# 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

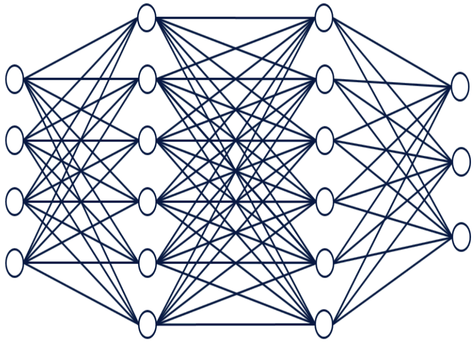
Peter Frazier

Ziv Scully

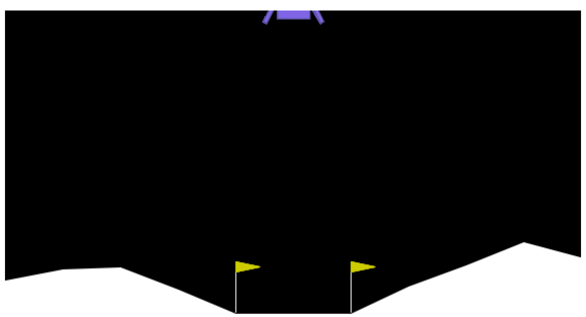
Alexander Terenin

# World of Parameter Optimization

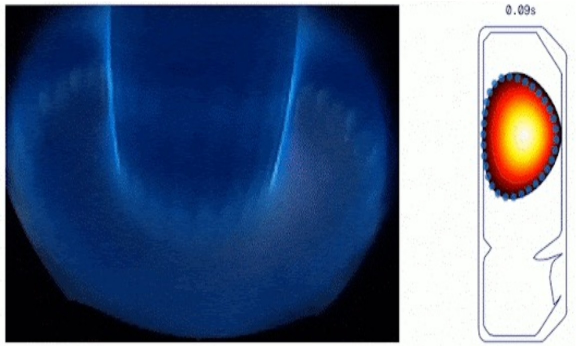
Hyperparameter tuning:

Training parameters →  → Accuracy

Control optimization:

Control parameters →  → Reward

Plasma physics:

Reactor parameters →  → Stability

# World of Parameter Optimization

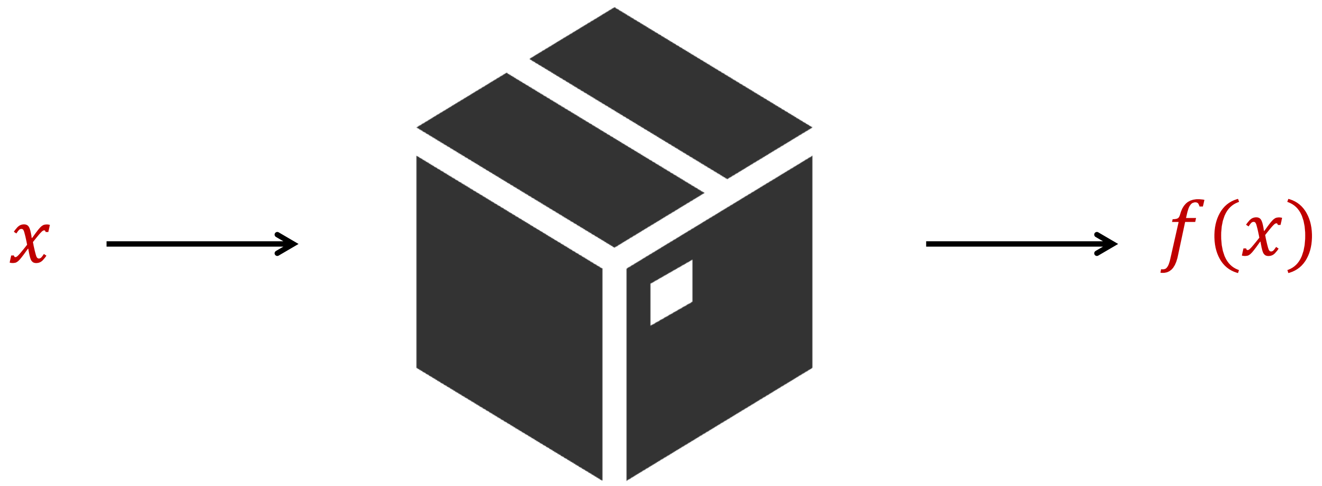
Black-box optimization:

Input parameters →

→ Performance metrics

# World of Parameter Optimization

Black-box optimization:



# Optimizing Black-box Functions

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

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

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$f \sim$Stochastic Process

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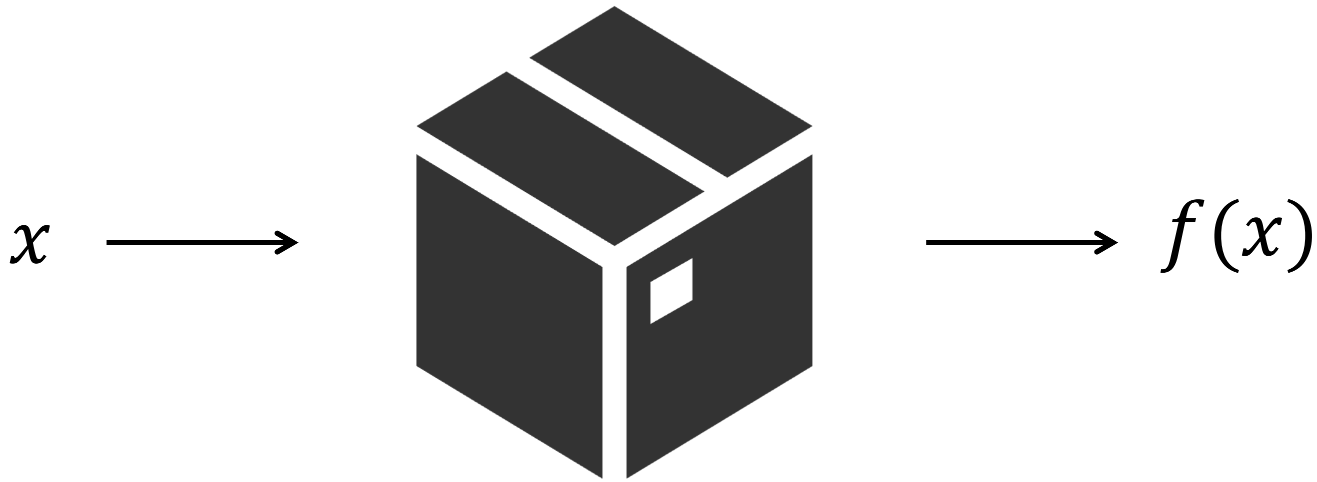
expensive-to-evaluate

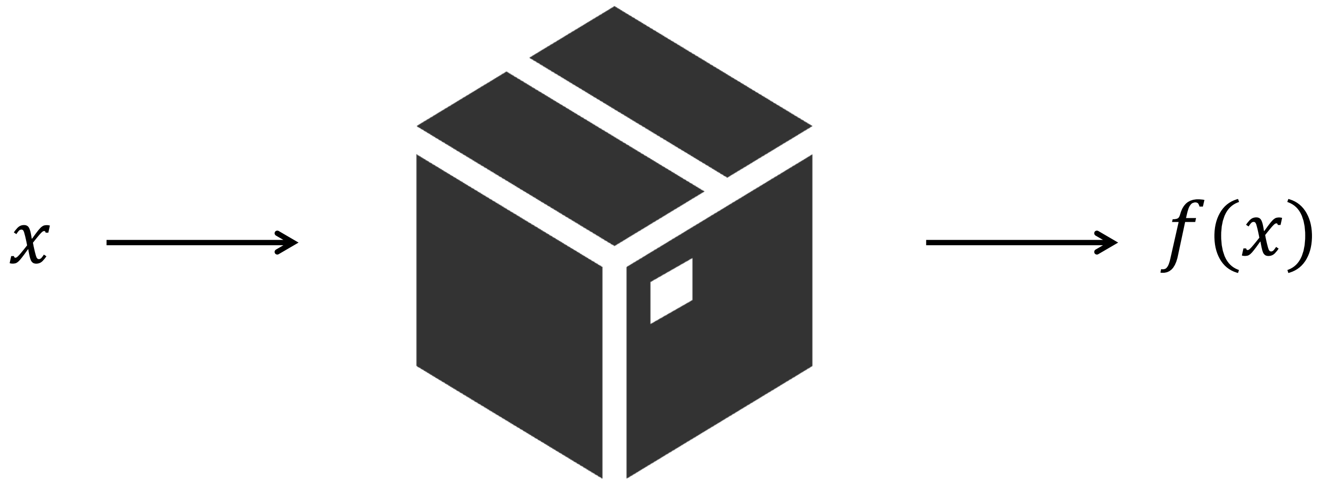
Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

# Optimizing Black-box Functions




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

# Optimizing Black-box Functions

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# Bayesian Optimization

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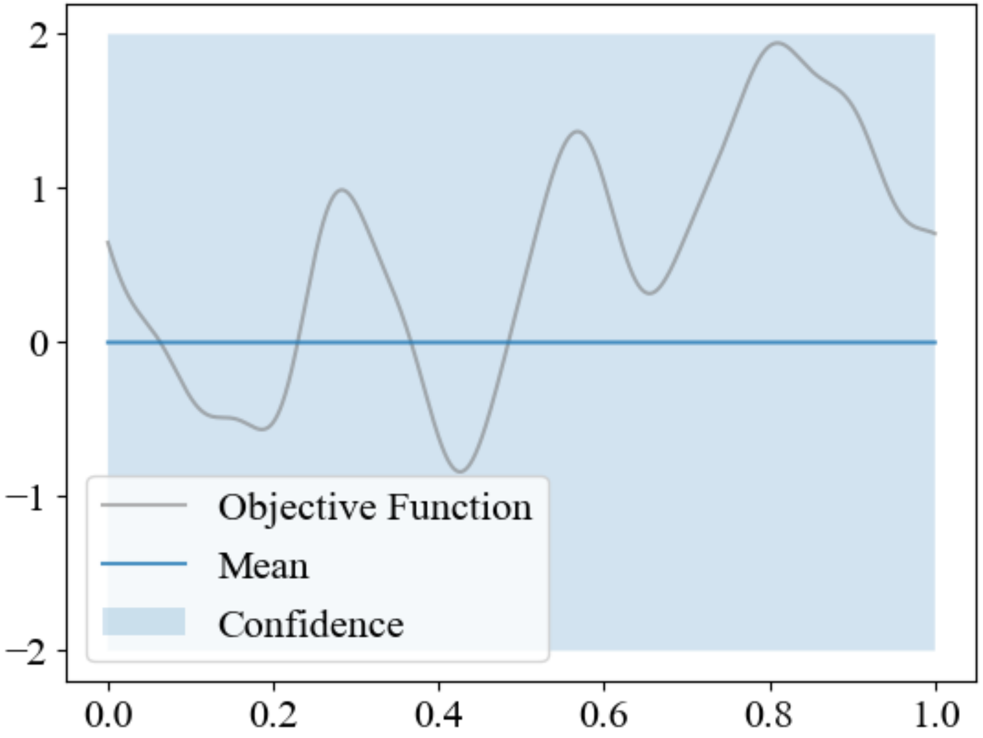


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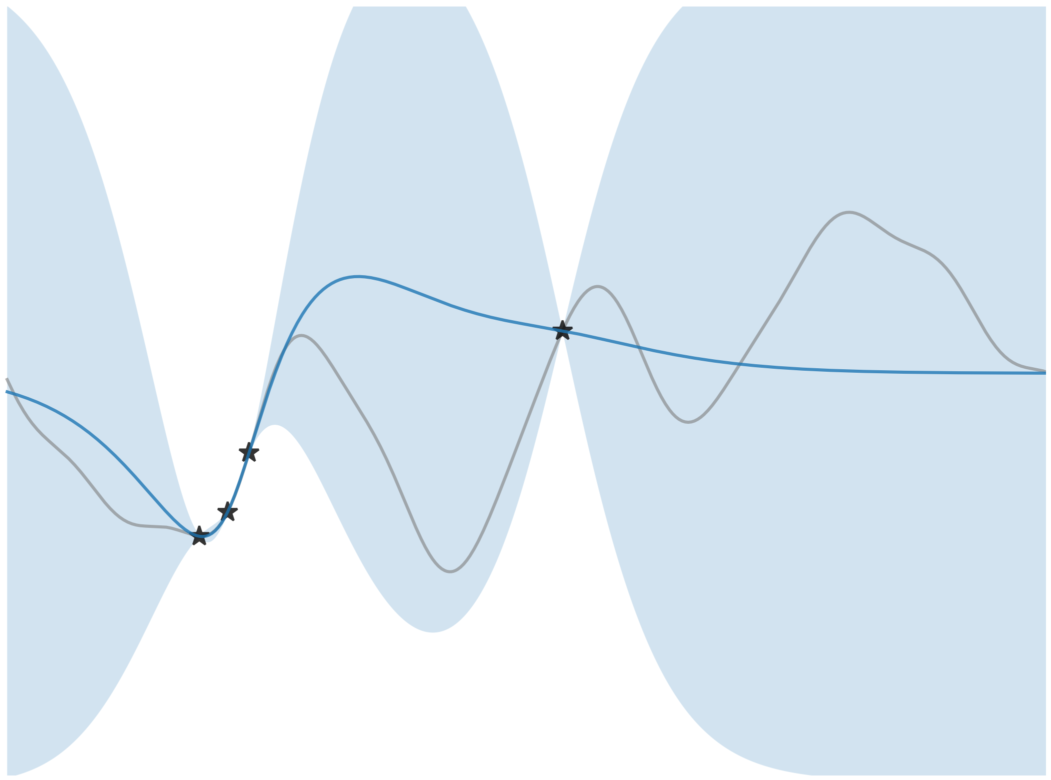
$f$ ~Gaussian Process

