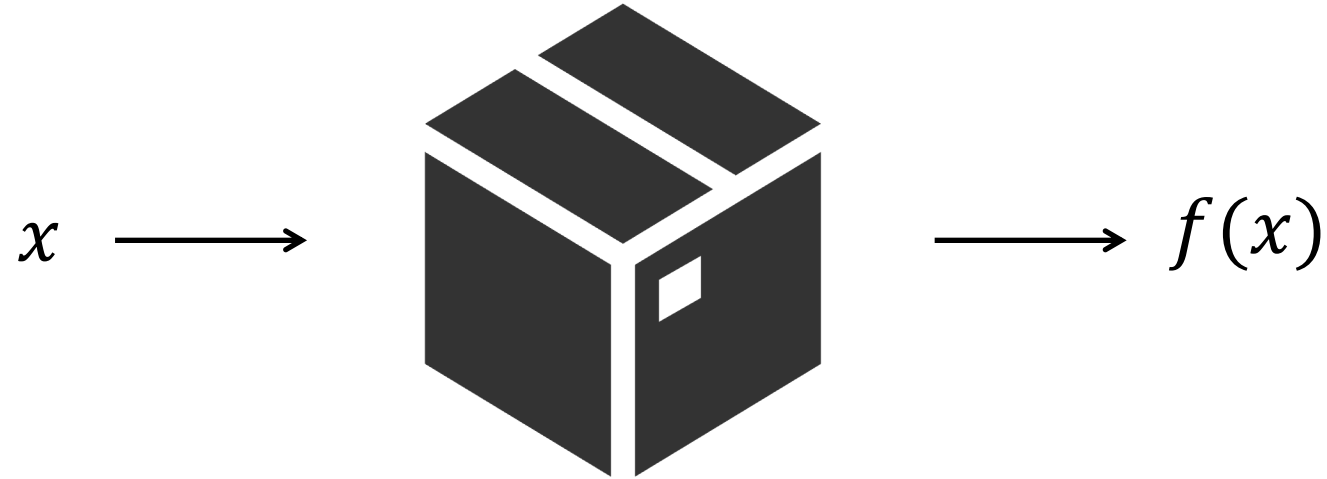
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$f \sim$ Gaussian Process

Bayesian Optimization

$$x \longrightarrow \boxed{} \longrightarrow f(x)$$

Goal: $\mathbf{max} \; \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$
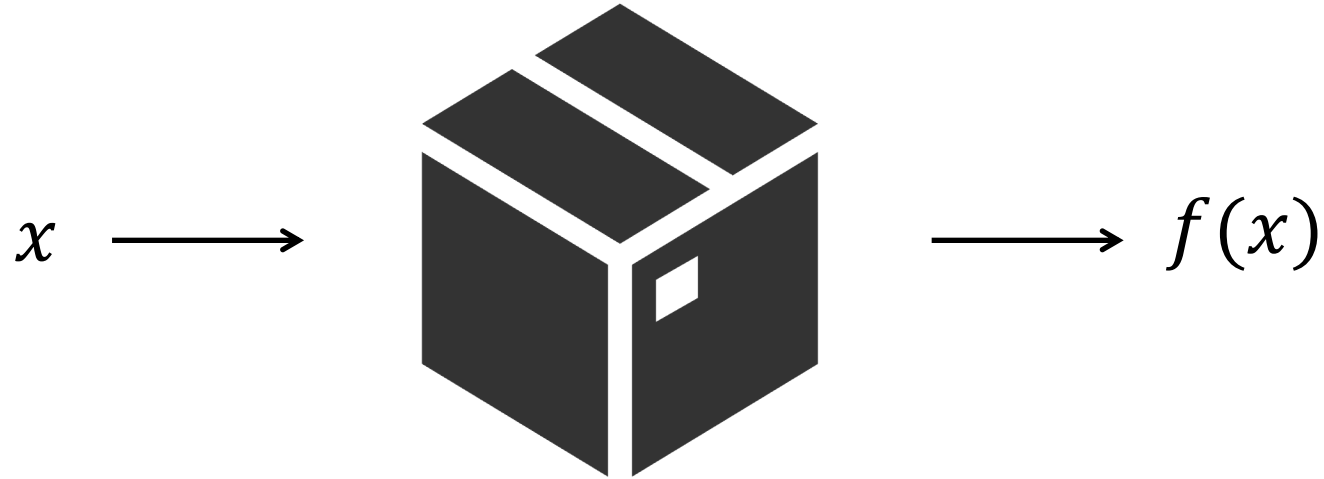
$f \sim$ Gaussian Process

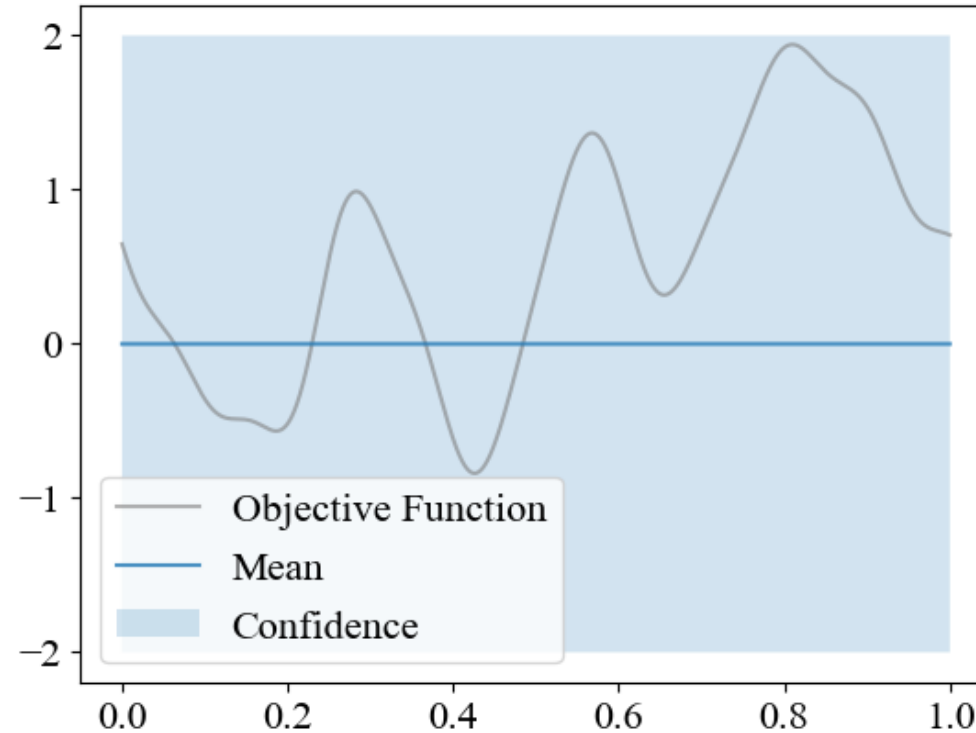# Bayesian Optimization
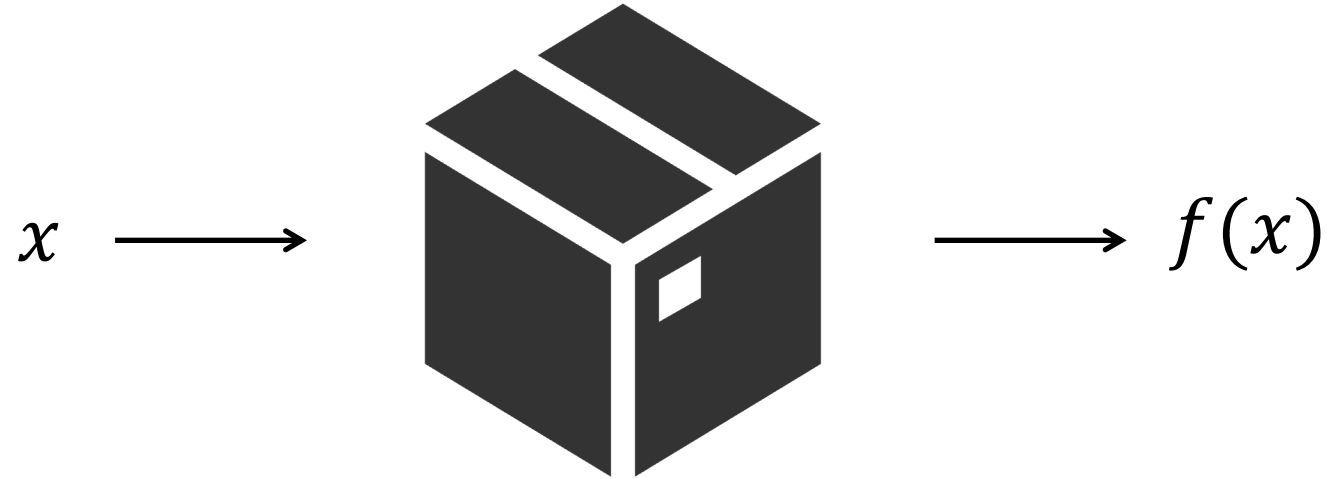
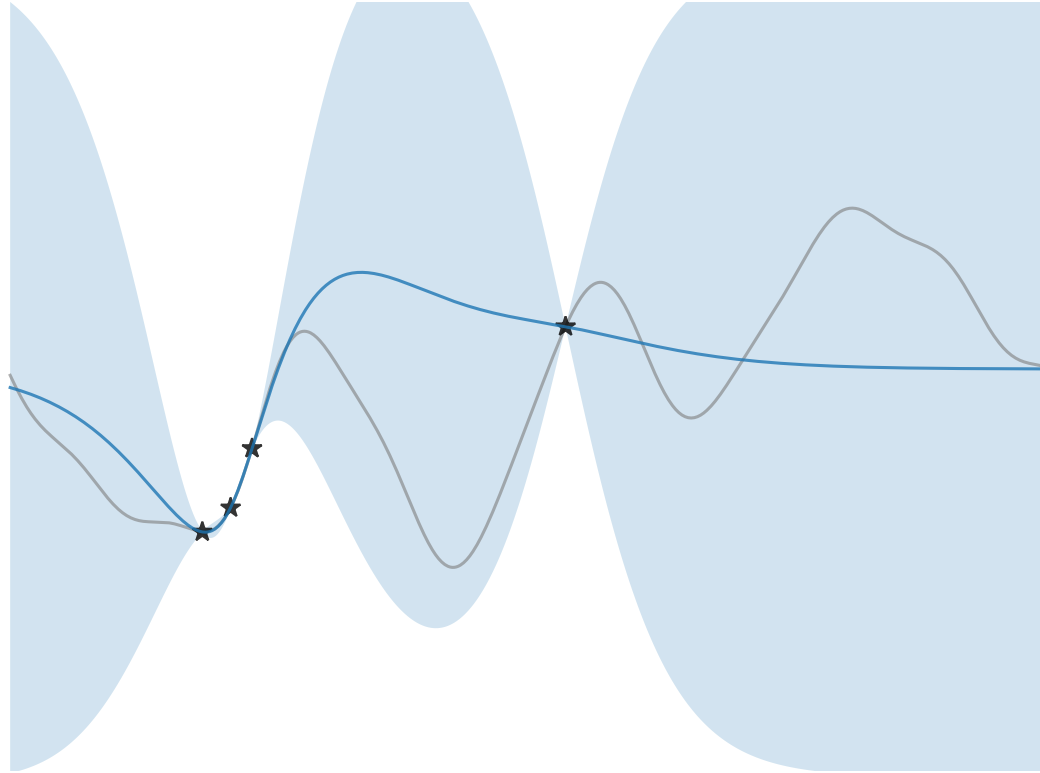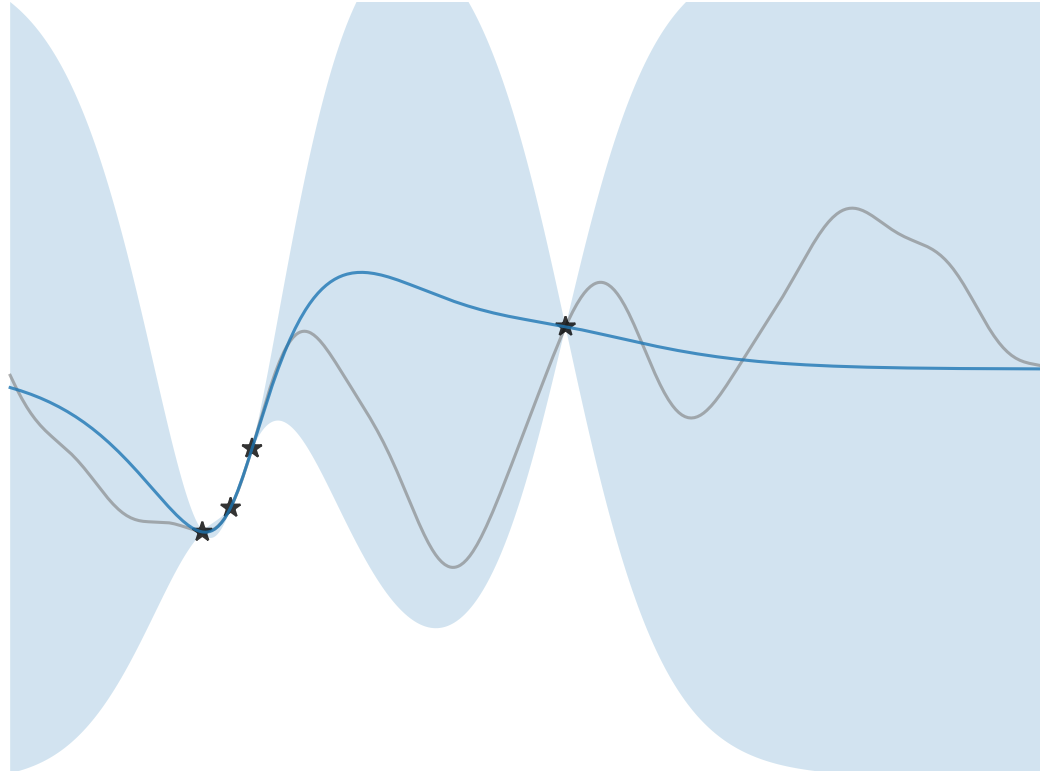Goal: $\max\ \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

