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
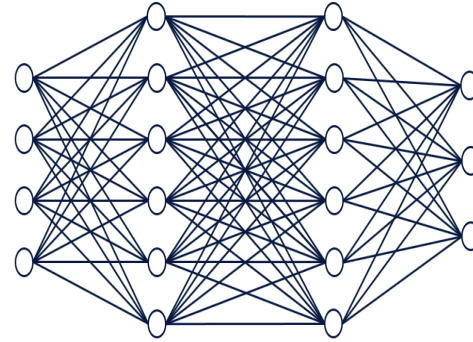

Raul Astudillo

Peter Frazier

Ziv Scully

Alexander Terenin

World of Parameter Optimization
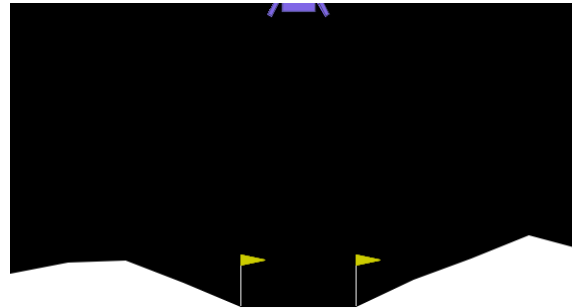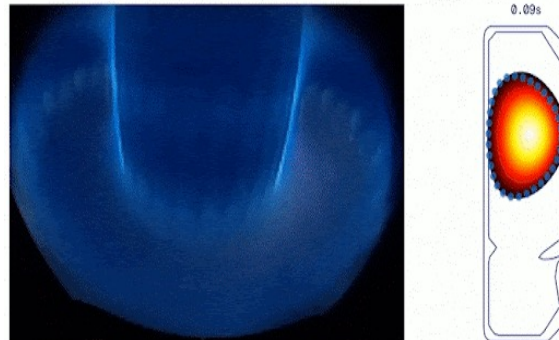
Hyperparameter tuning:

Training parameters $\longrightarrow$ $\longrightarrow$ Accuracy

Control optimization:

Control parameters $\longrightarrow$ $\longrightarrow$ Reward

Plasma physics:

Reactor parameters $\longrightarrow$ $\longrightarrow$ Stability

World of Parameter Optimization
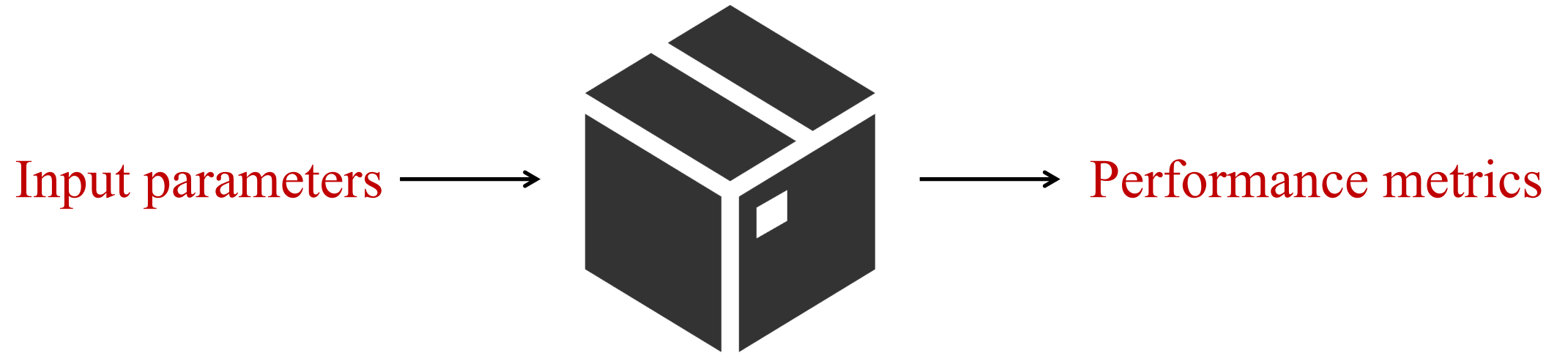
Black-box optimization:

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

World of Parameter Optimization

Black-box optimization:

x $\longrightarrow$ $f(x)$

Optimizing Black-box Functions

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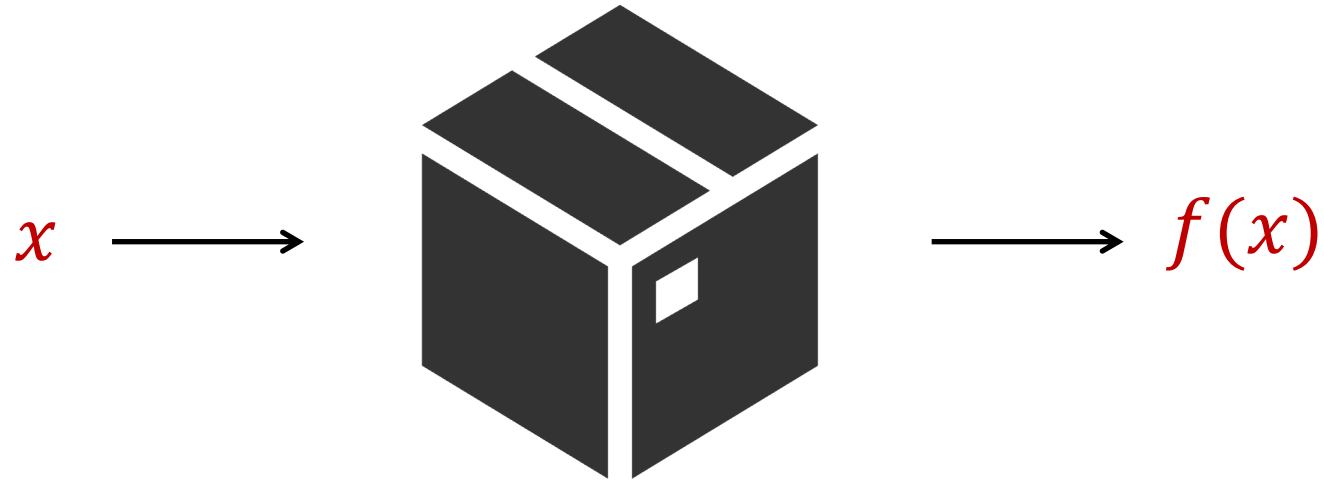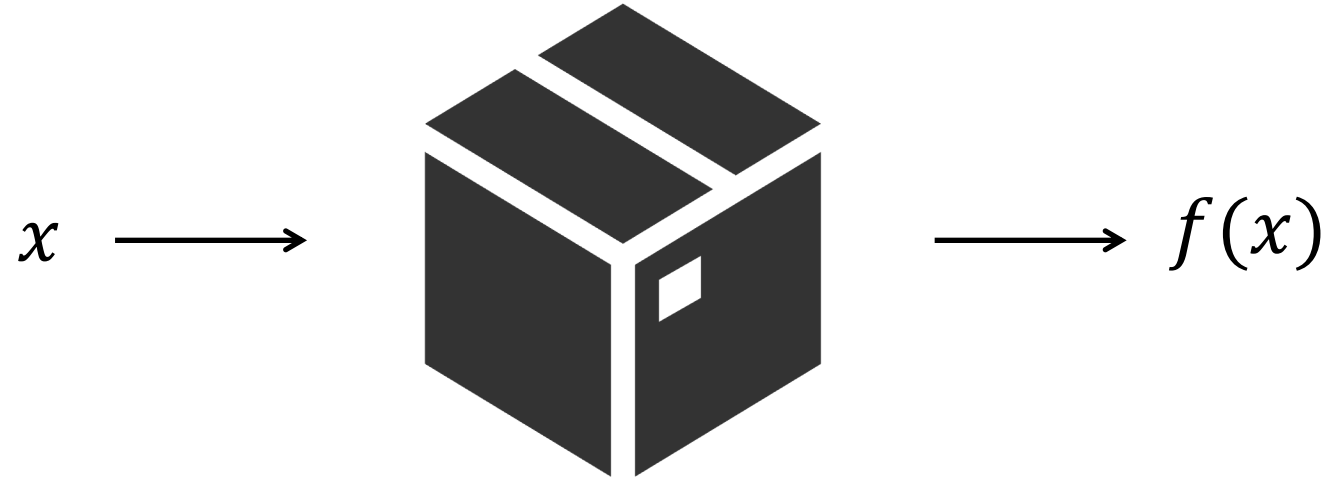
Goal: $\mathbf{max}_{x \in \mathcal{X}} \, f(x)$

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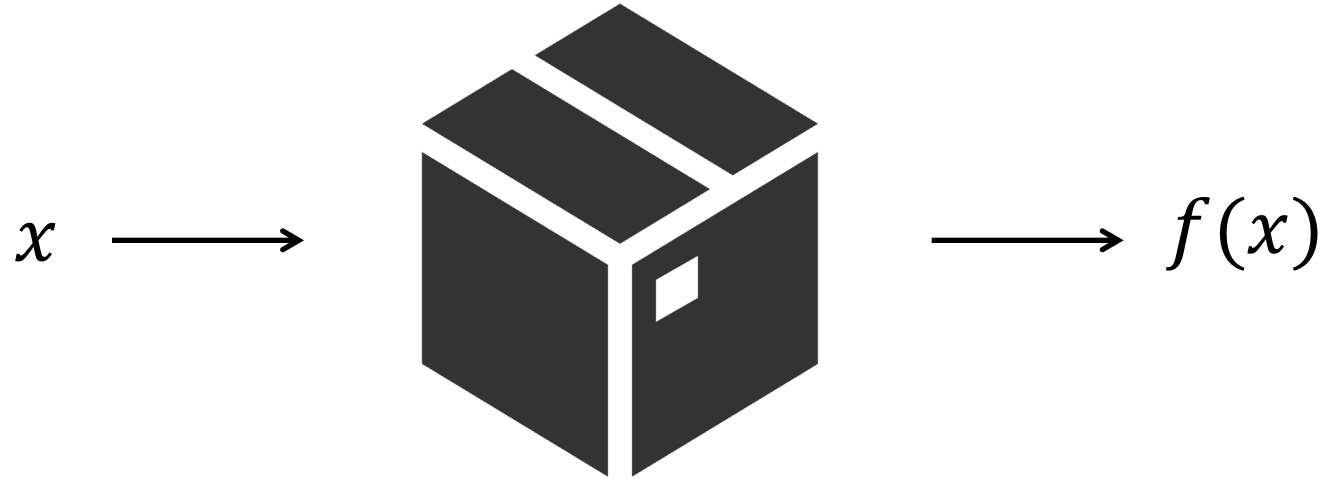
$x \longrightarrow$ [black box] $\longrightarrow f(x)$

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

$f \sim$ Stochastic Process

Optimizing Black-box Functions

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

expensive-to-evaluate

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

Optimizing Black-box Functions

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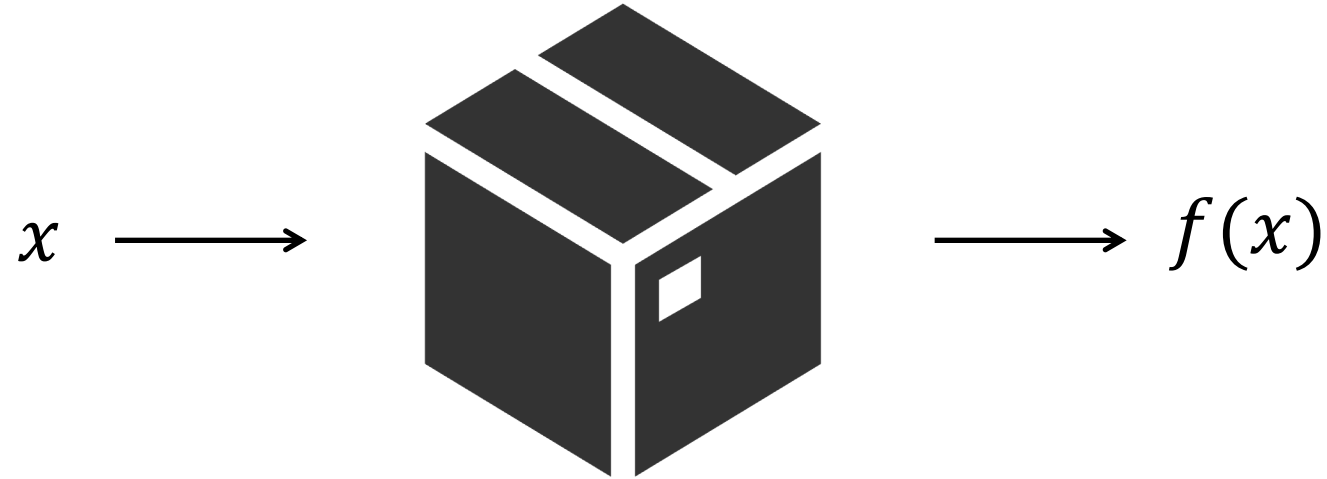
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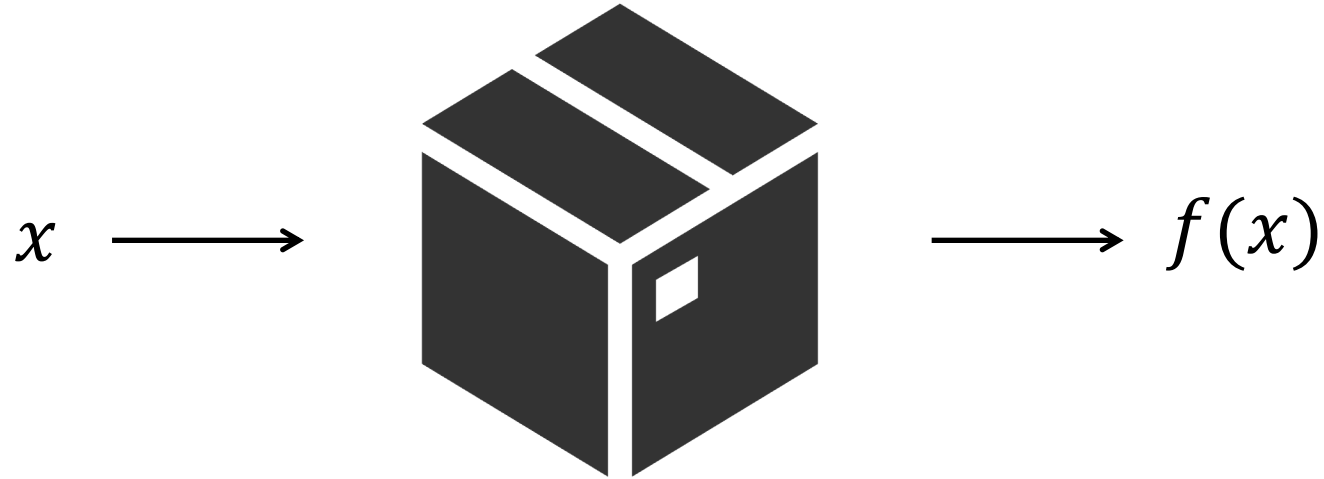
$$x \longrightarrow \boxed{} \longrightarrow f(x)$$