# Bayesian Optimization



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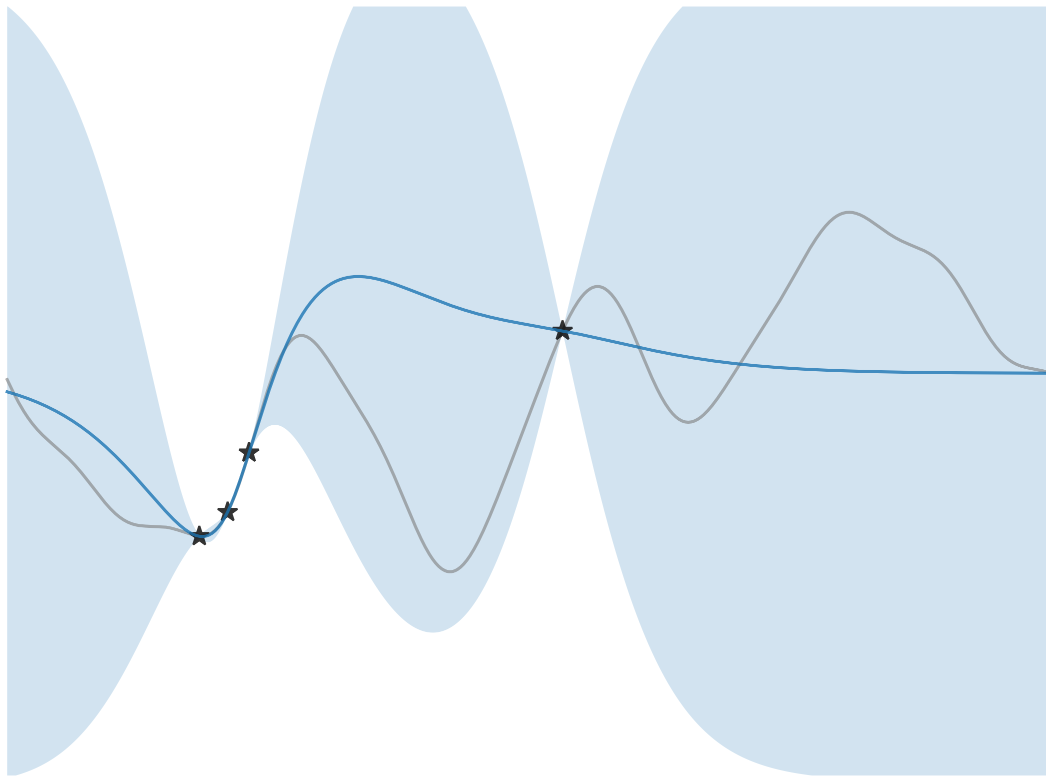
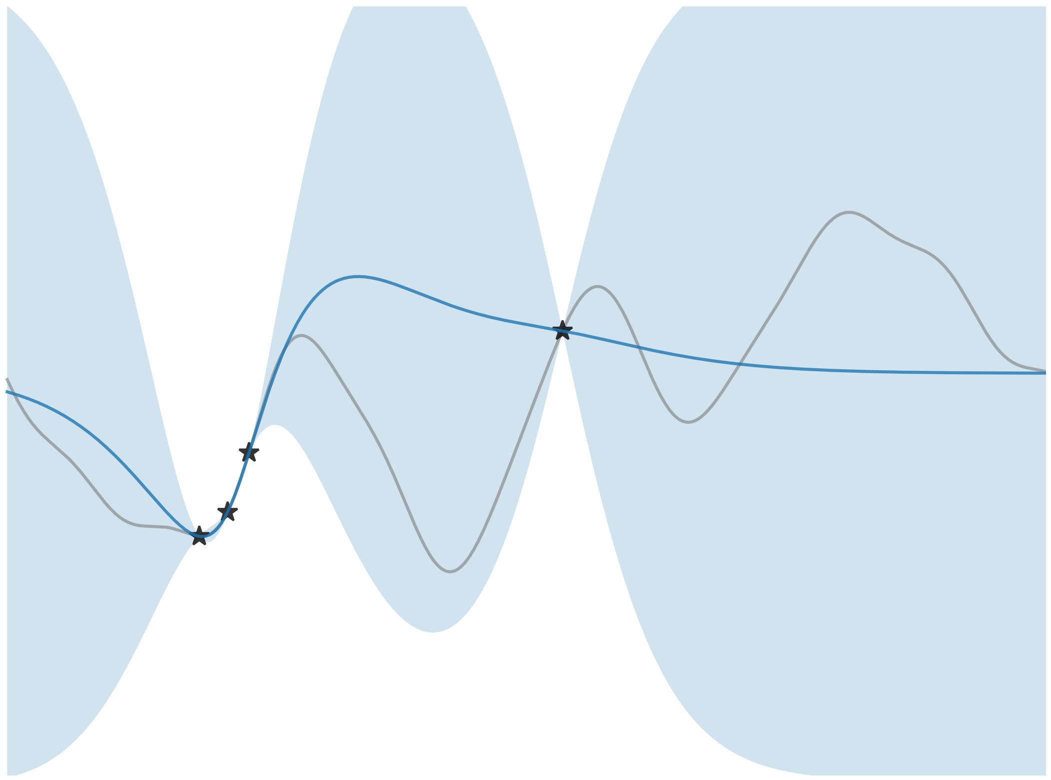


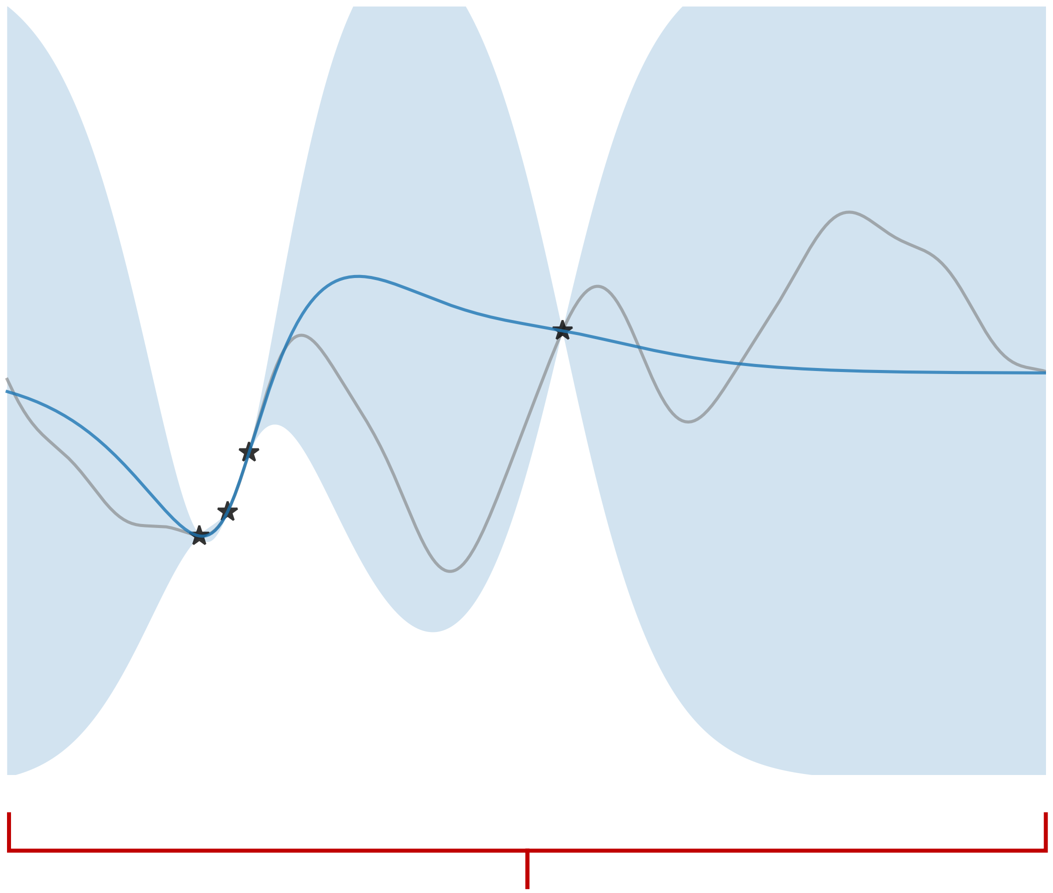
What to evaluate next?

# Bayesian Optimization



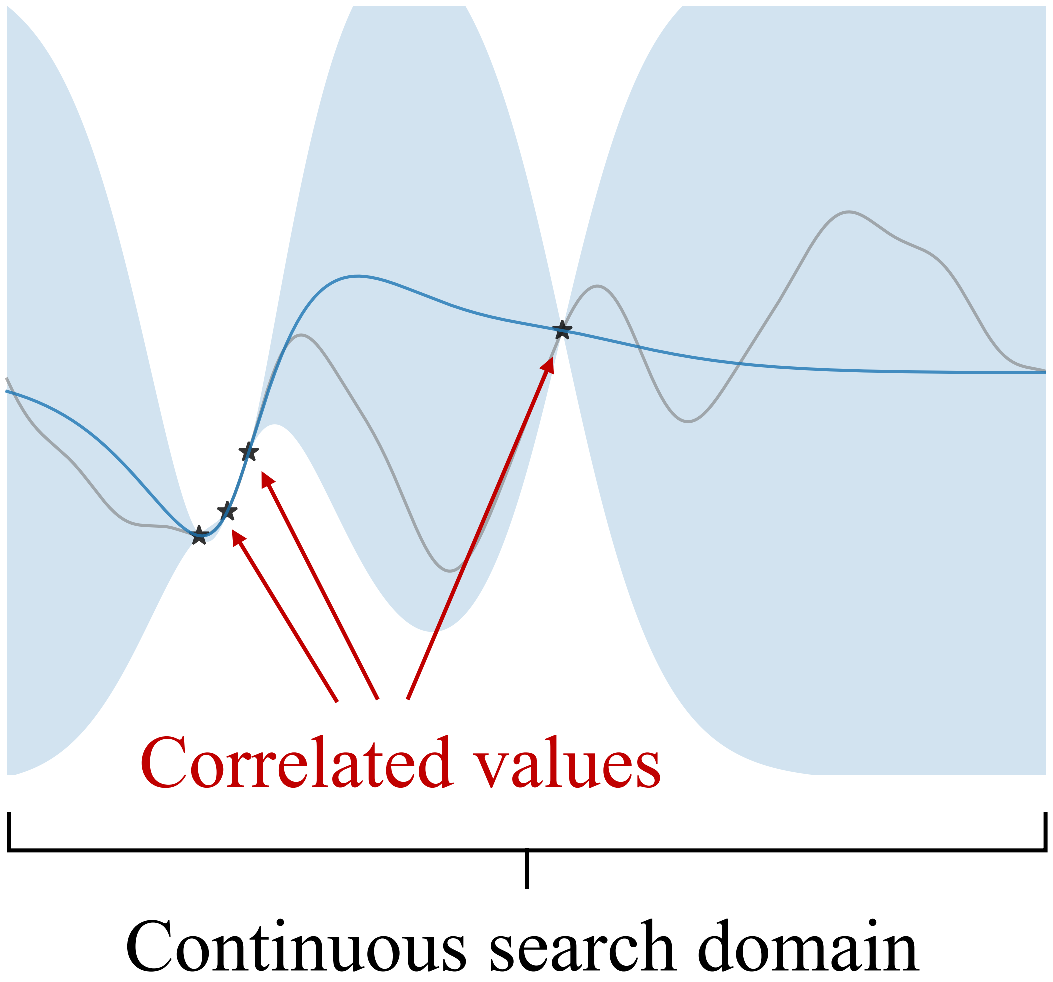
Optimal policy?