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Bayesian Optimization

$$\text{Goal: } \mathbf{max} \ \mathbb{E} \ \max_{t=1,2,\dots,T} f(x_t)$$
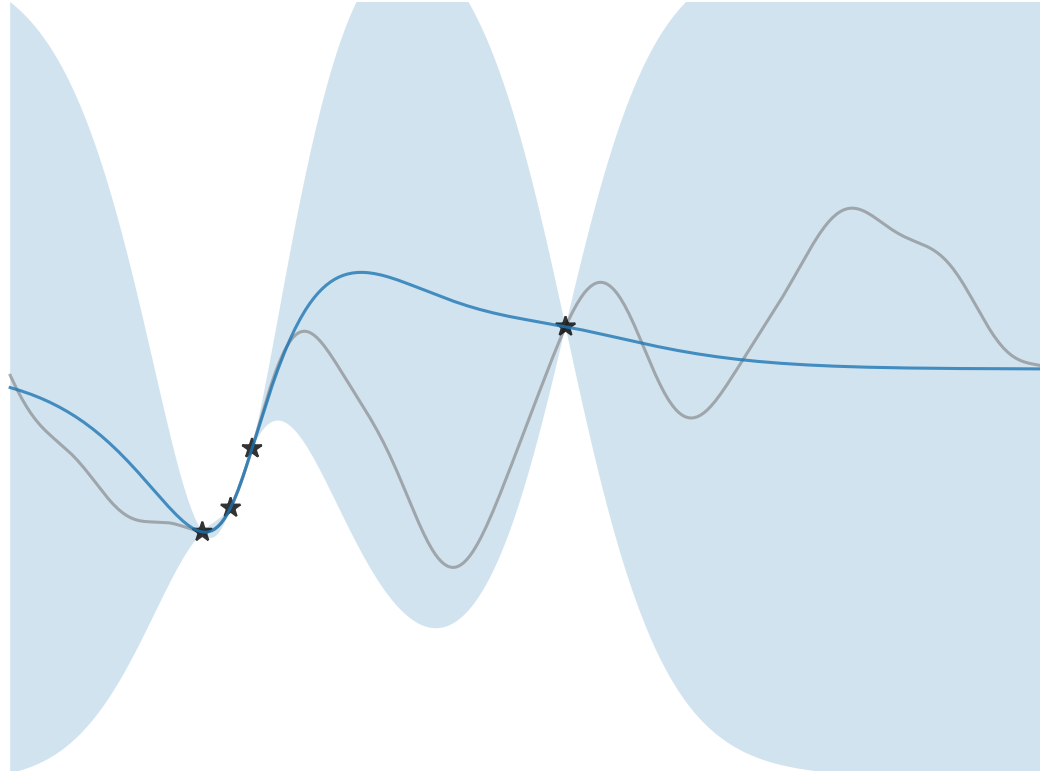
$f \sim \text{Gaussian Process}$

Bayesian Optimization
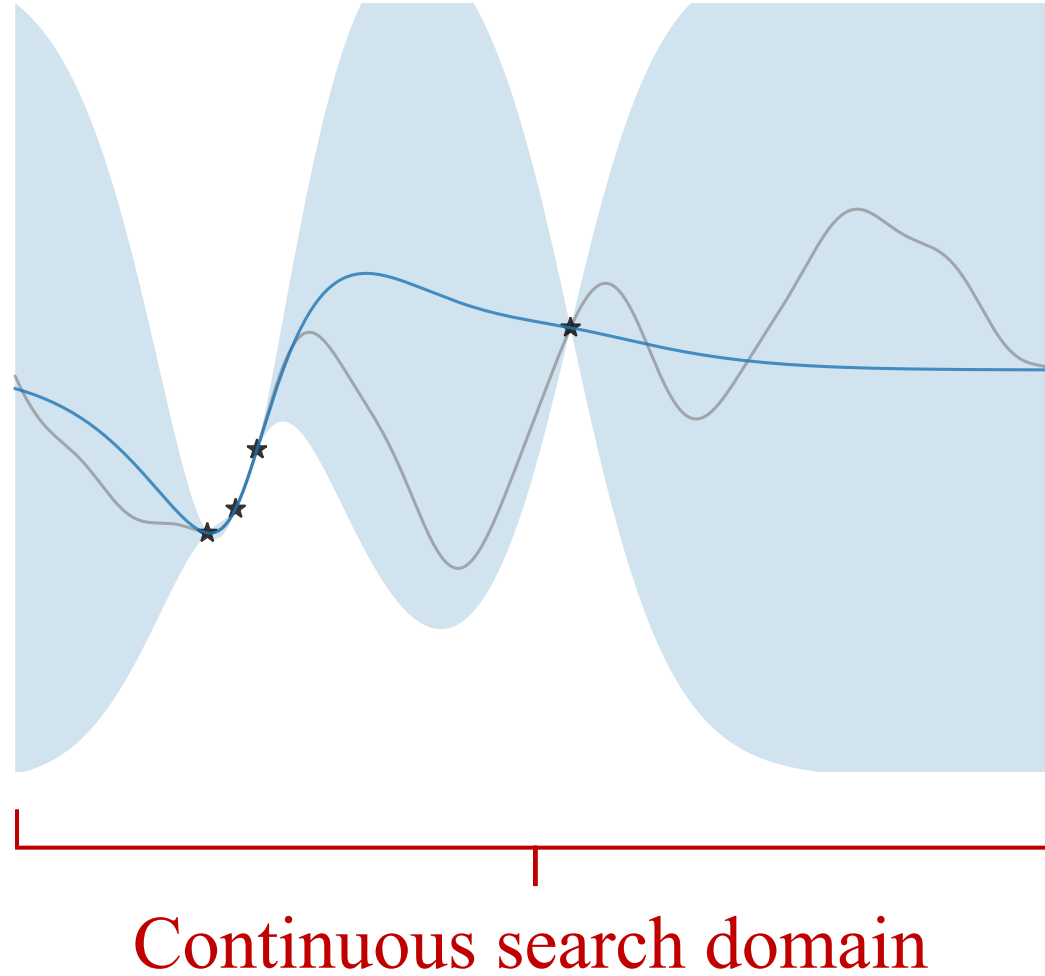

What to evaluate next?

Bayesian Optimization

Optimal policy?

Challenges of Bayesian Optimization

Continuous search domain

Challenges of Bayesian Optimization

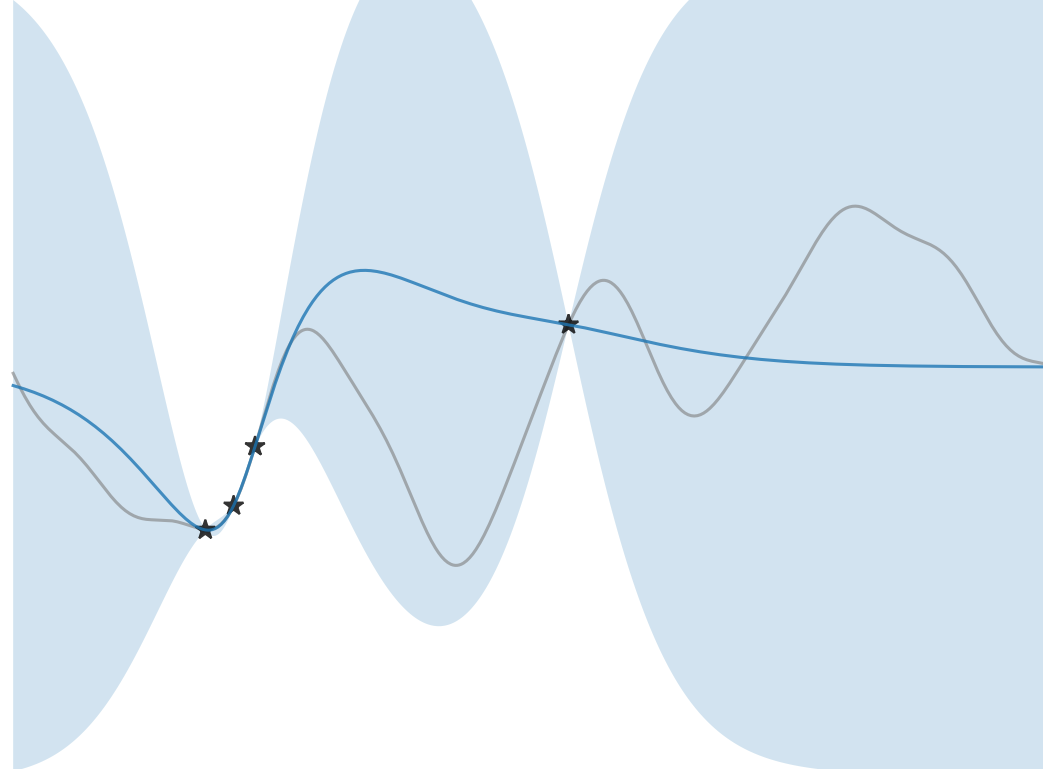Correlated values

Continuous search domain
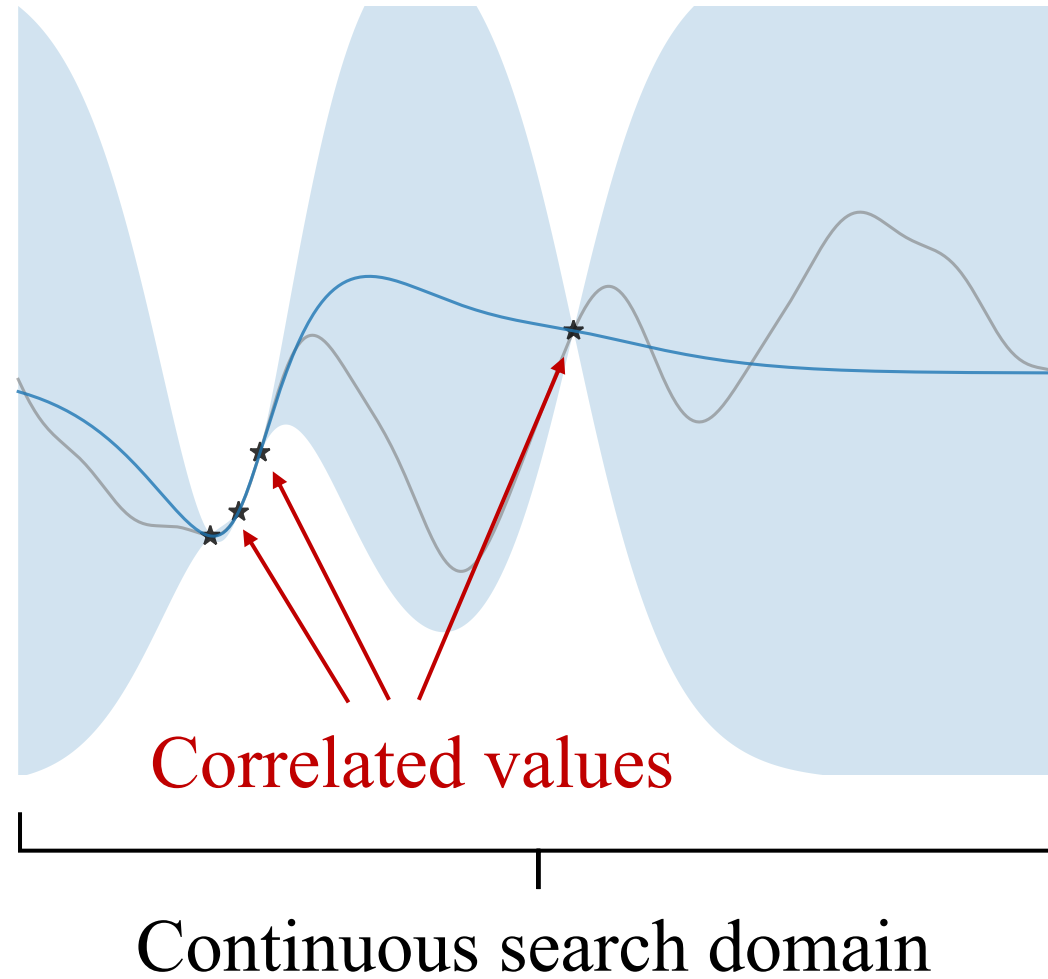
Challenges of Bayesian Optimization
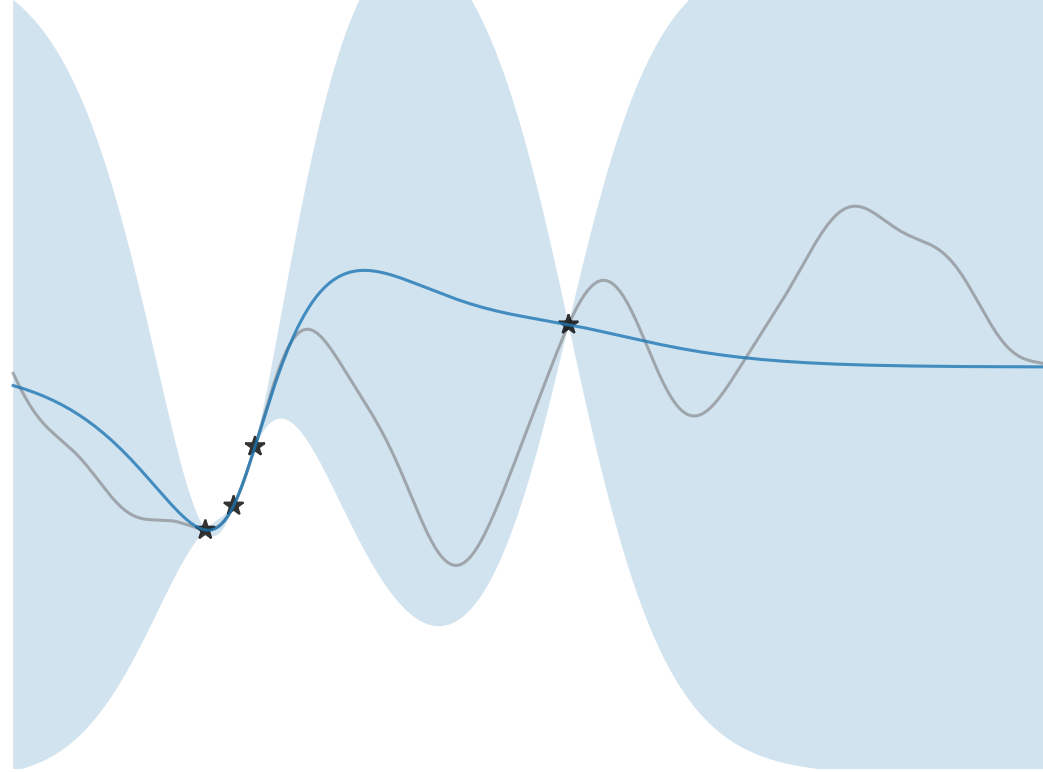
Correlation & continuity $\Rightarrow$ Intractable MDP