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

$f \sim$ Gaussian Process

Bayesian Optimization

$$x \longrightarrow \qquad \longrightarrow f(x)$$

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

$f \sim$ Gaussian Process

Bayesian Optimization

Legend:
- Objective Function
- Mean
- Confidence

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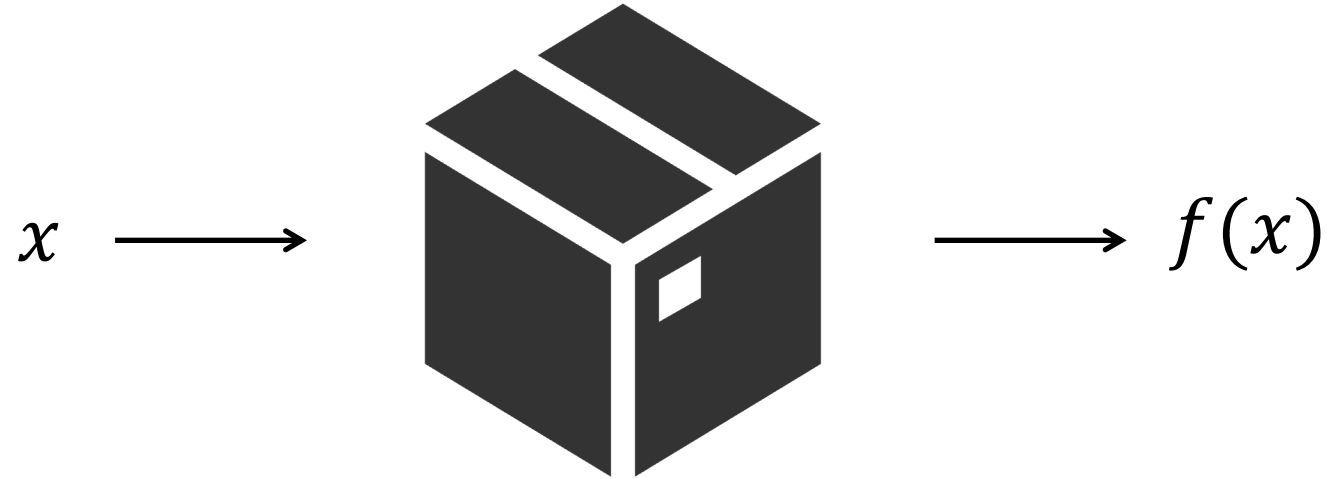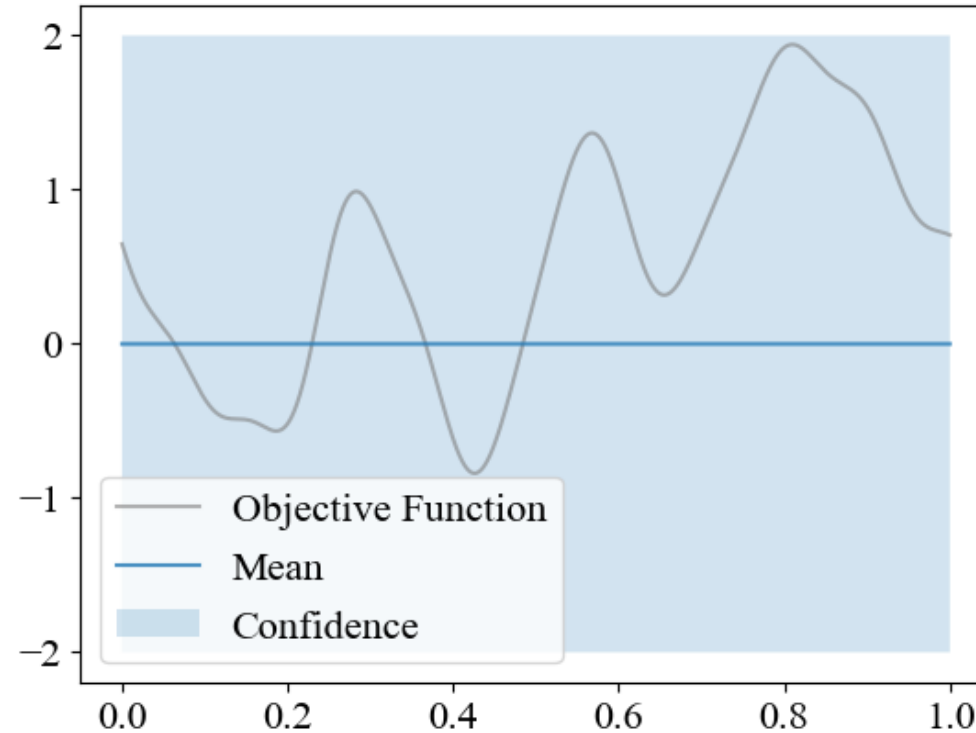
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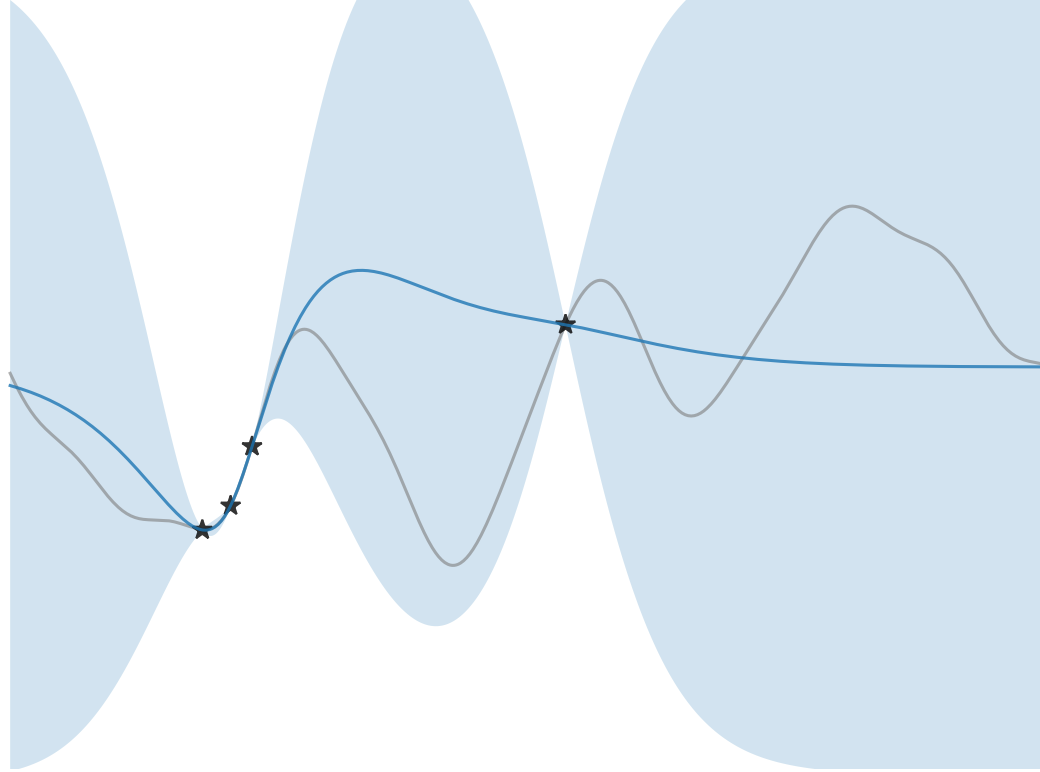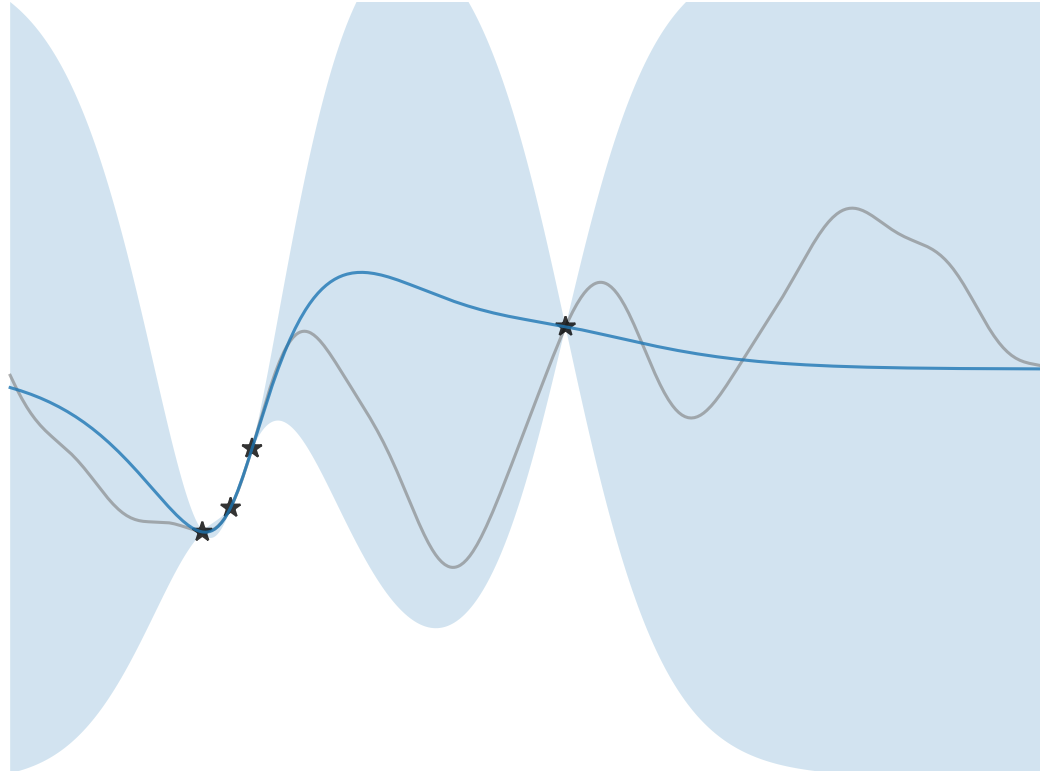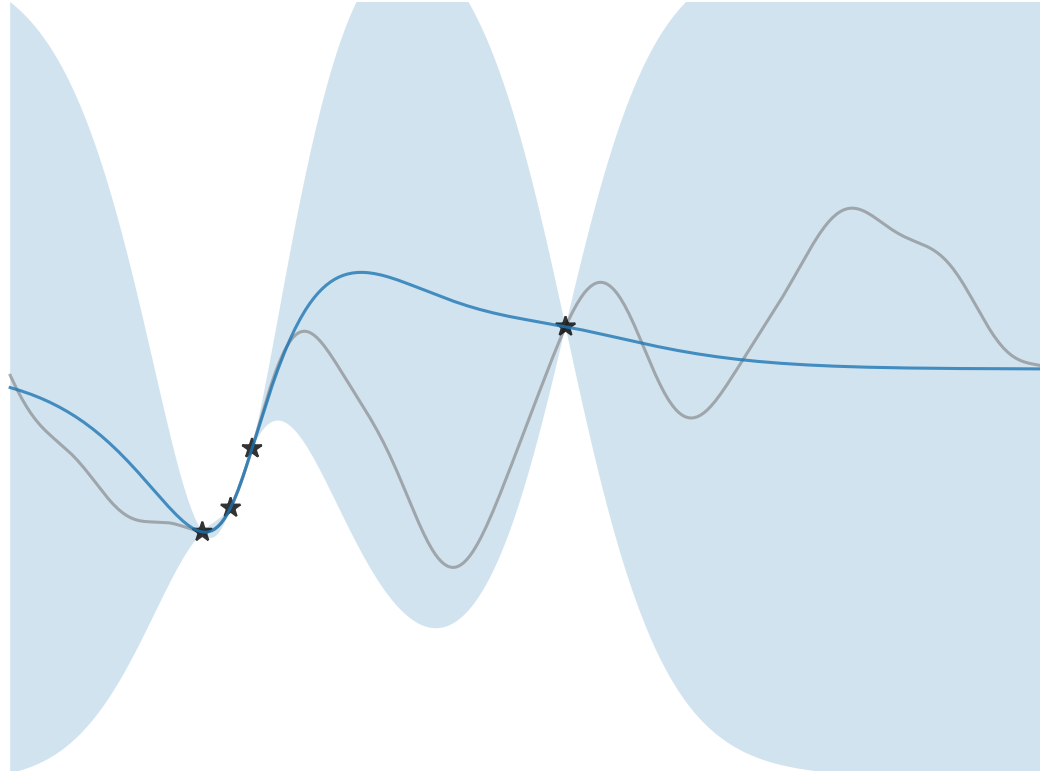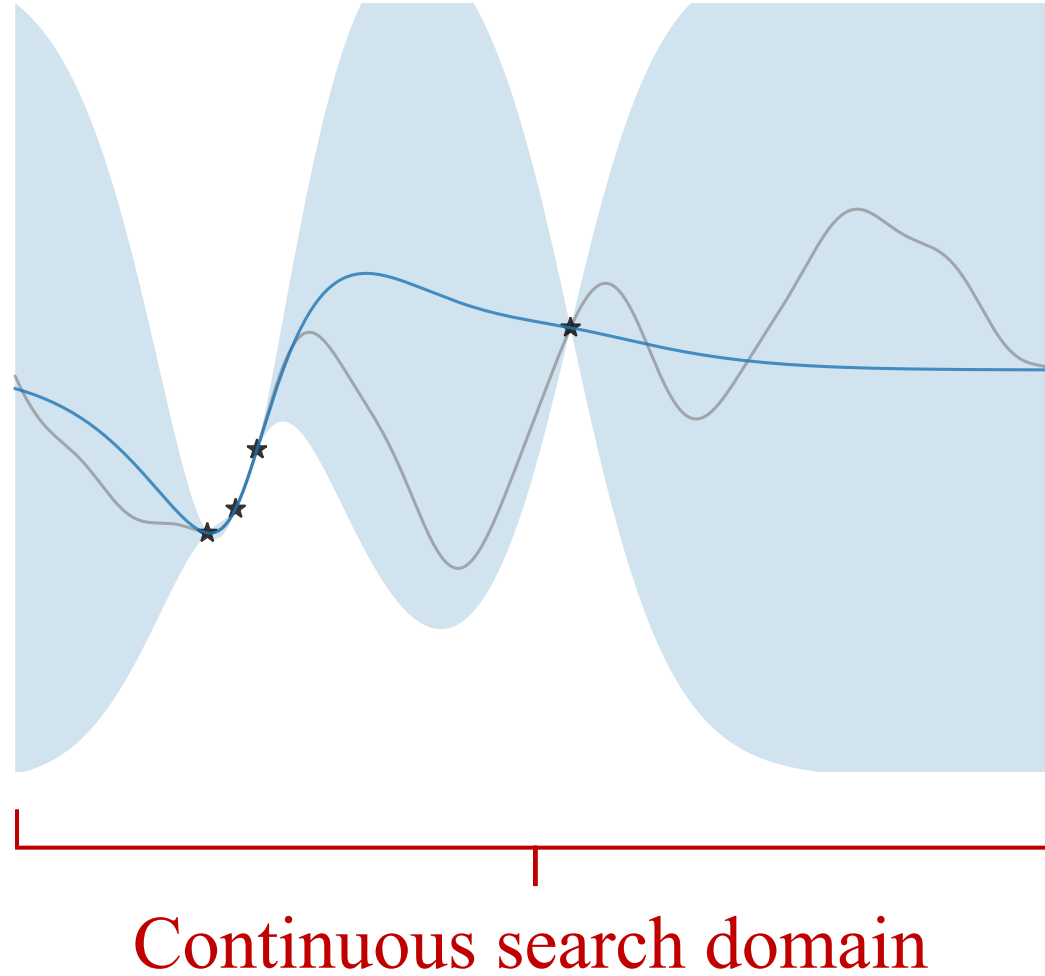
Bayesian Optimization