# Challenges of Bayesian Optimization



Continuous search domain

# Challenges of Bayesian Optimization



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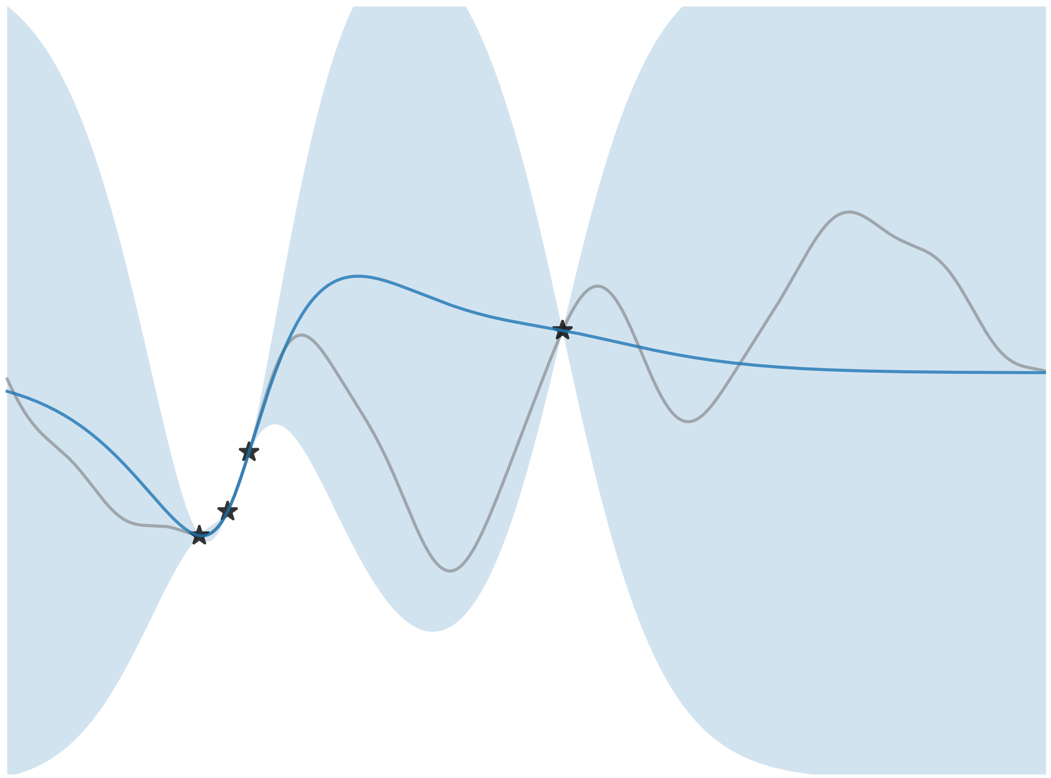
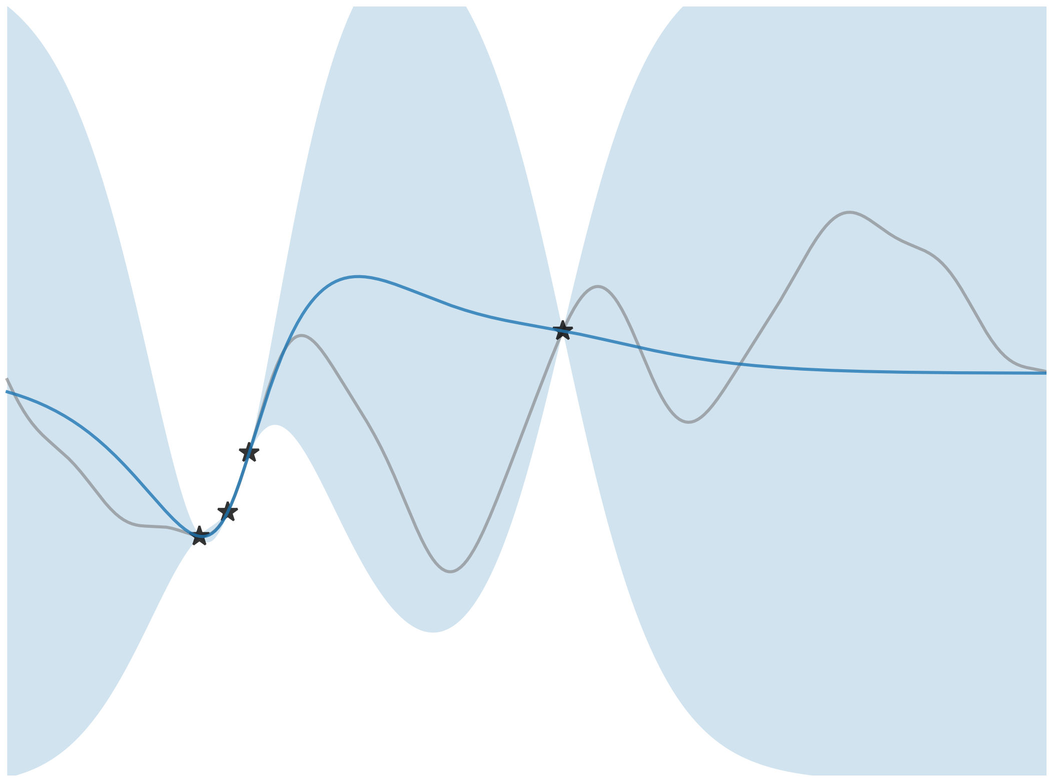


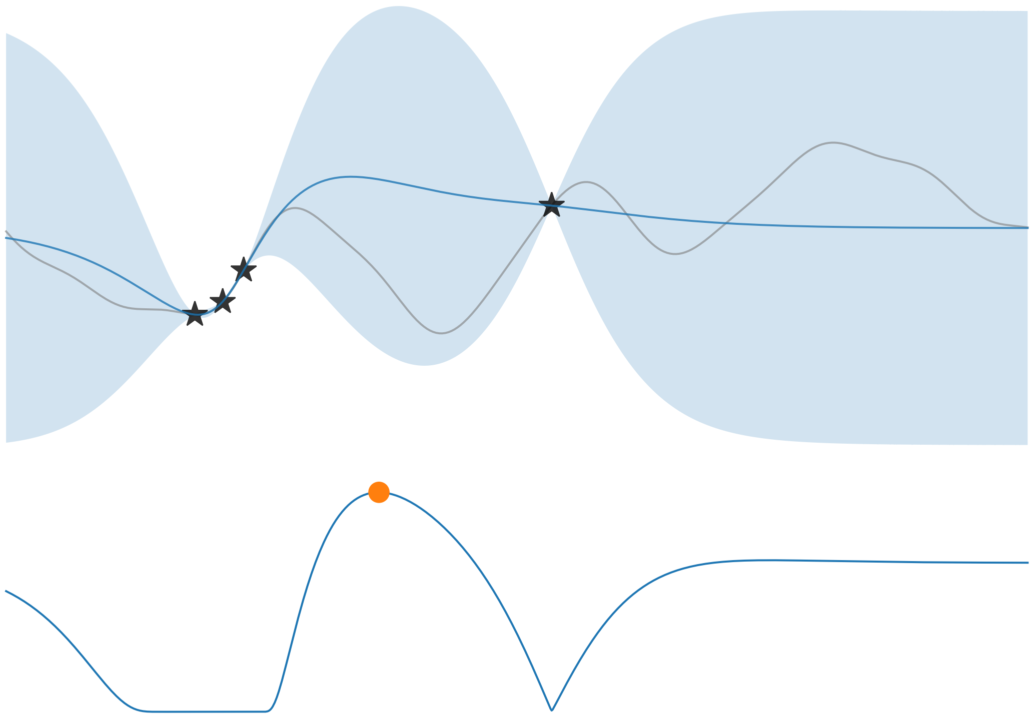
Correlation & continuity $\Longrightarrow$ Intractable MDP

# Challenges of Bayesian Optimization



Intractable MDP $\Longrightarrow$ Optimal policy unknown

# Popular Policy: Expected Improvement

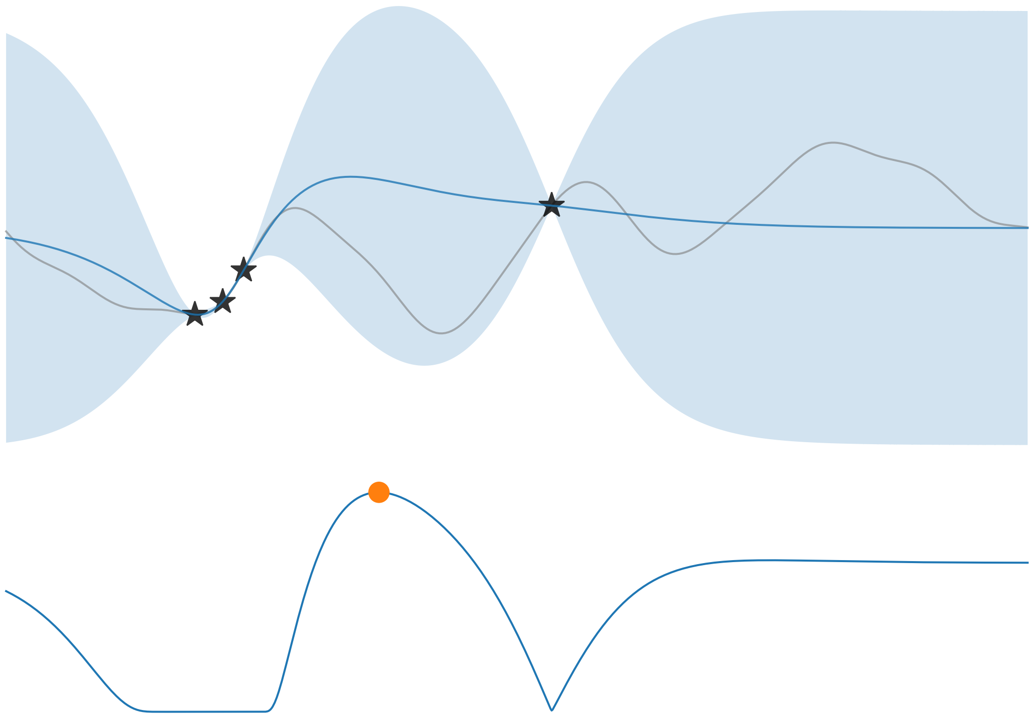


current best observed

data

$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{“improvement”}} \mid D]$$

# Popular Policy: Expected Improvement



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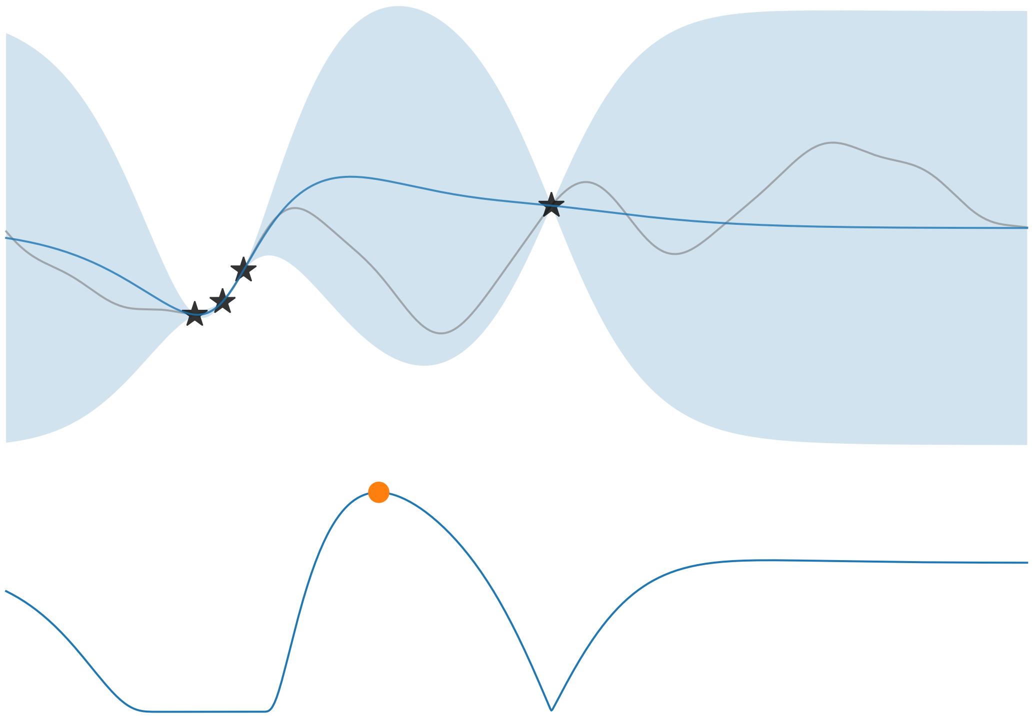

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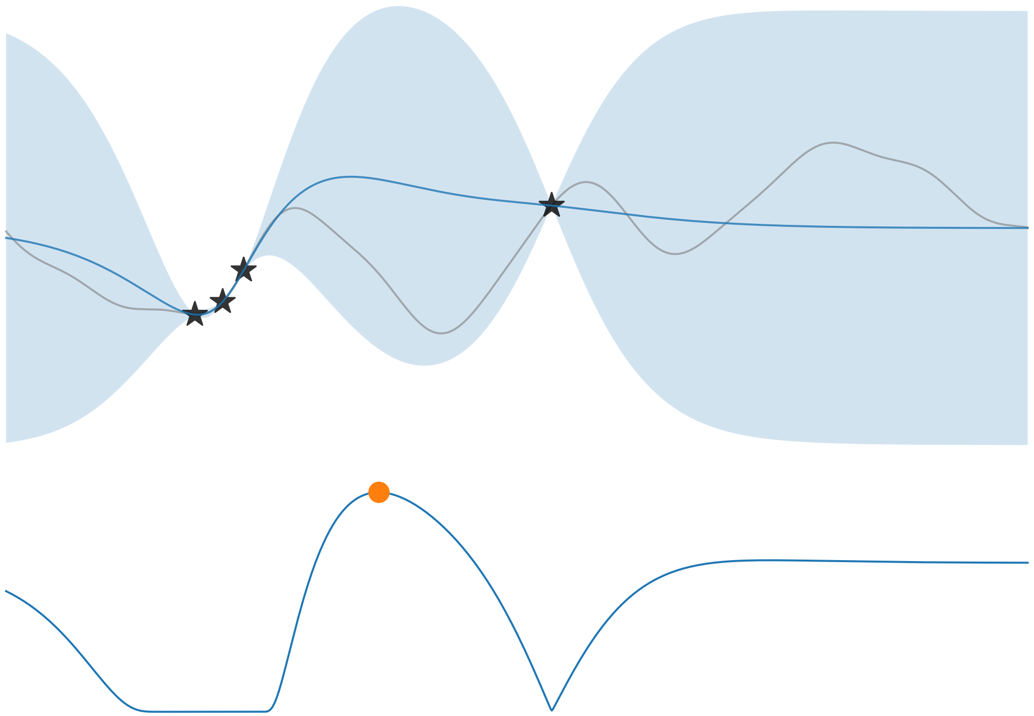

Other improvement-based policy:

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

# Approaches to Bayesian Optimization

- Improvement-based:
  - Expected Improvement
  - Probability of Improvement
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- Our work: Gittins Index

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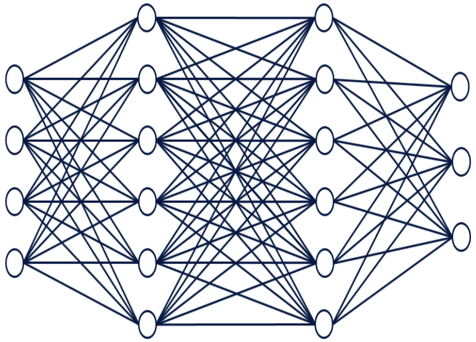
Why another approach?