Challenges of Bayesian Optimization

Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement
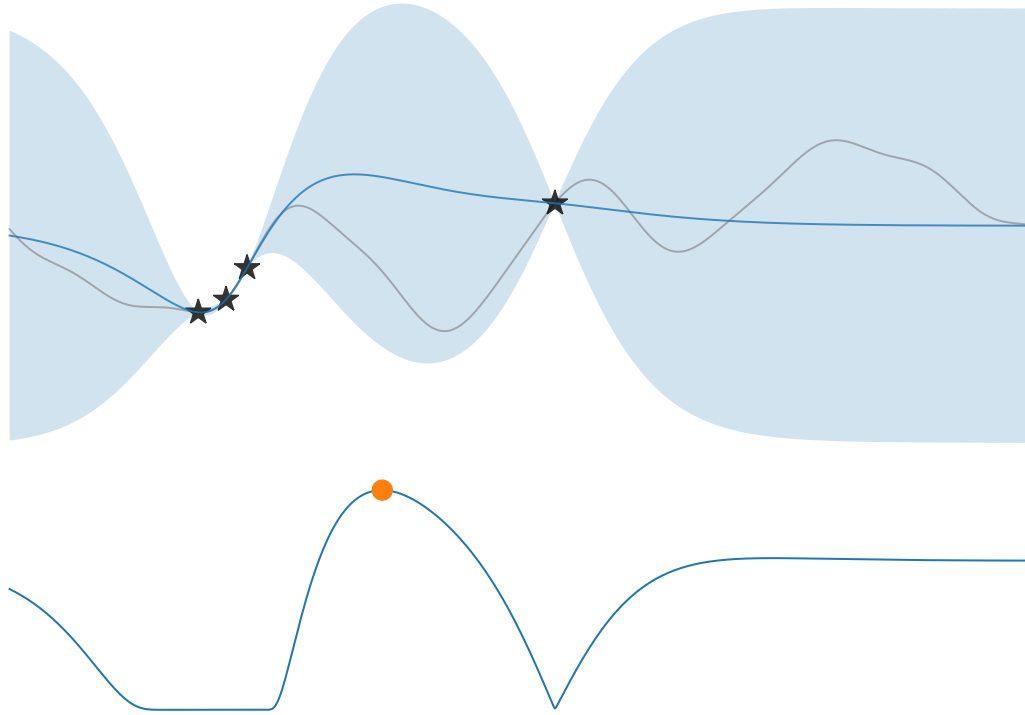
current best observed data

$$\mathrm{EI}(x) = \mathbb{E}[\max(f(x) - y_{\mathrm{best}}, 0) \mid D]$$

"improvement"

Popular Policy: Expected Improvement

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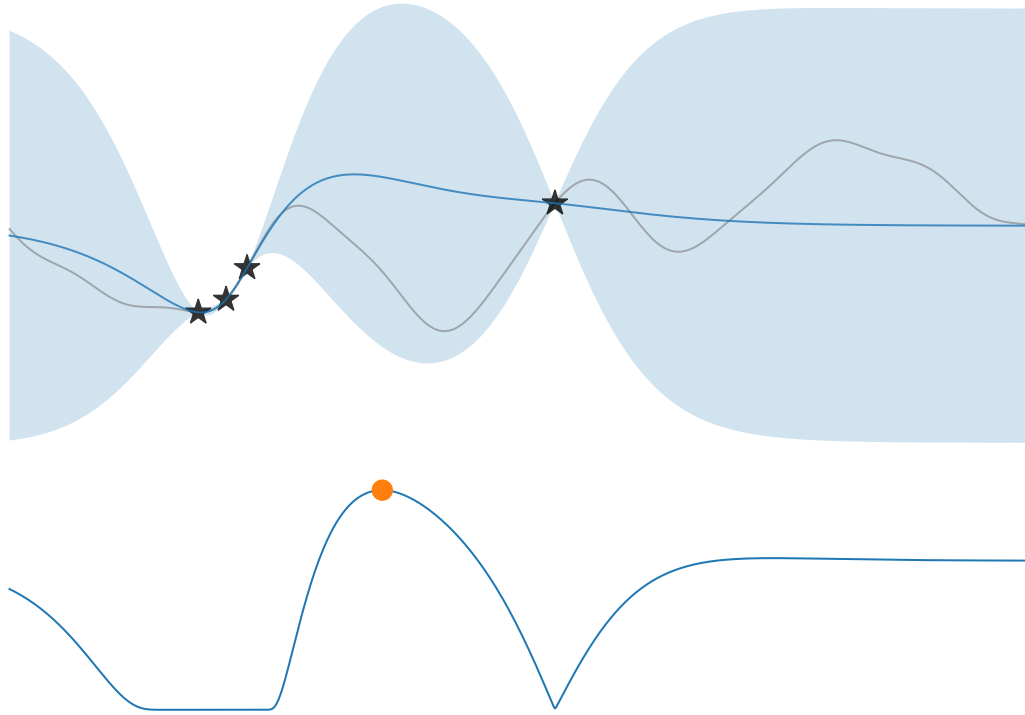
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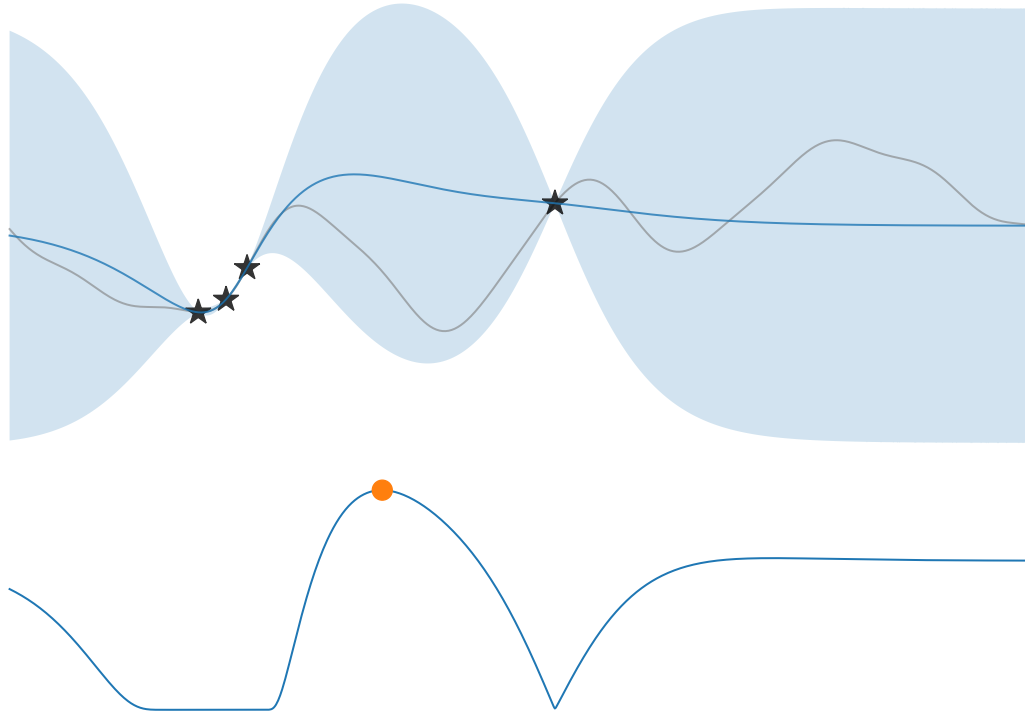
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One-step approximation to MDP

Popular Policy: Expected Improvement
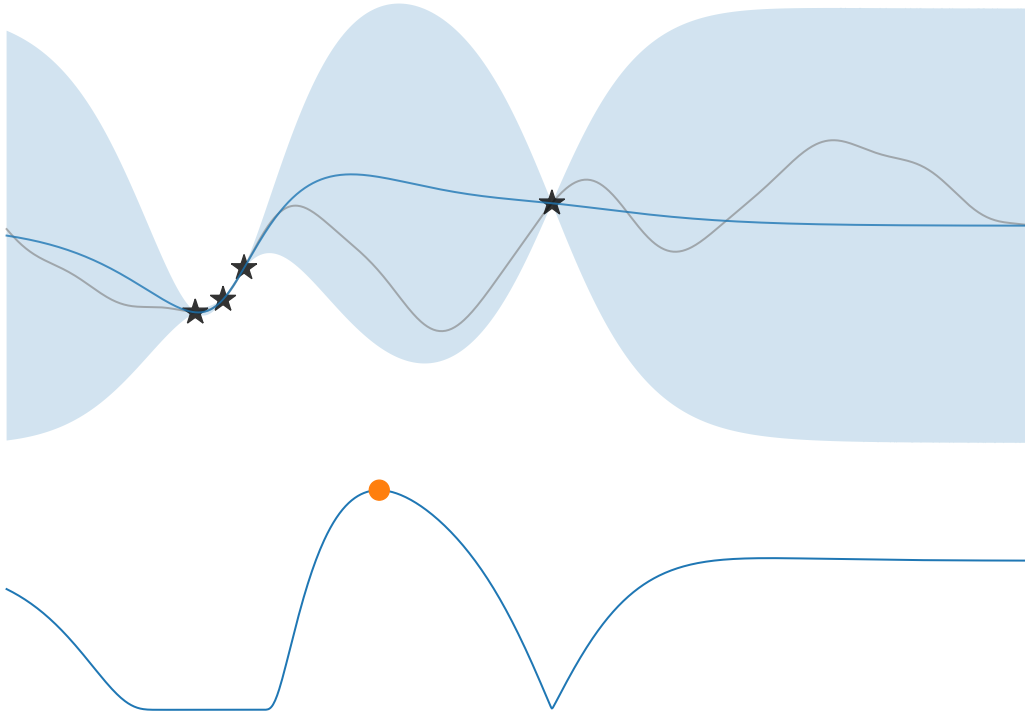
Other improvement-based policy:

- Probability of Improvement
- Knowledge Gradient
- Multi-step Lookahead EI
- …

Approaches to Bayesian Optimization

- Improvement-based:
  - Expected Improvement
  - Probability of Improvement
  - Knowledge Gradient
  - Multi-step Lookahead EI

Approaches to Bayesian Optimization

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    - Max-value Entropy Search
    - Predictive Entropy Search

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- Upper Confidence Bound

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Approaches to Bayesian Optimization

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- Our work: Gittins Index
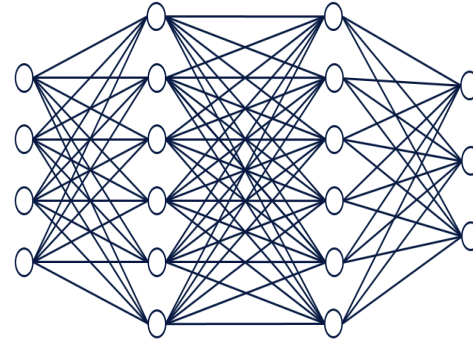
Approaches to Bayesian Optimization

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  Why another approach?