What to evaluate next?

Bayesian Optimization

Optimal policy?

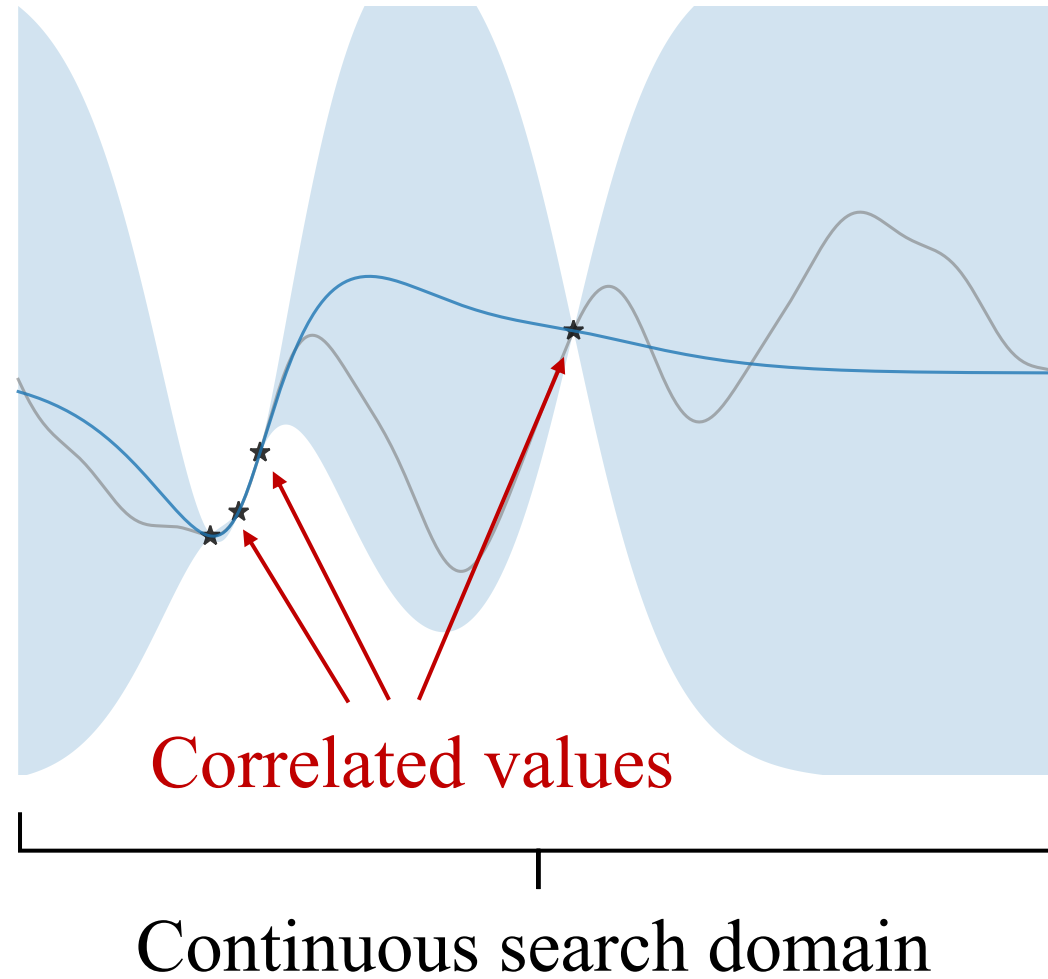# Challenges of Bayesian Optimization

Continuous search domain

Challenges of Bayesian Optimization

Correlated values

Continuous search domain
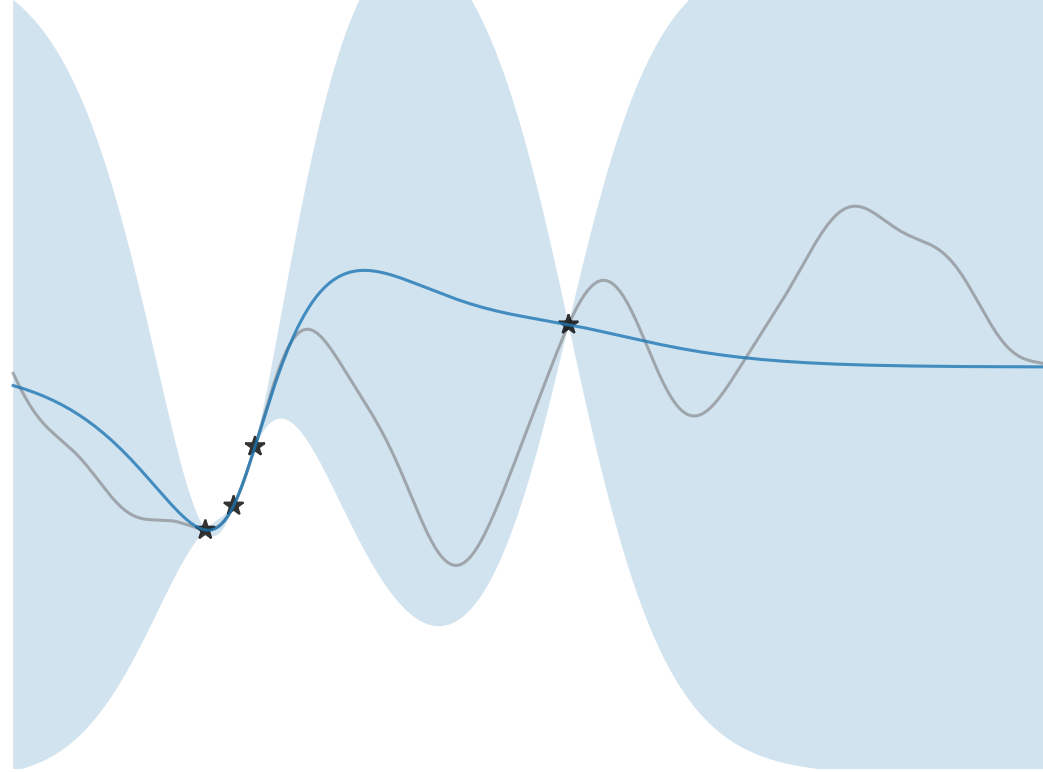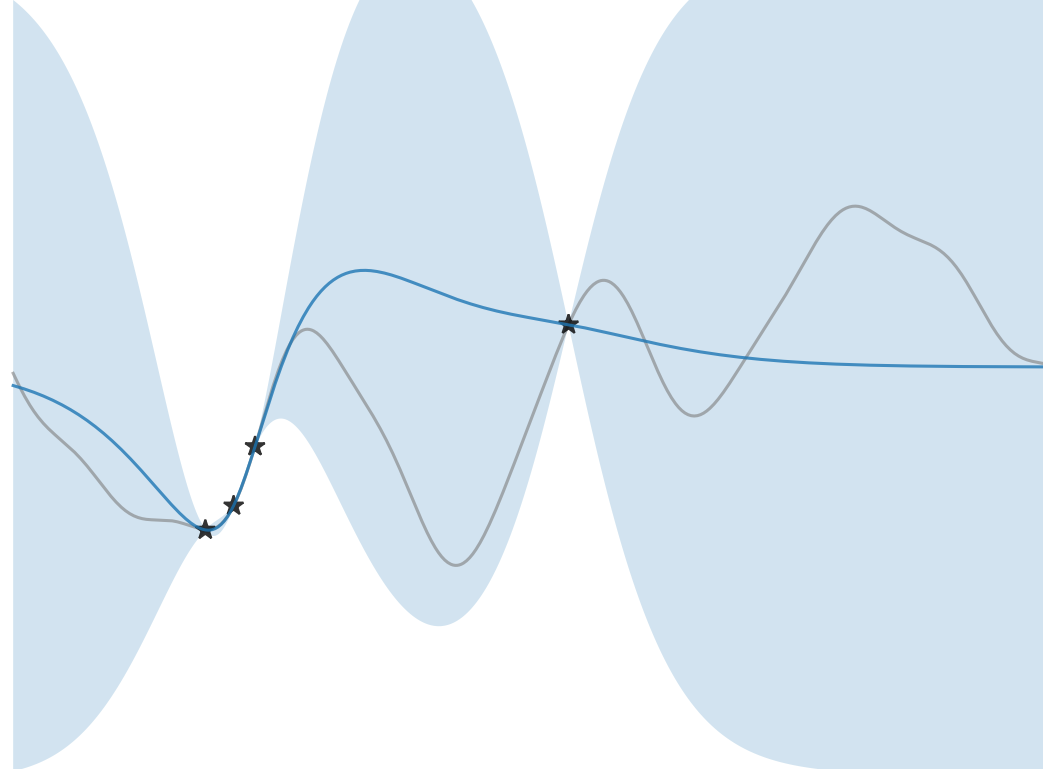
Challenges of Bayesian Optimization

Correlation & continuity $\Longrightarrow$ Intractable MDP

Challenges of Bayesian Optimization

Intractable MDP $\implies$ Optimal policy unknown

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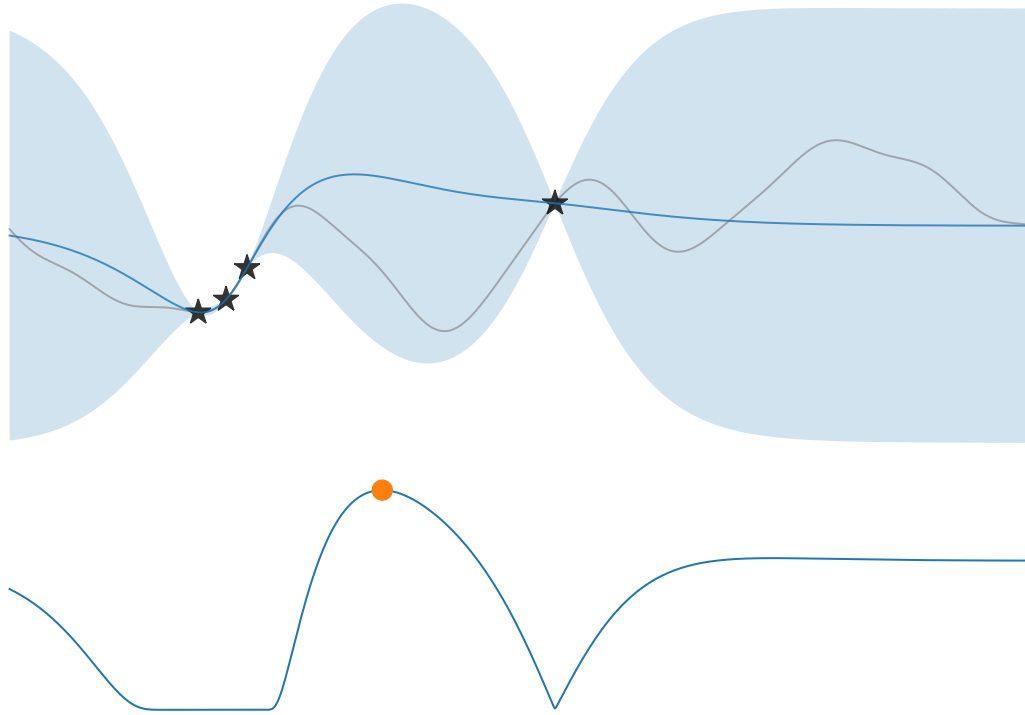
$$\text{EI}(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

current best observed

data

"improvement"