# Another Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters →  → Accuracy

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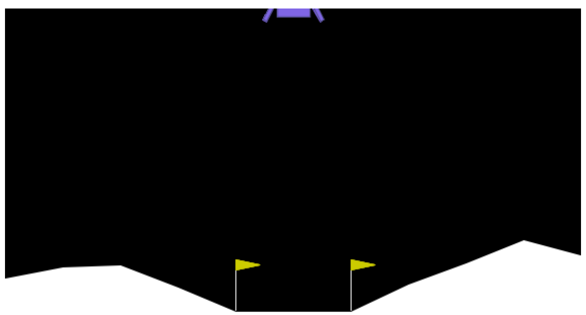
Control parameters →  → Reward

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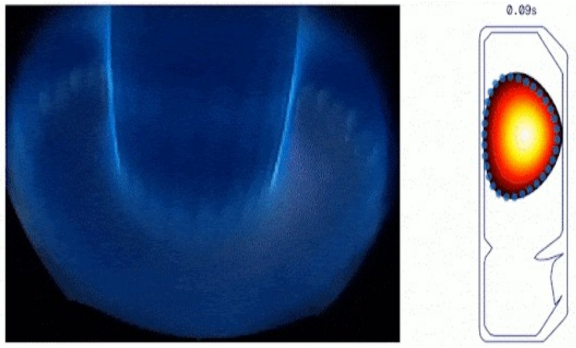
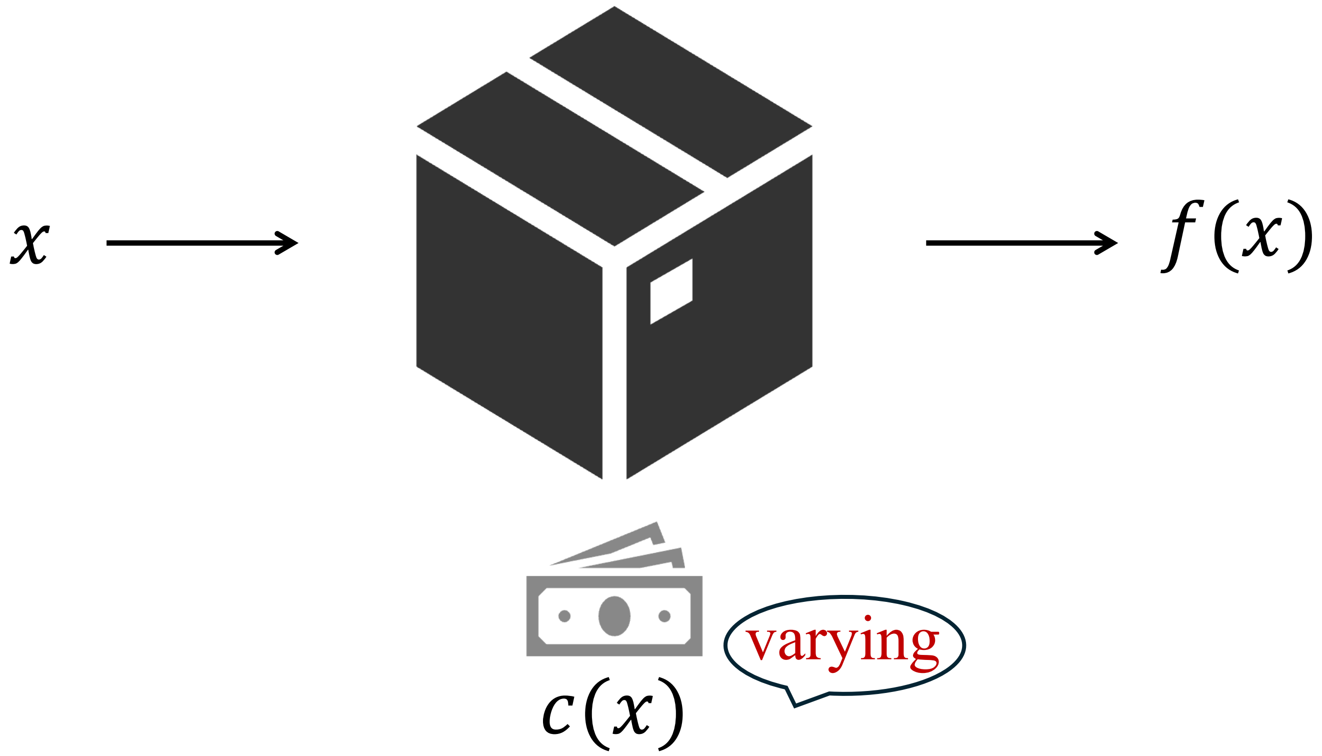
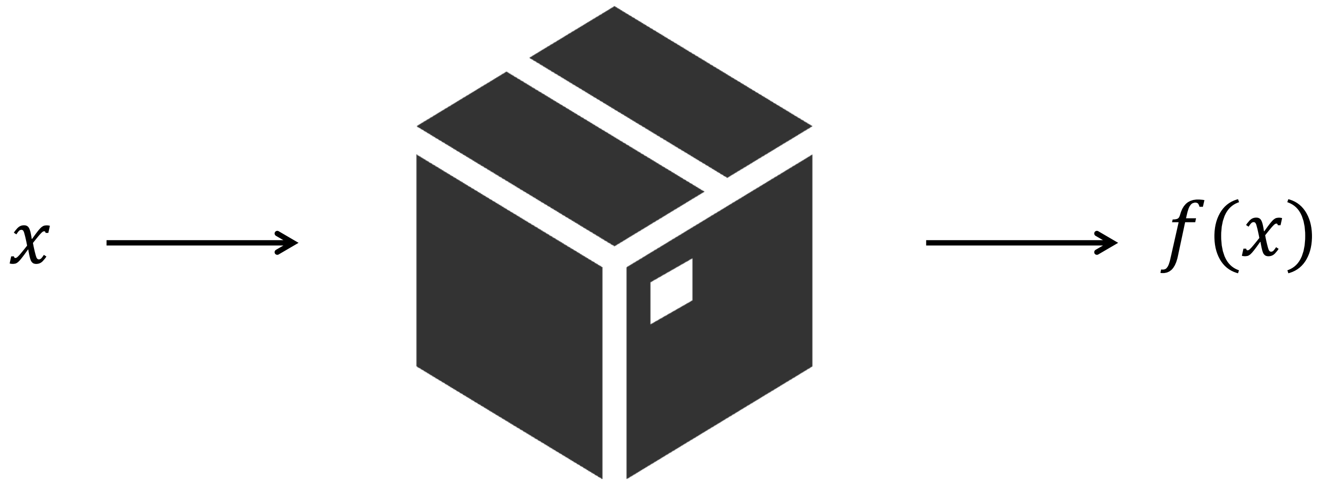
Reactor parameters → 

→ Stability

# Another Challenge: Varying Evaluation Costs



# Cost-aware Bayesian Optimization




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

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

[Lee, Perrone, Archambeau, Seeger’21]

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

# Cost-aware Bayesian Optimization

| | Uniform costs | Varying costs |
|---|---|---|
| One-step | Expected improvement<br>$\max_x \mathrm{EI}_{f\mid D}(x; y_{\text{best}})$ | |

# Cost-aware Bayesian Optimization

| | Uniform costs | Varying costs |
|---|---|---|
| One-step | Expected improvement | Expected improvement per cost |
| | $\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})$ | [Snoek, Larochelle, Adams'21] |

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Why divide?

# Cost-aware Bayesian Optimization

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

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

# Cost-aware Bayesian Optimization

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slow

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

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| | ⋮ | ⋮ |

Our view: lack of a guidance to incorporate costs

# Cost-aware Bayesian Optimization

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New design principle: Gittins Index

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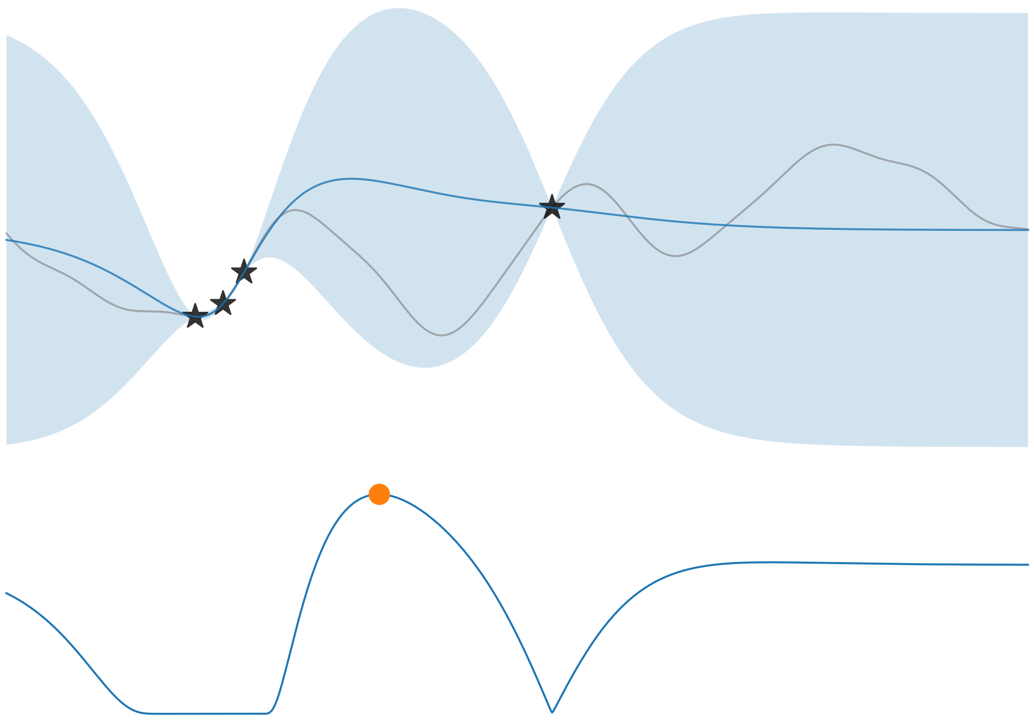
New design principle: Gittins Index