- Thompson Sampling

- Our work: Gittins Index

Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters $\longrightarrow$ $\longrightarrow$ Accuracy

Control optimization:

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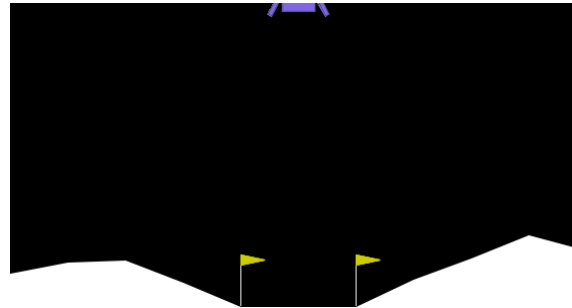
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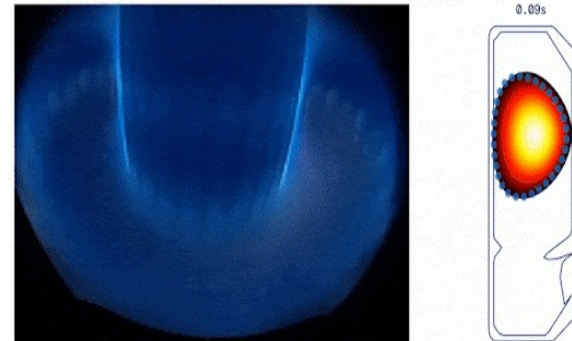
Reactor parameters $\longrightarrow$ $\longrightarrow$ Stability

Challenge: Varying Evaluation Costs

Black-box optimization:
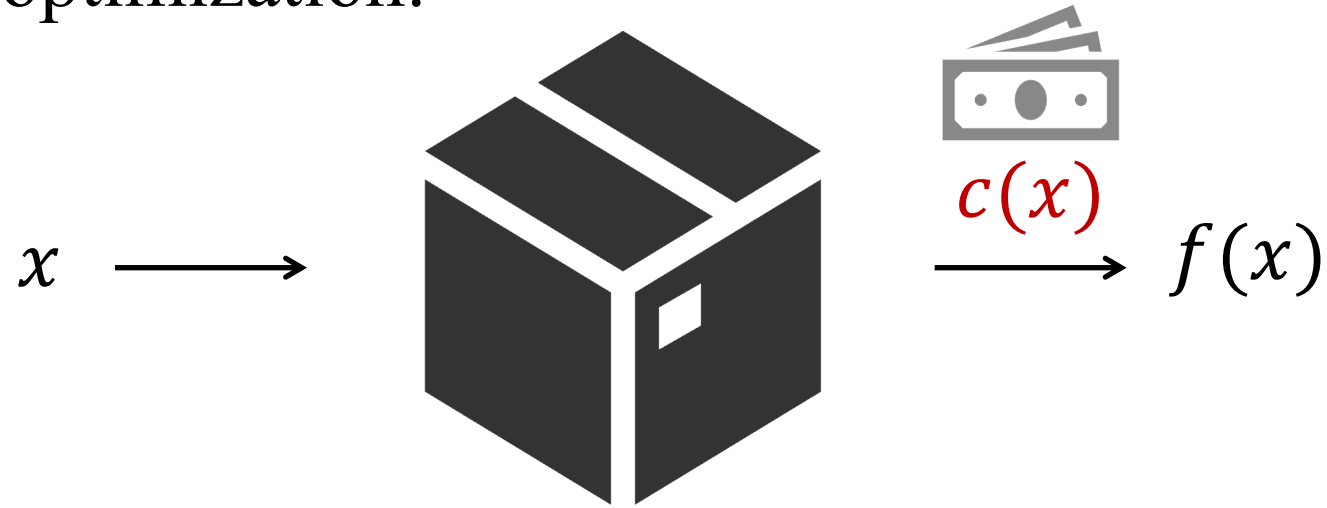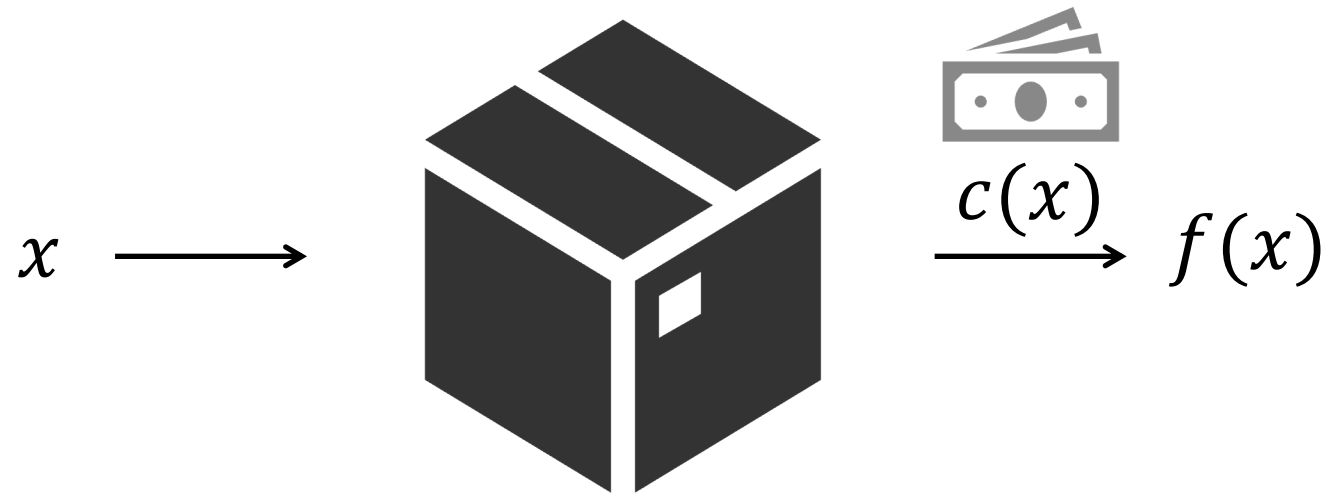
$x \longrightarrow$ [box] $\xrightarrow{\;\; c(x) \;\;} f(x)$

Challenge: Varying Evaluation Costs

Goal: $\mathbf{max} \ \mathbb{E} \ \max_{t=1,2,...,T} f(x_t)$

s.t. $\mathbb{E} \sum_{t=1}^{T} c(x_t) \leq B$

Cost-aware Bayesian Optimization

$$x \longrightarrow \boxed{} \xrightarrow{c(x)} f(x)$$
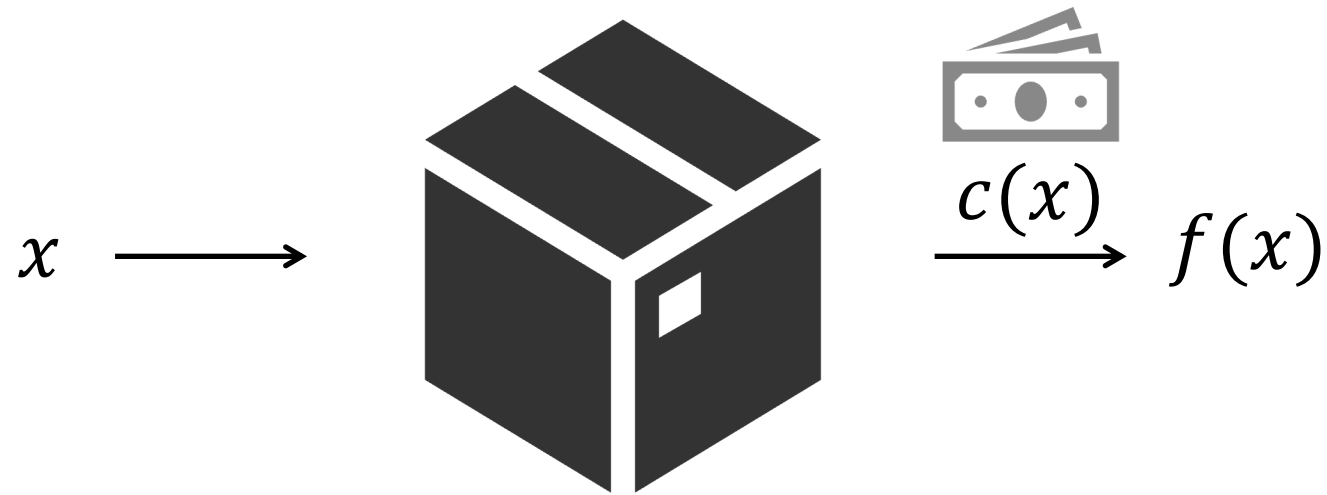
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[Lee, Perrone, Archambeau, Seeger'21]
[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

Uniform costs   Varying costs

Expected improvement

$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

$$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$$

Varying costs

Expected improvement per cost

$$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}}) \color{red}{/c(x)}$$

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

Varying costs

Expected improvement per cost

$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})/c(x)$$

Why divide?

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

Varying costs

Expected improvement per cost

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Why divide?

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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Varying costs

Expected improvement per cost

$$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})/c(x)$$

EI and EIPC policy can be arbitrarily bad under varying costs!

[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

Uniform costs

Varying costs

Expected improvement

Expected improvement per cost

Multi-step Lookahead EI

Budgeted Multi-step Lookahead EI

slow

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

Multi-step Lookahead EI

Upper Confidence Bound

Thompson Sampling

Varying costs

Expected improvement per cost

Budgeted Multi-step Lookahead EI

?

?

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
Expected improvement	Expected improvement per cost
Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
Upper Confidence Bound	?
Thompson Sampling	?
⋮	⋮

New design principle: Gittins Index

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
Expected improvement	Expected improvement per cost
Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
Upper Confidence Bound	?
Thompson Sampling	?
⋮	⋮