Popular Policy: Expected Improvement

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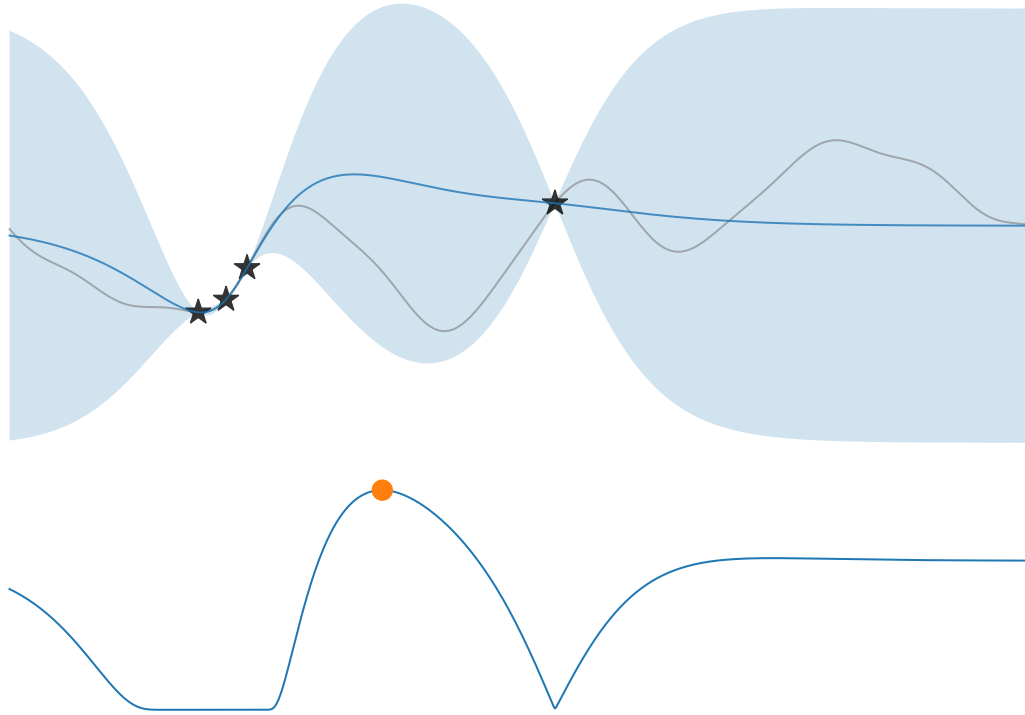
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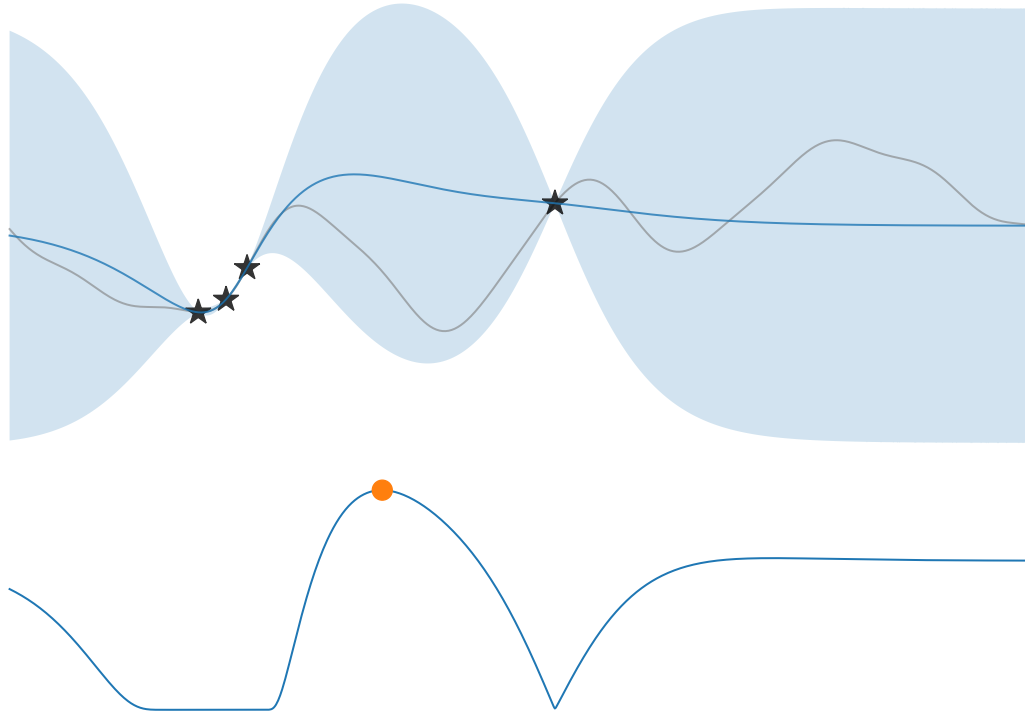
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One-step approximation to MDP

Popular Policy: Expected Improvement
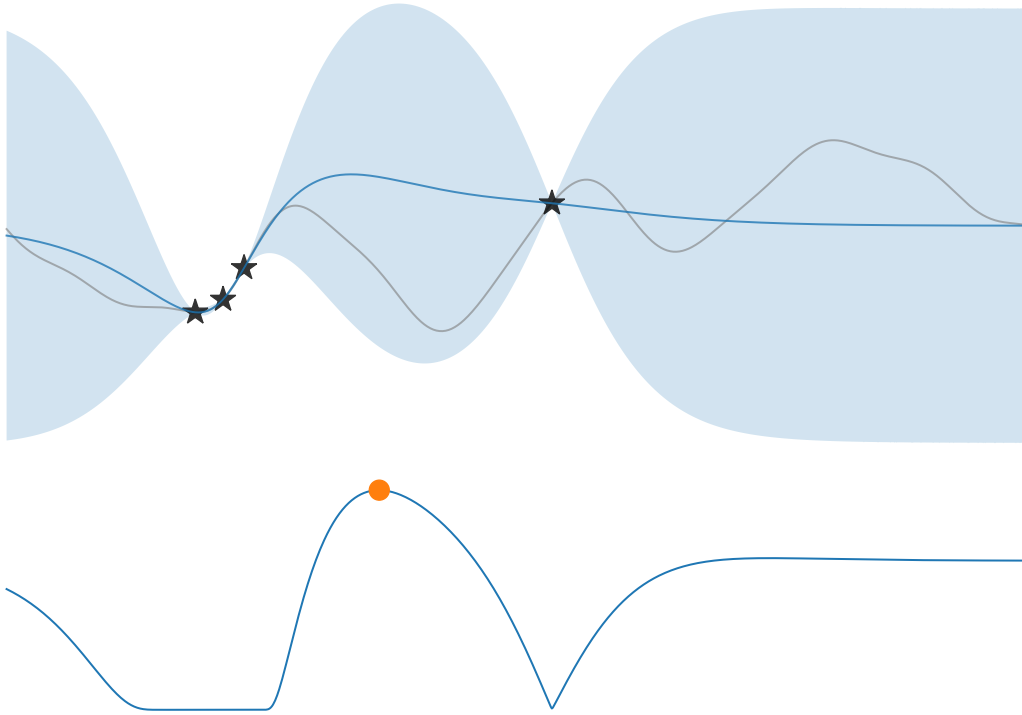
Other improvement-based policy:
- Probability of Improvement
- Knowledge Gradient
- Multi-step Lookahead EI
- …

Approaches to Bayesian Optimization

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

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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

- Improvement-based

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- Our work: Gittins Index
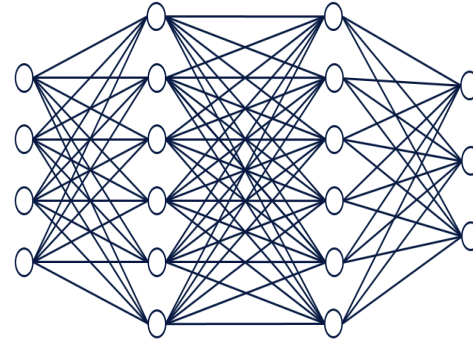
Approaches to Bayesian Optimization

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- Our work: Gittins Index

Why another approach?

Challenge: Varying Evaluation Costs
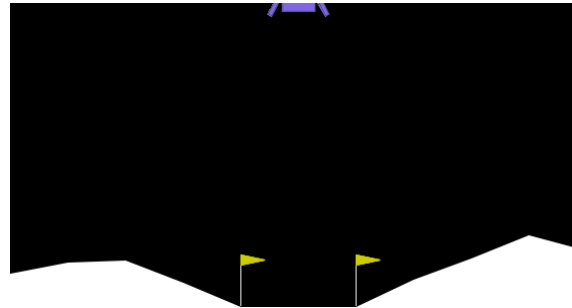
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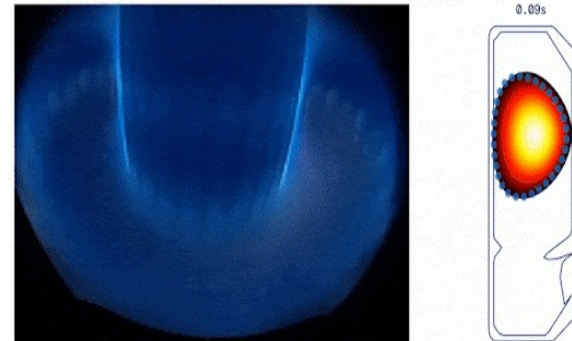
Control optimization:

Control parameters $\longrightarrow$ $\longrightarrow$ Reward

Plasma physics:

Reactor parameters $\longrightarrow$ $\longrightarrow$ Stability

Challenge: Varying Evaluation Costs

Black-box optimization:
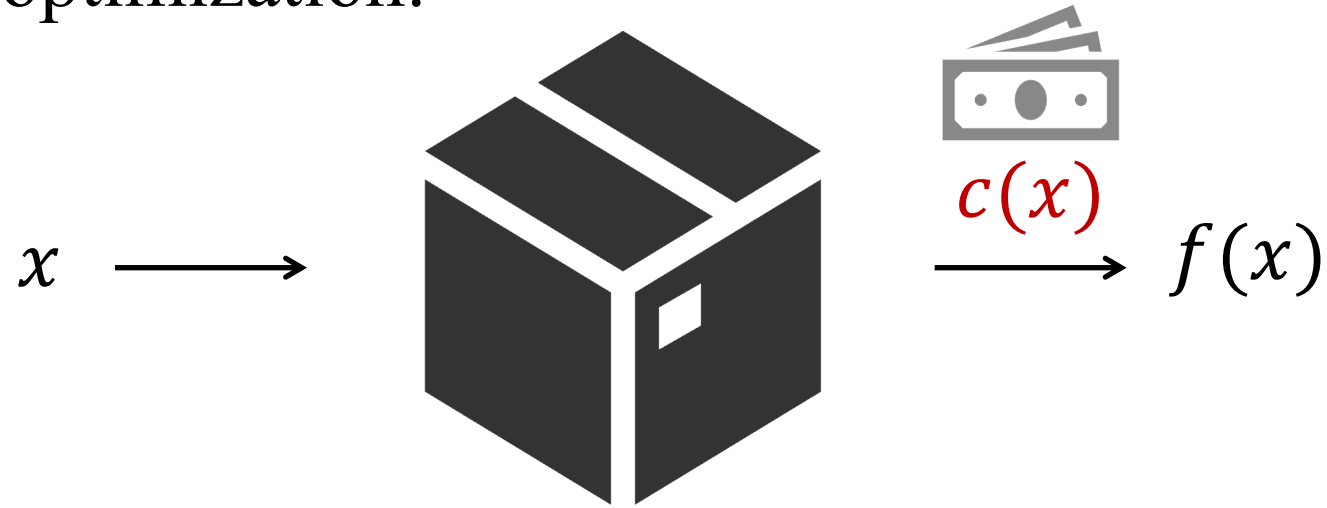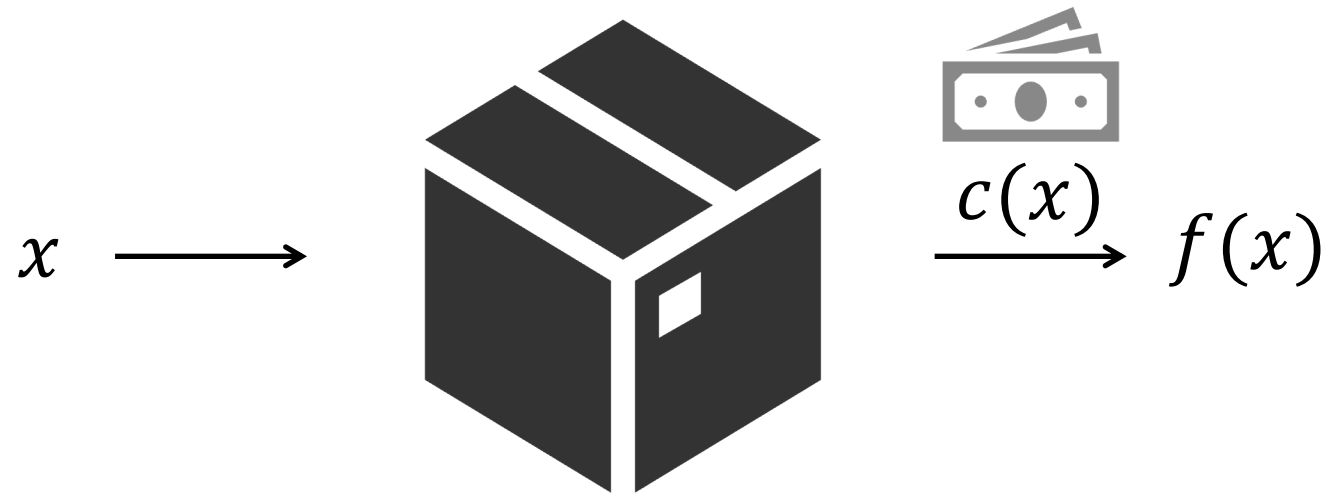
x ⟶ $\xrightarrow{\quad c(x) \quad}$ $f(x)$