naturally cost-aware

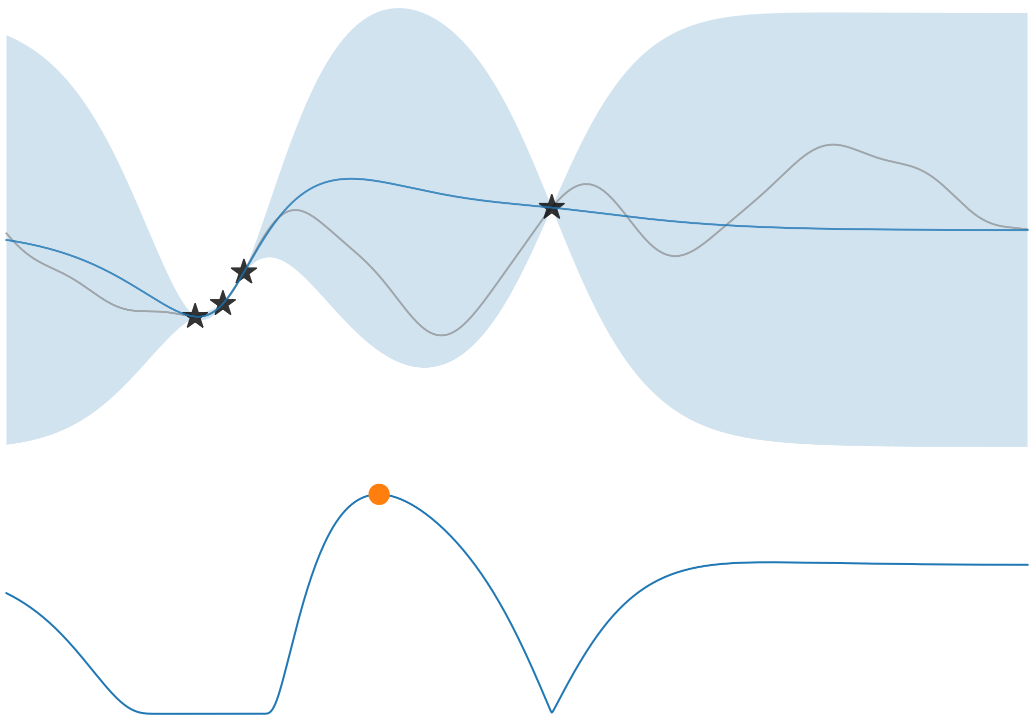
# Expected Improvement



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

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

## Expected Improvement



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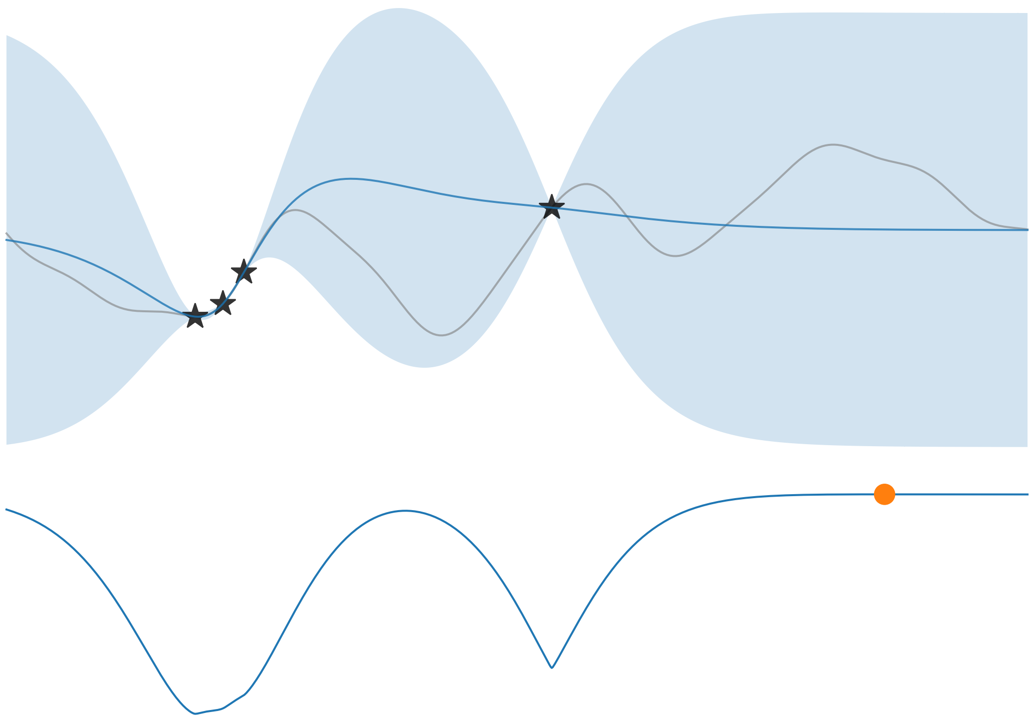
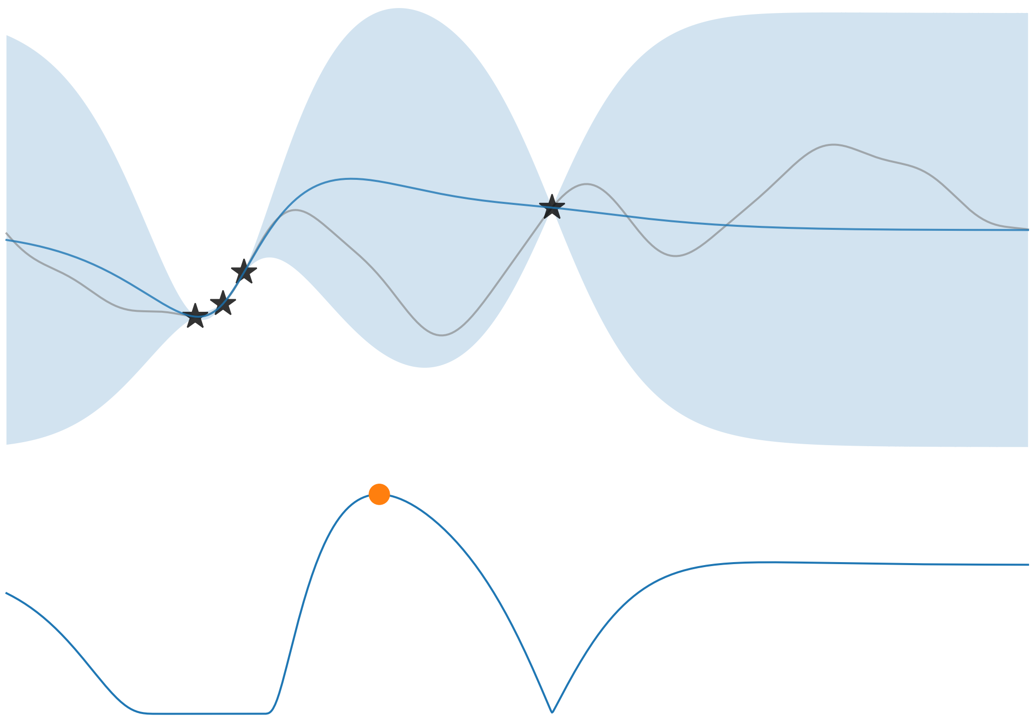
## Gittins Index



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

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

## Expected Improvement



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One-step approximation to MDP

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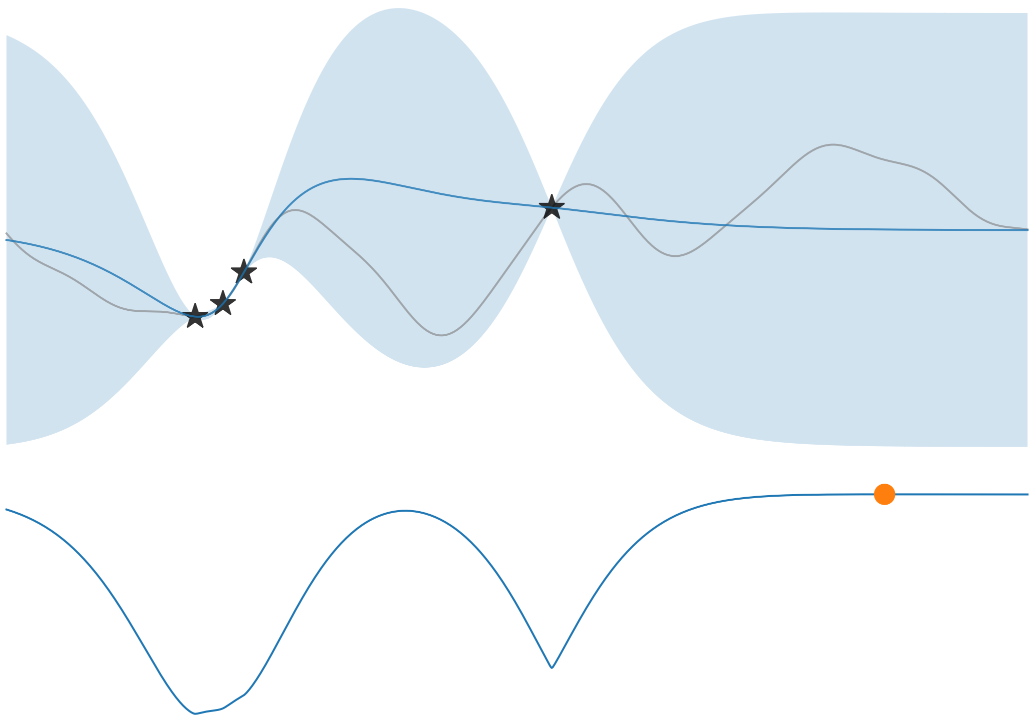

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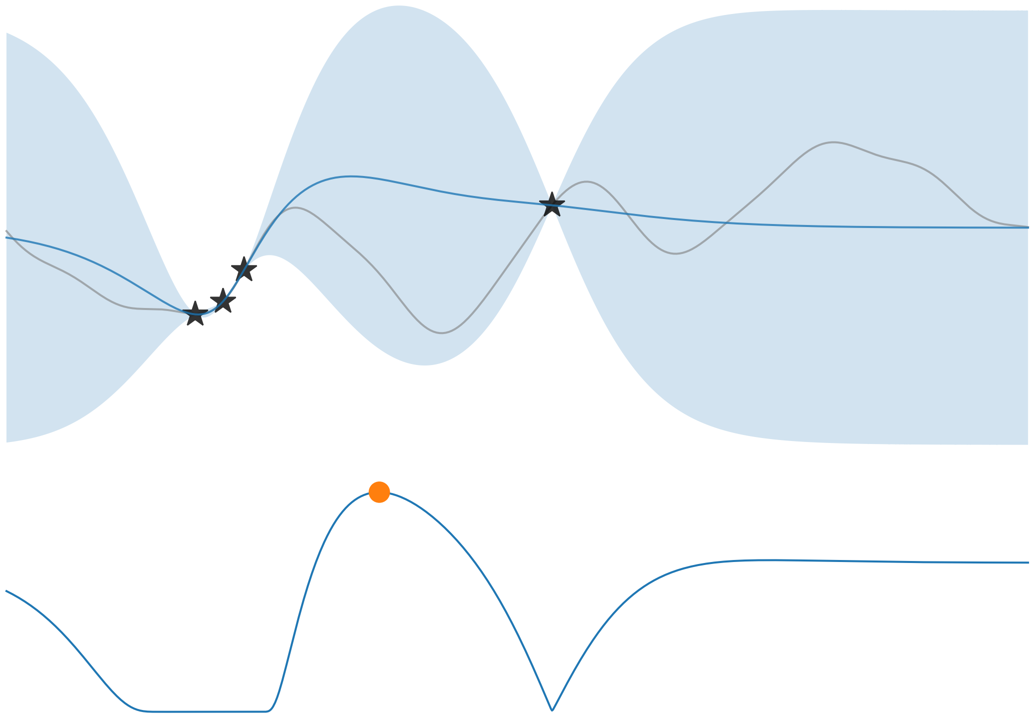

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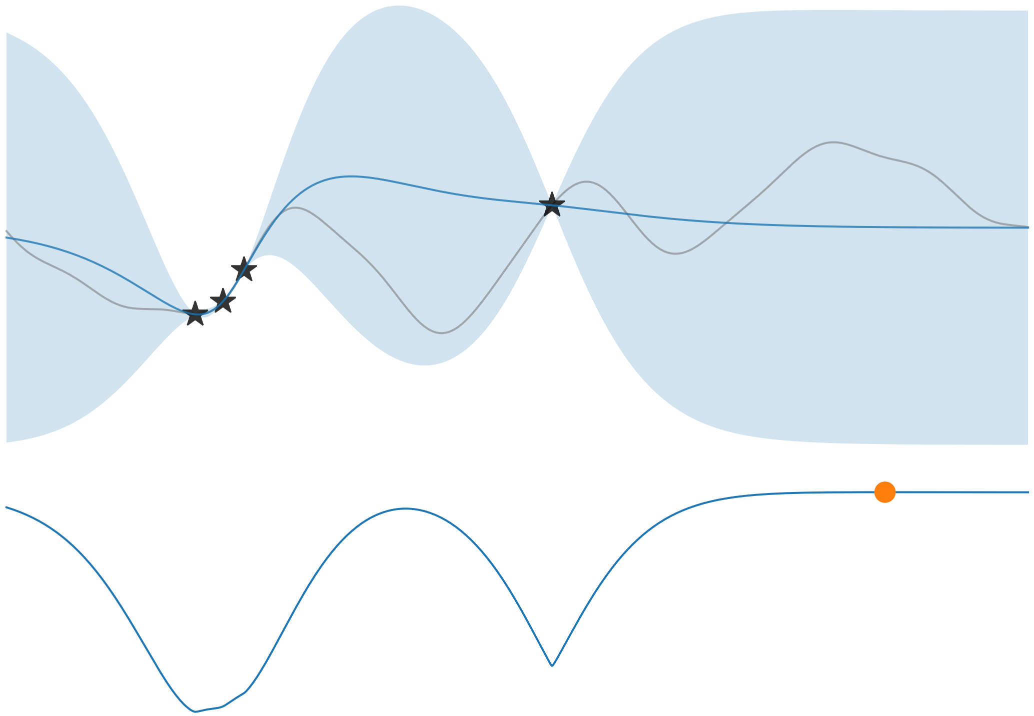
Temporal simplification to MDP

## Gittins Index



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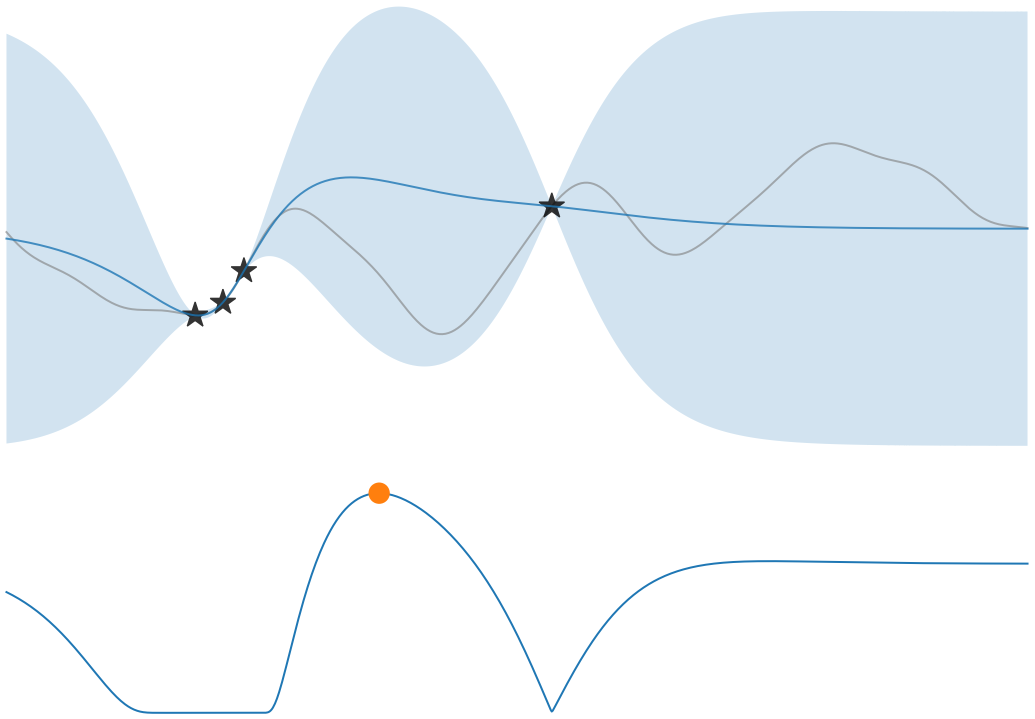