New design principle: Gittins Index

naturally cost-aware

Expected Improvement
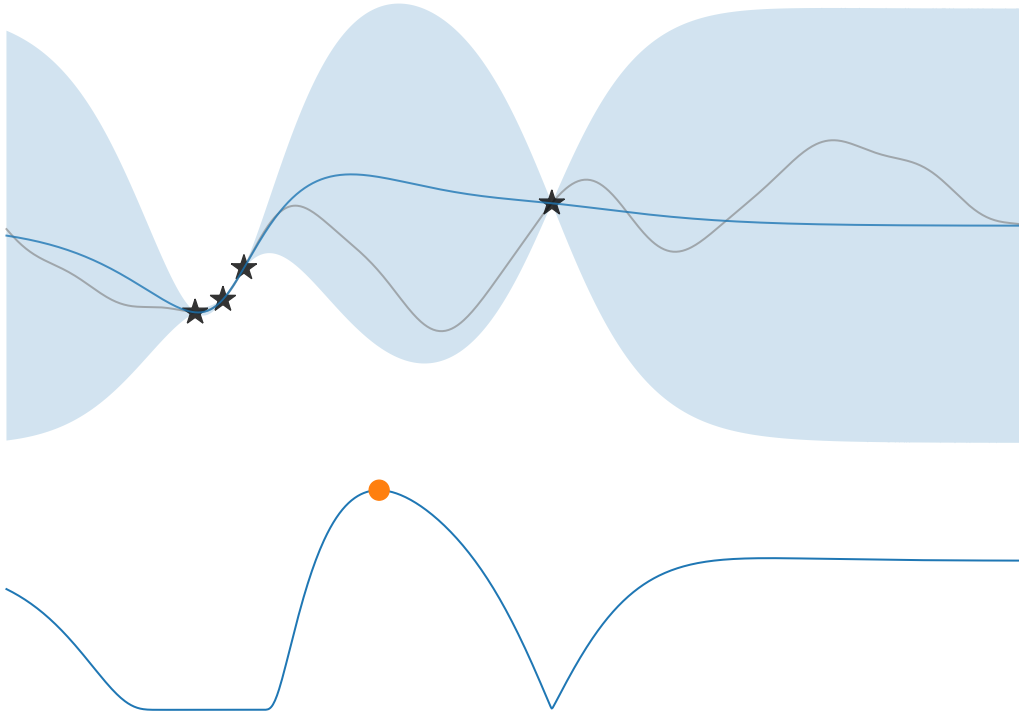
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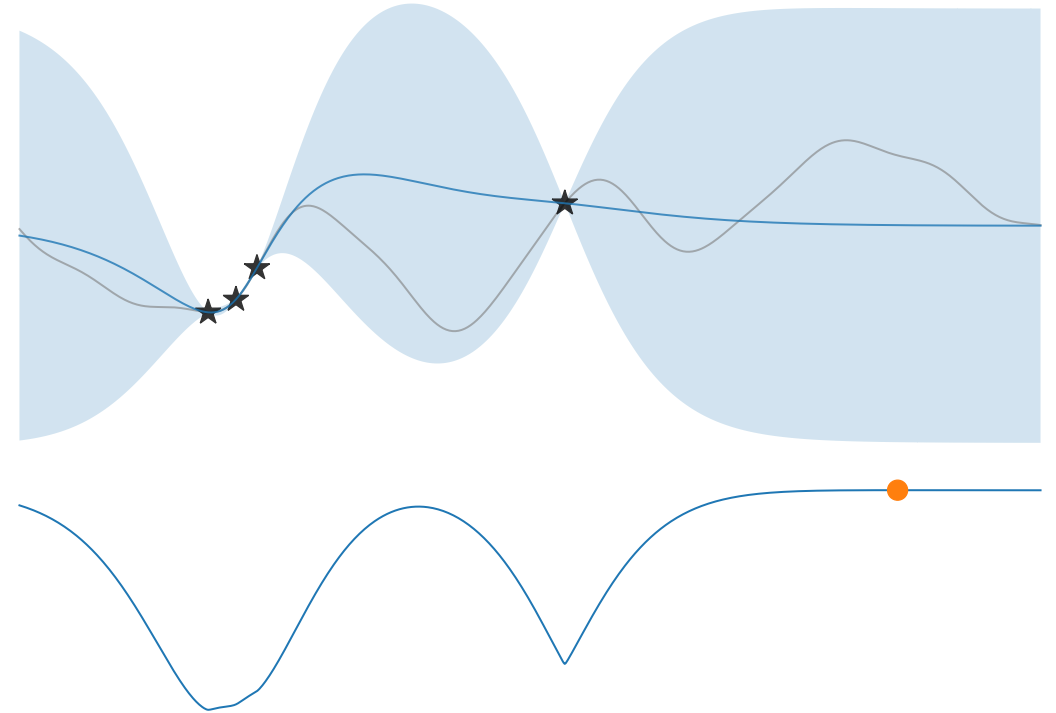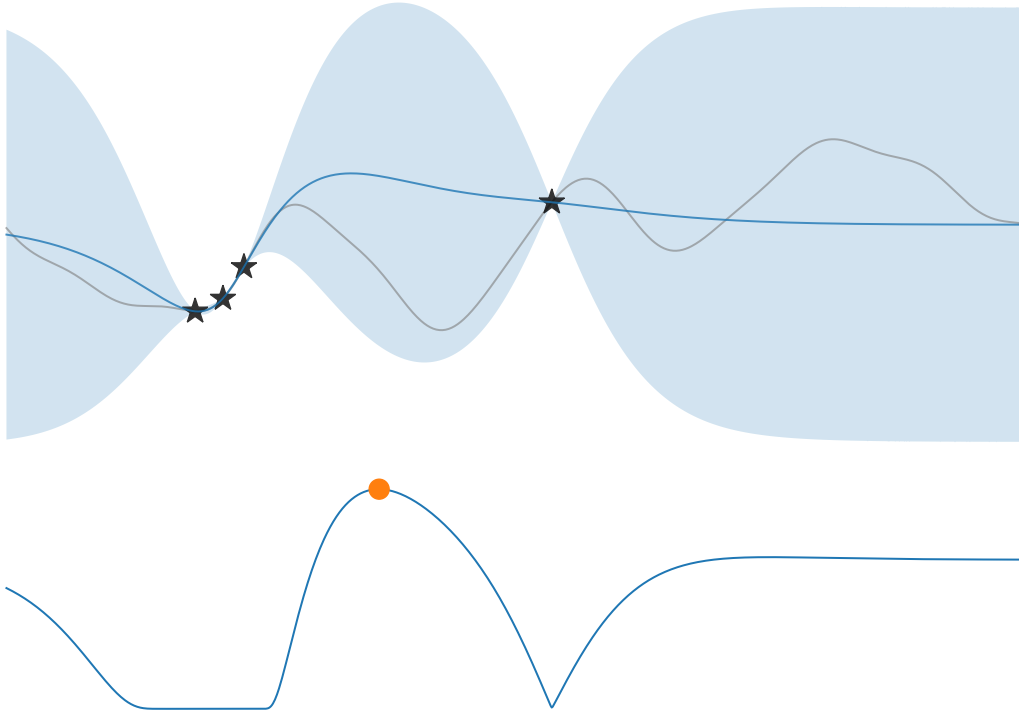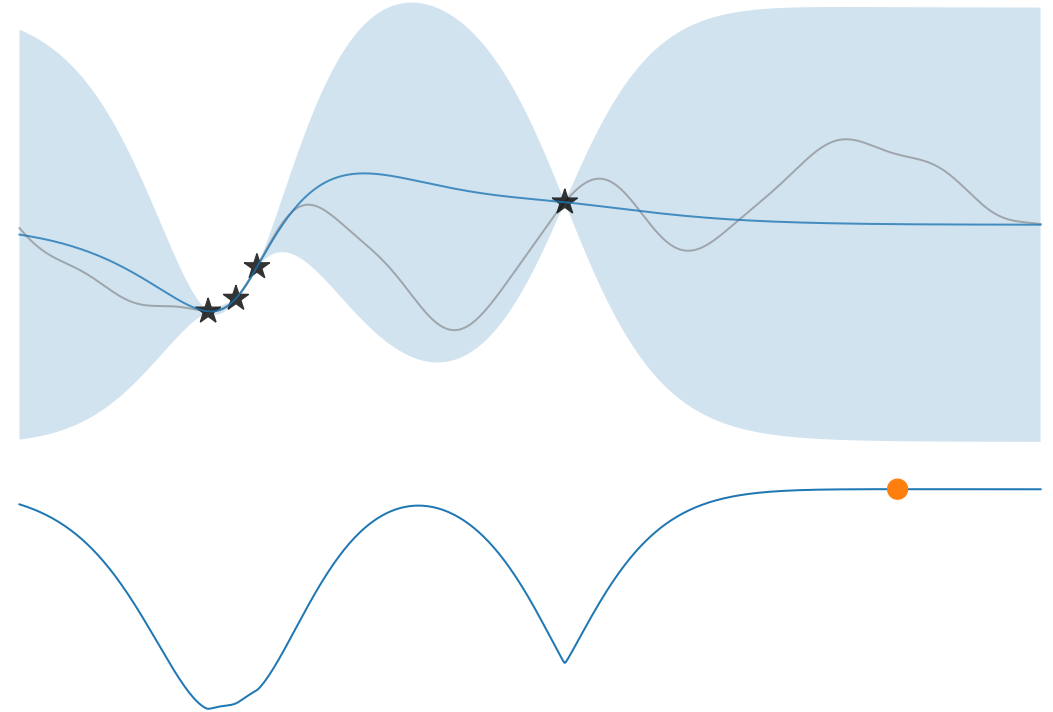
$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

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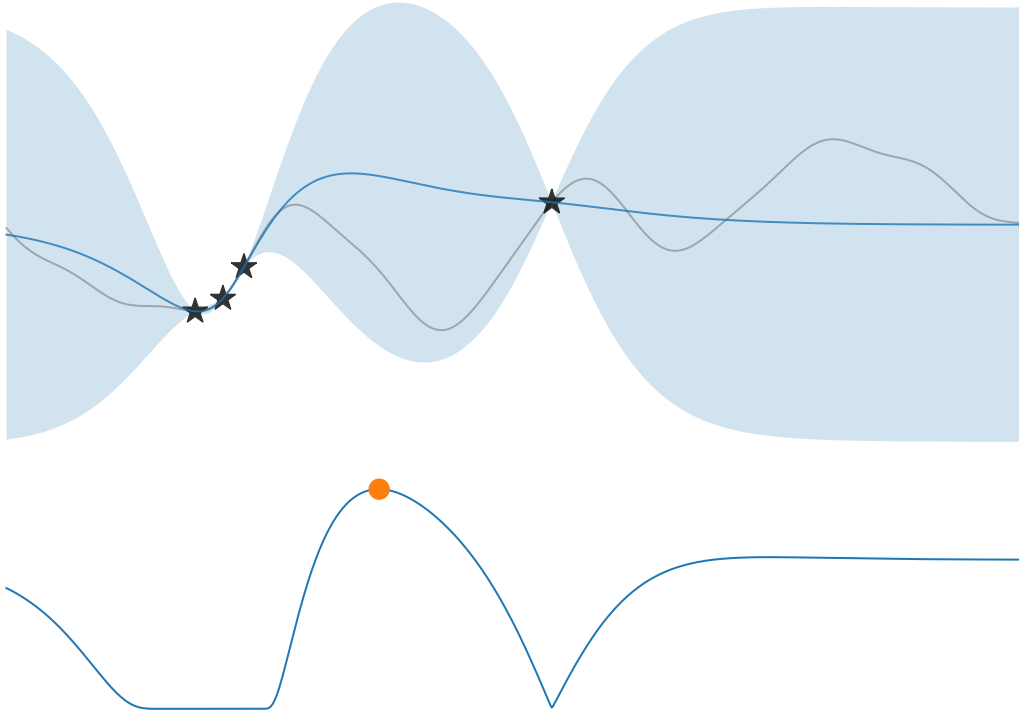
Gittins Index

$$\text{EI}(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

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$$\textcolor{red}{\text{GI}_{f|D}(x)} = g \text{ s.t. } \text{EI}_{f|D}(x; \textcolor{red}{g}) = c(x)$$
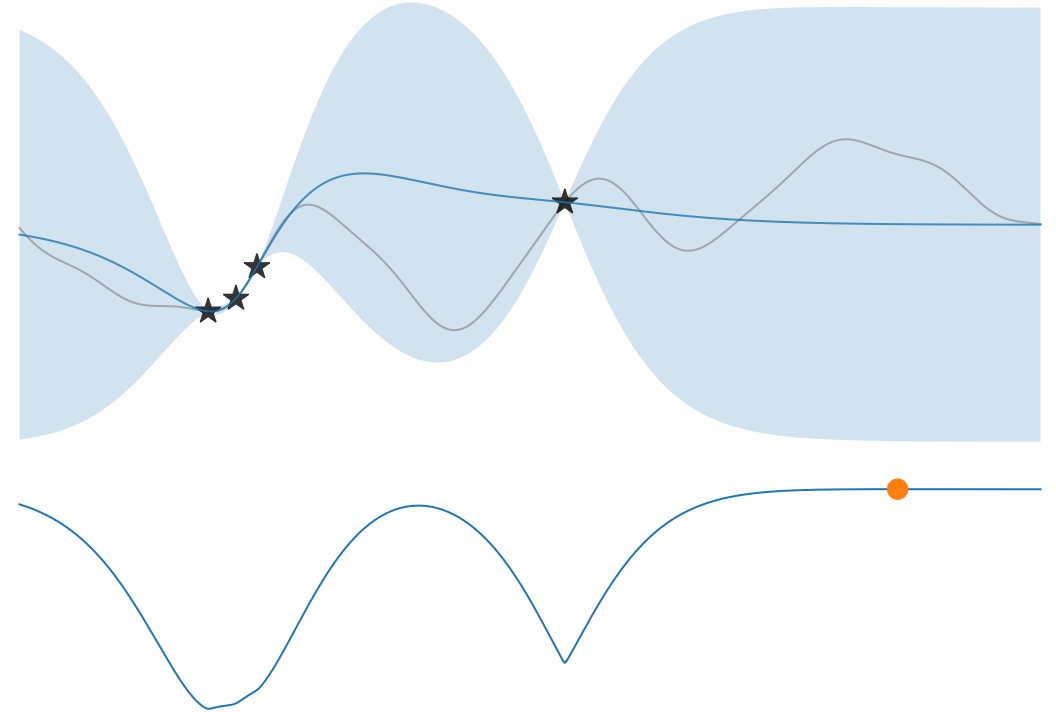
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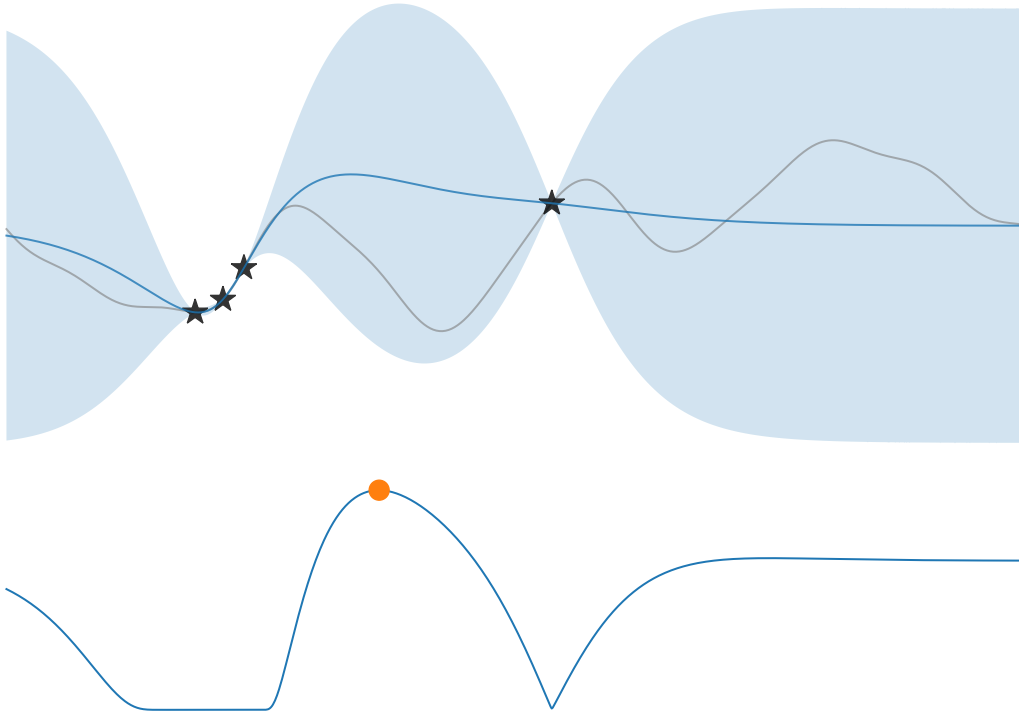
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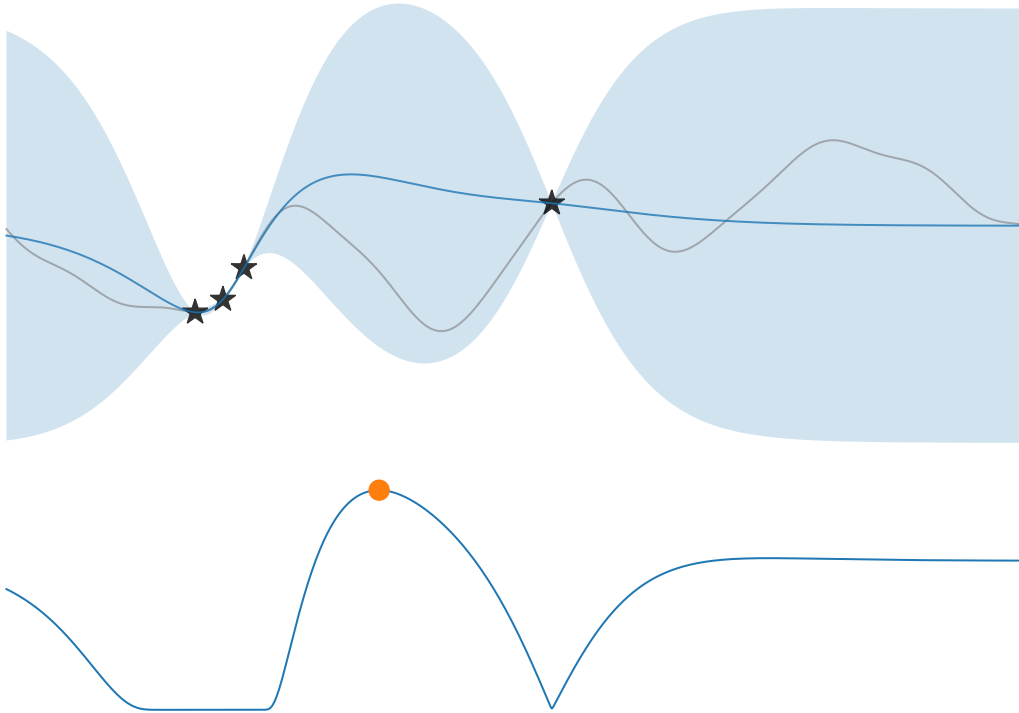$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