Challenge: Varying Evaluation Costs

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

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

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

Cost-aware Bayesian Optimization

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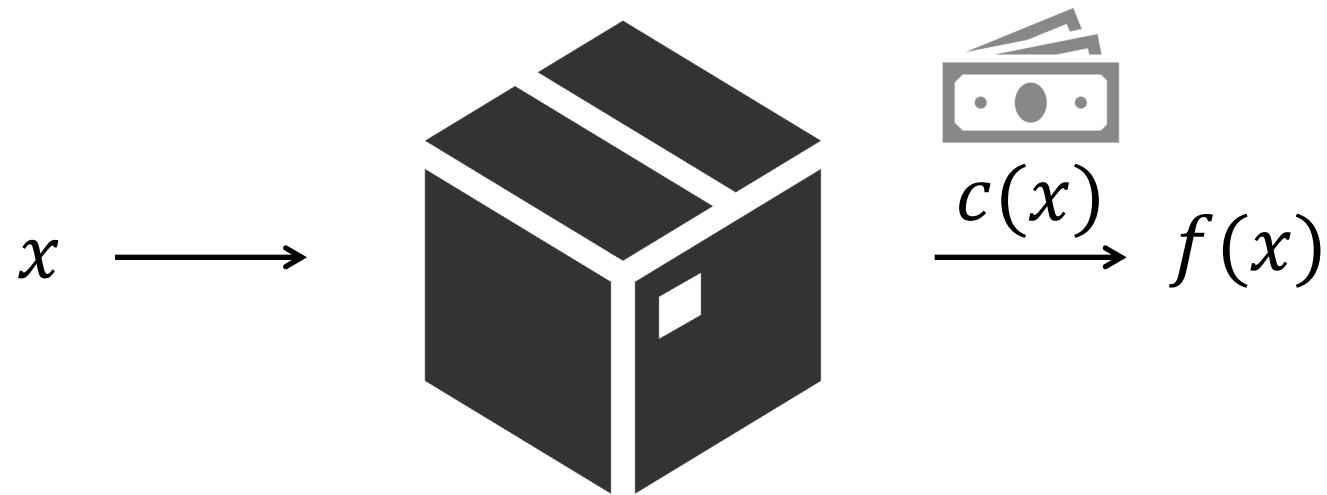
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[Lee, Perrone, Archambeau, Seeger'21]
[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

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

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

Varying costs

Expected improvement per cost

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

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

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Why divide?

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

<table>
<tr><td align="center">Uniform costs</td><td align="center">Varying costs</td></tr>
<tr><td align="center">Expected improvement</td><td align="center">Expected improvement per cost</td></tr>
<tr><td align="center">$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$</td><td align="center">$\max_x \text{EI}_{f|D}(x; y_{\text{best}})/c(x)$</td></tr>
</table>

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

Cost-aware Bayesian Optimization

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⋮	⋮

New design principle: Gittins Index

Cost-aware Bayesian Optimization

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

New design principle: Gittins Index

naturally cost-aware

Expected Improvement
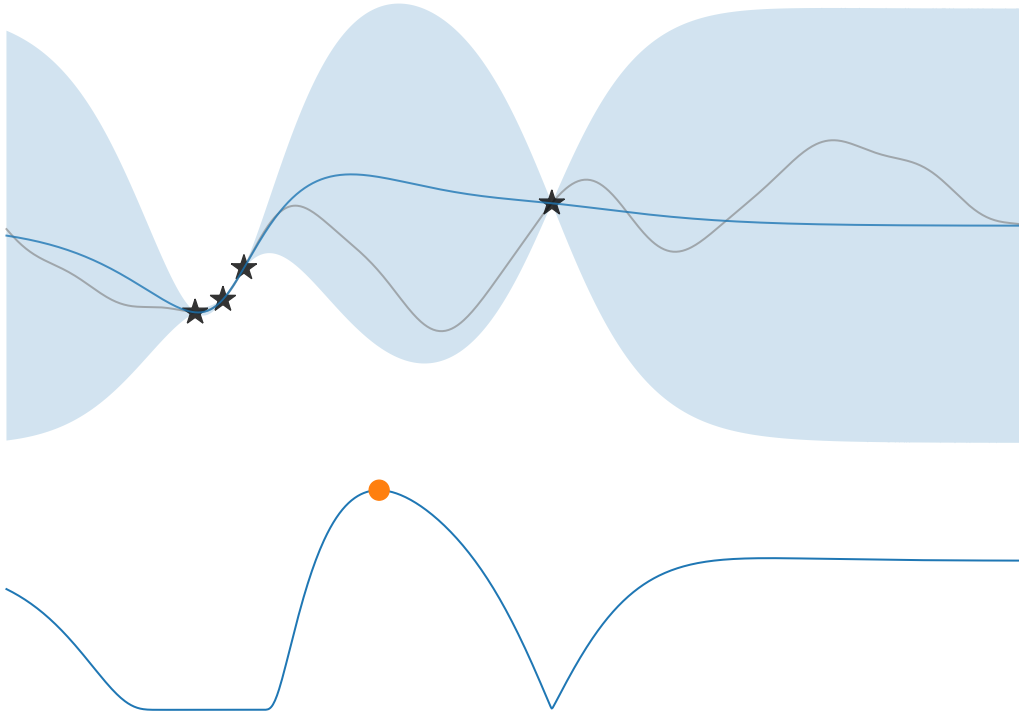
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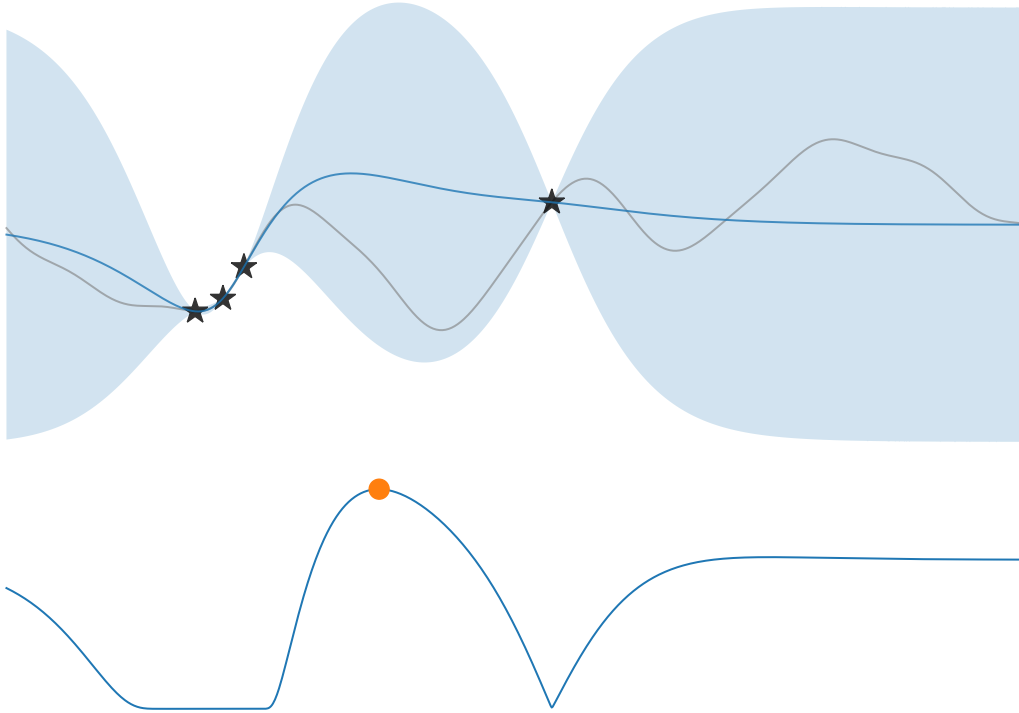
Gittins Index

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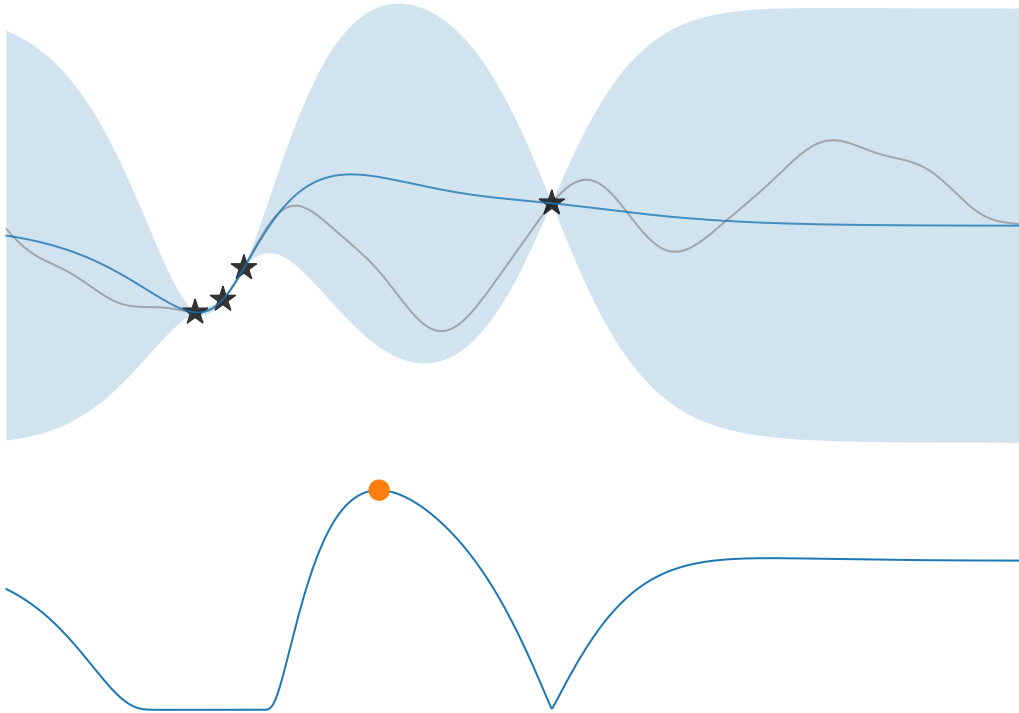
$$\max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

$$\text{GI}_{f|D}(x) = g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$
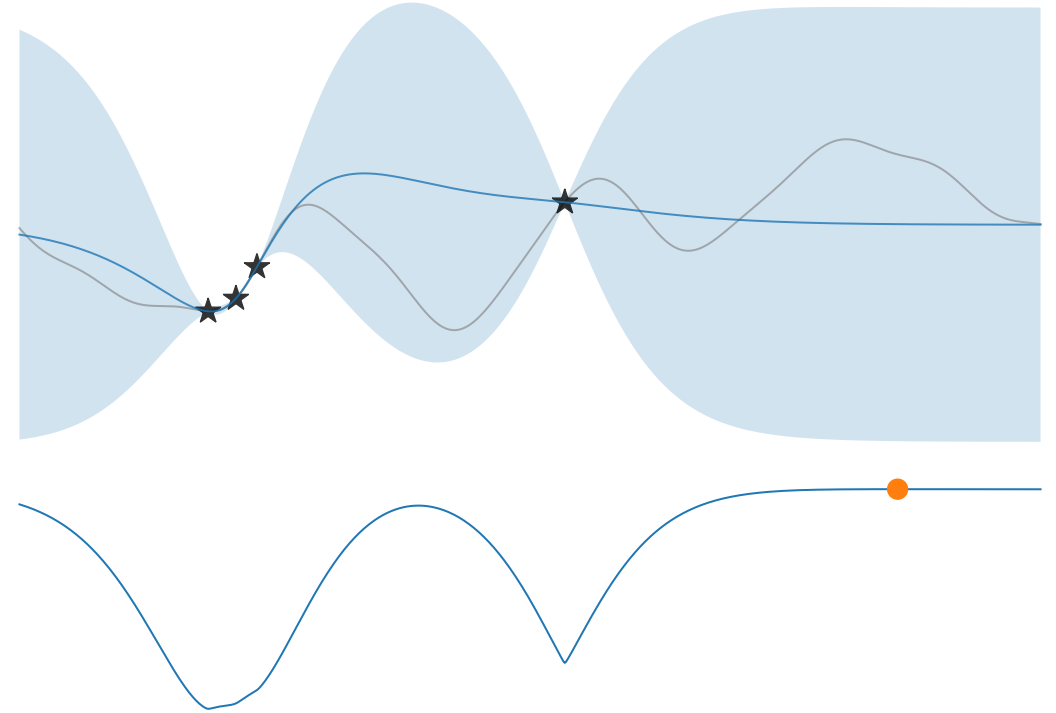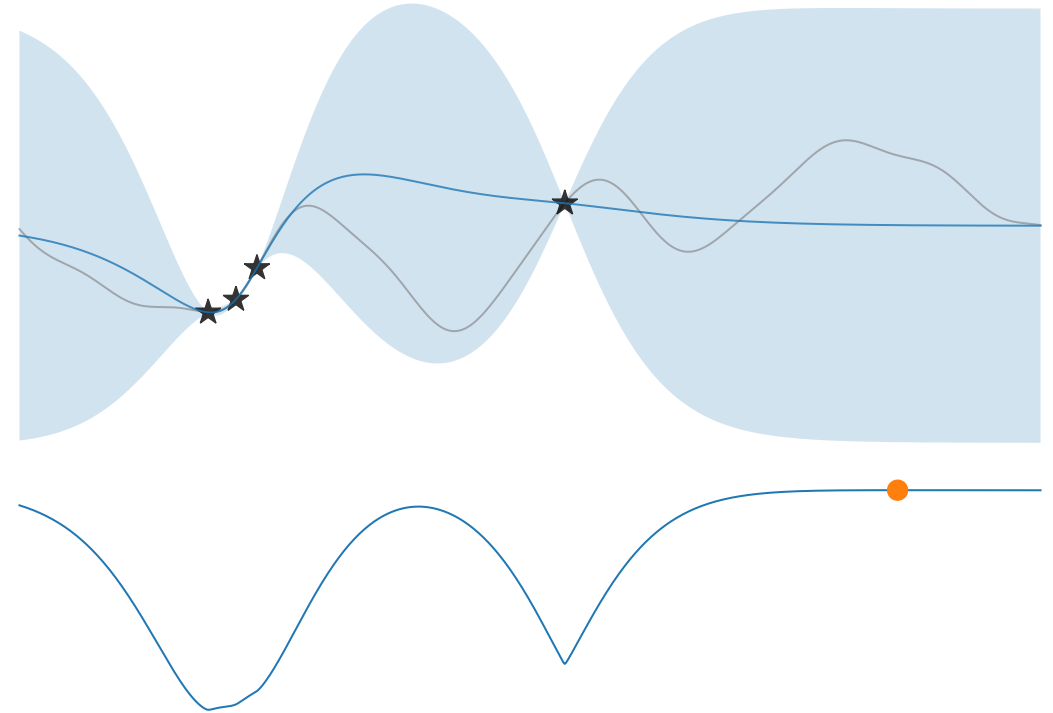
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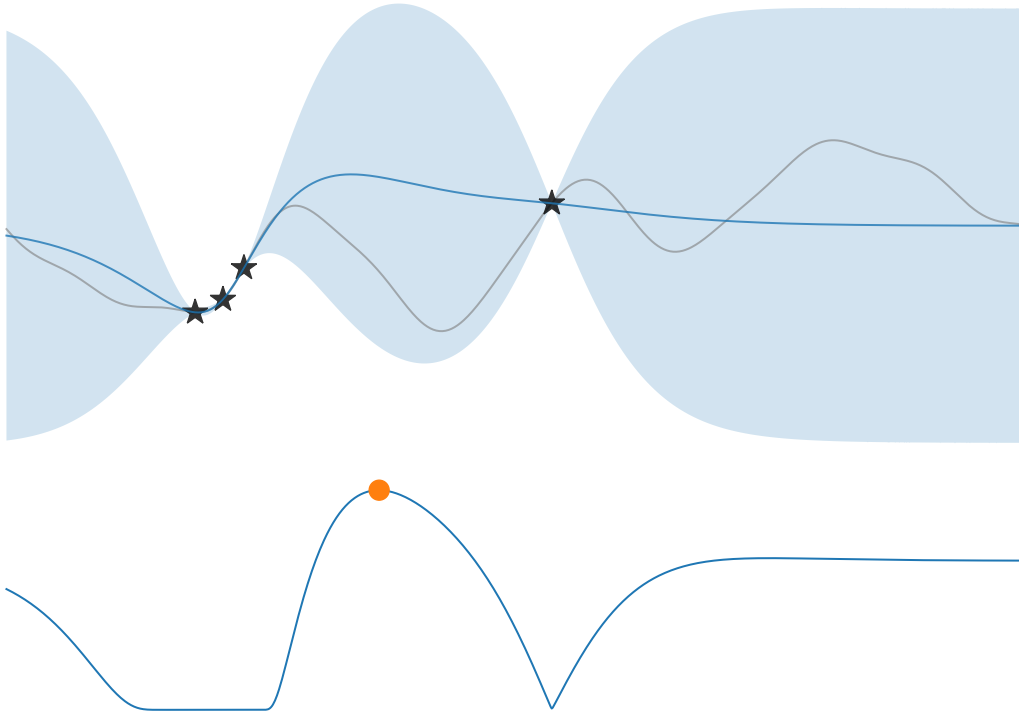
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One-step approximation to MDP