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Temporal simplification to MDP

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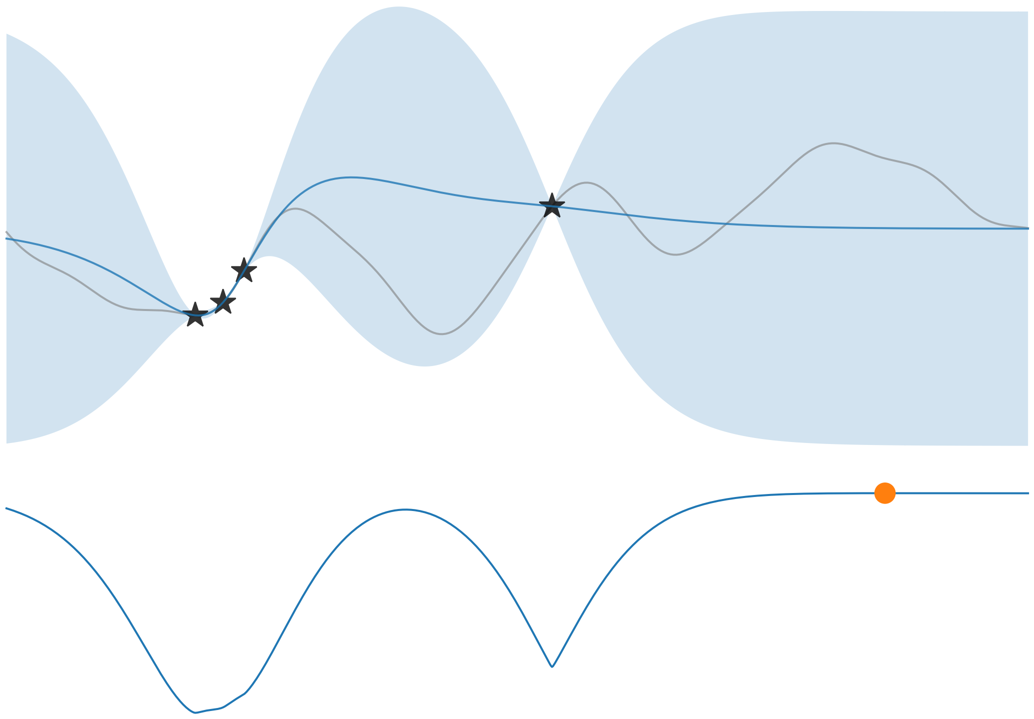
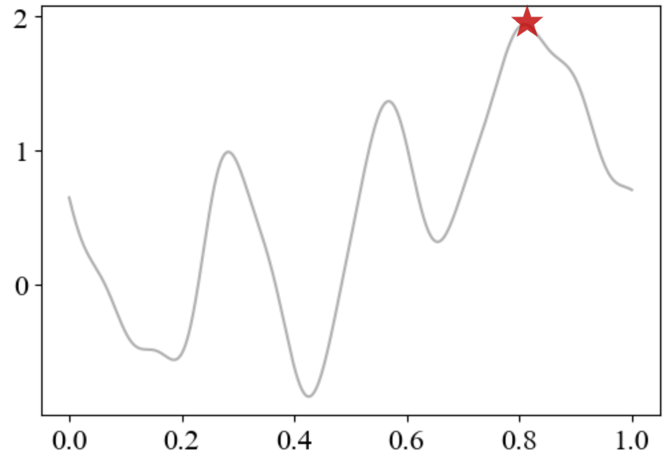


$$\mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$

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

Spatial simplification to MDP

# Our Approach: Spatial Simplification

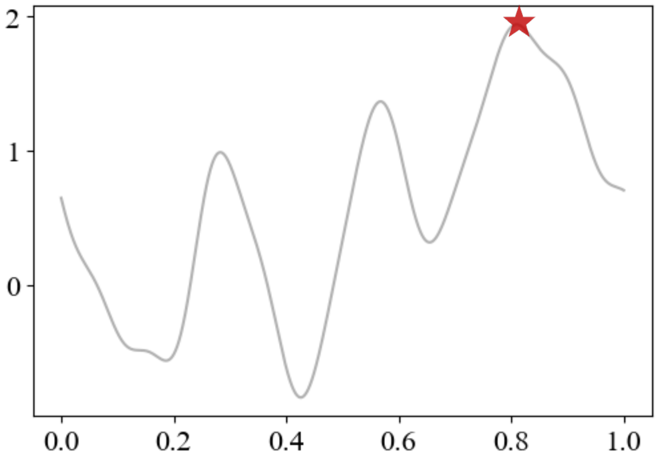



Bayesian Optimization

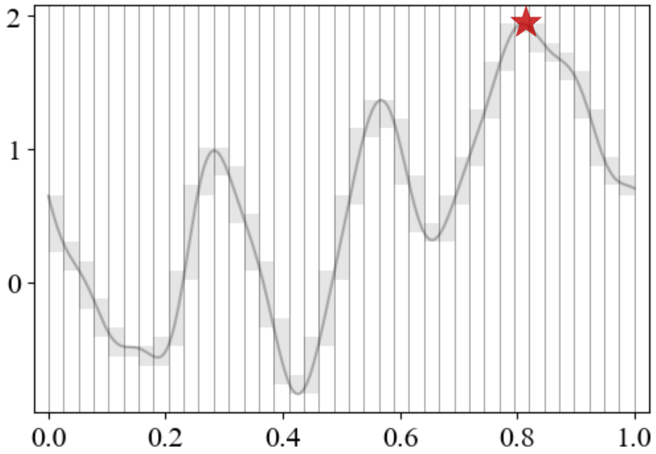
Continuous

Correlated

# Our Approach: Spatial Simplification




⟹

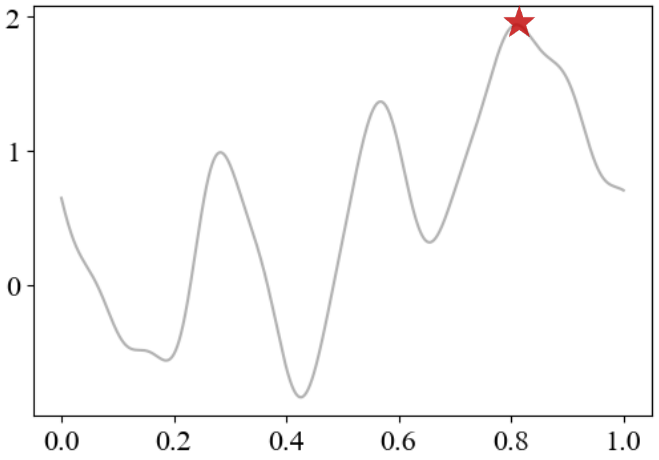



Bayesian Optimization

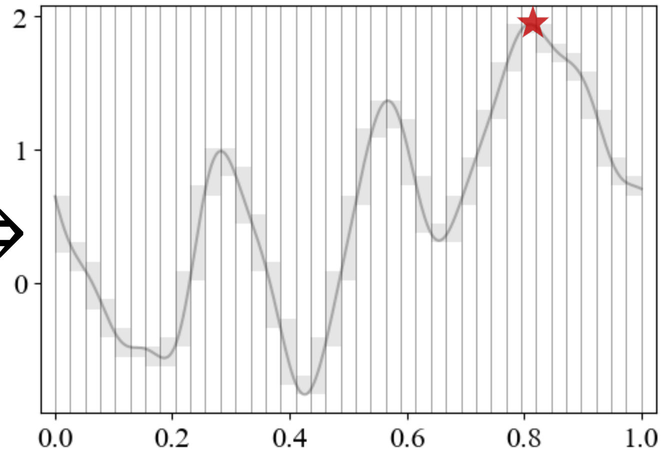
Continuous ⟹ Discrete

Correlated

# Our Approach: Spatial Simplification




$\Longrightarrow$




Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

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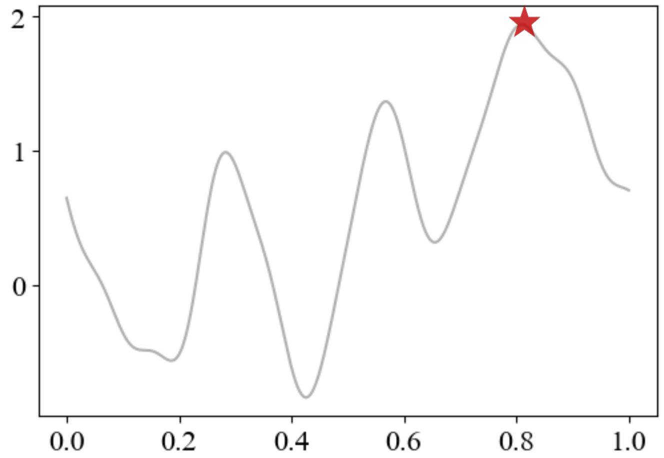


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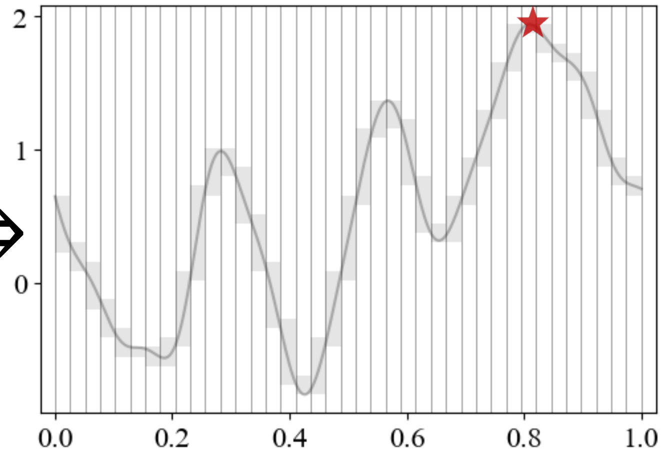


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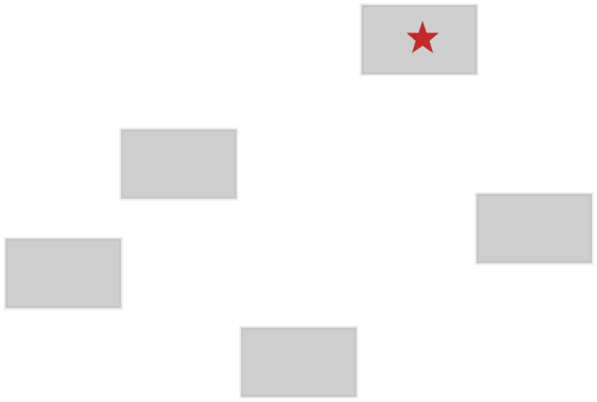

Bayesian Optimization

| | | |
|---|---|---|
| Continuous | $\Longrightarrow$ | Discrete |
| Correlated | $\Longrightarrow$ | Independent |

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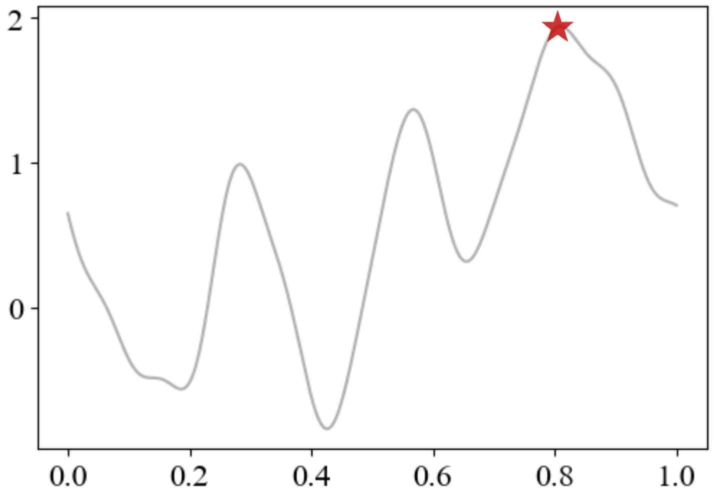


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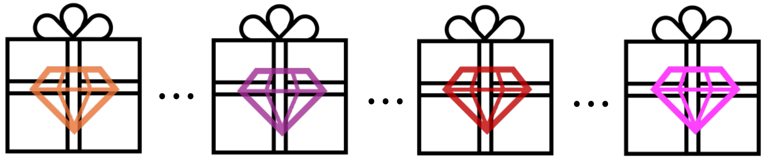

Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

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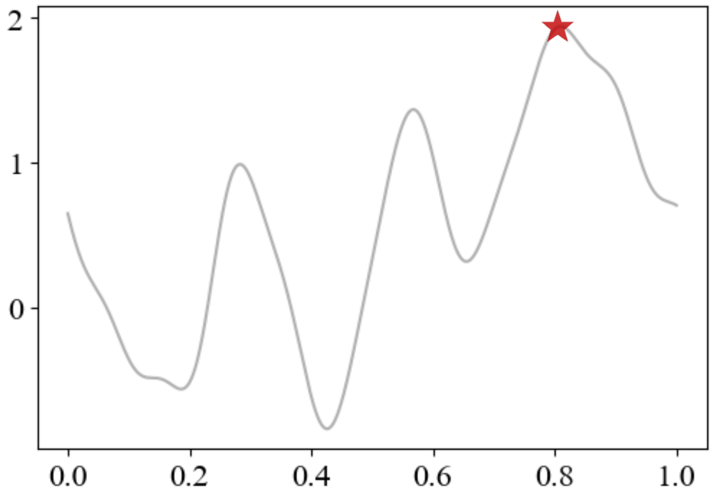