One-step approximation to MDP

Gittins Index

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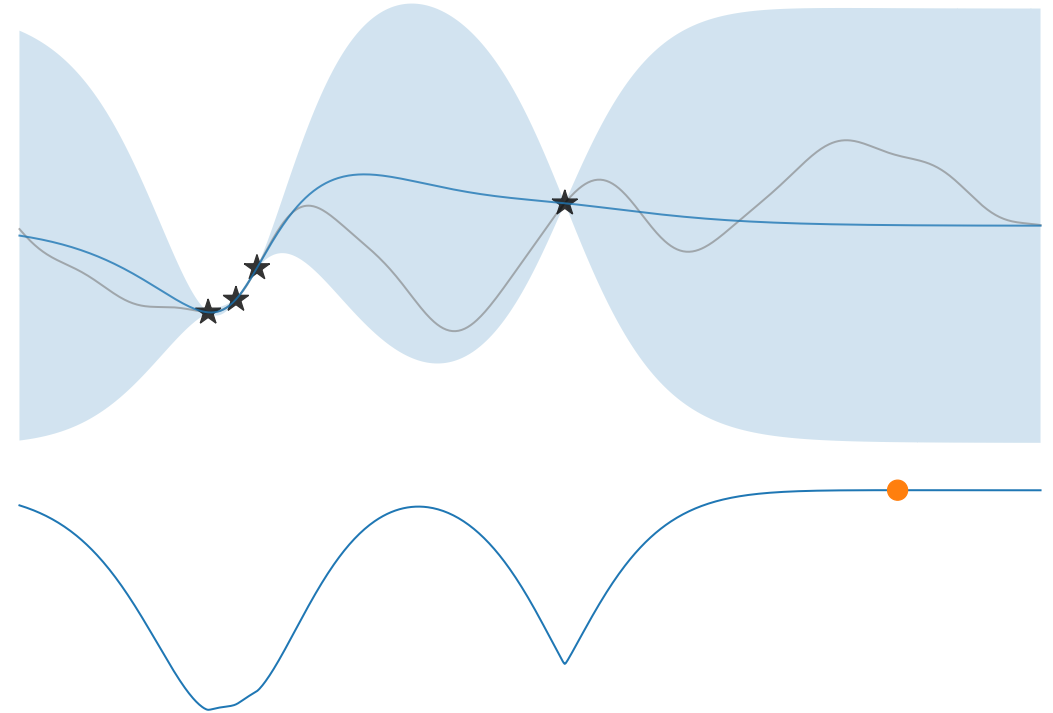
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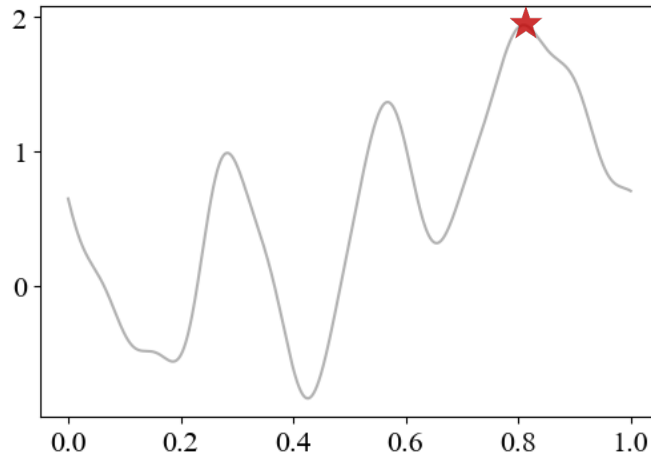
Temporal simplification to MDP

Gittins Index

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$$\max_x \mathrm{GI}_{f|D}(x)$$

Expected Improvement

$$\text{EI}(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

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Temporal simplification to MDP

Gittins Index

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$$\max_x \text{GI}_{f|D}(x)$$

Spatial simplification to MDP
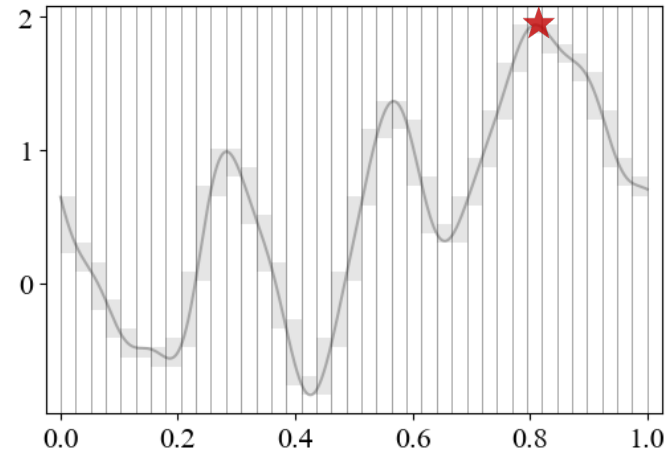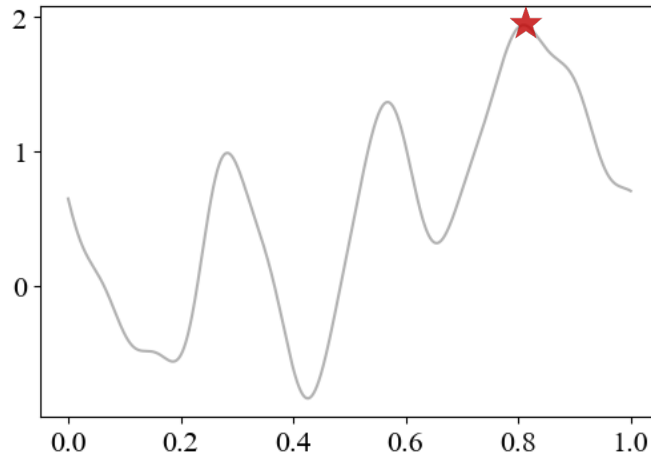
Our Approach: Spatial Simplification

Bayesian Optimization

Continuous

Correlated

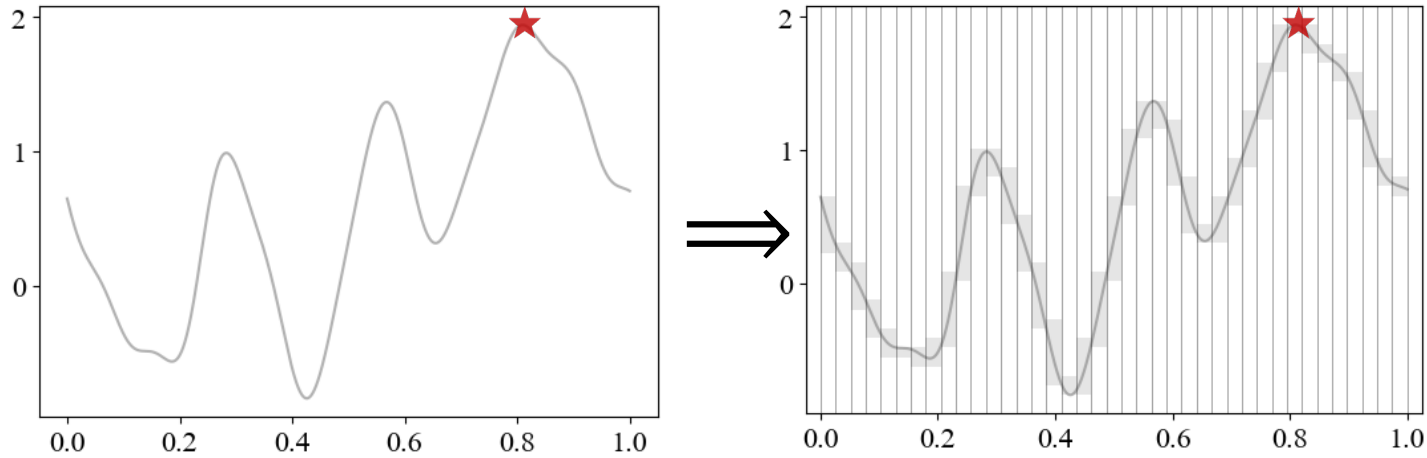# Our Approach: Spatial Simplification

Bayesian Optimization
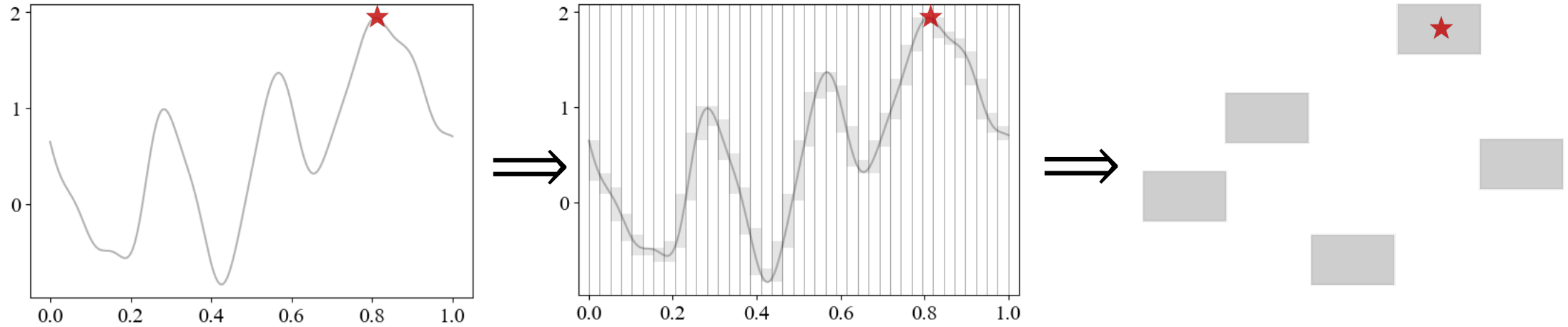
Continuous $\Longrightarrow$ Discrete

Correlated

Our Approach: Spatial Simplification
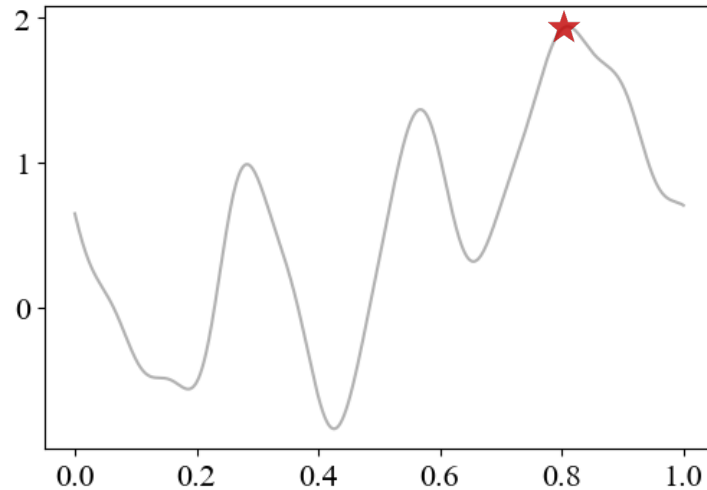

Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

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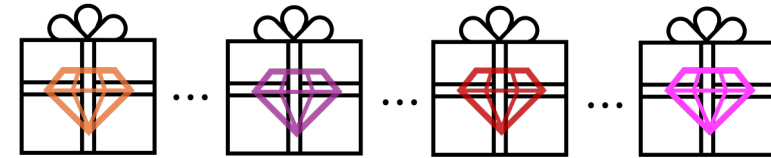
Continuous $\implies$ Discrete