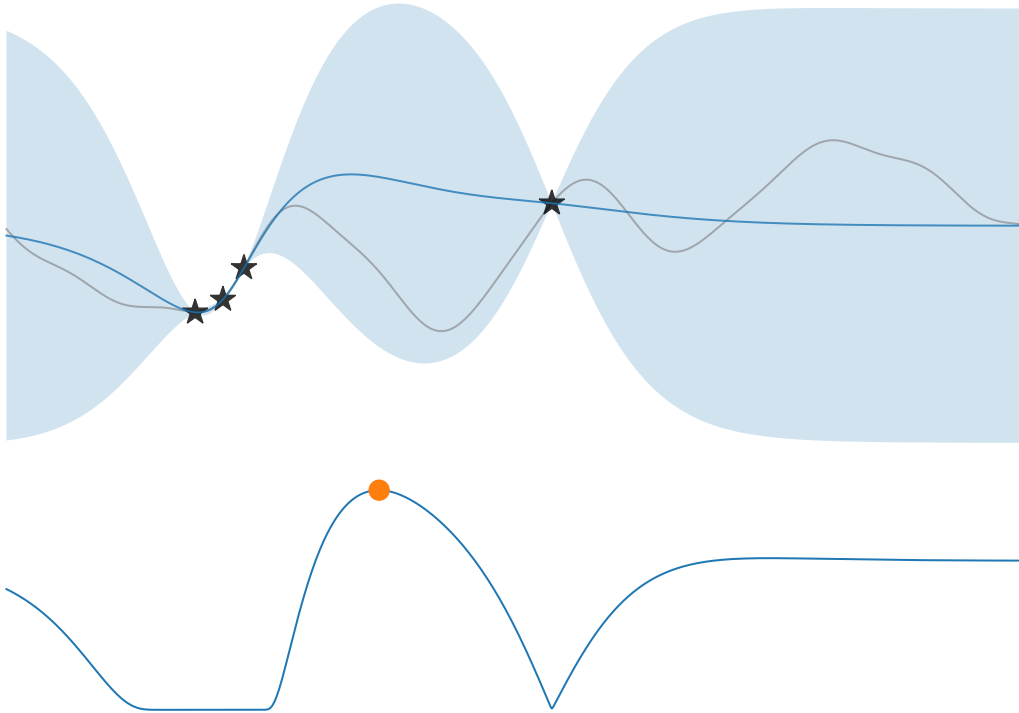# Gittins Index

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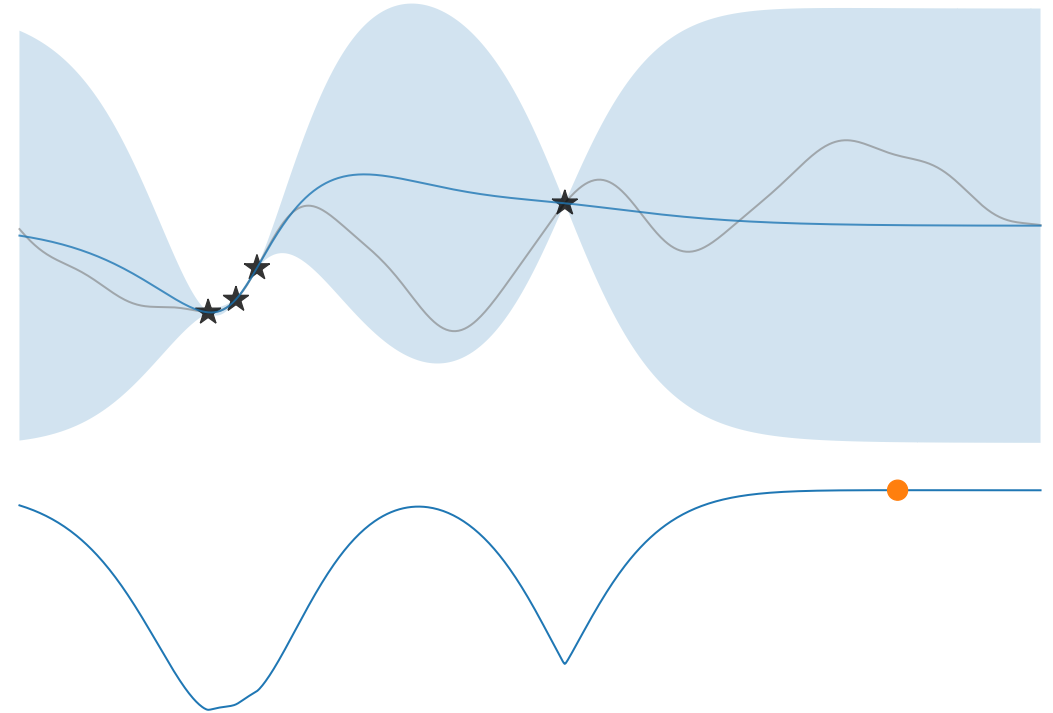
$$\max_x \text{GI}_{f|D}(x)$$

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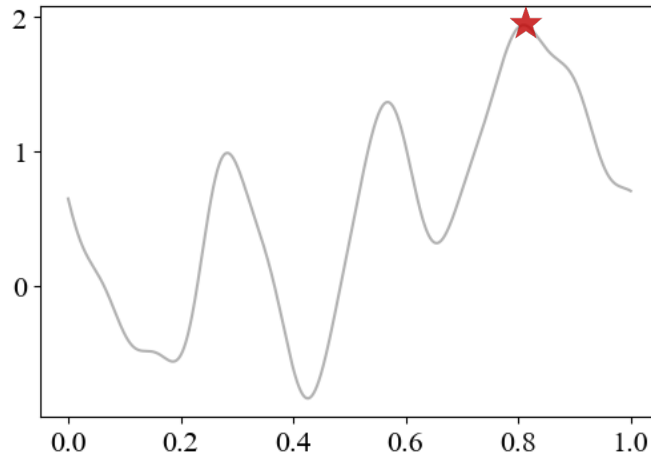
Temporal simplification to MDP

Gittins Index

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Temporal simplification to MDP

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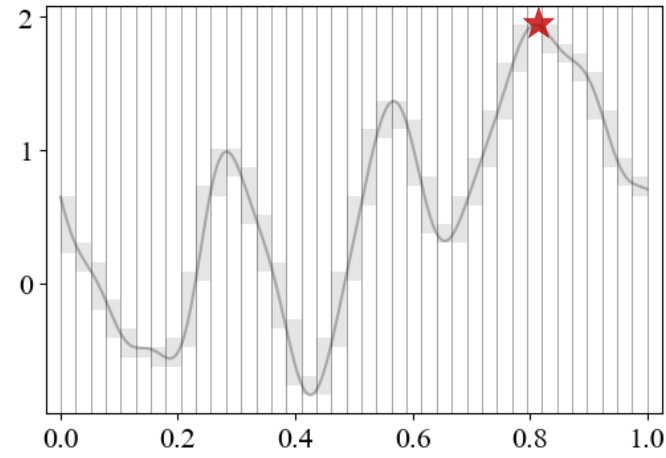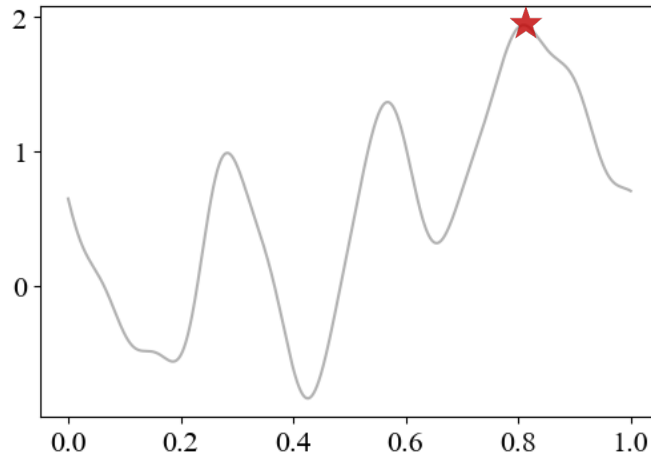Spatial simplification to MDP

Our Approach: Spatial Simplification

Bayesian Optimization

Continuous

Correlated

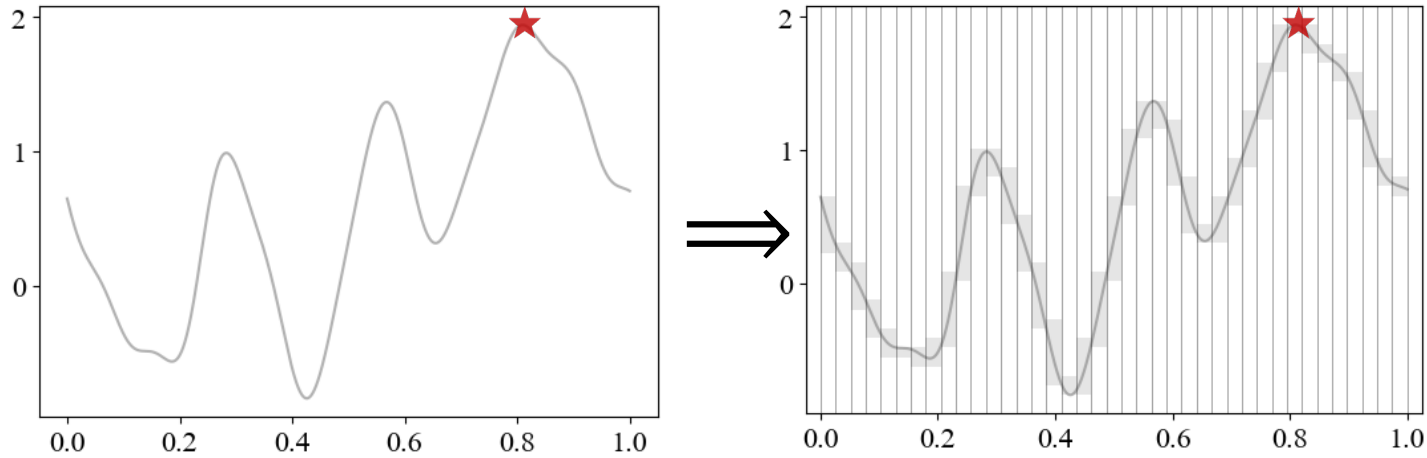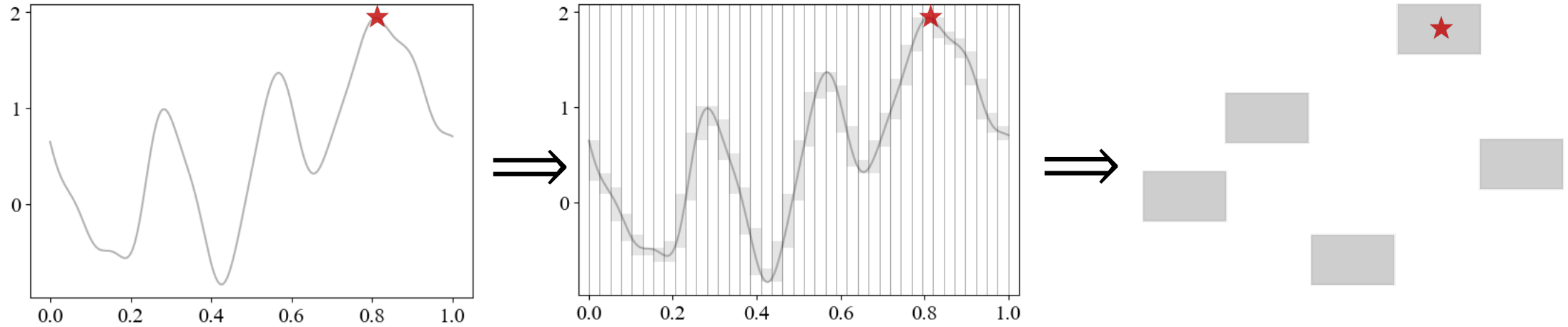# Our Approach: Spatial Simplification