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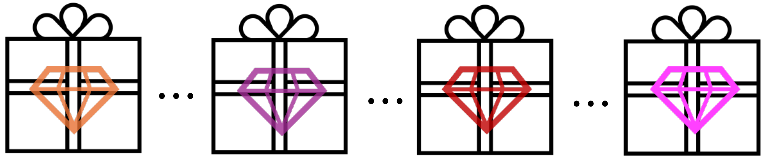

Bayesian Optimization

Pandora's Box [Weitzman'79]

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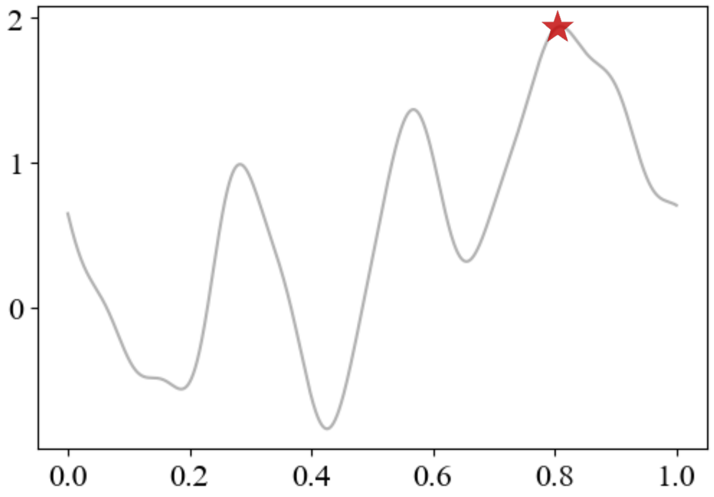
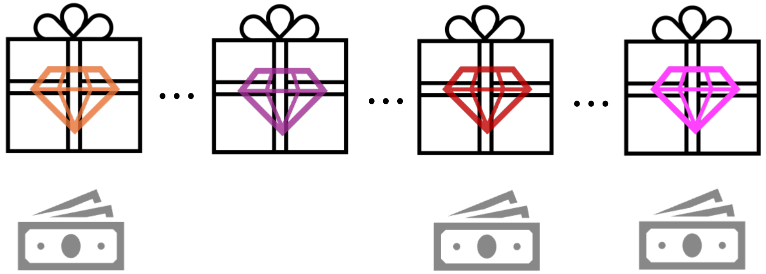
Optimal policy: Gittins index

# Our Approach: Spatial Simplification




$\Longrightarrow$



Bayesian Optimization

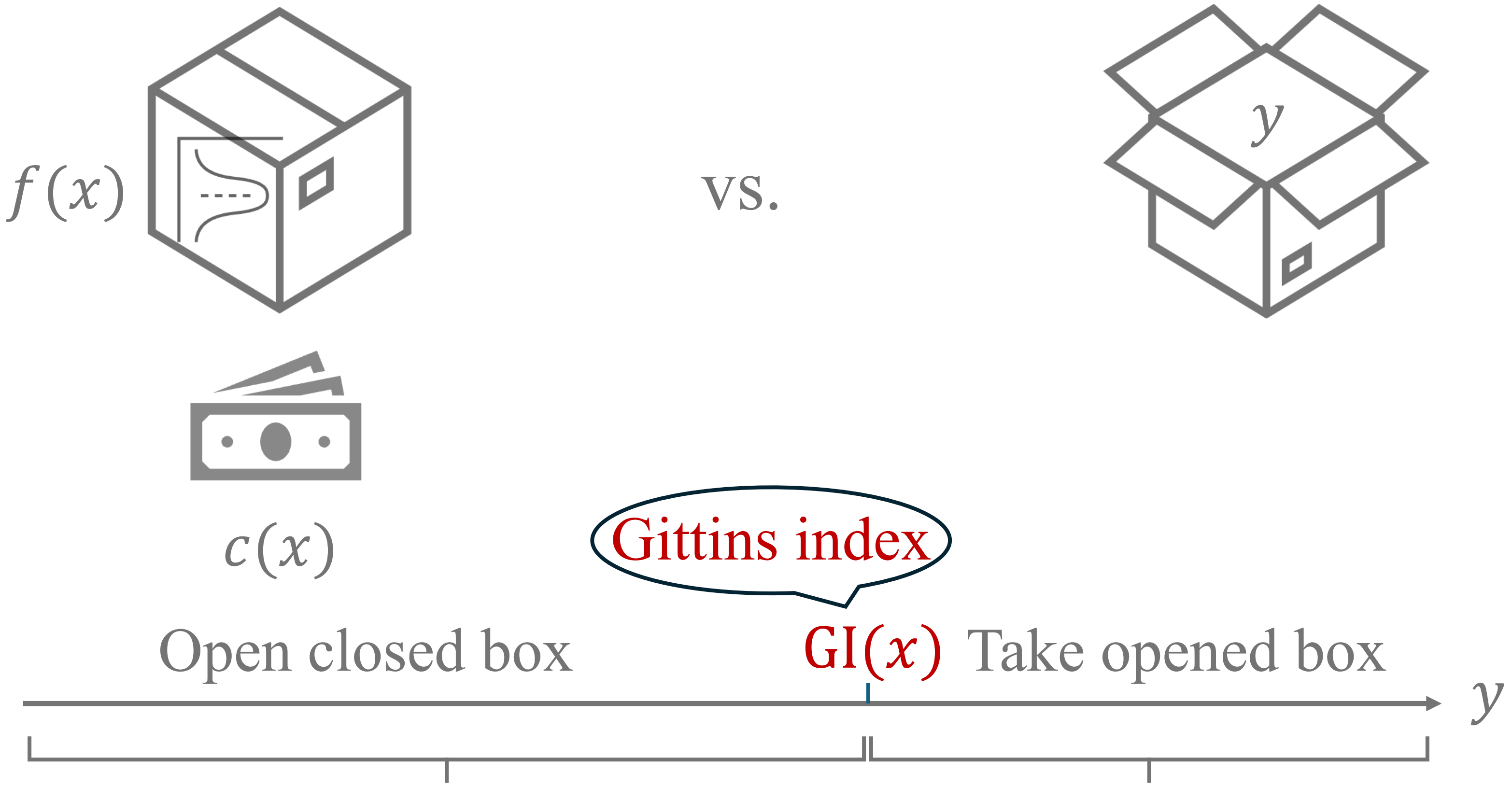
Pandora's Box [Weitzman'79]

| | | | |
|---|---|---|---|
| Continuous | $\Longrightarrow$ | Discrete | allow varying costs |
| Correlated | $\Longrightarrow$ | Independent | |

Optimal policy: Gittins index

# Intuition Behind Pandora's Box Gittins Index

## 1.5-box problem:

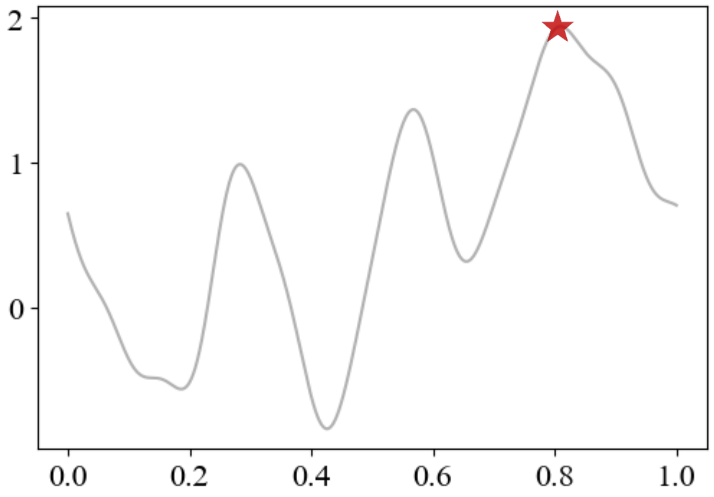



Profit: $\mathbb{E}[\max(f(x), y)] - c(x)$

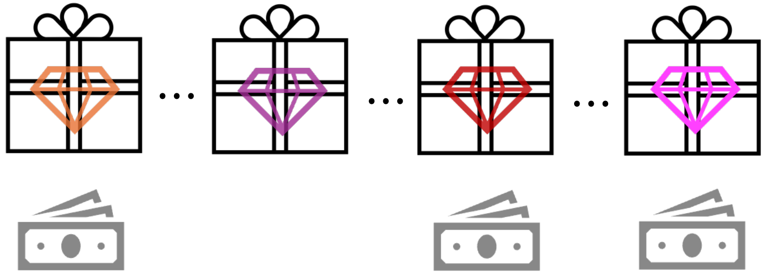
Profit: $y$

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

# How to translate Gittins index?




$\Longrightarrow$



Bayesian Optimization

Pandora's Box [Weitzman'79]

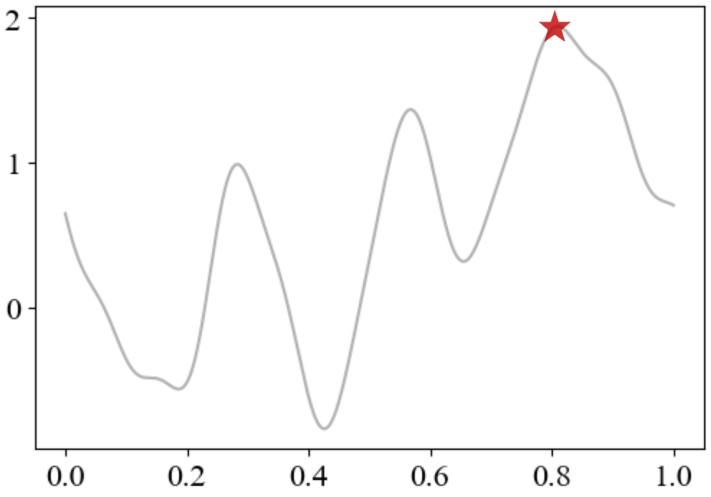
Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

How to translate?

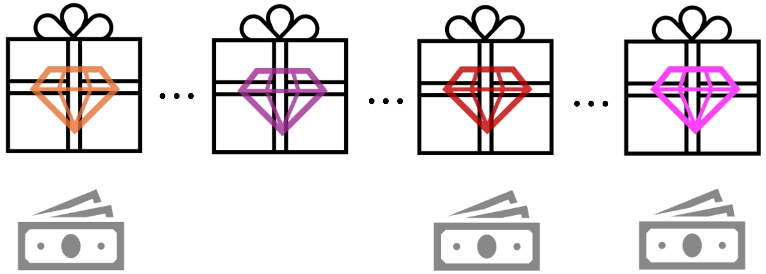
$\Longleftarrow$ Optimal policy: Gittins index

# How to translate Gittins index?




Bayesian Optimization

$\Longrightarrow$




Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

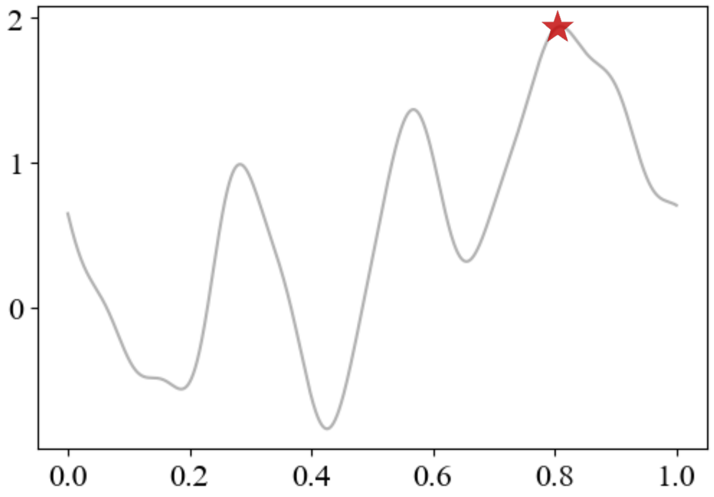
Correlated $\Longrightarrow$ Independent

incorporate posterior

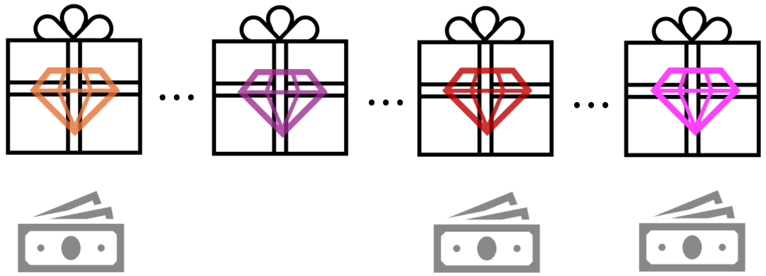
Our policy $\Longleftarrow$ Optimal policy: Gittins index

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

# Is Gittins good in Bayesian Optimization?




$\Longrightarrow$



Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Is Gittins index good? $\xLeftarrow{\text{incorporate posterior}}$ Gittins index is optimal