Correlated $\implies$ Independent

Our Approach: Spatial Simplification

Bayesian Optimization

Pandora's Box [Weitzman'79]

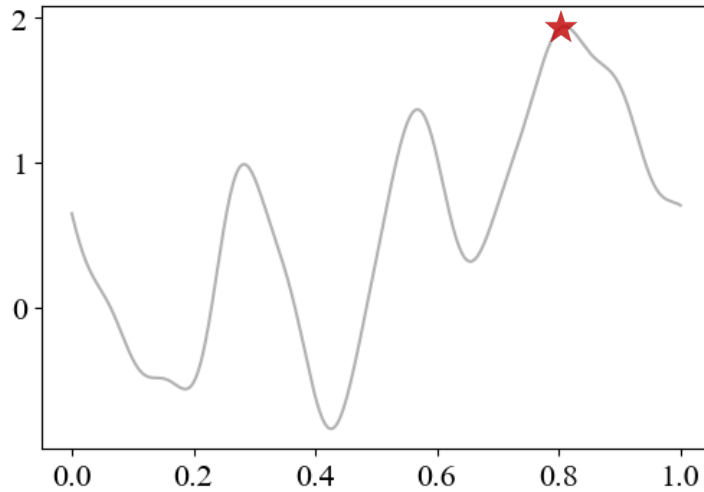Continuous $\implies$ Discrete

Correlated $\implies$ Independent

Our Approach: Spatial Simplification

Bayesian Optimization $\Rightarrow$ Pandora's Box [Weitzman'79]

Continuous $\Rightarrow$ Discrete

Correlated $\Rightarrow$ Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification

Bayesian Optimization

Pandora's Box

Continuous $\Rightarrow$ Discrete
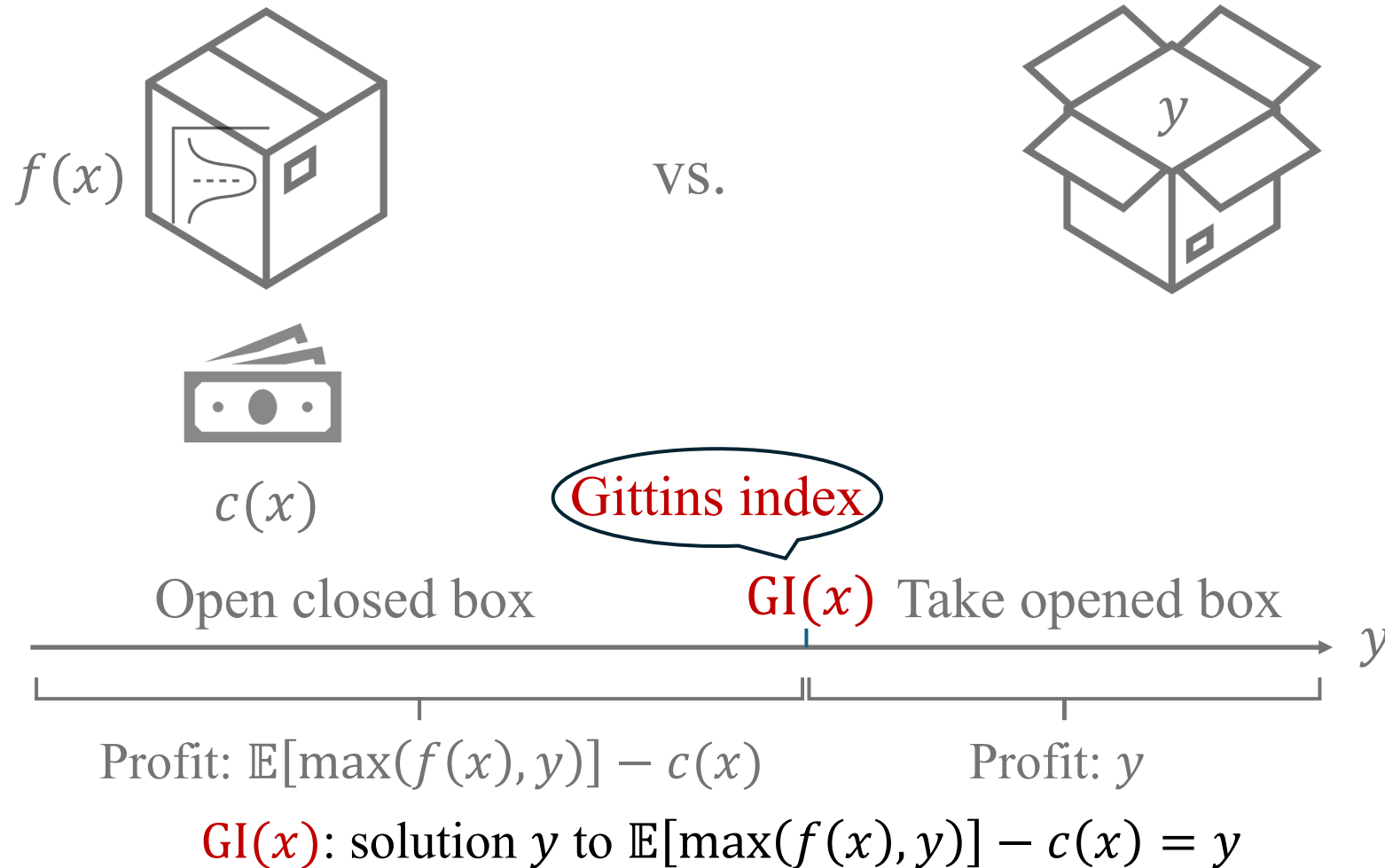
allow varying costs

Correlated $\Rightarrow$ Independent

Optimal policy: Gittins index

Intuition Behind Pandora's Box Gittins Index

1.5-box problem:

$f(x)$ vs. y

$c(x)$ Gittins index

Open closed box $\mathrm{GI}(x)$ Take opened box y

Profit: $\mathbb{E}[\max(f(x), y)] - c(x)$ Profit: y

$\mathrm{GI}(x)$: solution y to $\mathbb{E}[\max(f(x), y)] - c(x) = y$

How to translate Gittins index?
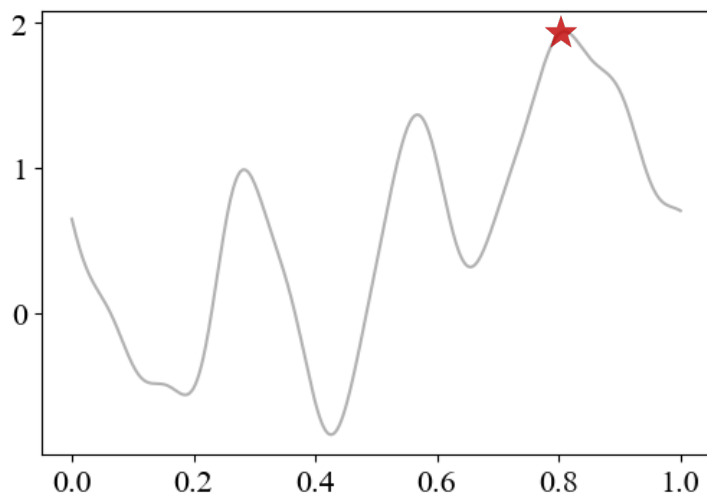
Bayesian Optimization $\Longrightarrow$ Pandora's Box
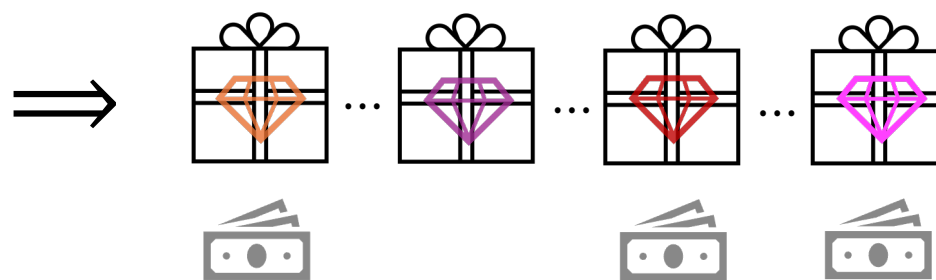
Continuous $\Longrightarrow$ Discrete

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How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

How to translate Gittins index?
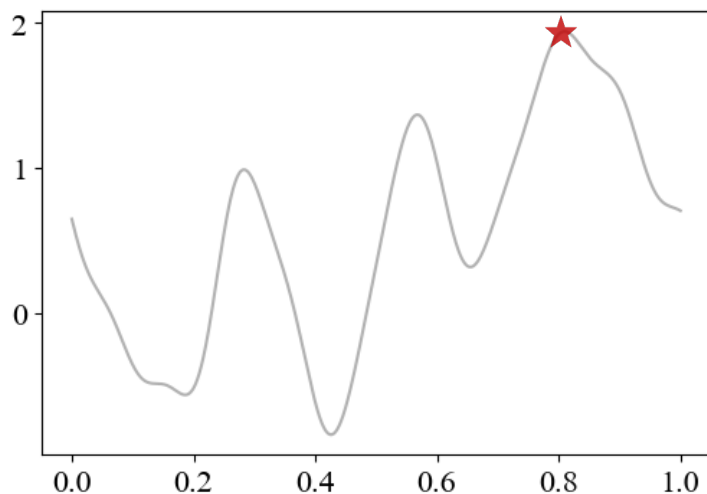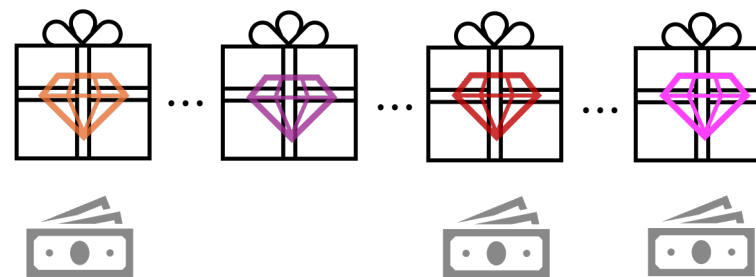
Bayesian Optimization $\implies$ Pandora's Box

Continuous	$\implies$	Discrete
Correlated	$\implies$	Independent

incorporate posterior

Our policy $\Longleftarrow$ Optimal policy: Gittins index
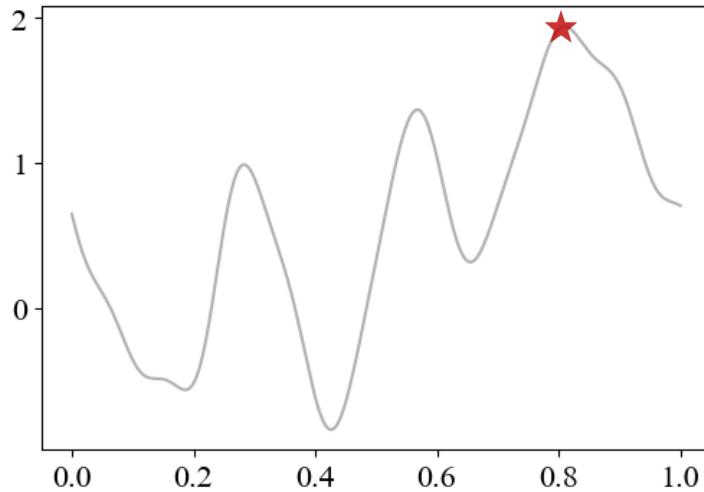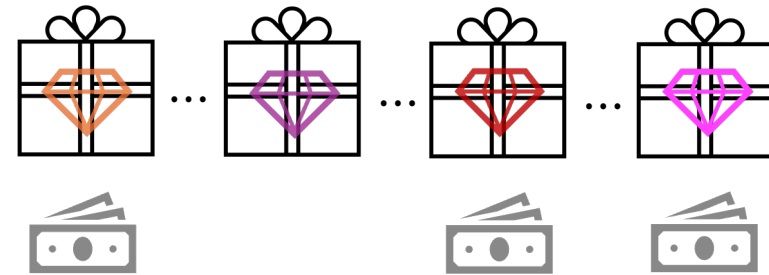
$\max_x \text{GI}_{f|D}(x)$ $\max_x \text{GI}(x)$

Is Gittins good in Bayesian Optimization?