Bayesian Optimization

Continuous $\implies$ Discrete

Correlated

Our Approach: Spatial Simplification

$\Longrightarrow$

Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

Correlated

Our Approach: Spatial Simplification

Bayesian Optimization

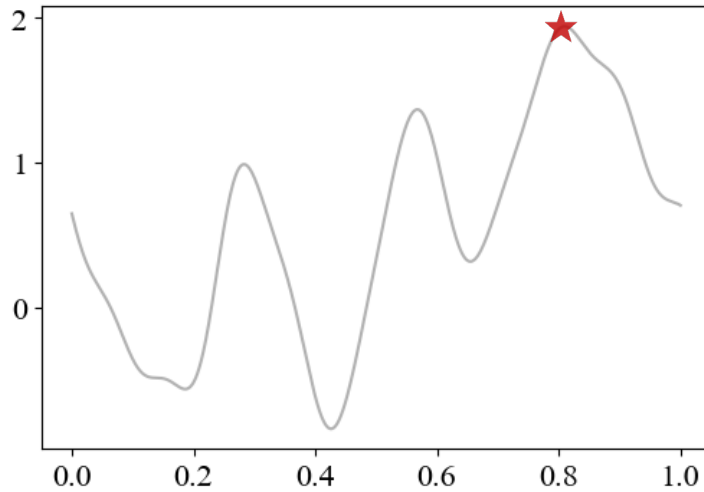|		
Continuous	$\Rightarrow$	Discrete
Correlated	$\Rightarrow$	Independent

Our Approach: Spatial Simplification

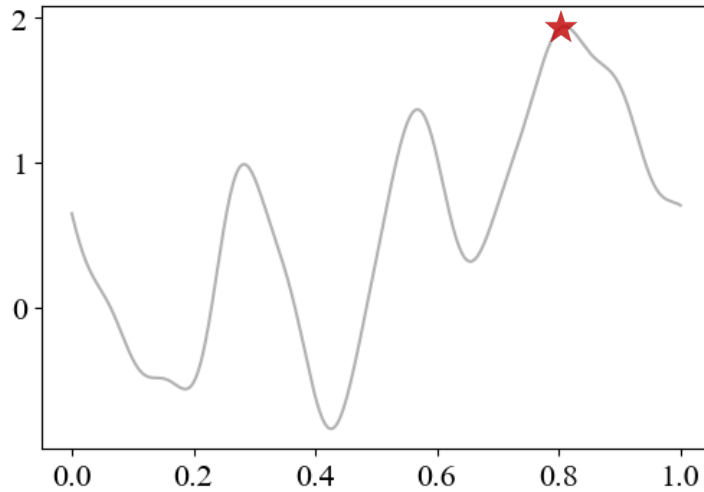Bayesian Optimization $\Longrightarrow$ Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Our Approach: Spatial Simplification

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

Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification

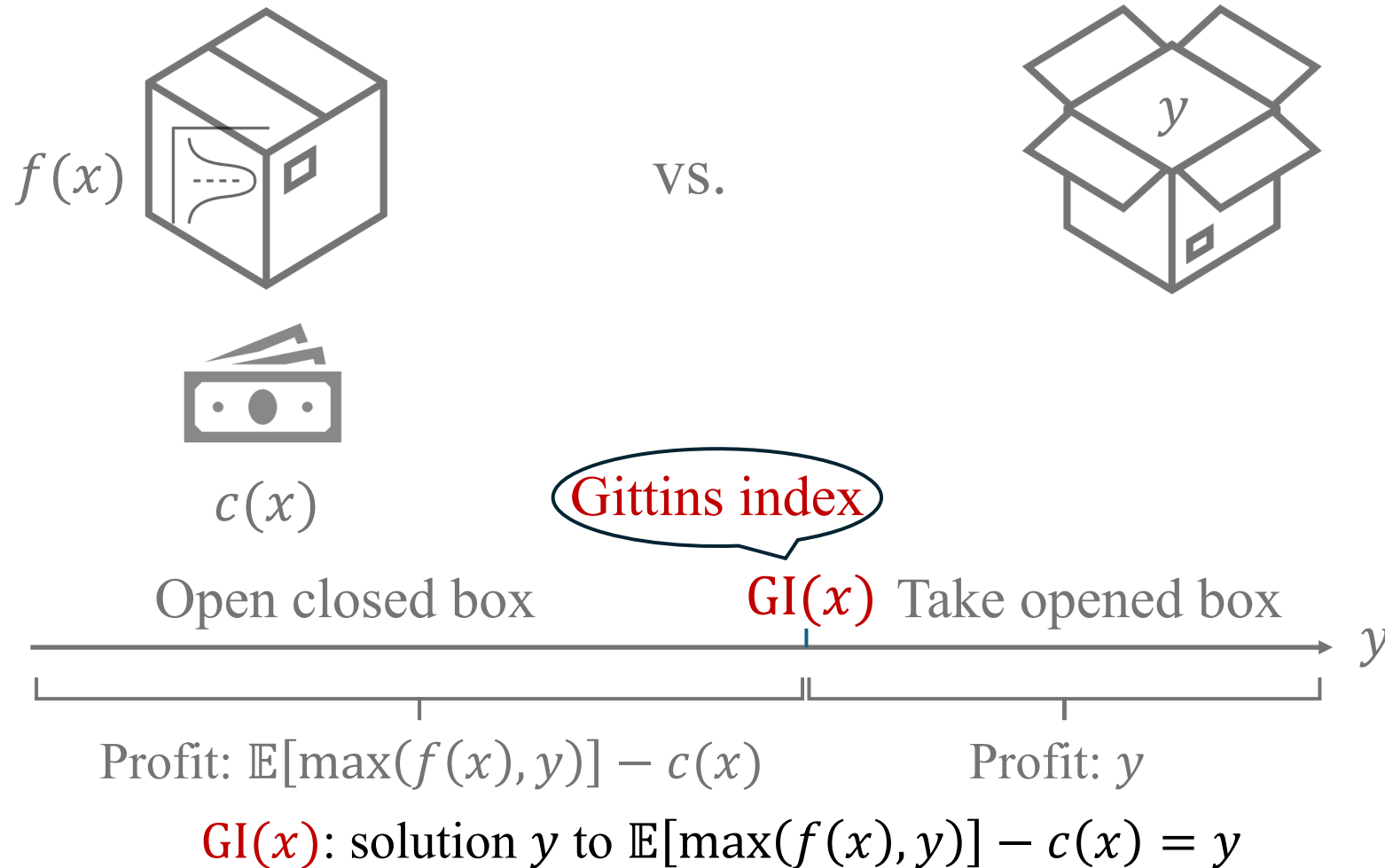
Bayesian Optimization   Pandora's Box

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 $GI(x)$ Take opened box
                                                                        y

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

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

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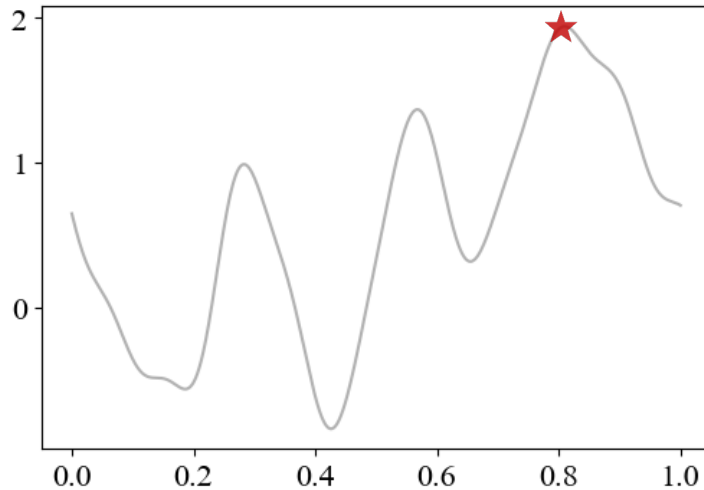
Bayesian Optimization   Pandora's Box
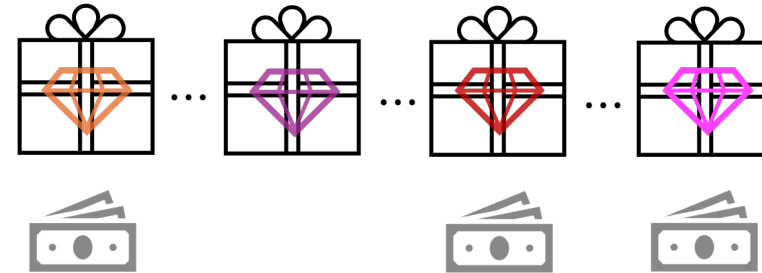
Continuous $\Longrightarrow$ Discrete

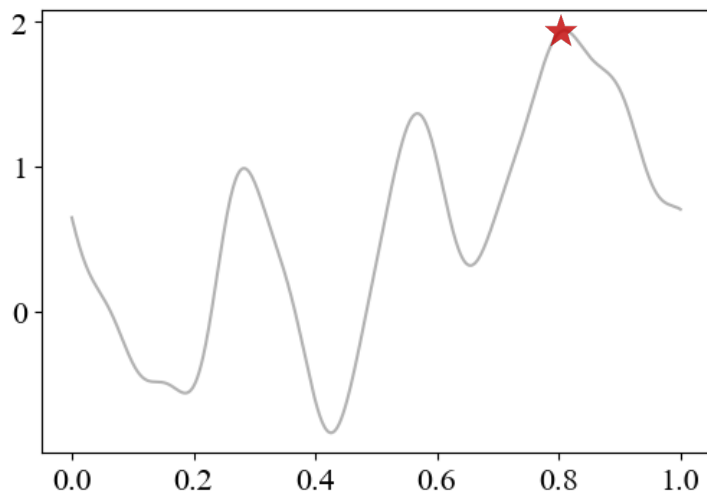Correlated $\Longrightarrow$ Independent

How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

How to translate Gittins index?
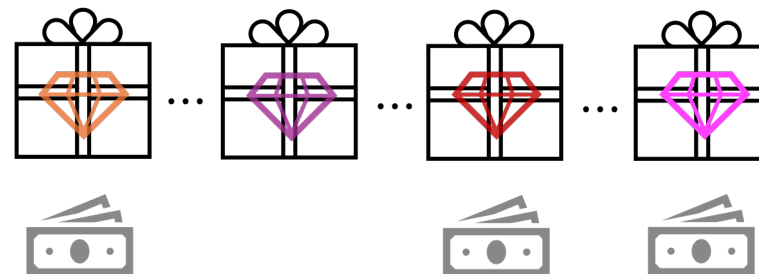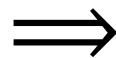
Bayesian Optimization