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

# Experiment Setup: Objective Functions

Synthetic

Samples from prior

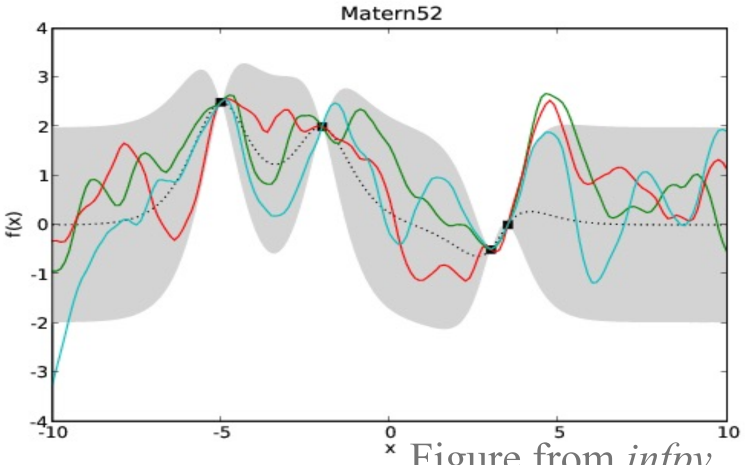



Figure from *infpy*

Ackley function

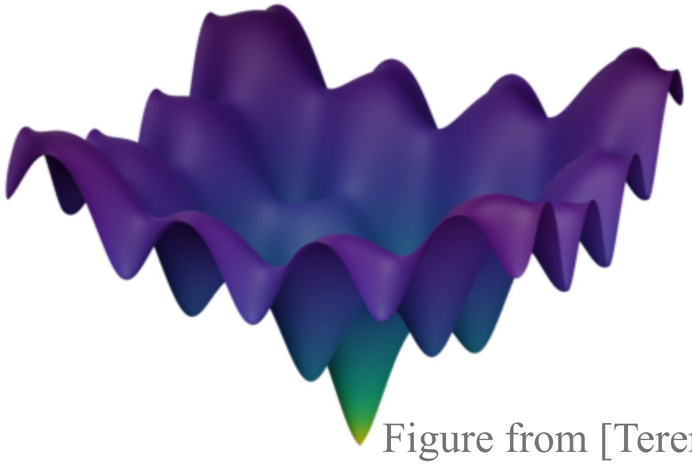


Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT

Lunar Lander

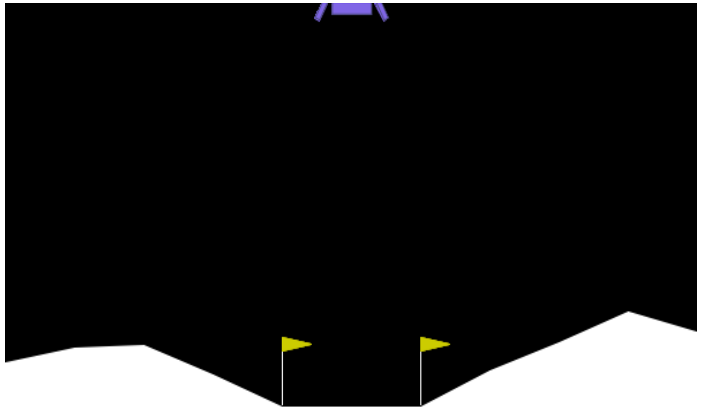
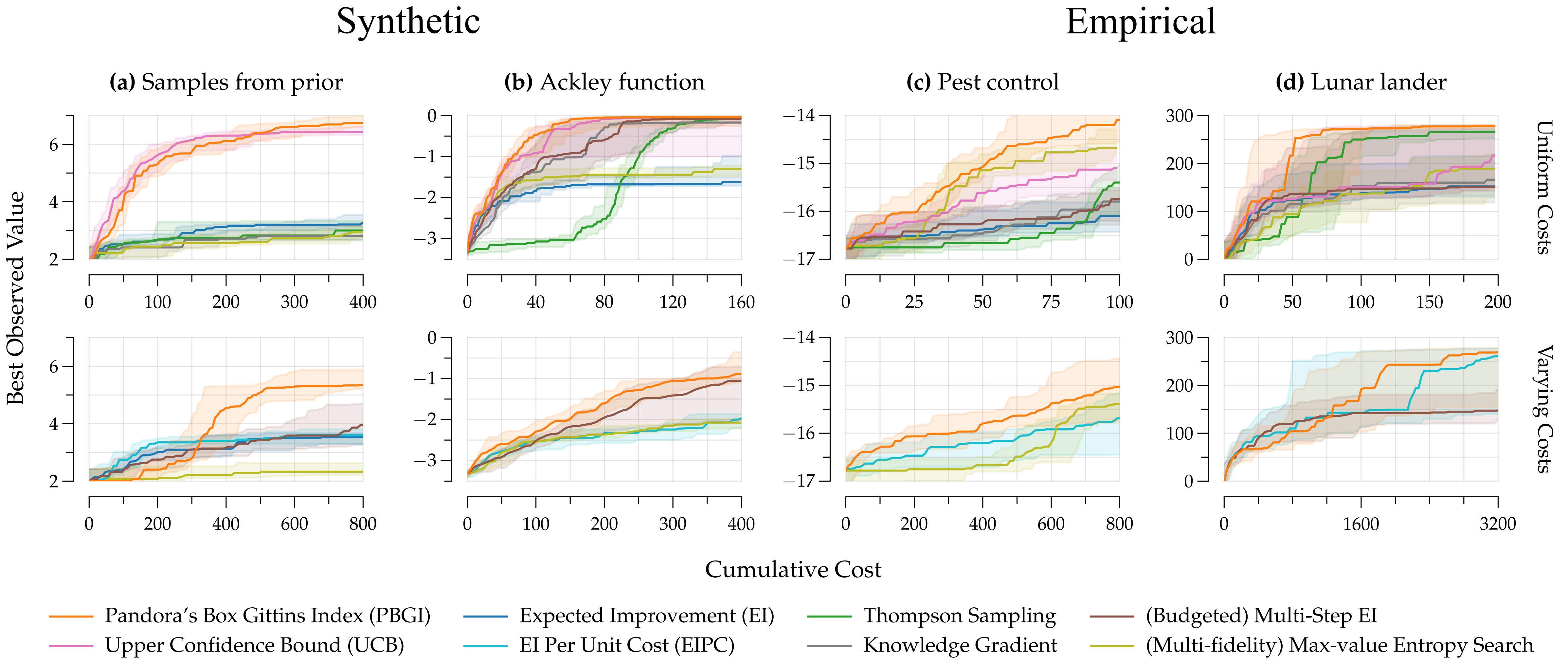


Figure from OpenAI Gym

# Experiment Results



# FAQ

- Easy-to-compute?

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  Yes, EI + bisection

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- Any theoretical results?

# FAQ

- Easy-to-compute?

  Yes, EI + bisection

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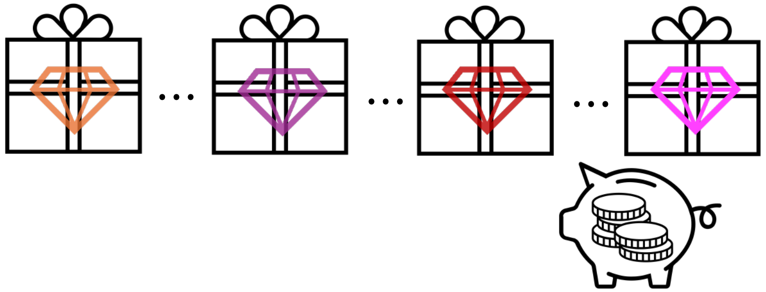
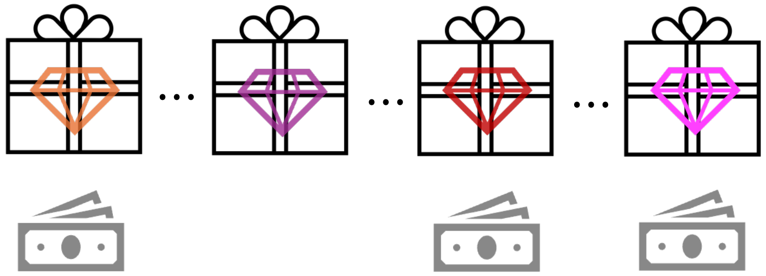
  Yes, expected-budget-constrained $\cong$ cost-per-sample

# Theoretical Result

**max** best observed under budget



**max** (best observed – costs)



Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

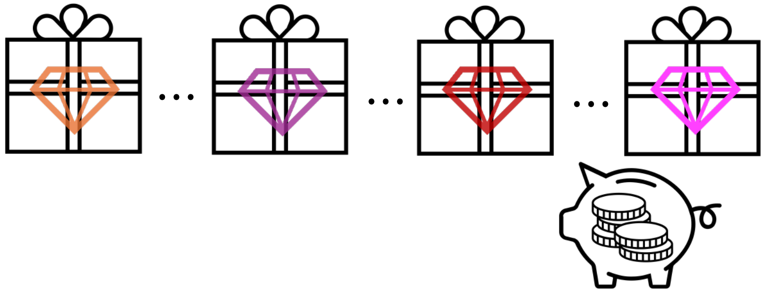
Pandora's Box

Cost per sample

Optimal policy: Gittins index

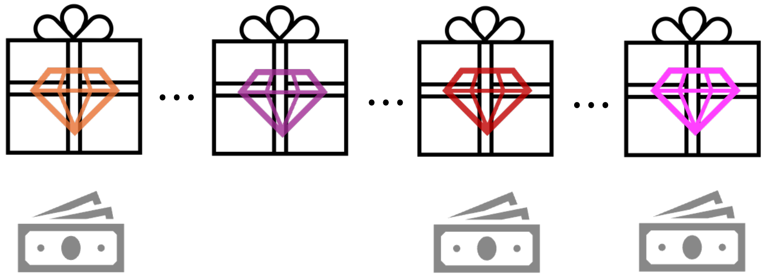
# Theoretical Result

**max** best observed under budget



$\Longleftarrow$

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



Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh'24]

Pandora's Box

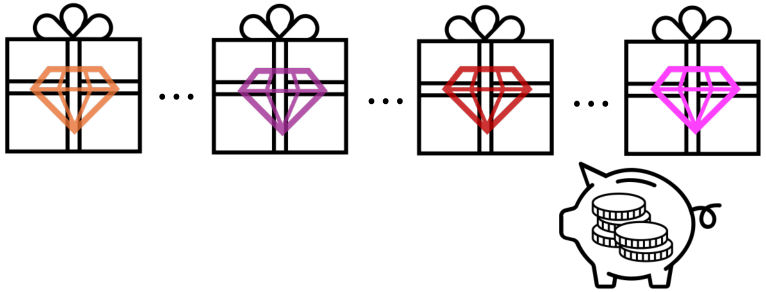
Cost per sample

Optimal policy: Gittins index

# Theoretical Result

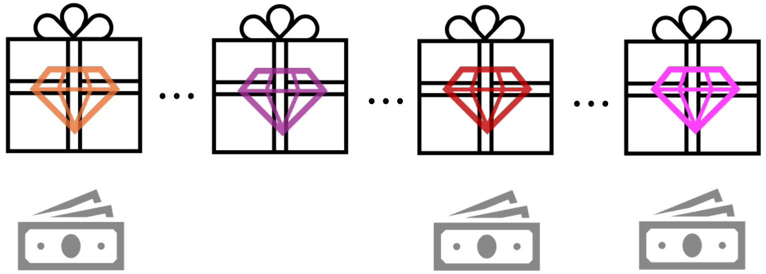
budget-dependent

**max** best observed under budget



$\Longleftarrow$

**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?

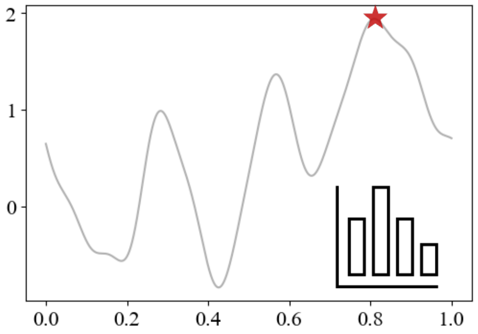
  Yes, EI + bisection
- Any theoretical results?

  Yes, expected-budget-constrained ≅ cost-per-sample
- Tuning parameters?

  Yes, control unit conversion

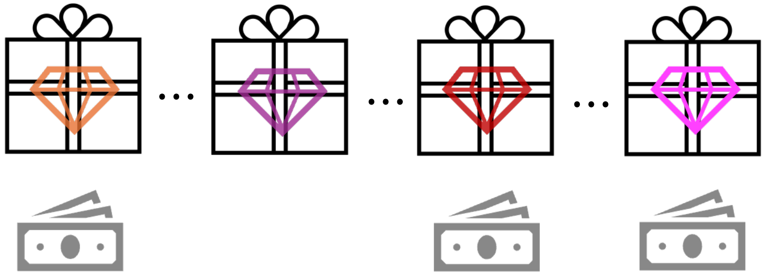
# New Design Principle: Gittins Index

## Problem



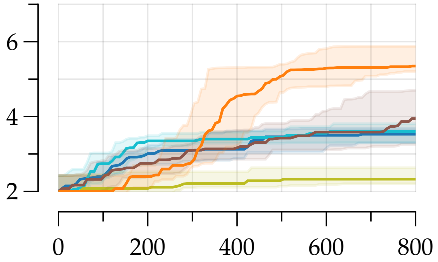

Bayesian optimization
with varying costs

## Key idea



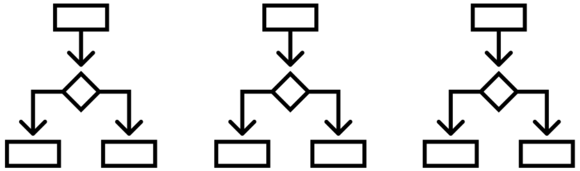
link to Pandora's box
and Gittins index theory

## Impact




competitive performance

## Future potential



black-box processes
with partial feedback

# Check our paper on ArXiv!

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