Bayesian Optimization $\implies$ Pandora's Box [Weitzman'79]

Continuous	$\implies$	Discrete
Correlated	$\implies$	Independent
Is Gittins index good? $\max_x \text{GI}_{f\|D}(x)$	$\impliedby$	Gittins index is optimal $\max_x \text{GI}(x)$

Experiment Setup: Objective Functions

Synthetic

Samples from prior

Figure from *infpy*

Ackley function

Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT
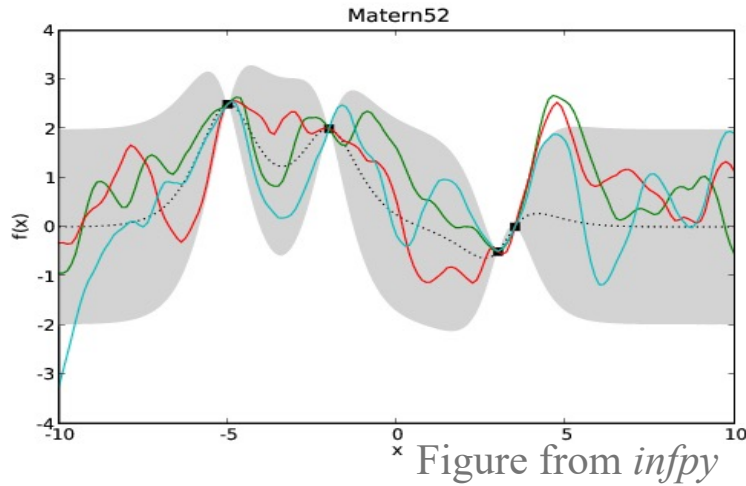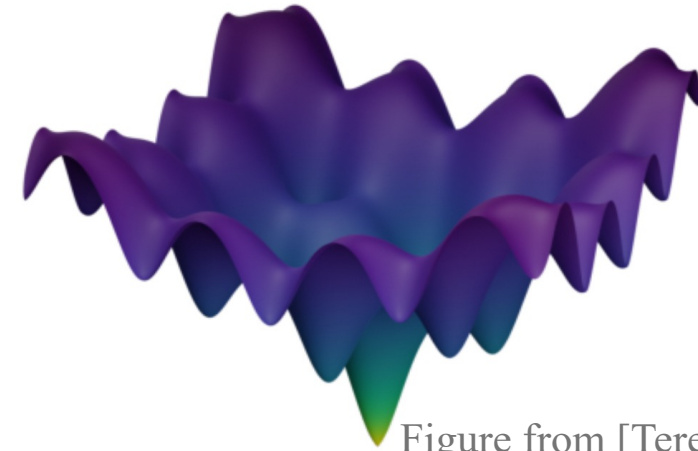
Lunar Lander
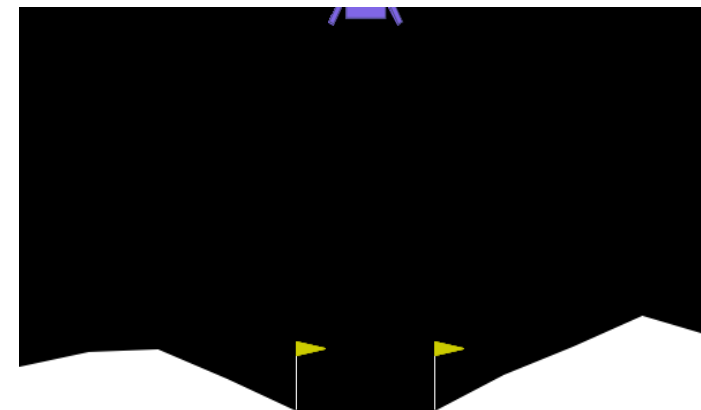
Figure from OpenAI Gym

Experiment Results

Synthetic

Empirical

(a) Samples from prior   **(b)** Ackley function   **(c)** Pest control   **(d)** Lunar lander

Uniform Costs

Varying Costs

Best Observed Value

Cumulative Cost

Legend:
- Pandora's Box Gittins Index (PBGI)
- Upper Confidence Bound (UCB)
- Expected Improvement (EI)
- EI Per Unit Cost (EIPC)
- Thompson Sampling
- Knowledge Gradient
- (Budgeted) Multi-Step EI
- (Multi-fidelity) Max-value Entropy Search
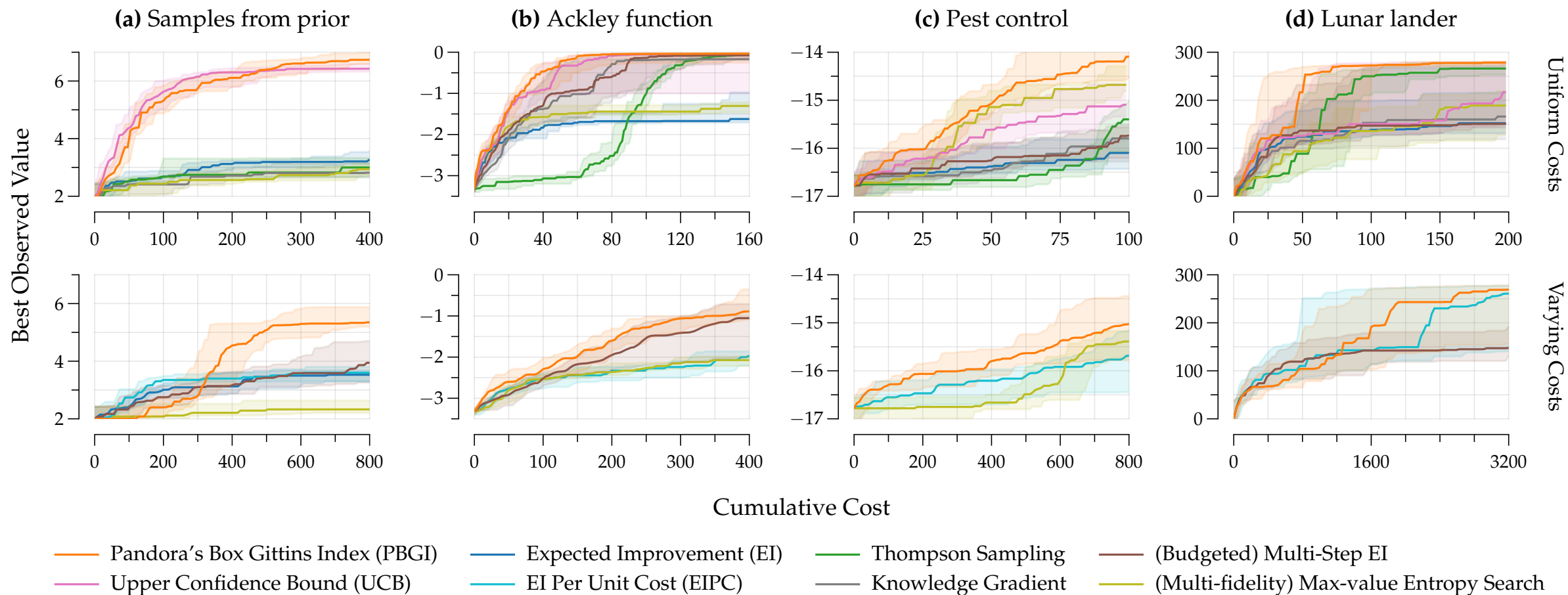
FAQ

- Easy-to-compute?

FAQ

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    Yes, EI + bisection

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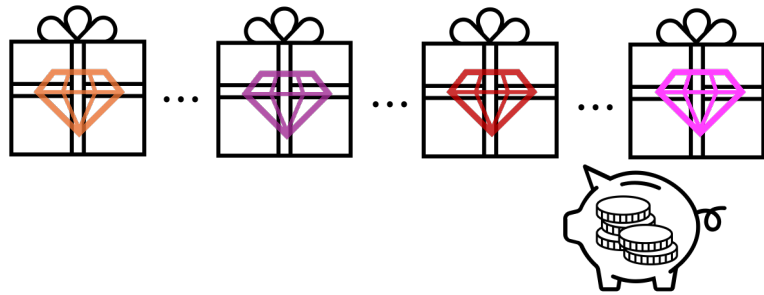
- Any theoretical results?

FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample

Theoretical Result
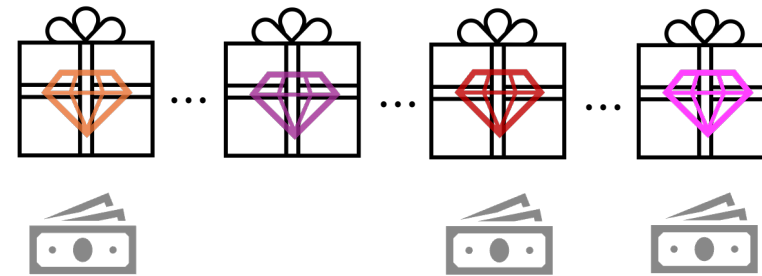

max best observed under budget

Budgeted Pandora's Box

Expected budget constraint

Optimal policy?
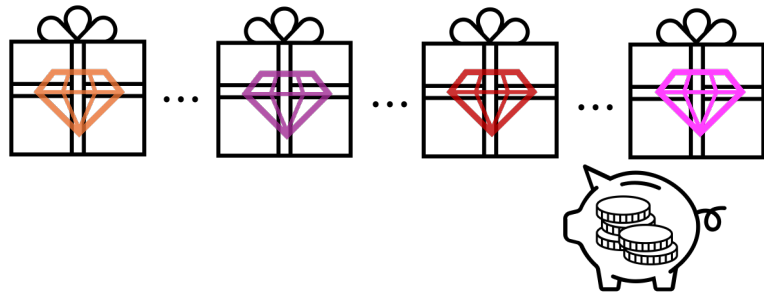
max (best observed – costs)

Pandora's Box

Cost per sample

Optimal policy: Gittins index

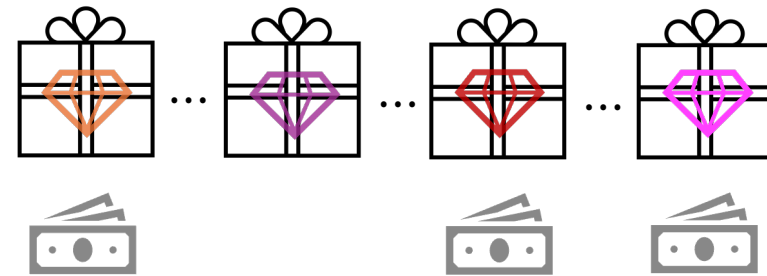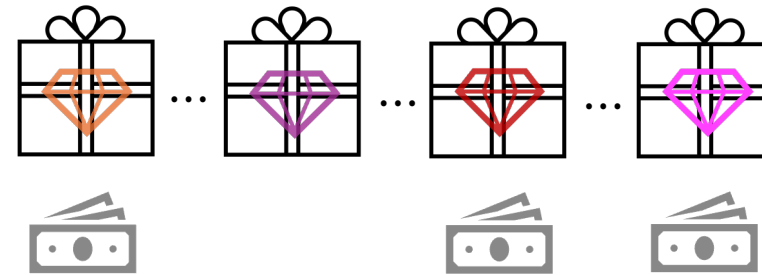# Theoretical Result

max best observed under budget   **max** (best observed – scaled costs)

Budgeted Pandora's Box   Pandora's Box

Expected budget constraint   Cost per sample

Optimal policy ✓   Optimal policy: Gittins index

extension to [Aminian, Manshadi, Niazadeh'24]

Theoretical Result

budget-dependent

max best observed under budget

max (best observed – scaled costs)

Budgeted Pandora's Box

Pandora's Box

Expected budget constraint

Cost per sample

Optimal policy ✓

Optimal policy: Gittins index

extension to [Aminian, Manshadi, Niazadeh'24]

FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample

- **Tuning parameters?**

FAQ

- Easy-to-compute?

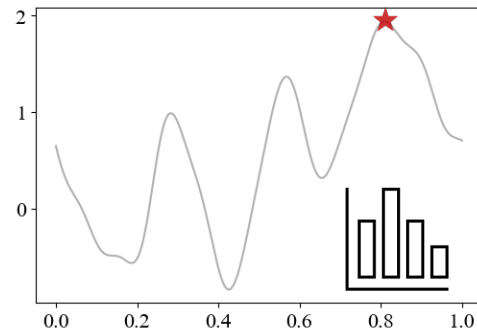   Yes, EI + bisection

- Any theoretical results?

    Yes, expected-budget-constrained $\cong$ cost-per-sample
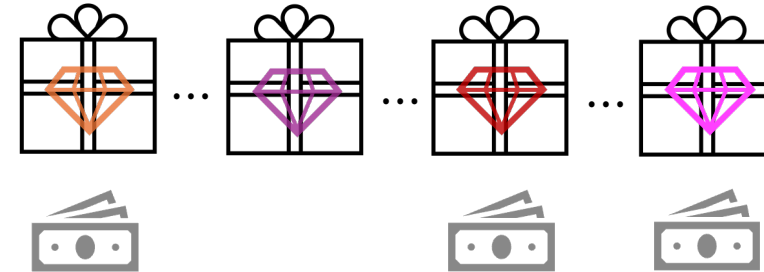
- **Tuning parameters?**

    Yes, control unit conversion
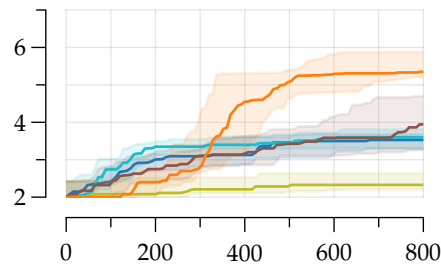
New Design Principle: Gittins Index

Problem

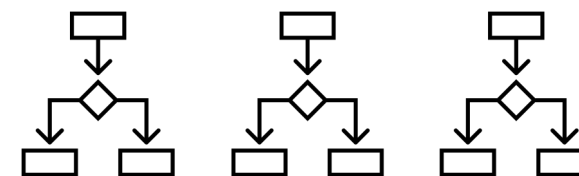Bayesian optimization
with varying costs

Impact

competitive performance

Key idea

link to Pandora's box
and Gittins index theory

Future potential

black-box processes
with partial feedback

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