Pandora's Box

Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

incorporate posterior

Our policy $\qquad \Longleftarrow$ Optimal policy: Gittins index

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

Is Gittins good in Bayesian Optimization?
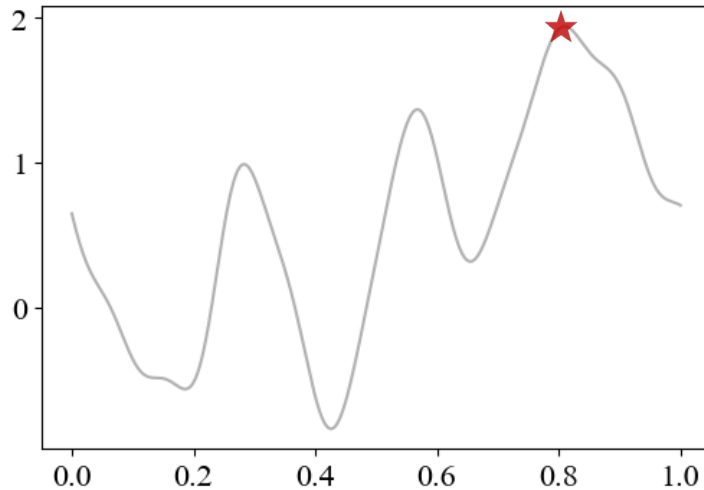
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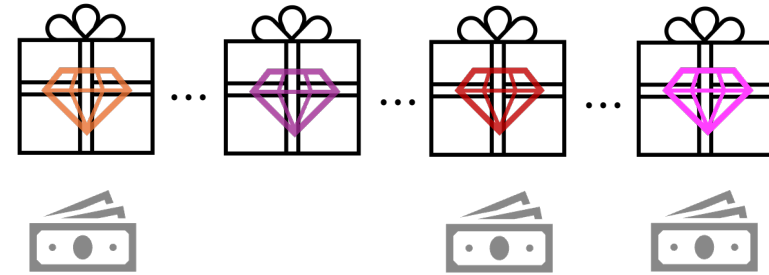
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

incorporate posterior

Is Gittins index good? $\quad\Longleftarrow\quad$ Gittins index is optimal

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

Experiment Setup: Objective Functions

Samples from prior

Ackley function

Synthetic

Matern52

Figure from infpy

Figure from [Terenin'22]
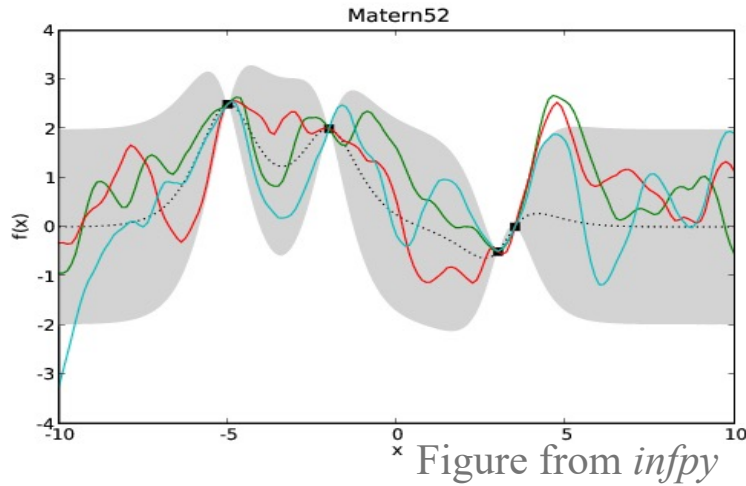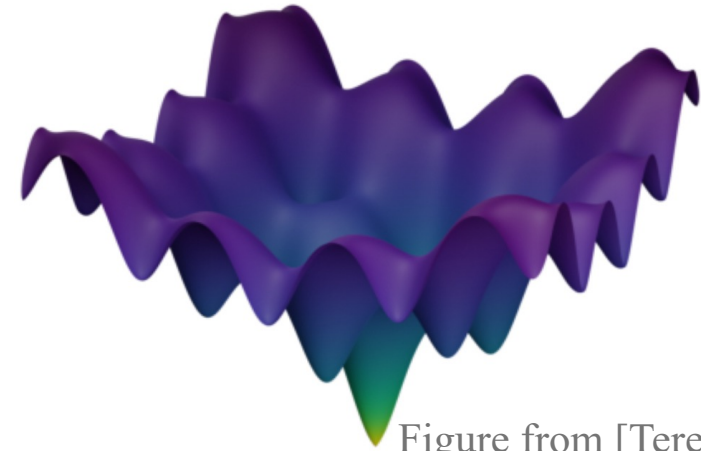
Pest Control

Lunar Lander

Empirical

Figure from ChatGPT
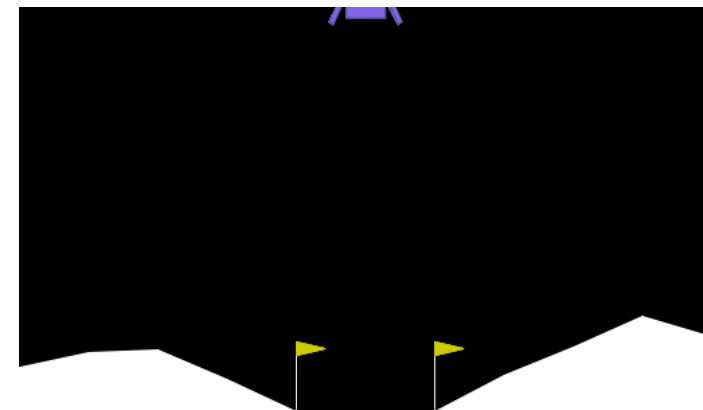
Figure from OpenAI Gym

Experiment Results

Synthetic | Empirical

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

Best Observed Value | Cumulative Cost

Uniform Costs | Varying Costs

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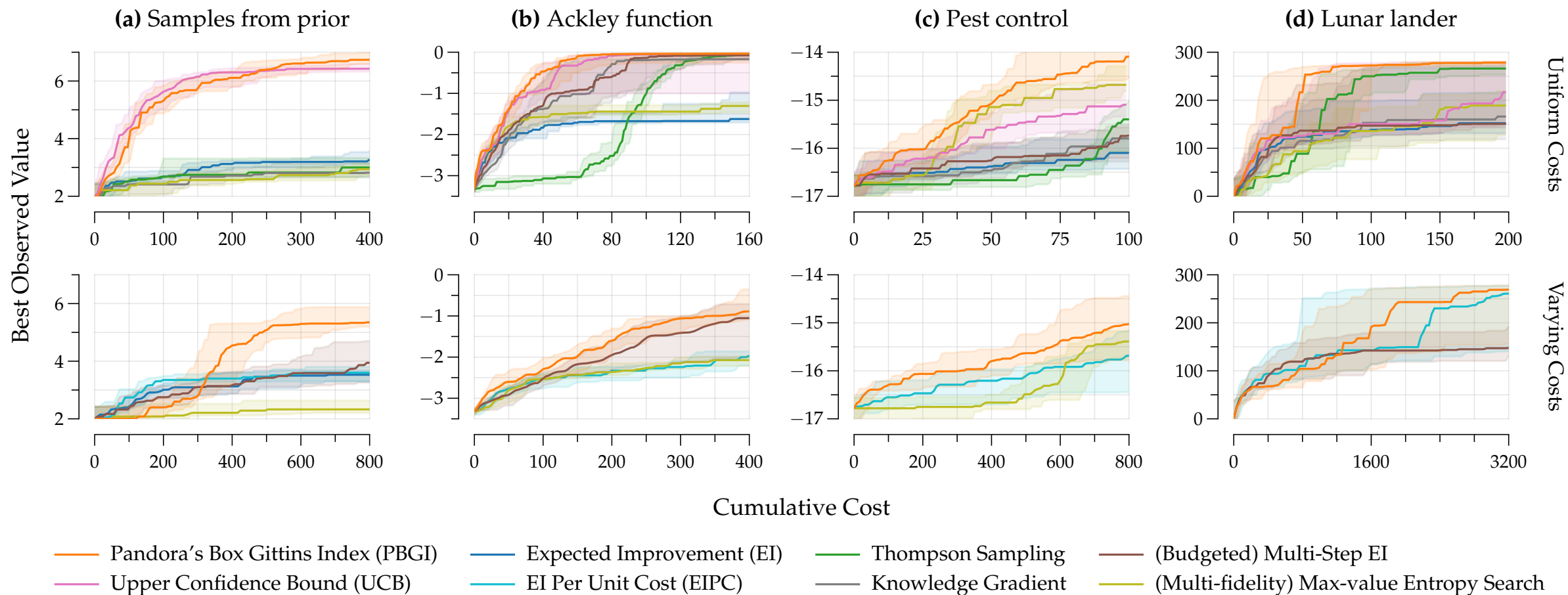
FAQ

- Easy-to-compute?

FAQ

- Easy-to-compute?

    Yes, EI + bisection

FAQ

- Easy-to-compute?

    Yes, EI + bisection

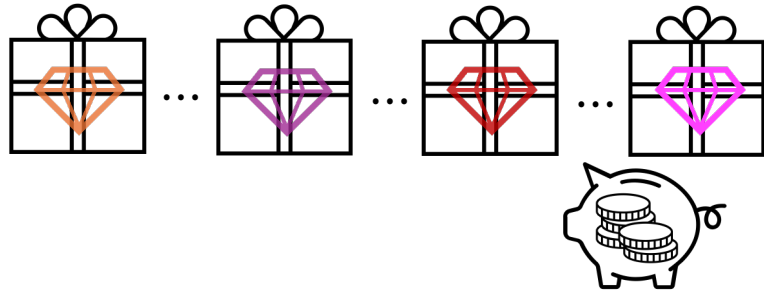- Any theoretical results?

FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

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

Theoretical Result

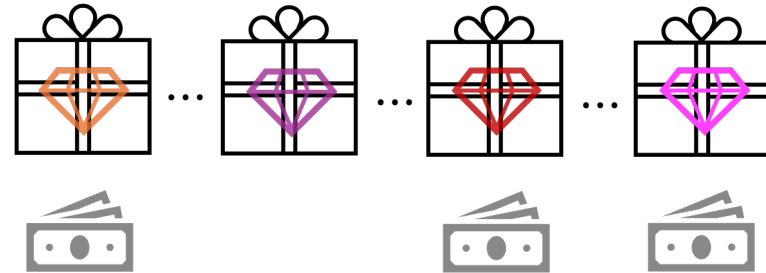**max** best observed under budget

Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

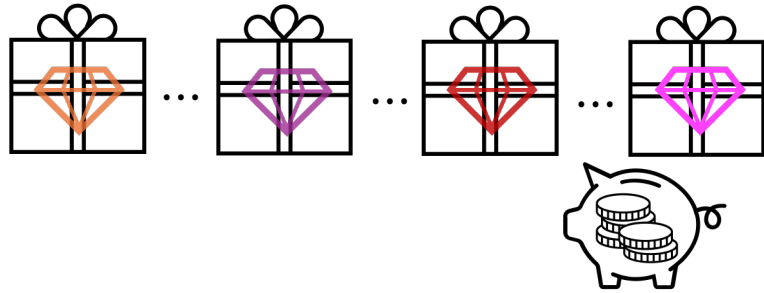**max** (best observed – costs)

Pandora's Box

Cost per sample

Optimal policy: Gittins index

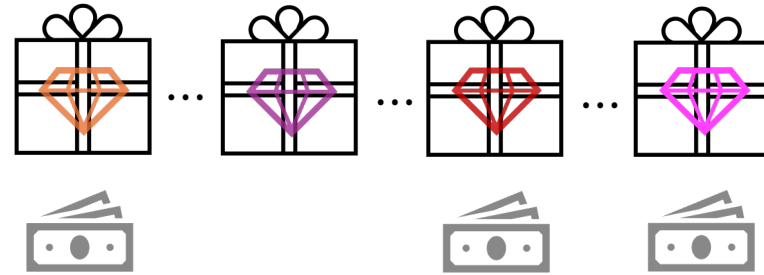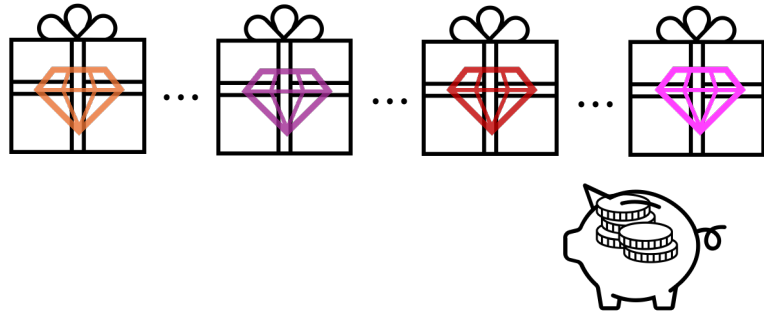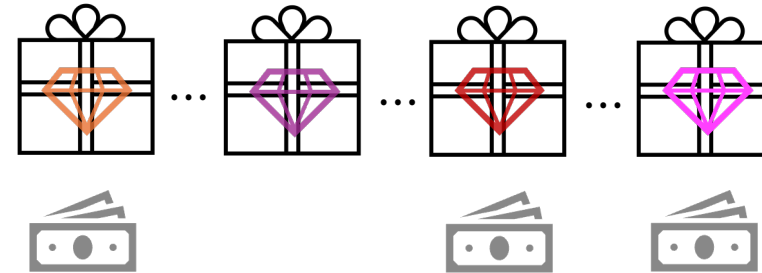# Theoretical Result

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

max best observed under budget

max (best observed – scaled costs)

budget-dependent

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?

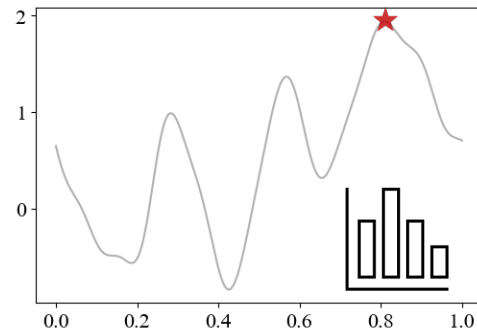 Yes, EI + bisection

- Any theoretical results?

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

- **Tuning parameters?**
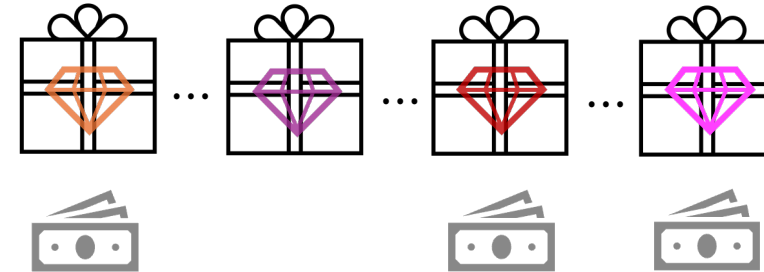
  Yes, control unit conversion

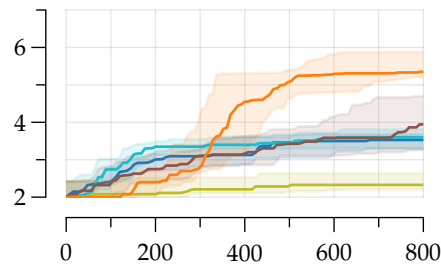# New Design Principle: Gittins Index

Problem

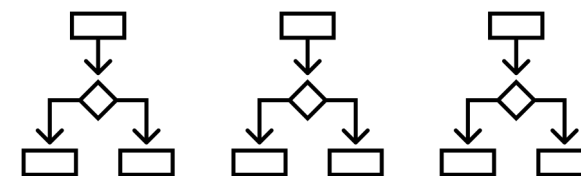Key idea

Bayesian optimization
with varying costs

link to Pandora's box
and Gittins index theory

Impact

competitive performance

Future potential

black-box processes
with partial feedback